PETRA IV.
Upgrade of PETRA III to the Ultimate 3D X-ray Microscope
Conceptual Design Report
PETRA IV

Upgrade of PETRA III to the Ultimate 3D X-ray Microscope

Conceptual Design Report
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General Information

Name: PETRA IV (acronym: PETRA IV)

Research field(s): Matter / From Matter to Materials and Life (MML)

Coordinating Helmholtz Centre: Deutsches Elektronen-Synchrotron DESY

Helmholtz centres and external partner institutions: Helmholtz Centre Geesthacht (HZG), European Molecular Biology Laboratory (EMBL), Max Planck Society (MPG)

Category B: Intended for the German National Roadmap for Large-Scale Infrastructures

Description: PETRA IV will be a synchrotron radiation source with ultra-low emittance and will be operated as a user facility (LK II).

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Executive Summary

PETRA IV – The Ultimate 3D X-ray Microscope

Sustainable technologies for the production, storage and use of energy, for environmentally friendly transport and for information systems will depend crucially on the development of novel materials with tailor-made functions. Realising these will require sophisticated materials design down to the atomic scale, which in turn can only be accomplished if suitable diagnostics tools are available. Among the most important challenges here are the investigation of the mechanisms of the desired material and molecular phases, the precise determination of nanoscale structures and the in-situ analysis of the dynamics of structural and electronic changes on relevant length and time scales. A revolutionary new analytical capability to observe the atomistic mechanisms of material synthesis with the highest precision is essential if we are to achieve a basic understanding that allows the transition from the previous empirical trial-and-error method of synthesis to knowledge-based rational materials and process design. This requires a new generation of photon sources with analytical capabilities that were previously unimaginable. With PETRA IV, this challenge will be met: PETRA IV is a conceptually new X-ray source in the hard X-ray range that enables highest resolution on relevant length, time and energy scales, with a very high degree of coherence, highest brightness, as well as with all options for in-situ/operando analysis required for the knowledge-based design of the next generation of multifunctional materials.
With nanoscale resolution PETRA IV will push the limits of X-ray imaging. For the first time, PETRA IV will make it possible to analyse individual nanoscale objects within their larger context and capture the atomic and electronic structure and function of individual molecular functional units, avoiding uncertainties by averaging over particle size, shape, orientation and defect distribution. These new possibilities of nano-control and X-ray imaging will have a disruptive impact not only for the development of new materials in information technology, future quantum technologies and sustainable energy concepts, but also for deciphering the complex, hierarchical structures and processes in life sciences to provide the ground for curing deceases and rational drug design.

The PETRA IV project comprises the upgrade of the present synchrotron radiation source PETRA III at DESY to an ultra-low-emittance source. At X-ray energies of about 10 keV, PETRA IV will generate beams that are close to the physical limits in terms of parallelism and smallest achievable source size, approaching the so-called diffraction limit. It will be an ideal source for 3D X-ray microscopy of biological, chemical and physical processes under realistic conditions, on length scales from atomic dimensions to millimetres and on time scales down to the sub-nanosecond regime. These novel analytical opportunities will enable groundbreaking studies in many fields of science and industry, addressing major societal challenges in fields like Energy, Health, Transport & Technology, Earth & Environment and Information Technology.

The main goal of the PETRA IV project is to replace the PETRA III storage ring with a state-of-the-art multibend achromat (MBA)-based ultra-low-emittance storage ring. The upgrade includes the renewal of parts of the existing preaccelerator chain and of the storage ring infrastructure, the civil construction of a new experimental hall in the western part of the DESY campus and the upgrade and relocation of existing beamlines, including the construction of new beamlines. The new storage ring can store relativistic electrons in a beam that is 50 to 100 times more focused and less divergent than currently possible at PETRA III. By generating synchrotron radiation in specialised new undulators, a photon beam can be obtained with a spectral brightness that is 100 to 1000 times higher than achievable today. Up to an X-ray energy of about 10 keV, this beam is nearly diffraction-limited and can thus be efficiently focused down to nanometre dimensions. In addition, the high degree of coherence can be exploited for X-ray microscopy with coherent light, pushing the spatial resolution limit to the single-digit nanometre range. The coherent beam is also ideal for studying the dynamics in complex matter. At PETRA IV, dynamics from hours down to the nanosecond range can be covered in this way. The highest gains in brightness are obtained for high-energy X-rays, enabling new kinds of microscopic studies in biology and materials science. Thanks to the large penetration depth of hard X-rays, PETRA IV is ideal for investigating samples in their natural environment or inside special sample environments. The combination of highest spatial resolution and sensitivity and the possibility to measure various physical and chemical properties in-vivo, in-situ and operando makes PETRA IV the ultimate 3D X-ray microscope for biological, chemical and physical processes.

The planning of PETRA IV started in 2016 with the conceptual design phase, which came to a conclusion in 2019 with the publication of this conceptual design report (CDR). In the following technical design phase, which will be completed by the end of 2022, a detailed technical design for the upgraded facility will be developed, including project management plans, logistics, robust financial estimates and a detailed risk assessment. In parallel, several steps in the approval process for PETRA IV are being carried out, such as the Helmholtz Roadmap for Large-Scale Infrastructures (FIS) process, a coordination of photon science infrastructures on the national and European level (LEAPS) and the preparation of a proposal for the National Roadmap of large-scale research infrastructures of the German Federal Ministry of Education and Research (BMBF). After financial approval of PETRA IV, approximately three years will be needed to prepare and produce all the components and plan the civil construction, installation and commissioning of the new facility. Until shortly before the start of civil construction and installation of PETRA IV, PETRA III will continue regular user operation. The civil construction, installation and commissioning of the new storage ring...
and beamlines are scheduled to last about two years and will be followed by the commissioning and operation of PETRA IV. Like PETRA III, PETRA IV will be operated as a user facility (LK II) for the production of synchrotron radiation for about 5000 hours per year. PETRA IV is expected to be used by more than 3500 scientists and engineers from various fields of science covering all Helmholtz programmes and ranging from physics, chemistry, biology and biomedicine to geological, environmental and materials sciences as well as nanoscience and technology. Access to beamtime for scientific users will be based on external peer-review similar to the procedure established at PETRA III. Special access modes for industrial users with support from DESY’s ITT group are foreseen to foster innovation and the industrial applications of the extraordinary capabilities of PETRA IV. The facility is expected to be operated beyond 2050.

PETRA IV – Local, National and International Scientific Landscape

The DESY campus in Hamburg-Bahrenfeld hosts many strategic partners of DESY, making the site most attractive for research, education and innovation. Around the photon sources PETRA III, FLASH and the European XFEL, a vibrant scientific environment has been established on the campus including partner institutions like the European Molecular Biology Laboratory (EMBL), the Max-Planck-Society (MPG) or the Universities of Hamburg (UHH, TUHH). Recently, the City of Hamburg, the University of Hamburg and DESY started the urban planning project Science City Bahrenfeld with support from BMBF. The project comprises significant construction activities on the Bahrenfeld campus premises, the relocation of parts of the natural sciences of the University of Hamburg to the Bahrenfeld campus, the integration of complexes for start-ups and industry and the creation of more than 2000 apartments. The project will span at least two decades with investments of the order of one billion Euros. Eventually, the Science City Bahrenfeld will host more than 15 000 scientists and students from all over the world. It will be a benchmark campus for the 21st century, combining science, education, industry and residential areas. PETRA IV is a cornerstone for this project, ensuring world-class analytical opportunities for an interdisciplinary and international user community.

Today, PETRA III at DESY is the high-energy synchrotron radiation source with one the smallest horizontal emittances worldwide and plays a leading role in research using tender to hard X-ray synchrotron radiation. With the multibend achromat (MBA), a new storage ring technology has become available, and many synchrotron radiation sources around the world plan upgrades based on this technology to achieve better horizontal emittance and thus higher brightness. Upgraded, they will surpass PETRA III by a factor of 3 to 30 in emittance and spectral brightness, and thus PETRA III will lose its leading role in photon science. Owing to the worldwide largest circumference for a synchrotron radiation source of the PETRA storage ring tunnel, the upgrade to PETRA IV permits a much stronger reduction in emittance, by at least a factor of 50 compared to PETRA III, enabling PETRA IV to again assume a world-leading position in photon science: PETRA IV will offer unique possibilities to investigate complex matter on all relevant length and time scales from atomic dimensions to millimetres and from sub-nanoseconds to hours. For this reason, DESY must make every effort to implement the MBA technology as quickly as possible in order to maintain the worldwide leading position of DESY, the Helmholtz Association and Germany in this dynamically developing field in the coming decades.
PETRA IV – Strategic Importance (National, International)

PETRA III caters to a large national user community from all fields of science, in particular to all major scientific organisations and institutions in Germany, i.e. the Helmholtz Association, the Max Planck Society, the Leibniz Association, the universities and many other institutes. In particular, PETRA IV is in line with the mission of the Helmholtz Association and meets the goals of the German High-Tech Strategy, as it links German research to the needs and grand challenges of society, fosters new technological revolutions with its new transformative beam properties and forms a creative space for innovation with its integrative innovation and technology transfer concept. The mission of the Helmholtz Association is to contribute to solving the major challenges facing society, science and the economy by conducting top-level research within six research fields: Energy, Earth & Environment, Health, Aeronautics, Space and Transport, Matter, and Key Technologies. PETRA IV will position the Helmholtz topic Research on Matter with Brilliant Light Sources in an international leadership position, enabling its scientists to address highly complex systems in all the aforementioned fields in close cooperation with the national and international user community. Covering the needs for highly brilliant tender and hard X-rays in Germany, it will ideally complement the proposed future VUV and soft X-ray synchrotron radiation source BESSY III at Helmholtz-Zentrum Berlin, as detailed in the German National Photon Science Roadmap (NPSS) that is in preparation. From a European perspective and together with the upgraded ESRF-EBS source in Grenoble, France, PETRA IV will ensure that the European user community has access to an unprecedented quality of tender to hard X-ray beams for the most demanding science projects and thus enabling Europe to stay at the forefront of this field of science. As a partner in the League of European Accelerator-based Photon Sources (LEAPS), DESY collaborates with its European partners to promote science and technology at the European light sources. The long-standing partnership with EMBL will guarantee optimum conditions for the use of synchrotron radiation in the Life Sciences. With its extraordinary beam parameters, PETRA IV will provide unique experimental conditions that are complementary, especially in the time domain, to free-electron laser sources, such as FLASH and the European XFEL, and to many other probes, such as electrons and neutrons.
The major global challenges in the fields of Energy, Health, Transport & Technology, Earth & Environment and Information Technology include for example the fight against cancer and infectious diseases, the supply of clean and sustainable energy as well as the reduction of greenhouse gases. From a scientific and engineering point of view, solutions to these problems rely on understanding the often complex structures and processes in matter and on gaining control over them by tailoring the properties of new materials to specific needs. Currently, the microscopic origin of macroscopically complex behaviour is often unknown, preventing significant progress and further development in these areas.

With its exceptional brightness, PETRA IV will provide scientists and engineers with the means to gain insight into the structures and processes in matter on all length scales from atomic distances to macroscopic dimensions and thus to understand the emergence of complexity in nature and technical processes. The extremely bright tender and hard X-rays provided by PETRA IV are the ideal probe for structures and dynamics under in-vivo and in-situ/operando conditions.

In the following, we will discuss selected examples from the aforementioned fields to showcase the unique potential of PETRA IV to tackle these global challenges. Each of the following five examples elucidates the respective scientific question, explains why PETRA IV can make decisive contributions and describes what particular X-ray methodology gives PETRA IV a cutting edge in the respective field.
The transition to climate-friendly, renewable energies for electricity, heat and mobility requires durable and safe energy storage systems. It will only succeed with the development of improved or new energy storage devices, for which batteries are a prominent example. PETRA IV will provide revolutionary insights into the processes occurring in batteries during their operation – into the smallest structures and processes that determine how the battery functions. PETRA IV can thus be used to optimise innovative developments for industry-relevant applications – for example, by developing nanotechnology for electromobility.

A View into the Working Battery
High-capacity sustainable batteries as energy storage devices play a key role for the phase-out of fossil fuels and for our digital, mobile way of life. Concepts for new types of batteries are being researched worldwide. Innovative materials are to increase the capacity and service life of batteries, shorten charging times and conserve scarce resources. However, no suitable experimental approach has been available so far to investigate in more detail which factors could increase the storage capacity of batteries and enhance their lifetime. PETRA IV will overcome this methodological limit.

For the first time, experiments at PETRA IV will provide detailed insights into the inner workings of functional batteries. The hard X-rays penetrate the entire working battery, e.g. while it is charging or discharging. Thus, with the nanofocused X-ray beam of PETRA IV, even the smallest electrochemical changes can be scanned and detected inside the battery, showing how these disturbances influence the battery’s function and cause it to age. Comparable studies are not possible with any technique today. For this to work, the probe needs to be sensitive to the structure and chemistry...
Executive Summary

of the relevant elements, e. g. lithium, inside the battery. The techniques of choice, pair distribution function analysis and inelastic X-ray scattering, can reveal the structure and chemical properties inside a battery without the need to cut it open. Only the brightest X-ray beams provided by PETRA IV are able to make these techniques work with the resolution necessary to understand the actual origin and formation of defects from atomic to mesoscopic scales. For many branches of industry, the demand for light and very safe batteries is increasing – for example for electromobility. All in all, batteries are becoming smaller and smaller, making their nanostructuring increasingly important. However, the higher the energy density, the more likely it is that defects will occur that will destroy the battery. PETRA IV offers the necessary resolution to investigate the smallest structures in the materials to unravel chemical reactions on the nanoscale and thus provides the necessary information to optimise the material properties.

PETRA IV Technology:
Sharper Vision with Highly Intense and Coherent X-rays

- The X-rays of PETRA IV can scan a fully functional battery and allow internal processes to be monitored under operating conditions. With the finely focused X-rays that can penetrate the whole battery, it will become possible to record the relevant processes on all length scales and display their temporal evolution.

- Experiments at PETRA IV will analyse the interaction of selected chemical elements in the battery with their environment in order to determine their role for the process of energy storage. Only the very coherent and intense hard and high-energy X-ray light from PETRA IV provides a sufficiently high signal to track such processes with sufficient spatial resolution.

- Complementary questions about the course of ultra-fast chemical processes can be answered with the European XFEL.
Tumour Research

Through unique studies of molecules, cells and tissues in their natural environments, PETRA IV can help to develop new treatments for cancer and infectious diseases. The very high screening throughput possible at PETRA IV will enable clinically relevant studies. The excellent experimental possibilities and outstanding interdisciplinary expertise in Hamburg offer research, clinics and industry optimal conditions for the analysis of biological samples.

New Agents Against Tumour Growth

In our ageing society, the incidence of cancer is increasing. Targeted therapies will advance the fight against cancer with fewer side effects for the patients: While chemotherapy and radiotherapy attack damaged and healthy tissue alike, targeted therapies are directed towards specific tumour mechanisms. However, they are only known for some tumour types and are usually not free of side effects. In order to improve active pharmaceutical ingredients, tumour growth and the effect of drugs on cells and tissue have to be better understood, new targets have to be found, and already known therapeutic principles have to be optimised. In the future, PETRA IV will enable studies with the necessary level of detail, efficiency and statistical reliability to systematically improve and expand targeted therapies.

One example of a targeted therapy is the use of angiogenesis inhibitors, which suppress the formation of micro blood vessels inside a tumour, a key mechanism of tumour growth. The new blood vessels enable the tumour to meet its increasing demand for oxygen, sugar and nutrients. Thus, if the formation of blood vessels can be prevented, the spread of the tumour is also slowed down. However, basic research on this subject is still in its infancy, and open questions abound: How exactly are...
PETRA IV will provide answers to these and other questions by enabling biological samples to be analysed experimentally in their natural form.

The new PETRA IV measurement capabilities will provide insights from the molecular level to larger tissue structures. Experiments will analyse individual cell components, such as proteins and molecules, and whole cells as integral parts of larger samples. In this way, mechanisms in tumour cells, interactions of the cells with their environment and the effect of drugs introduced into the tissue can be observed across the board. In addition to primary mechanisms of action, possible desirable or undesirable side effects of drugs can also be investigated, for example the coupling of the active substance to other receptors in the environment. With PETRA III, researchers currently still depend on investigating isolated effects in crystallised samples. In contrast, the high brightness, coherence and rapid signal detection at PETRA IV will allow studies of biological systems from the molecular to the tissue level and also enable a very high throughput, e.g. for screening investigations.

Even beyond cancer research, the new imaging possibilities offered by PETRA IV are a milestone for health research in an ageing society. They will help us to better understand neurodegenerative diseases such as Alzheimer’s or bone diseases such as osteoporosis. PETRA IV can for example map the communication process of individual neurons in the brain and link these findings with the ability of associative learning, which is partly lost through disease. In bones, X-rays can already detect defects on the nanoscale. Various projects in Hamburg are specifically expanding the interdisciplinary cooperation between medical research, clinics and the life sciences, e.g. with the University Hospital in Hamburg-Eppendorf.

The Bahrenfeld campus offers a unique research environment with dedicated expertise and support ranging from sample preparation to theoretical modelling. In the future research building HARBOR of the University of Hamburg, users will receive competent assistance in preparing experiments for PETRA IV. The strong interdisciplinary research landscape at DESY includes the Centre for Structural Systems Biology (CSSB), the Center for Hybrid Nanostructures (CHyN), the NanoLab of the Centre for X-ray and Nano Science (CXNS) and the European Molecular Biology Laboratory (EMBL).

**PETRA IV Breakthrough:** Imaging Cells in their Environment

- Experiments at PETRA IV will analyse cells as part of their natural environment (e.g. tumour tissue, healthy tissue, tissue in the brain) with highly brilliant X-ray light.

- PETRA IV will enable scientists to examine large samples in which biological processes take place. Experiments at PETRA IV will routinely take images that were previously only possible with extraordinary experimental effort and at considerably lower spatial resolution. Key to these outstanding experimental opportunities are the brightness and coherence of the X-rays as well as the speed with which the detectors at PETRA IV can pick up signals.

- For the analysis of the composition and chemistry of biological samples, instruments such as cryo-microscopy and the European XFEL can be used to complement PETRA IV.
Reducing Fine Dust and Particulate Matter

The mechanisms of how fine dust is generated by abrasion are still largely unexplored. PETRA IV can be used to experimentally quantify the formation of biologically relevant fine dust particles during friction processes. The interdisciplinary usage strategy of PETRA IV combines findings from physics and materials research with those from health research.

Fine Dust from Abrasion
Friction processes are primarily responsible for the release of fine dust and particulate matter in road traffic in Germany. Around 70% of the fine and ultra-fine particles originate from the abrasion of tyres, brake linings and road surfaces, only the rest from the exhaust gases of combustion engines. However, systematic scientific studies on the generation of fine dust are rare. At the same time, they are urgently needed for a fact-based debate and for new industrial solutions. PETRA IV will provide new analysis possibilities to understand fine dust from abrasion, measure its health potential and counteract it.

X-ray sources are ideal for the experimental observation of fine dust from abrasion. The place where the friction occurs – the contact surface between two materials – is naturally not visible at the moment the abrasion occurs. X-rays, on the other hand, penetrate the materials and provide images of friction in action. Already today, some experiments of this kind are possible in principle at PETRA III. However, its beam quality is not sufficient to detect the smallest and most relevant fine dust particles. The upgrade of PETRA III to PETRA IV will make the X-ray focusing more than 100 times more efficient, enabling scientists to view particles from a few micrometres in size to the smallest nanoparticles in ultra-fine dust. This especially fine fraction of fine dust is considered to be particularly harmful to health.
In future, innovative materials whose abrasion contains significantly smaller quantities of tiny particles could reduce the potential risk from fine dust. Friction experiments at PETRA IV can investigate the distribution of particle sizes and differentiate between particulate matter contents that are hazardous to health. They will allow researchers to understand how fine dust particles are released from the tyre when a car tyre comes into contact with road surfaces, for example, and how the particles are distributed in the environment. The very high measurement throughput at PETRA IV will also enable large-scale industrial studies for new material developments. DESY plans to support industrial users in this area with the preparation and post-processing of the experiments.

The smaller the fine dust particles, the deeper they can penetrate into the human body, into the lungs or, as nanoparticles, into the bloodstream and the brain. They can cause chronic inflammatory reactions and possibly also trigger neurodegenerative diseases. With PETRA IV, health research has the opportunity to use the great penetration depth of X-rays to examine the biological effect of the fine dust particles in tissues as precisely as possible: How do the particles spread? Which transport mechanisms do they use? Already today with PETRA III, researchers investigate transport processes of special and easily detectable nanomarkers in biological samples in order to find out to what extent they are suitable for tracking drug transport or labelling diseased tissues. With PETRA IV, they will be able to transfer this type of investigation to the transport of ultra-fine dust particles in tissues.

**PETRA IV Technology:**
**Coherent Light for High-Contrast Images**

- The highly brilliant X-rays from PETRA IV penetrate matter and can reveal the formation of fine dust particles at the contact surface between two materials during abrasion. Their high degree of coherence guarantees the necessary high image contrast for time-resolved detection of even the smallest particles.
- With the high sensitivity and resolution of biological imaging at PETRA IV, fine and ultra-fine dust particles can be tracked inside biological organisms to reveal pathways of uptake and potential mechanisms of disease.
- In the Science City Bahrenfeld, scientists and engineers will find a rich environment to solve problems related to fine dust, ranging from support in engineering materials science (GEMS) to structural and systems biology (EMBL, CSSB).
The Role of Water for Life, Technology and the Environment

Water is elementary for life on Earth, for technology and for the environment. Water research creates the basis for new findings in health research, opens up new sources of energy and enables sustainable resource management. PETRA IV will make the molecular network of water molecules visible and relate it to the macroscopic properties of water.

Understanding the Extraordinary Properties of Water

Water is the essential constituent of all life on Earth. Biological processes do not function without water. Water in seas, rivers and glaciers shapes our planet, and water is omnipresent in technical applications. However, many extraordinary characteristics of water that distinguish it from other fluids still remain a mystery. PETRA IV will be the instrument of choice for deciphering the structure and dynamics of water at the molecular level. The results of water research will bring advances in health research and accelerate technical innovations, such as the production of hydrogen as an energy carrier. Water molecules play an important role in the biochemistry of living systems and influence how the cells of organisms behave. In cells, proteins work tirelessly in their water environment. In the future, PETRA IV will enable scientists to follow the individual movement and interaction of the proteins within the cell, which measure only a few nanometres. If, for example, the proteins are concentrated in groups, this can have positive or negative biological effects. In diseases such as Alzheimer’s, disturbing protein plaques that no longer dissolve are observed in the brain. Researchers want to understand exactly how such protein accumulations develop and whether it is possible to specifically intervene in this process. The high coherent flux of PETRA IV can be used to deci-
pher the protein dynamics in the aqueous environment of the cell. Compared to PETRA III, the dynamics in these complex systems can be followed on time scales that are a hundred to several ten thousand times faster. For the first time, PETRA IV will give access to the dynamics in aqueous solutions and other complex matter on time scales down to the nanosecond range. In these measurements, the X-ray light from PETRA IV can be dosed so precisely that the proteins do not suffer any radiation damage during the measurement.

The experimental conditions at PETRA IV will enable a fundamental breakthrough in the understanding of water and its special properties. According to today’s knowledge, the anomalies of water are decisive for the existence of life on Earth. However, there is still no satisfactory model that explains why water shows characteristics unlike those of any other liquid. One theory posits that water is not a homogeneous liquid at all, but actually consists of two liquid components of different density. Investigations of strongly supercooled water with PETRA III have already provided indirect evidence of the possible coexistence of two such components of water. PETRA IV will make this theory directly verifiable: The very fast detection method could separate the dynamics of the two liquid states from each other. The direct detection of two liquid components of water would be a scientific sensation and have far-reaching consequences for biology and chemistry, for the health sector and for technical applications alike.

In the future Science City Bahrenfeld, the Centre for Molecular Water Science (CMWS) will be established, which will bring together several research groups with Europe-wide expertise in water research. The centre will focus on the investigation of the fundamental properties of water and the relationship between its microscopic and macroscopic properties and play a leading role in Europe. It will promote and facilitate exchange with related disciplines, such as chemistry and biochemistry, geosciences, astrophysics and nanotechnology. The CMWS will also support future users in the preparation of their highly complex experiments, for example through sample environments for the generation of microdroplets. The future access to PETRA IV in combination with the European XFEL makes Hamburg a unique centre of attraction for research on water.

PETRA IV Technology:
Coherent Light for Measurements on Multiple Length and Time Scales

- The complex dynamics of water and aqueous solutions can be followed using the highly coherent X-rays of PETRA IV on time scales ranging from nanoseconds to hours.
- The role of water in natural and technological processes can be followed in detail, such as diffusion in the cell or photocatalytic water splitting for energy harvesting.
- For studies of the dynamics in complex matter, PETRA IV and the European XFEL in combination cover the full range of time scales, from femtoseconds to hours.
Superconductivity

Materials that conduct electricity without loss at room temperature would mean a technological revolution – with applications ranging from energy supply to information technology. Today’s well-known superconductors lose their electrical resistance only at very low temperatures, and the high cooling requirement prevents them from being widely used. PETRA IV will bring an experimental breakthrough enabling researchers to decipher the basic physical mechanisms of high-temperature superconductors with the aim to develop new materials.

Innovative High-Temperature Superconductors

Materials that conduct electricity without loss close to room temperature and ambient pressure are the ultimate goal of research into high-temperature superconductors. Potential applications range from lossless power transport for sustainable energy supply to extremely fast switches for data processing or highly sensitive sensors and lossless information storage in quantum computers. For many years, intensive efforts have been made worldwide to find solutions. However, in order to tailor materials so that they can be used for broad technical applications, fundamental physical processes must first be better understood. The future experimental possibilities at PETRA IV promise a breakthrough: For the first time, the local electronic structure in high-temperature superconductors can be made visible on the nanoscale. In contrast to conventional superconductors, the physical processes that cause high-temperature superconductivity to emerge below a certain transition temperature have not yet been satisfactorily explained. There are many indications that important parameters of superconductivity are not yet experimentally accessible. Without such a “recipe” for high-
temperature superconductivity, however, the systematic further development of new materials towards higher transition temperatures is difficult to achieve.

The new insights from measurements at PETRA IV could reveal what a material must consist of in order for the critical temperature to approach room temperature. If this succeeds, new high-temperature superconductors can be developed for a broad range of applications.

Superconducting copper oxides are currently known to reach maximum transition temperatures of around \(-135\, ^\circ\text{C}\). It has long been assumed that these high-temperature superconductors have a rather homogeneous structure. However, recent investigations with X-rays have provided initial indications that instead, a heterogeneous electronic structure – a sort of disorder – in the copper oxides could be the key to high-temperature superconductivity: The superconducting phase transition seems to take place when most electrons have come together in certain complex, group-wise arrangements – “puddles of electrons” of different sizes – around which the remaining electrons move in pairs on geometrically complex paths from one point to another. However, today’s experiments are limited. Even the analysis of a single material requires enormous effort and can only distinguish local phenomena down to about one micrometre, while the observed puddles of electrons measure an average of a few nanometres.

Experiments at PETRA IV will be able to distinguish the local distribution of electrons with a spatial resolution down to the nanometre range. It will also be possible to check whether the explanatory approach of disorder can be generalised to other materials. Analyses with PETRA IV can provide the necessary information to specifically tailor new superconducting materials at the nanolevel, for example by “inserting” puddles of electrons into the material by oxygen bombardment.

**PETRA IV Technology:**

**X-Ray Nano-Spectroscopy of Quantum Materials**

- PETRA IV will make differences in the electronic structure of materials directly visible, quantifiable and ultimately controllable on the local, atomic level. Processes in functional materials can be observed in live action.

- PETRA IV will shift the limits of today’s X-ray spectroscopic methods from a spatial resolution in the micrometre range to the nanometre range.

- The combination of high energy and high spatial resolving power at PETRA IV has the potential to revolutionise the understanding of functional materials whose macroscopic properties are based on quantum states. High-temperature superconductivity is a prime example.

- Complementary to PETRA IV, the European XFEL makes very fast electronic processes visible by combining spectroscopic energy resolution with highest time resolution.
PETRA IV – Conceptual Design

The Accelerator

Originally built for high-energy physics starting 1976, the PETRA storage ring at DESY was operated first as an electron-positron collider and later as a pre-accelerator for the HERA electron-proton collider. Since end of 2009, the PETRA storage ring has been operated as part of the third-generation synchrotron radiation source PETRA III. Starting in 2014, the experimental programme at PETRA III was extended, accommodating 12 additional beamlines in two new experimental halls.

With the conceptual design presented here, a next, fourth-generation synchrotron radiation source is proposed: PETRA IV. It will deliver photon beams close to the physical limits in terms of parallelism and smallest achievable source size, approaching the diffraction limit in the hard X-ray range. This limit is reached when the size of the entire electron beam and its divergence are matched to the natural size and divergence of X-rays emitted by a single electron. With increasing X-ray energy, it becomes more and more difficult to reach this diffraction limit. A diffraction-limited beam implies that (nearly) the full X-ray beam is laterally coherent and can be focused to the diffraction limit, effectively making PETRA IV the ultimate X-ray microscope.

The product of the beam size and divergence of the electron beam, the electron beam emittance, is characteristic for a given storage ring. It results from quantum excitation and radiation damping during the orbital motion of the electrons and the interaction of the electrons with each other. To reach the diffraction limit at about 10 keV, an emittance of 10 pm rad or smaller is needed. While the vertical emittance of PETRA III is already close to this value, the horizontal emittance of 1300 pm rad is about two orders of magnitude larger than the diffraction limit in the hard X-ray range. The aim of the PETRA IV project is to reduce the horizontal emittance to a value in the range of 10 pm rad to 20 pm rad close to the diffraction limit. Due to its large circumference, which exceeds that of all other synchrotron radiation sources worldwide, the PETRA storage ring is particularly well suited to reach this exceptionally small emittance, making PETRA IV the world-leading hard X-ray source for decades to come.

The PETRA storage ring has an overall circumference of 2304 m and consists of eight arcs with a total length of 1612.8 m as well as two times four straight sections with lengths of 64.8 m and 108 m, respectively. Originally designed for high-energy physics experiments, this geometry was very beneficial for PETRA III, since the straight sections could be used to install damping wigglers and thus improve the beam quality significantly. The large circumference and large bending radius are also very beneficial for PETRA IV, since the beam emittance scales with the third power of the bending angle per arc cell. The long straight sections provide space to accommodate highly optimised 10 m long insertion devices, reaching brightnesses exceeding that of other planned synchrotron radiation sources by an order of magnitude. In addition, they ease the layout of the injection and extraction sections and provide sufficient space for other subsystems. Nevertheless, to meet the requirements for the injection into the PETRA IV storage ring, it will be necessary to also upgrade the injector complex. A new booster synchrotron will provide a low-emittance beam that is suitable for injection into PETRA IV. These advantages, together with the considerable cost saving related to reusing most of the existing ring tunnel and the existing experimental halls, make it possible to design a sustainable diffraction-limited hard X-ray source within the existing geometry of the storage ring. A comparison of the design parameters of the PETRA III and PETRA IV storage ring is summarised in the following table.

The conceptual design of the PETRA IV storage ring foresees a new design for the magnet arrangement that keeps the electrons on their orbit. This new design of the electron optics is based on a hybrid seven-bend achromat (H7BA) lattice, a variant of the multibend achromat, which was developed at the European Synchrotron Radiation Facility for the ESRF-EBS upgrade. Due to the larger bend-
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Design parameter | PETRA III | PETRA IV
---|---|---
Operation mode | Continuous | Timing | Brightness | Timing
Energy / GeV | 6 | 6 |
Circumference / m | 2304 | 2304 |
Emittance (horz. / vert.) / pm rad | 1300 / 10 | < 20 / 4 | < 50 / 10 |
Total current / mA | 100 | 200 | 80 |
Number of bunches | 960 | 40 | 1600 | 80 |
Bunch current / mA | 0.1 | 2.5 | 0.125 | 1.0 |

The ing radius of PETRA IV compared to the ESRF-EBS and other planned fourth-generation synchrotron radiation sources worldwide, PETRA IV can reach by far the smallest emittance.

While the design of the lattice entails similar requirements as for the ESRF-EBS, the sextupole and octupole magnets in the PETRA IV lattice have to be stronger than those in the ESRF-EBS storage ring, and a new design of these magnets will be necessary for PETRA IV. Prototypes of these magnets will be built during the technical design phase. For most of the other magnets, the proven ESRF-EBS magnet designs demonstrate the feasibility of the magnet lattice of PETRA IV.

The PETRA IV magnet lattice also requires a very precise alignment of the accelerator components (magnets and beam position monitors). This is due to the fact that the sensitivity of the beam dynamics to alignment errors at PETRA IV compared to PETRA III or other third-generation light sources is increased significantly due to the very strong focusing of the electron beam. Establishing the circulating beam and recovering the dynamic aperture require an iterative procedure that involves several correction steps, similar to the procedure implemented for other upgrade projects. Simulations of these procedures for PETRA IV were performed based on a statistical model of alignment errors, which generates random seeds representative of possible alignment scenarios in the PETRA tunnel. The simulations demonstrate that the alignment can be achieved to the required precision.

The demands on magnet alignment for the operation of PETRA IV are 30 µm (rms) for the transverse magnet offsets for selected / the most delicate magnets. The alignment precision achieved at PETRA III nearly reaches the range of PETRA IV requirements. Simulations of the measurement procedure show that the required accuracy of the magnet alignment on the girders can be achieved by introducing a larger number of reference points and improved metrology.

The ambitious performance goals of PETRA IV are approaching the limits of the present state of the art of accelerator physics and technology. Therefore, a strategy for risk mitigation in this highly complex project is mandatory. The risk of serious conceptual flaws is counteracted very efficiently by thorough analyses and detailed studies performed by the accelerator design team. A continuous exchange with other colleagues in the worldwide accelerator community and with DESY’s Machine Advisory Committee (MAC) is extremely valuable to avoid overlooking design flaws or missing opportunities for further design optimisation.

The technical risk mitigation strategy is based on two pillars: (i) building and testing of prototypes and (ii) the possibility of testing prototypical PETRA IV components or diagnostics, correction concepts and controls with beam in the PETRA III ring and the present injector complex. The risk mitigation strategy is covering all subsystems of PETRA IV, including the magnets, alignment and stability of components, power supplies and utilities, the vacuum system, the radio frequency system and the beam diagnostics, to name only the most important subsystems.
Photon Beamlines

PETRA IV will enable groundbreaking and transformative new experiments. In addition, established experimental techniques will be significantly boosted by the new source. The concept foresees 30 undulator beamlines distributed over four experimental halls, one of which is to be built within the project. The long straight sections at the entrance of each hall allow for optimising an undulator source with a length of up to 10 m, matching the electron beam parameters. In this way, a spectral brightness can be delivered to the experiments that exceeds that of all other existing and planned future sources by an order of magnitude. All other beamlines will have a 5 m undulator source.

The beamline portfolio of PETRA IV will be developed together with the user community during the coming technical design phase. The definition of beamlines will be based on the science drivers of PETRA IV and the resulting experimental requirements, the boundary conditions from the storage ring and on the existing beamlines at PETRA III, their user base and their scientific output.

To fully exploit the capabilities of the ultra-low-emittance storage ring, new technologies have to be developed in areas such as radiation sources, X-ray optics, sample environments, mechanical stability, precision and scan speed, detectors and data management. These aspects will be addressed within the coming technical design phase, and an optimised and standardised toolbox of beamline components will be developed that will help to streamline the construction and operation of the upgraded beamlines.

The major risks in this part of the project lie in the market development of the construction sector and in the market fluctuation of certain special materials, e.g. magnetic materials for the undulator sources. Both risks will be mitigated by long-term planning during the first three years of the project phase.

With the new suite of beamlines, PETRA IV will be ready to address the most pressing societal challenges, helping scientists and engineers from all fields of science to understand the structure and function of complex matter on all relevant length scales by directly looking at biological, chemical and physical processes under *in-vivo* and *in-situ/operando* conditions. Thanks to these insights, it will be possible to develop novel materials solutions and drugs with tailored local structures ultimately designed atom by atom.
PETRA IV
The Ultimate 3D X-ray Microscope
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1. PETRA IV Project

Synchrotron radiation sources are among the most versatile analytical tools used to study the structure, dynamics and function of the different states of matter. Since their first use in the late 1960s, synchrotron radiation technologies have been developed and diversified, and many scientific disciplines now strongly depend on their availability. The techniques developed at these facilities are indispensable in many scientific fields, ranging from physics, chemistry, biology and materials science to medicine, environmental science and nanotechnology. The increasing success of synchrotron radiation experiments and the corresponding user requirements have led to continuous improvements in source quality, mostly in source brightness and stability. The dramatic increase in brightness during the last two decades has triggered the development of a wealth of new experimental techniques that allow for a deeper and more detailed view of the structure and dynamics of matter. The increasing demands of the user community for ever brighter X-ray sources have triggered the development of novel magnetic lattices for synchrotron storage rings, called multibend achromat (MBA) lattices, which will enable another significant leap in source performance, bringing the brightness close to the physical limits of storage ring sources. This increase in brightness comes along with an about two orders of magnitude higher coherent fraction of the beam in the high-energy X-ray regime, which will allow these beams to be focused efficiently to the sub-ten nanometre range. As a result, coherence-based techniques will become highly efficient and allow revolutionary new insights into the molecular machinery of advanced materials and biological systems. This conceptual design report (CDR) discusses the transformation of PETRA III into the MBA-lattice-based synchrotron radiation source PETRA IV, which, thanks to the unique size and geometry of the PETRA storage ring, will be the brightest synchrotron radiation source worldwide.

1.1. PETRA IV Project Scope

The PETRA IV project comprises the upgrade of the present synchrotron radiation source PETRA III at DESY into an ultra-low-emittance source. At X-ray energies of up to 10 keV, PETRA IV will generate beams that are close to the physical limits in terms of parallelism and smallest achievable source size, approaching the so-called diffraction limit. It will be an ideal source for 3D X-ray microscopy of biological, chemical and physical processes under realistic conditions and on length scales from atomic dimensions to millimetres and time scales down to the sub-nanosecond regime. The efficient focusing to nanometre beams will enable the investigation of complex multifunctional materials at the nanoscale. This will facilitate groundbreaking studies in many fields of science and industry, such as health, energy, earth & environment, transport and information technology. PETRA IV will be operated as a user facility (LK II) for the production of synchrotron radiation for about 5000 hours per year. The assignment of beamtime to users will be based on an external peer-review system similar to the one established at PETRA III.

The main goal of the PETRA IV project is the replacement of the PETRA III storage ring with a state-of-the-art MBA-based ultra-low-emittance storage ring. This includes the renewal of parts of the existing accelerator chain and of the storage ring infrastructure, the civil
construction of a new experimental hall in the western part of the storage ring and the upgrade and relocation of existing beamlines including the construction of three new beamlines.

1.1.1. Upgrade of PETRA III into a Storage Ring Source with Ultra-low Emittance

In recent years, a new (fourth) generation of synchrotron light sources has emerged based on new storage ring lattice types, i.e. the MBA lattice in several variants. The new concept allows for a significant reduction of the horizontal emittance compared to existing facilities. The synchrotron radiation source MAX IV in Lund, Sweden, is the first light source to be successfully commissioned with this new lattice type. The new technique allows an increase in spectral brightness by one to two orders of magnitude, which will dramatically change the landscape of synchrotron radiation facilities in the next decade (cf. Figure 2.4). In this way, PETRA IV can be transformed into the world’s leading X-ray microscope, which, by operating at the theoretical limits, would enable users to follow biological, chemical and physical processes in complex materials in-situ/operando and on length and time scales from atomic dimensions to millimetres and from nanoseconds to hours, respectively. Figure 1.1 shows the layout of the planned synchrotron radiation facility PETRA IV.

The target parameters for PETRA IV are summarised in Table 1.1. For comparison, the parameters of the existing synchrotron radiation source PETRA III are shown as well. The conceptual design of the storage ring is presented in Chapter 6 in Part III.
Table 1.1.: PETRA IV parameters. PETRA IV will have two modes of operation, one optimised for highest brightness and one enabling time-resolved experiments.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>PETRA IV Brightness mode</th>
<th>PETRA IV Timing mode</th>
<th>PETRA III</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy / GeV</td>
<td>6</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>Circumference / m</td>
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<tr>
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<tr>
<td>Number of bunches</td>
<td>1600</td>
<td>80</td>
<td>40 . . . 960</td>
</tr>
<tr>
<td>Emittance</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>Horiz. $\epsilon_x$ / pm rad</td>
<td>$&lt; 20$</td>
<td>$&lt; 50$</td>
<td>1300</td>
</tr>
<tr>
<td>Vert. $\epsilon_y$ / pm rad</td>
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<td>$&lt; 10$</td>
<td>10</td>
</tr>
<tr>
<td>Number of undulator beamlines</td>
<td>30</td>
<td>21(26)</td>
<td></td>
</tr>
</tbody>
</table>

1.1.2. Experiments and Beamlines at PETRA IV

Today’s experiments and beamlines at PETRA III are state-of-the-art and in many aspects at the forefront of developments. They are continuously being enhanced in terms of instrumentation and methods. PETRA IV, however, will enable groundbreaking and transformative new experiments that require new specialised instrumentation. Hence, to exploit the full capability of the ultra-low-emittance storage ring PETRA IV, new technologies in areas such as X-ray optics, ultra-precision mechanics, detectors, data evaluation and data management have to be developed. These new technologies are described in detail in Chapter 7 and are reflected in the respective work packages of the PETRA IV project (cf. Figure 1.3).

During the construction phase of PETRA IV (cf. Section 1.3), the existing beamlines need to be realigned to the new storage ring geometry. Some of the beamlines need to be shifted within the existing experimental halls, and for some a relocation to the new experimental hall will be necessary. To fully exploit the new ultra-low emittance of the storage ring in view of highest brightness, each beamline providing nanofocus or coherence capabilities will be allocated to an individual 5 m straight section. The first beamline in each octant of the ring allows for installation of an undulator source up to 10 m in length optimised for ultimate brightness. These ultra-bright flagship beamlines can push X-ray analytics to its limits in terms of spatial, temporal and spectral resolution (cf. Chapter 7.2).

In the technical design report (TDR) preparation phase (see Section 1.3 and Figure 1.4), the scientific requirements for the beamlines will be investigated in detail, which will in turn result in definitions of the corresponding technical requirements for the instrumentation. Moreover, additional new beamlines are to be constructed in the new experimental hall (see Figure 1.1). The beamlines will be defined in more detail in the TDR phase in cooperation with the user community, the KFS\(^1\) and the DESY advisory committees.

New PETRA IV Experimental Hall

The technical requirements of the new storage ring imply that the current close spacing of the beamlines cannot be maintained. A new experimental hall is therefore needed, which will be built in the western part of PETRA (see Figure 1.1). This building has similar specifications to the present experimental halls and will follow the curvature of the storage ring. It will be about 600 m long and offer space for 16 beamlines including all infrastructure, eleven of which will presumably host existing beamline instrumentation by relocation. Of the five additional beamlines, three are planned to be new beamlines as part of the PETRA IV project and two will be kept open for upcoming new

\(^1\)The Komitee Forschung mit Synchrotronstrahlung (KFS) is an elected body of representatives of the German synchrotron and FEL user community.
ideas. Like for the other experimental halls, special mechanical and temperature stability is required. Both user laboratories for the experiments at the beamlines and offices for beamline staff are also foreseen in this hall. The technical requirements of the hall result in a building placed outside the current campus.

It will be situated in the Lise Meitner Park. Interference with the well understood importance of this park as part of the Hamburg ecological urban planning endeavours will be restricted to the minimum. Additional resources are foreseen to guarantee this condition.

1.2. Planned Governance Structures during Construction and Operation

The *Deutsches Elektronen-Synchrotron* DESY is a foundation under private law and a member of the Helmholtz Association. It is organised in five divisions (Accelerators, Photon Science, Particle Physics, Astrophysics Physics, Administration, see Figure 1.2). DESY is governed by a directorate consisting of a chairman and the five division directors. The directorate is supervised by a Foundation Council (*Stiftungsrat*) consisting of representatives from the funding bodies and four members from industry and society. DESY is advised on scientific and strategic matters by a Scientific Council (**Wissenschaftlicher Rat**, WR), which also reports to the Foundation Council. Each division has its own advisory body that reports to the WR. As the PETRA IV project is pursued mainly by the Accelerator (M), Photon Science (FS) and Administration (V) divisions, the most relevant advisory bodies will be the DESY Machine Advisory Committee (MAC), the Photon Science Committee (PSC) and the Administrative Advisory Committee (AAC). Additional advice will be provided by the Innovation Advisory Committee (IAC). Each division is subdivided in groups and in some cases in subgroups responsible for particular tasks and headed by a group leader.

Figure 1.2.: Organisation chart of DESY (June 2019).
Coordination with the European Molecular Biology Laboratory (EMBL) is facilitated by regular meetings at the managerial and at the working level. The scientific staff of DESY and of the external working groups on site also elect representatives to the Scientific Committee (Wissenschaftlicher Ausschuss, WA), which advises the directorate on scientific and strategic matters.

All scientific activities of DESY are part of the Helmholtz research field Matter. DESY’s photon science activities, the user operation of PETRA III and the FLASH free-electron laser facility are part of the Helmholtz Programme From Matter to Materials and Life.

1.2.1. Management during the PETRA IV Project Phase

The responsibility for the PETRA IV project lies with the DESY directorate. For the PETRA IV project, the directorate has appointed a project leader (PL) and deputy project leaders from the Accelerator and Photon Science divisions to constitute the PETRA IV project management. In addition, a PETRA IV steering board with members from the directorate and the project management team has been installed in order to deal with overarching matters such as contacts to funding bodies and authorities. Following the positive experience with earlier DESY projects — especially the PETRA III project — the PETRA IV project has been subdivided into four main work packages (Strategy and Management, Accelerators and Storage Ring, Photon Science Experiments, Infrastructure and Integration) as can be seen in Figure 1.3. These four main work packages are further subdivided into work packages dealing with specific tasks. For each work package (WP), a responsible WP leader (WPL) has been appointed. The personnel for the individual WPs is recruited from the responsible DESY groups. To carry out the project, the PETRA IV PL and WPLs will conclude written agreements with the DESY group leaders (GL).

Figure 1.3.: PETRA IV project structure showing all work packages for the PETRA IV technical design phase (November 2019). For the coordination of work packages to be run by DESY’s partners, like EMBL or HZG, suitable structures will be implemented.
and division directors on the provision of personnel and resources for the project as well as on additionally required resources, interfaces to other WPs, deliverables and the schedule. This practice was successfully implemented in the PETRA III project. The PETRA IV project management will be assisted by a group of technical and scientific coordinators as well as by a project office on matters concerning scheduling, change management, budget control and documentation. The entire organisational structure of the PETRA IV project is shown in Figure 1.3. As for PETRA III, a number of work packages will be under the responsibility of DESY partners such as EMBL or the Helmholtz Centre Geesthacht (HZG). These WPs will be managed using established and further optimised models.

The project is supported by central infrastructure groups on technical and administrative matters. The project status is regularly reported to DESY’s advisory and supervisory bodies, who give their advice and feedback to the directorate, as well as its partners.

1.2.2. Management During the Operation Phase

In the same way as PETRA III, PETRA IV will be operated as a LK II facility within the Helmholtz research programme From Matter to Materials and Life (MML) in the Helmholtz research field Matter. As such, all the rules for Helmholtz LK II facilities will apply. About 80% of the beamtime at PETRA IV will be made available either through an open peer-reviewed access mode for academic users or through privileged access for a fee for industrial users or privileged access groups (for details cf. Section 2.2).

Like PETRA III, the PETRA IV facility will be operated within the established DESY matrix structure and again jointly with DESY’s partners EMBL and HZG. There will be a lead scientist who is responsible for the scientific management of the facility and reports directly to the director of the Photon Science (FS) division. This scientist will be in charge of the scientific-strategic development of the facility and act as representative of the facility within the research and user community. The experiments and beamlines at PETRA IV as well as the organisation of the user support are the responsibility of the FS division and of the respective groups in charge of the operation and maintenance of the PETRA beamlines. The operation of the accelerator is the responsibility of a machine coordinator who will report directly to the director of the Accelerator (M) division. This coordinator is supported by the technical groups through the matrix structure of the M division. IT support will be provided by DESY’s central IT group (Particle Physics division) and administrative support by the central Administration (V) division. For PETRA IV beamlines to be operated by EMBL, models for management and operation established during the past four decades of cooperation will be used.

1.3. Schedule

DESY has a long tradition and extensive experience in designing, building and operating large-scale facilities, such as PETRA III and the accelerator of the European XFEL. Based on this experience and in order to both minimise the downtime for users between the shutdown of PETRA III and the start of operation of PETRA IV and ensure a reliable course of the upgrade project and a robust financial plan, the project has been divided into several phases, as illustrated in Figure 1.4:

**CDR Phase**
The conceptual design was developed together with a detailed analysis of the science case and the societal impact. This phase has just come to an end with the completion of this conceptual design report (CDR) (Milestone 1).

**TDR Phase**
Immediately following the CDR phase, a detailed technical design for the upgraded facility will be developed. During the TDR phase, first prototypes of mission-critical components will be designed, built and tested. As the basis
for the realisation of the PETRA IV project, the technical design report (TDR) will contain all project management plans, technical specifications, logistics, robust financial estimates and a detailed risk assessment. We expect that the risk assessments and financial estimates will be available at the latest by the end of 2020 to serve as input for a submission to the National Roadmap for large-scale facilities (Milestone 2.1). At the end of this phase, in 2022, a detailed TDR will be available (Milestone 2.2).

Project Approval Phase
In parallel to the TDR phase, several steps have to be taken for the approval of the project on various levels:

- Approval within the Helmholtz Association by the Forschungsinfrastruktur (FIS) Commission: This process was started at the end of 2018 and is expected to be completed in mid-2020.
- Coordination at the European level: Inclusion of PETRA IV in the LEAPS\(^2\) Roadmap.
- Coordination with partners like EMBL and HZG about potential contributions to PETRA IV.

- Submission of the project to the National Roadmap for large-scale facilities will presumably be ready beginning of 2021 (Milestone 3). The final project approval is granted with the admission to the National Roadmap.

Project Phase (Construction Phase)
Provided the financial approval of the full project in 2022, starting 2023, approximately two years will be needed to prepare and produce all the components and plan the civil construction, installation and commissioning of the new facility (Milestone 4). During this phase, operation of PETRA III will continue in regular user mode. Just before the start of civil construction and installation, PETRA III will be shut down. The civil construction, installation and commissioning of the new storage ring and the beamlines are scheduled to last about two years, i.e. from the beginning of 2025 to the end of 2026, and end with Milestone 5.

Operation Phase
This phase, which will follow the commissioning of PETRA IV, is planned to start in 2027. The facility is expected to be operated beyond 2050.

\(^2\)League of European Accelerator-based Photon Sources
1.4. PETRA IV Project Alternatives

To make the best use of the new MBA accelerator technology and create a leading synchrotron radiation facility with parameters similar to those in Table 1.1, DESY has analysed several possibilities in view of performance, practical implementation, sustainability and costs. Three alternatives have been analysed and are briefly described here.

**New Facility on a Green-Field Site**
Such a facility would provide maximum freedom in the choice of parameters, allowing for the lowest possible emittance and best beam parameters (optimal length of the straight sections, matching of electron and photon beam parameters, optimal stability of the stored beam). The number of beamlines could be significantly extended, and the “dark time” between the shutdown of PETRA III and the startup of the new facility could be minimised. However, this would require significant additional resources for all the infrastructure that needs to be built as part of the project. An integration into the growing Science City Bahrenfeld (cf. Section 2.1) would not be possible, and synergies due to the proximity to this rich scientific environment would be lost. Building the facility in parallel to PETRA III operation to avoid an extended dark time would require a significant increase in the number of expert employees for the time of construction, who might not be available within the international community.

**Optimum Storage Ring on the DESY Premises**
The PETRA III storage ring has eight long straight sections (cf. Figure 1.1), which reduces its circular parts to about 1.6 km compared to its overall circumference of 2.3 km. A circular storage ring within the PETRA footprint would have several advantages: Its larger bending radius and high symmetry would allow for ultra-low emittances and best beam parameters (optimum length of the straight sections, matching of electron and photon beam parameters, optimal stability of the stored beam) similar to the green-field option. As part of the Science City Bahrenfeld, a high level of synergy could be exploited. However, none of the existing PETRA infrastructure including the experimental halls could be reused, all of it would have to be demolished and rebuilt. This also includes some of the buildings on top of the ring tunnel, which would have to be rebuilt as well. The demolition and construction work would result in a longer shutdown of PETRA and a significant disruption of the activities on the DESY campus.

**Upgraded PETRA within Existing Infrastructure**
Upgrading PETRA III to an ultra-low-emittance storage ring would still allow worldwide exceptional beam parameters to be reached (cf. Table 1.1 and Figure 2.4). Optimum matching of the electron and photon beam parameters would be possible at five special flagship beamlines in the long straight sections (cf. Section 7.1). The brightness of all other beamlines at PETRA IV would exceed that of any other planned source worldwide (cf. Figure 4.3). Most of the PETRA III infrastructure could be reused, and the facility would be fully integrated into the rich scientific environment of the Science City Bahrenfeld. The boundary conditions of this storage ring design require special care in its realisation. Some parameters, such as alignment tolerances and magnet strengths, need to be pushed to the limits, leading to some technical challenges and requiring careful risk analysis. The upgrade requires a shutdown of PETRA III for the construction of PETRA IV, resulting in a dark time of about two years for users.

While the first two alternatives would provide optimum beam parameters for all beamlines, they have significant drawbacks compared to the third alternative. The green-field option comes with a more than twice higher construction costs and would forfeit the synergies with the partner institutions on campus and within the Science City Bahrenfeld. The optimal-storage-ring solution on the DESY campus would be highly disruptive to the campus life and operation, require about 50% higher in-
vestment costs and make many of the current investments obsolete. Upgrading PETRA III within the existing infrastructure leads to an only slightly reduced overall performance compared to the other two options, reuses a large portion of the investments in the DESY campus and fits in an ideal way into the scientific environment of the Science City Bahrenfeld. It requires by far the least additional resources and is thus the most sustainable. Therefore, we will pursue only this option in this Conceptual Design Report (CDR).
2. PETRA IV as Part of the Local, National and International Scientific Landscape

2.1. DESY, the Science City Bahrenfeld and the City of Hamburg

In 2018, largely on the initiative of DESY and its collaboration partners on the Hamburg-Bahrenfeld campus, the Free and Hanseatic City of Hamburg, the University of Hamburg and DESY started the urban development project Science City Bahrenfeld (Figure 2.1) with strong support from the German Federal Ministry of Education and Research (BMBF). The project comprises significant construction activities on the Bahrenfeld campus premises, the relocation of the Departments of Physics, Chemistry and Biology of the University of Hamburg to the Bahrenfeld campus, the integration of at least two complexes for startups and industry and the creation of more than 2000 apartments. The Science City Bahrenfeld, officially announced by Hamburg’s First Mayor Peter Tschentscher and Hamburg’s Minister of Science, Research and the Equalities, Katharina Fegebank in January 2019, will span at least two decades with investments of the order of more than one billion Euros. Eventually, the Science City Bahrenfeld will host over 15,000 scientists and students from all over the world. It will be a benchmark campus for the 21st century, combining science, industry and residential areas. The scientific infrastructures of DESY and in particular PETRA IV are a cornerstone for the project, ensuring world-class analytical opportunities for an interdisciplinary and international user community.

Already today, the Bahrenfeld campus hosts many strategic partners of DESY, making the site attractive for research, education and innovation. Around the unique photon sources at DESY, a vibrant scientific environment has been established. With the synchrotron radiation source PETRA III, the vacuum ultraviolet (VUV) and soft X-ray free-electron laser FLASH [1] and the European XFEL hard X-ray free-electron laser [2], the Bahrenfeld campus is a unique landmark in photon science.

Hubert Grimm
Managing Director, Hamburg Industry Association

“We actively follow the DESY project PETRA IV and support it explicitly! PETRA IV will strengthen research cooperation between industry and science and open up further innovation potential. This is an aspect that should not be underestimated in terms of location development. With PETRA IV, the research campus in Bahrenfeld can reach a unique international radiance. It will be an important contact point for science and industry not only for the Hamburg metropolitan region but also for Germany and on an international level.”

2.1.1. Science

In operating beamlines at PETRA III, DESY is collaborating closely with two partner institutions, the European Molecular Biology Laboratory (EMBL) [3] and the Helmholtz Centre Geesthacht [4]. Both operate outstations on campus as well as beamlines at PETRA III providing user access to their respective scientific communities. Activities at the EMBL Hamburg [5] include the integrated facility EMBL@PETRA III for applications in structural biology. The activities focus on state-of-the-art structural biology methods, making optimum use of the high-brightness synchrotron radiation source PETRA III and exploring novel opportunities at the European XFEL. EMBL is combining cutting-edge technology with an ambitious research programme on structures
of multifunctional proteins and protein complexes of biomedical relevance. The Helmholtz Centre Geesthacht (HZG) runs the German Engineering Materials Science Centre (GEMS) [6] on campus, with a strong focus on in-situ and operando characterisation of engineering materials both with X-rays and neutrons. HZG operates several beamlines at PETRA III, including general user support.

In addition to these partners, close collaboration in using the analytical capabilities at PETRA III exists with several institutes of the Max Planck Society.

To drive the science and development at the photon sources in Hamburg, two science centres were established, the Center for Free-Electron Laser Science (CFEL) [7] and the Centre for X-ray and Nano Science (CXNS), which also comprises the DESY NanoLab [8]. Their mission is to push photon science both for fundamental and applied research, develop new methods and instrumentation and directly support users with sample preparation and complementary analytical tools. Within CFEL, scientists from DESY, the Max Planck Institute for the Structure and Dynamics of Matter (MPSD) and the University of Hamburg collaborate in studying – with the help of the free-electron laser sources on campus (FLASH and the European XFEL) – the properties and behaviour of matter down to the atomic level and at attosecond to femtosecond time scales. In particular the structure and function of biological materials and solids and their electronic and structural dynamics. Being part of CFEL, MPSD is currently expanding, with a new building available in 2020. Materials synthesis techniques and complementary techniques for sample handling and characterisation on the nanoscale are provided within the DESY NanoLab as part of CXNS in order to support the users of the DESY photon sources.

The University of Hamburg [9] is the largest scientific partner on site. The Department of Physics [10] is present with several institutes: the Institute of Experimental Physics [11], the Institute of Laser Physics (ILP) [12], the Center for Optical Quantum Technologies (ZOQ) [13], and the II. Institute for Theoretical Physics [14]. The latest additions to the campus are the Center for Hybrid Nanostructures (CHyN) [15] and the Hamburg Advanced Research Centre for Bioorganic Chemistry (HARBOR) [16] whose building is currently under construction. The University of Hamburg and DESY have partnered in one former cluster of excellence (Hamburg Centre for Ultra-fast Imaging (CUI) [17]) and two new such clusters (Advanced Imaging of Matter (AIM) [18] and Quantum Universe (QU) [19]).
DESY also has a very close relationship to the Christian-Albrechts-Universität zu Kiel (CAU) [20] through the Ruprecht Haensel Laboratory (RHL). In this framework, CAU will also become a partner of CXNS and share space in the new building.

Attracted by the unique analytical capabilities on campus, the Centre for Structural Systems Biology (CSSB) [21] has been established as a further research activity. As a joint initiative of ten research partners from Northern Germany, including three universities and six research institutes from the Leibniz and Helmholtz Associations and EMBL as an intergovernmental research institution, CSSB is devoted to infection biology and medicine. The purpose of the centre is to unravel the underlying molecular mechanisms of important pathogenic processes in order to develop more effective treatment options against bacterial and viral pathogens and parasites. CSSB complements the analytical facilities on campus by a state-of-the-art cryo electron microscopy (EM) facility.

DESY and its collaboration partners plan several additional centres in the future, i.e. the Centre for Molecular Water Science (CMWS), the Wolfgang Pauli Centre (WPC) [22] for theoretical physics and the Centre for Data and Computing in Natural Science (CDCS).

The Centre for Molecular Water Science (CMWS) will bring together key experts from different areas of water-related research to develop a detailed molecular understanding of water. This includes dynamic processes in water and at water interfaces, which are highly relevant for chemistry, biology, earth and environmental science, as well as for technology. The research programme will build on the suite of enabling technologies available at PETRA IV, FLASH and the European XFEL, complemented by theoretical modelling.

The Centre for Data and Computing in Natural Science (CDCS) aims at tackling the growing data challenge that the Science City Bahrenfeld faces due to the ever advancing analytical capabilities on campus, both at the large-scale photon sources and at the other science centres. CDCS is a joint interdisciplinary effort of DESY and the local universities to foster technology transfer from informatics to fundamental and applied physics and vice versa. It will position data science as a new research field on campus. Within this framework, information scientists and domain scientists will work together on the pressing challenges in large-scale data treatment and analysis. In connection with CDCS, it is planned to establish the Interdisciplinary Data Analysis Facility (IDAF) as a user facility (Helmholtz LK II) in order to establish a complete data evaluation chain for DESY’s user facilities, in particular for PETRA IV.

On an international level, JNCASR (Bangalore, India) on behalf of the Indian user community and the University of Linköping (Sweden) on behalf of the Swedish materials science community cooperate with DESY in operating scientific instruments at PETRA III. The Ada Yonath experimental hall hosts the Swedish Materials Science Beamline (SMS) [23], while India contributes to the operational budget of PETRA III in exchange for privileged access [24].

### 2.1.2. Education

Education and training of students and young scientists are key to bringing interdisciplinary research facilities such as PETRA IV to fruition. DESY scientists are extensively engaged in university programmes. Many lead scientists and group leaders at DESY and at the partner institutions also have an affiliation with a university and are lecturing for bachelor and master study programmes, teaching lab courses, or supervising theses. This represents an important and successful recruitment channel. In addition, thanks to its world-class analytical facilities and its international and interdisciplinary environment, DESY is very attractive for Ph.D. students and postdocs. For the systematic training and career development of Ph.D. students, the PIER Helmholtz Graduate School (PHGS) [25], a graduate education programme of the University of Hamburg [9] in collaboration with DESY, plays a central role by participating in international fairs or publishing online calls and offering soft-skill training. Additionally, the international DESY summer student programme [26], during which students from about 30 different countries are hosted in DESY research groups, helps DESY to attract over 100 talented young people every year, with many coming back to DESY for a master or Ph.D. thesis later on.
The PHGS is mandated by the DESY directorate to develop and offer interdisciplinary qualification and development measures to Ph.D. students. Training courses and regular events allow for a vivid exchange between students from different research fields and guarantee a centre-wide homogeneity of general competencies. Additional graduate schools and structured Ph.D. programmes by the cluster of excellence Advanced Imaging of Matter (AIM), the International Max Planck Research School for Ultra-fast Imaging and Structural Dynamics (IMPRS-UFAST) [27], the graduate school “Data Science in Hamburg — Helmholtz Graduate School for the Structure of Matter” (DASHH) [28], the Max Planck School of Photonics and the EMBL International Ph.D. Programme constitute a well-structured portfolio of Ph.D. programmes which ensure all necessary help, regular monitoring and timely completion of the theses. The large community of postdoc on the DESY campus is a well-established source of competent personnel for synchrotron-based and related institutions world wide.

2.1.3. Innovation

DESY is at the core of a constantly growing research and innovation campus in Hamburg-Bahrenfeld. According to its innovation strategy, DESY is systematically opening up to industry and has set itself the goal of becoming a starting point for innovations in the high-tech sector. To achieve this goal, DESY is currently building a suitable ecosystem for knowledge-based high-tech startups, established technology-oriented companies and applied-research institutes on the DESY campus in Hamburg. The establishment of a high-quality infrastructure for high-tech spin-offs is an essential part of the future Science City Bahrenfeld.

The Science City Bahrenfeld is a holistic concept aiming at closely connecting excellent science, teaching and business in an urban setting. Such an international, highly connected district has a high potential to develop into a German science and business centre. DESY and the scientific departments of the University of Hamburg form the core institutions in the project, which is supervised by the Hamburg Authority for Urban Development. As part of the project, the City is developing an Innovation Park, which will be located 800 metres from the DESY campus and where companies fitting to the innovation profile of DESY will be settled.

The DESY Innovation Village, which was opened in February 2019, is a first important milestone in the development of complementary high-quality infrastructure for high-tech startups and young research groups on the Bahrenfeld campus. The objective is to attract startups to the DESY campus and the entire science and technology ecosystem in Bahrenfeld. The Innovation Village offers modern office, workshop and laboratory space for founders and innovative projects (approx. 1000 m²). Existing startups currently use the Innovation Village as a transitional solution until the Innovation Centre on the DESY campus is built. In the long term, it will provide space for innovation projects, e.g., validation projects or teams in the pre-start-up phase.

The next major building block is the Innovation Centre, a joint project of the University of Hamburg, the City of Hamburg and DESY. The aim of this large-scale project is the construction of a high-quality complex for startups and companies working in the fields of the life sciences, biotechnology, nanotechnologies and new materials. The centre is designed to provide tailor-made infrastructure in particular for newly founded high-tech companies that are challenged by long and costly incubation periods. The complex infrastructure will combine co-working space with laboratory space (more than 2000 m²) and support the startups with consulting services and a favourable rent. It will offer S1 biological laboratories, clean-rooms, workshops as well as office space and high-quality event rooms. In addition to providing in-house laboratory units, the Innovation Centre will also make the infrastructure of DESY and its partners accessible for startups. An integrative approach that connects innovation projects and research activities aims at systematically interlinking science and business. Establishing research and industry multipliers (such as the Universitätsklinikum Hamburg-Eppendorf (UKE), Life Science Nord) near the campus might be one important aspect in this mission. Moreover, DESY is trying to involve further strategic partners. The construction phase for the Innovation Centre started in spring 2019 and is expected to be finished by the end of 2020.
2.2. The User Facility PETRA IV

In the same way as PETRA III at present, PETRA IV is to be operated as a user facility (LK II). As such, a large fraction of the beam-time (≈ 80%) will be made available to external user groups including industrial users. The internal users of DESY’s photon science research programme (LK I) also have access to the infrastructures through the peer-review proposal system.

The users of the present synchrotron radiation source PETRA III are from many areas of science and engineering, ranging from physics, chemistry, biology and biomedicine to geological, environmental and materials sciences as well as nanoscience and technology. Research at PETRA III covers activities within all Helmholtz programmes (cf. Section 2.4.1) and contributes in various ways to the grand societal challenges (see Figure 2.2a). Beam-time at PETRA III is highly requested, with an overbooking factor between two and three. In 2017 and 2018, DESY and its partner institutions organised 13 workshops on the science case for PETRA IV. More than 700 users as well as interested scientists who had so far not used synchrotron radiation for their research participated in these workshops and expressed their interest in the new experimental opportunities at PETRA IV, which are detailed in Chapters 3, 4 and 5 in Part II. The more than 170 oral contributions covered all the scientific fields mentioned above. As a result, many of the participants of the workshops are actively helping to shape the science case of PETRA IV. In comparison with all other synchrotron radiation sources worldwide, PETRA IV will offer significantly better – and in many ways unique – experimental conditions. An increased demand by users from other regions of the world is therefore expected. In view of the targeted number of 30 beamlines and their improved performance, it is expected that PETRA IV can at least double the number of user visits compared to PETRA III today.

2.2.1. Access Management for Scientific Users

DESY has many decades of experience in access management to synchrotron radiation sources. User access is organised by the DESY user office, whereby access for Structural Biology is operated by EMBL. Access to PETRA IV will be organised in the same way as access to PETRA III. The existing administrative procedures will be adapted to the needs of the growing PETRA IV user community. Access is open to the worldwide scientific community and is granted on the basis of scientific excellence assessed in a peer-review process. Industrial access is also possible via a separate procedure described below. After passing an internal safety and feasibility review, all scientific proposals are evaluated by international Proposal Review Panels (PRP). The EMBL runs an additional Proposal Evaluation Committee (PEC) for Structural Biology proposals. That brings the total numbers to 85 reviewers and 11 PRPs. For PETRA III, the proposal review is currently carried out by
about 85 external reviewers in 11 PRPs. In the future, the PRPs will be organised by groups of beamlines that cover similar scientific topics or methods in order to improve grading and scheduling of user proposals. Beamtime is allocated based on scientific excellence to the top-rated projects. Like for PETRA III, it is planned to allocate approximately 4000 hours of the annual 5000 operation hours of PETRA IV to user experiments. For non-proprietary research by publicly funded institutions, the access to the facility is free of charge.

As part of the user programme, other DESY and EMBL facilities such as the DESY NanoLab or the EMBL Sample Preparation and Characterisation facility, can be accessed for sample preparation, handling and use of complementary characterisation tools. The scientific output of the user facility is regularly reviewed by DESY’s advisory bodies. The users’ interests are represented by the DESY Photon Science User Committee, which is elected by the users in regular intervals.

2.2.2. Access Management for Industrial Users

Next to academic users, DESY also offers beamtime to commercial clients and industrial users. They can obtain direct and rapid access to DESY’s large-scale facilities against payment. In this case, no scientific review process is required. The following services are offered:

- Feasibility studies in order to check the applicability of methods,
- Access to beamlines against payment and
- Additional services, such as sample preparation, conducting of experiments, data analysis and sample mail-in service.

The prices for these services are fixed annually on the basis of a full-cost model. Discounts are possible either by ordering a large amount of beamtime or publishing of results.

DESY’s activities to promote the use of its photon sources by industrial users are managed by the Innovation and Technology Transfer (ITT) group of DESY and for access to the beamlines and facilities run by EMBL via EMBLEM. The industrial projects at PETRA IV are organised in close collaboration between ITT and the Photon Science division to ensure a professional service to industrial clients. This includes a “one face to the customer” policy, which is ensured by the ITT group. By offering an efficient and professional service for industrial users, DESY wants to increase the commercial beamtime as a mid-term goal to 5% of the total beamtime available for users at PETRA IV.

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1https://embl-em.de/
2.3. PETRA IV in the International Context

PETRA III is currently the high-energy synchrotron radiation source (6 GeV) with the smallest horizontal emittance worldwide. It thus plays a leading role in research using tender to hard X-ray synchrotron radiation. However, there are already a number of upgrade projects for other synchrotron radiation sources that will reach a better horizontal emittance by means of a new storage ring technology (multibend achromat, MBA). The first source of this type is MAX IV in Lund, Sweden, a 3 GeV storage ring that started operation in mid-2016. The horizontal emittance of the European Synchrotron Radiation Facility (ESRF, 6 GeV) in Grenoble, France, will be significantly reduced with the completion of the ESRF-EBS project in mid-2020, which will improve the brightness of the source by roughly an order of magnitude relative to PETRA III. Worldwide, all major synchrotron radiation source operators are pursuing upgrade plans to exploit this new MBA technology for dramatically improving the horizontal emittance of their facilities. Examples of high-energy storage rings (6 GeV) are the APS-U project at the Advanced Photon Source in Chicago, USA, SPring-8-II in Japan, the planned new source HEPS in Beijing, China, and the new USSR source in Protvino, Russia.

In the lower electron energy range (<3.5 GeV), there are SIRIUS in Brazil, ALS-U at LBNL, USA, DIAMOND II in the UK, SLS II in Switzerland, Elettra II in Italy and SOLEIL II in France. The brightness of all these sources will be improved in the next 10 years. They will thus surpass the existing source PETRA III by a factor of 3 to 30 in emittance and reach the diffraction limit at correspondingly higher X-ray energies (cf. Figure 2.4). Owing to the worldwide unique circumference of the PETRA ring tunnel, the upgrade to PETRA IV will permit a much stronger reduction in emittance (by about a factor of 100 in comparison to PETRA III), enabling PETRA IV to again assume a world-leading position and reach the physical limits for the generation of synchrotron radiation at storage rings in the X-ray range at a photon energy of up to about 10 keV.

As a consequence and as detailed in Chapter 3 and Chapter 4, PETRA IV will offer unique possibilities to investigate complex matter on all relevant length and time scales from atomic dimensions to millimetres and from sub-nanoseconds to hours. PETRA IV will outperform its strongest competitors (e.g., APS-U and HEPS) by about an order of magnitude in brightness. Hence, it will be the ultimate 3D microscope for investigating biological, chemical and physical processes under realistically conditions. DESY and the Helmholtz Association will thus assume an international leading role in this field of research for decades to come. The Helmholtz-Zentrum Berlin (HZE) is operating the synchrotron radiation source BESSY II in Berlin-Adlershof. This source is run at an electron beam energy of 1.7 GeV and is therefore excellently suited for experiments at lower photon energies in the UV, VUV and soft X-ray range. Within the German National Photon Science Roadmap (NPSS), HZB is also planning an MBA upgrade of BESSY with a storage-ring energy of about 2 GeV. Since PETRA IV, just like PETRA III, will be operated at 6 GeV electron beam energy and cover the tender to hard X-ray range, these two sources will be widely complementary to each other.

2.3.1. Complementarity to Free-Electron Laser Sources

The individual photon pulses at synchrotron radiation sources are, with a few exceptions, at least 100 ps long or longer. Consequently, these sources can be used to investigate processes with longer time scales on the microscopic level, e.g. the dynamics of large atomic or molecular groups during a reaction. The domain of fast and ultra-fast atomic and molecular processes is that of free-electron lasers (FELs), which operate with up to 10000 times shorter photon pulse lengths. The FLASH free-electron laser at DESY in Hamburg (photon energy in the EUV and soft X-ray range) and the European XFEL X-ray laser with photon energies in the medium and hard X-ray range are complementary to the synchrotron radiation sources with respect to temporal resolution. The close proximity of PETRA and the free-electron lasers FLASH and European XFEL...
Figure 2.4.: Diffraction-limited photon energy for some synchrotron radiation sources and their future upgrades. PETRA IV will be the first source worldwide to reach the diffraction limit for hard X-ray energies. The diffraction-limited X-ray energies were calculated based on emittance values from Table 1 in [29] and updated according to [30–37].

on the DESY campus generates both administrative and scientific synergies. According to a recent assessment of the American Basic Energy Science Advisory Committee (BESAC) of the US Department of Energy (DOE), the future demand for X-ray analyses will be covered ideally by the complementary development of high-brightness storage ring sources and X-ray free-electron lasers.

2.3.2. Complementarity to Other Analytical Techniques

There are many different analytical techniques both at other research facilities using laser light, electrons, neutrons and ions or in the laboratory. The following brief overview over the most relevant techniques aims at placing science at PETRA IV into a broader analytical context [38].

Lasers play an important role in many fields of science. The LASERLAB-EUROPE consortium [39] involves leading institutions providing light pulses for research projects that explore dynamic processes from attosecond to picosecond time scales. Experiments at these facilities are mostly complementary to those at PETRA IV in a similar way as for FEL sources (cf. Section 2.3.1). This holds in particular for the European Extreme Light Infrastructure (ELI), which hosts the most advanced lasers with beamlines starting up to open for users in 2019.

In general, due to the energy of their photons, laser sources probe the electronic structure of the valence and outer electrons. VUV and X-ray sources, in contrast, can address the element-specific core electron levels of lighter and heavier elements, respectively. Thanks to their short wavelengths, X-rays can also provide spatial information on atomic positions. Neutron-based techniques offer many opportunities that are complementary to the photon-based ones at PETRA IV. As the absorption cross section for neutrons is lower than that of X-rays, neutrons are ideal probes for very thick samples. In scattering and diffraction experiments, due to isotope-specific atomic...
scattering cross sections, they yield contrasts different to X-rays, enabling e.g. studies of heavier atoms. Their spin makes them very sensitive to the magnetic structure of a sample, and since the energy of thermal neutrons is of the same order of magnitude than the one of vibrational states in matter, inelastic neutron scattering is the prime tool to study their properties. Due to their complementarity in contrast, it is quite frequent to find experiments in the literature in which both neutron- and photon-based techniques are used to provide an answer to cutting-edge scientific questions. However, the brightness of neutron sources is extremely low compared to today’s and future photon sources. The application of neutrons therefore requires relatively large samples, and neutrons are not very well suited for microscopy techniques. For decades, electron microscopy (SEM and TEM) has been a very important tool for characterising the structure and composition of matter with very high spatial resolution. In general, electron microscopes provide a real-space resolution far superior to that of X-ray microscopes. However, to obtain high spatial resolution, they require thin object sections and highly specialised thin sample environments for in-situ or operando studies. Meanwhile, transformative technological advances in detector technology allow cryo-EM-based techniques to be used to solve the structures of larger biological macromolecules without the need for crystallisation. In the future, the combination of cryo-EM and synchrotron-radiation-based techniques – with high-resolution images of individual macromolecules or smaller macromolecular complexes provided by macro-molecular crystallography using synchrotron radiation, medium-resolution images of large macromolecules up to large complexes using cryo-EM and lower-resolution images of entire cells using X-ray imaging – will very likely revolutionise our understanding of complex biological processes over a large resolution range.

Nuclear magnetic resonance (NMR) spectroscopy is used in chemistry to identify various compounds, mainly containing hydrogen (\(^1\)H). It can be extended to other elements, but requires isotopes with a net nuclear spin (e.g. \(^{13}\)C and \(^{15}\)N). The structure of smaller biomolecules can be identified using NMR from solution, without the need for any crystallisation. NMR requires larger specimens, e.g. high concentrations of soluble molecules with limited dimensions, and is not applicable to large proteins. In this way, it is complementary to cryo-EM and macromolecular crystallography using synchrotron radiation. NMR imaging is extensively used in clinical medicine and physiological chemistry, enabling in-vivo studies of soft tissues and human organs in action. It can provide 3D images of physiological processes in living organisms. However, the method is limited in spatial resolution by magnetic-field gradients to several tens of micrometres and is thus complementary to X-ray microscopy techniques, in particular those at PETRA IV.

A large number of other analytical and microscopy techniques, such as optical microscopy, scanning probe techniques (e.g. atomic force (AFM) and scanning tunneling microscopy (STM)), lab-based X-ray imaging and tomography, X-ray powder diffraction, X-ray diffraction (XRD), small-angle X-ray scattering (SAXS), X-ray photoelectron spectroscopy (XPS), ellipsometry, chromatography and mass spectrometry, provide invaluable complementary information to synchrotron-radiation-based techniques. As many of these techniques are required for a comprehensive pre-characterisation of the samples to be investigated at the photon science experiments at DESY, they are also made available to users close to the beamlines or in the DESY NanoLab. At PETRA IV, these off-line tools for sample preparation, manipulation and pre- or post-characterisation will be an integral part of the facility infrastructure.
2.4. Strategic Importance of PETRA IV

At present, there are only four synchrotron radiation sources worldwide operating at electron energies of 6 GeV or more with the capability of delivering highly brilliant photon beams up to the hard X-ray regime. These are, in the order of their realisation, ESRF (Grenoble, France), APS (ANL, Chicago, USA), SPring-8 (Harima, Japan) and PETRA III. Applications for hard X-rays are manifold. Due to their high sample environment penetration capabilities, they enable for example in-situ or operando studies or, in materials science, the investigation of the interior of larger workpieces. All three high-energy sources outside of Germany have plans to upgrade to multibend achromat (MBA) technology that are at different stages of completion. The ESRF-EBS upgrade project is presently being realised, the APS-U project is in a very advanced state of preparation, and SPring8-II is in its final planning stage. In addition, plans for two completely new sources of this class are being pursued, one in Protvino, Russia, and a second one in Beijing, China (HEPS). Construction work for the latter has already started. As soon as the first of these new sources starts operation, the request for analytical techniques using these extremely bright beams will rise quickly. For this reason, DESY has to make all possible efforts to realise the PETRA IV project in MBA technology as timely as possible in order to keep the world-leading position of DESY and of the Helmholtz programme From Matter to Materials and Life in this field. In this way, each region of the world has at least one high-energy synchrotron radiation source in addition to a number of lower-energy (1.5 – 3 GeV) sources in order to cover the entire spectrum of photon energies with the necessary synchrotron-radiation-based analytical tools. Within these regions, Europe has the largest synchrotron user community with over 25 000 annual users at the various European sources.

2.4.1. Strategic Importance for Germany

Within Europe, the German community is the largest and best organised one, dating back to the early days of synchrotron radiation at DESY/HASYLAB and BESSY. The German user community is very diverse, and PETRA III caters to all major scientific organisations and institutions, i.e. the Helmholtz Association, the Max Planck Society, the Leibniz Association, the universities and many other institutes (cf. Figure 2.3a). In this context, the BMBF-Verbundforschung also plays a crucial role, enabling university groups to actively contribute to new methods and to the further development of experimental techniques. For the German synchrotron radiation community, PETRA and the German share of 24% at the ESRF are crucial to enabling science programmes for which techniques in the tender to hard X-ray regime are needed. As far as possible, the experimental techniques at PETRA III were selected such as to maximise the degree of complementarity to the ones at the ESRF, carefully taking the demands of the different user communities into account. Many of the German user groups are at the forefront of methods and instrument development, in particular in the fields of X-ray nanoscience and X-ray imaging at the nanoscale. For these user groups, the projected PETRA IV beam parameters will give a huge thrust to their scientific work. The strategic importance of PETRA IV for the German and European user community was demonstrated by the overwhelming resonance to the PETRA IV workshops in preparation of the science case (cf. Chapter 5 for details).

As a technologically ground-breaking project, PETRA IV perfectly meets the goals of the German High-Tech Strategy. Within this strategy, the German government formulated three main goals:
• Link German research to the needs and
grand challenges of society
(cf. Section 3),
• Foster new technological revolutions and
• Create a creative space for innovation
(cf. Section 2.5).

PETRA IV is fully in line with these goals. As
a user facility, it will address all the decisive
questions of society in all the fields covered
by the mission of the Helmholtz Association.
Within the scope of the PETRA IV project, spe-
cial emphasis will be laid on increasing the
industrial use of synchrotron radiation in Ger-
many. In addition, the technological develop-
ments within this project will lead to new in-
novative products (cf. Section 2.5), which will
be transferred to industry in a structured and
efficient way.

Strategic Importance of PETRA IV for the
Helmholtz Association

Within the German science system, only the
Helmholtz Association has the resources, ex-
pertise and mission to operate large-scale sci-
ence infrastructures such as synchrotron radia-
tion sources for the entire science community.
The dedication of the Helmholtz Association to
excellent science and infrastructures requires
these facilities to be upgraded in regular inter-
vals in order to maintain international compet-
itiveness and attractiveness, not only for the
scientists within the Association but also for
the national and international user community.
At present, a large fraction of the user commu-
nity of PETRA III are scientists from Helmholtz
centres (see Figure 2.3a).
The PETRA IV project exactly follows these
lines by opening up the perspective of a world-
class analytical X-ray facility that will stay inter-
nationally competitive for the foreseeable fu-
ture. With its advanced analytical capabilities,
PETRA IV will contribute to the key Helmholtz
mission of solving the major challenges fac-
sing society, science and the economy (see
e.g. Figure 5.1) and to the research in all the
strategic programmes within the six Helmholtz
research fields: Energy, Earth & Environment,
Health; Aeronautics, Space and Transport;
Matter; Key Technologies.
In the focus of the Helmholtz programme From
Matter to Materials and Life (MML), within the
research field Matter, is, on one hand, the de-
velopment, construction and operation of world-
class user facilities in photon, neutron, ion and
high electromagnetic field science (Helmholtz
LK II) and, on the other hand, the research
activities to further develop these facilities, en-
hance their experimental capabilities and con-
tribute to solving scientific questions relevant
to basic research and to society (Helmholtz
LK I). PETRA IV as photon source will be im-
portant for the Helmholtz research field Matter.
Among the photon science facilities, the strate-
gic role of PETRA III/IV within the Helmholtz
Association and MML is and will be to cover
the required experimental techniques from
the tender to hard X-ray photon energy range,
while BESSY II and its future upgrade focus on
the UV to soft and tender X-ray regime.
In this way, together with the German share of
24% of the ESRF, both these facilities serve
the German and in part the European and in-
ternational synchrotron user community in an
ideal way with state-of-the-art experimental
capabilities covering the entire photon energy
range.

2.4.2. Strategic Importance for
Europe

In synchrotron radiation science today, it is
almost impossible to distinguish between a Eu-
ropean and a German perspective. This fact
was also taken into account when establishing
the League of European Accelerator-based
Photon Sources (LEAPS) in order to promote
an even stronger coordination between the dif-
frent European light sources. As a European
institution, the ESRF clearly has the largest
international user community, simply because
of its mission. However, synchrotron scientists
in general seem to “ignore borders” – the Eu-
ropean and international use of PETRA III was
about 44% in 2018 (see Figure 2.3b). This is
not a singularity, as all other synchrotron radia-
tion sources in Europe feature a 15 – 25%
share of German users alone. For the international Life Science community using synchrotron radiation in their research, the EMBL facilities at DESY have traditionally been a hub and will continue to do so on PETRA IV. Because of this multinational nature of the use of synchrotron radiation in Europe, all arguments for the strategic importance of PETRA IV for Germany made in the previous paragraph (Section 2.4.1) hold to a somewhat lesser extent also for Europe. Together with the upgraded ESRF-EBS, PETRA IV will ensure that the German and European user community has access to an unprecedented quality of tender to hard X-ray beams for the most demanding science projects and thus that Europe stays at the forefront of this field of science.

2.4.3. PETRA IV as Part of the DESY Strategy

DESY is one of the world’s leading laboratories for accelerator development, as it recently demonstrated again with the successful completion of the European XFEL, the most powerful FEL-based source for hard X-rays. In addition to operating the linear accelerator of the European XFEL, DESY also runs PETRA III as one of the world’s brightest synchrotron radiation sources for the tender and hard X-ray regime and FLASH as the most powerful FEL in the EUV to soft X-ray photon energy range. During the last two years, DESY has conducted a detailed strategic analysis to determine its future direction. The development, construction and operation of advanced accelerators are a central part of this strategy and one of DESY’s unique selling points. Today, the accelerators at DESY are almost entirely used to generate intensive, high-brightness synchrotron and FEL radiation as a unique tool to study the structure, dynamics and function of matter in a broad spectrum of applications. More than 80% of the beamtime for experiments available at the DESY facilities is being granted to external users mostly through a peer-review proposal system.

DESY’s research activities in photon science support its competence in the design, construction and operation of world-leading X-ray instruments at these facilities by exploring new areas in synchrotron radiation / FEL science, developing new methods in X-ray science and exploring and designing novel X-ray technologies. A central part of this strategy is the development of the necessary technologies for both the accelerators and the experimental techniques as well as for handling and evaluating the huge amounts of data made available by increasingly more complex experimental techniques. This strategy is implemented by establishing the Centre for X-ray and Nano Science (CXNS) and the planned Centre for Data and Computer Science (CDCS). The CXNS will be home to the DESY NanoLab, providing experimental facilities to produce, handle and characterise samples for experiments at the DESY photon sources. The CDCS will target the development of innovative data management and evaluation techniques to cope with the expected future data rates. In this way, DESY will enable first-class research at its photon sources both for in-house researchers and for academic and industrial users from all over the world. DESY will thus further strengthen its position as an international hub for top-level science and technology developments, as demonstrated by the successful establishment of the Centre for Structural Systems Biology (CSSB) close to PETRA III on the DESY campus and by the planned Centre for Molecular Water Science (CMWS).

In this strategic plan, the upgrade of DESY’s high-energy synchrotron radiation facility PETRA III to PETRA IV plays the most important role. On one hand, it will open up new and unique analytical capabilities (cf. Chapter 4) and scientific opportunities (cf. Chapter 3 and Chapter 5), especially where high spatial resolution X-ray analytics are required for a wide range of scientific areas. On the other hand, it will address the requirements of a large number of users and a broad science community. PETRA IV will not only vastly expand the analytical capabilities towards smaller length scales, but will also ensure DESY’s international competitiveness and attractiveness in the field of X-ray photon diffraction and spectroscopy, given the fact that almost every major synchrotron radiation facility operator worldwide is performing or planning similar improvements to their facility (cf. Section 2.3).

With PETRA IV, thanks to the large circumference of the existing PETRA ring tunnel, DESY will be in the unique position to regain the lead in brightness and beam quality, as has been
the case with PETRA III for third-generation synchrotron radiation sources. PETRA IV will outperform all currently planned future sources by about an order of magnitude in brightness, with all its implications (cf. Chapter 4 and Chapter 5).

Compared to FELs such as FLASH and the European XFEL, storage ring sources such as PETRA IV and BESSY III are mostly complementary with respect to their beam parameters. While FELs target experiments that explore extremely short time scales or extremely high pulse intensities, for example to record a “molecular movie” (see e.g. [40]) or to study matter under extreme conditions in ways not achievable by other means on Earth, experiments at storage ring sources in general address static and slower dynamical properties and functions of matter down to the sub-nanosecond regime.

Figure 2.5 illustrates the complementarity of the analytical capabilities for structural studies at DESY, the European XFEL and on the DESY campus. In this context, the new cryo-EM facility at CSSB ideally complements the analytical capabilities of the photon sources in the field of static analyses of biological systems using single-particle imaging and tomography.
2.5. Economic Importance, Innovation and Technology Transfer

PETRA IV will address various aspects of technology transfer and scientific services for commercial users. In this way, it will generate regional and supra-regional impact on the economy and society in general. This impact will start with the construction of the new facility, to which specialised suppliers will provide some of the necessary high-tech components and technological solutions, and continue with a structured exploitation of new technological developments for the accelerator complex and at the beamlines. It will end with offering commercial access to companies to analytical methods at PETRA IV and the expertise of its personnel to address challenges in their own market-driven innovation chains. In addition, the PETRA IV project will also act as cradle for new businesses. In its strategy, DESY includes the foundation of spin-off companies as a potential part of the exploitation chain. To support and promote this strategy, DESY has implemented the new position of Chief Technology Officer (CTO), associated to the directorate. All the goals and measures are regularly reviewed by the DESY Innovation Advisory Committee (IAC), in which industry representatives and partners advise the DESY directorate.

Enabling Suppliers through Knowledge and Technology Transfer

A complex high-tech facility such as PETRA IV generates high demands towards industry concerning the technological components of the accelerator complex, the synchrotron beamlines including the detector and IT infrastructure. Many of these high-tech components are not yet available on the market, and a dedicated R&D programme is required to bring the application readiness of the technology to such a level that it can be implemented at PETRA IV. The R&D programme (e.g. for special magnets) is conducted by DESY; the series production of the components, however, needs to be carried out by industrial partners. DESY will therefore protect its intellectual property (IP) and transfer the knowledge and technology to companies, thereby qualifying the industry to produce high-tech components for the PETRA IV project. The companies can then add the corresponding components to their product portfolio. This procedure has already been followed for the PETRA III project and the European XFEL, and it turned out to be a true success story for the technology transfer activities of a research centre such as DESY. For the European XFEL, for example, the production of components for the superconducting accelerator technology, which were developed at DESY, have been entirely transferred to industry. Nowadays, specialised companies successfully sell these products to many accelerator projects in the world.

Henning Fehrmann
CEO/Owner of Fehrmann GmbH, Deputy Chairperson of Family Businesses of the Hamburg Metropolitan Region, Spokesperson of the DESY Innovation Advisory Committee (IAC)

“The Innovation Advisory Committee (IAC) will support and accompany DESY and in particular its innovation and technology transfer in the coming years in the implementation of its strategic reorientation. Findings from the fields of basic research must be brought into the focus of industrial application much more quickly. The importance of new materials is increasing rapidly, and this will become even more apparent in the future. In order to understand the complexity and the possibilities of these new materials and to develop them further, it is necessary to advance to spatial scales that will only be made accessible by PETRA IV. It is indispensable for Germany as a location for innovation that cutting-edge research in close cooperation with industry opens the way for the technologies of the future.”

Exploiting Technological Developments at PETRA IV

DESY has worked out an innovation strategy and implemented performance indicators to exploit innovative DESY technologies. The indicators aim at detecting technological developments that are highly interesting for certain markets in order to bring them to a state
of being attractive for companies and eventually introduce the technology successfully into the market. To this end, DESY has implemented a scouting process that reveals the best ideas and developments from the research groups. Once identified, the technology can be supported through the DESY Generator Programme, which DESY has set up for early-stage funding in the technology transfer business. The global goal of the programme is to bring the technology to a stage where third-party funding or even private money can be attracted for developing a prototype. During these two stages, all relevant intellectual property (IP) will be protected. Usually, after the first two hurdles are cleared, collaboration with industry can help to properly address the challenges of the market. If the impact on the market is clear, the technology can be licensed to well-experienced companies, or a new company can be started within the DESY start-up programme. PETRA III triggered already the foundation of three companies exploiting techniques and developments at the facility. PETRA IV is expected to generate a similar indirect impact on the economy and society. As a primary benefit to society, the results of all academic research are published and thus made available to the public. Academic users at PETRA III today consider about one fourth of their proposals as pertaining to the applied sciences (23 %) or being industrially relevant (4 %) (cf. Figure 2.2b)

Commercial Access to PETRA IV
Like PETRA III, PETRA IV will be open for commercial users from industry. The facility can serve as an analytical tool to address challenges within industrial innovation chains and product development. Industrial research and cooperations with industry are being taken into account already today, at the very beginning of the PETRA IV project. Our goal is to establish a new commercial user community with its own share of beamtime alongside the academic users. In contrast to the scientific users of PETRA IV, commercial users will not have to pass a peer-review process but will have to pay for beamtime, scientific expertise and consulting.
DESY will be a professional and reliable partner for industry, helping the companies to solve scientific and technological questions be means of the excellent analytical power of PETRA IV. Commercial users will be offered direct and flexible access to PETRA IV beamtime, instruments and laboratories. The service will cover free feasibility studies to evaluate whether synchrotron radiation experiments can be effectively used to solve the user’s problem, sample preparation, beamtime and the support of scientific experts to conduct the experiments and analyse the experimental data. In addition, the offer will include mail-in service and remote access to the PETRA IV beamlines. If desired, all experiments and results will be treated with full confidentiality. Thanks to the close collaboration of DESY with the other scientific partners on the campus, commercial users will also benefit from special scientific expertise and experimental equipment. The commercial access to PETRA IV is expected to be used by industrial companies working in the fields of nanotechnology and nanomaterials, biomaterials, catalysis, batteries, energy generation, health, information technology and environmental protection. Prominent examples of research that are highly relevant for the industrial partners of DESY are described in Part II, especially in Chapter 5 at the end of each section. In order to implement new measures to increase the attractiveness of DESY as a service provider for industry, DESY plans to found a spin-off that will deal with all the requests from industry in a business-to-business model. The key to success in terms of industrial usage of PETRA IV is to act like an entrepreneur and therefore to belong to the same community as our clients.

PETRA IV as a Cradle for new Businesses
DESY welcomes and encourages spin-off projects of its employees and provides support throughout the whole process – from the first idea to the development of a business plan and the legal formation of the start-up company. It is our goal to inspire scientists’ entrepreneurial activities in the context of the PETRA IV project. A spin-off offers an alternative career option and transfers people and ideas to industry. This transfer enhances the interconnection and interaction between science based on the excellent large-scale facility PETRA IV and industry and technology. As a service for spin-offs, DESY offers consult-
In addition, DESY takes part in regional, national and international networks to strengthen its strategy and support its start-up companies. The foundation of startups is supported by two incubator institutes, the Start-up Labs Bahrenfeld and the Technology Centre (see Figure 2.6). Both institutes will be located on or in close vicinity of the DESY campus to stimulate a lively interaction between the scientific community, the large-scale research infrastructures and the start-up companies. Overall, this will strengthen the innovative culture on the DESY campus and within the Science City Bahrenfeld (cf. Section 2.1).

2.6. Sustainability

PETRA IV will not only be technically designed to the highest standards, it also will incorporate comprehensive sustainability concepts. The development tools and measures to support the long-term sustainability in a wide range of topics play a major part in the development of the PETRA IV proposal. In terms of sustainability, the PETRA IV project group is working along the LeNa\textsuperscript{2} guidelines and their management ideas, which focus on good governance and responsibility. This includes aspects of organisational development and research orientation as well as technical design questions and thus covers all three dimensions of sustainability: ecological, societal and economical.

The German and European user community participated in the development of the science case for PETRA IV (see Section 2.4.1 and Section 2.2). In terms of sustainability, it is very important to identify the demands of different interest groups and incorporate them into the development plans. Therefore, participation of a wide range of stakeholders over the

\textsuperscript{2}The LeNa guidelines on sustainability management for non-university research institutions were developed jointly by the Fraunhofer Society, the Helmholtz Association and the Leibniz Association; see \url{https://www.nachhaltig-forschen.de/startseite/}
complete cycle of development and usage of PETRA IV will be ensured. This includes aspects of the proposal review process, open access to the research facility as well as open-access data. The high brightness of PETRA IV will enable the science community to carry out research and make progress on the pressing questions of our time. Many areas profit from PETRA IV: Energy supply and efficiency (see Section 5.1), Life & Health (see Section 5.2), Transport & Technology (see Section 5.3), Earth & Environment (see Section 5.4) as well as Information Technology (see Section 5.5).

To go beyond fundamental research, DESY and the City of Hamburg are investing heavily into the establishment of innovation facilities and corresponding support to help young scientists and start-ups to develop their ideas towards application readiness. At the same time, access to PETRA IV will also be offered to the industry itself. These measures will ensure a sustainable development of the research results made with PETRA IV (see Section 2.1.3). DESY’s socio-economic impact on the region (Bahrenfeld, Hamburg and beyond) is already significant. The development of PETRA IV will ensure that DESY stays at the forefront of scientific development and research (see Section 2.5). This will boost the socio-economic impact even more and ensure employment and education within and around DESY (see Section 2.4 and Section 2.1.2).

To support DESY’s commitment to sustainability, as much hardware as possible will be reused or recycled (e.g. the present beamlines, see Section 7.1). New technologies, such as novel compact, energy-efficient (albeit not yet mature) injection systems based on emerging laser wakefield accelerator (LWA) techniques, will be evaluated in the Technical Design phase. DESY has been developing this novel accelerator technology for the past five years and has established itself as one of the world’s leading institutions pursuing this promising technology. Significant progress has been made in the achievable beam energy (up to 7.8 GeV from a 20 cm long structure [41]) and the long-term reproducibility and, with the rapidly evolving laser technology, LWAs could become a suitable complement to conventional accelerator-based injection systems. Questions such as how to match the beam into the storage ring and to what duration the intrinsically femtosecond-long bunches from the LWAs must be stretched to avoid strong coherent synchrotron radiation emission will be analysed during the Technical Design Report (TDR) phase. In addition, system reliability and robustness must be improved and demonstrated experimentally in the next five years. Investigations should be supported to develop the most energy-efficient technical elements for the synchrotron (without limiting its performance) and to study the possibility of using renewable energy. An energy demand calculation for the construction and especially for the usage phase can help to bring such ideas forward.

In cooperation with other research facilities that currently develop similar infrastructures, the project will strive for the highest possible efficiency (see Section 2.3). The development of prototypes in the next phase of the project, for example, should incorporate sustainable measures as mandatory. In this phase, incentives should also be developed to support the implementation of the latest technologies with highest efficiency.

The usage of waste heat as well as sustainable construction standards that are currently being developed for all DESY facilities will also be incorporated into the PETRA IV development. Emphasis should be put on possible synergies between the general DESY campus development and the PETRA IV plans. This includes for example the greening of buildings, improved insulation, LED lighting and controlled ventilation. PETRA IV will also be incorporated into the existing mobility arrangements at DESY and within the planned Science City Bahrenfeld3. This encompasses electric cars including charging stations, cargo bikes, Hamburg City bikes, improved public transport connections and more.

The ambition at PETRA IV is to open up to 30 beamlines on just one storage ring. More beamlines render an accelerator more efficient, as a single acceleration can support several beamlines. At the same time, there are limitations to building ever more beamlines, as the PETRA ring is situated in an established surrounding. Existing buildings and infrastructure limit the possibilities for new experimental halls.

3https://www.hamburg.de/sciencecity/
The only place where a new experimental hall could be built touches an existing park. The TDR therefore needs to put special emphasis on the incorporation of the facility into this environment. Sustainability also comprises topics essential for running an infrastructure as a large-scale user facility. Issues such as the handling of chemicals and problematic substances, the disposal of dangerous waste, the reduction of emissions as well as the handling of accidents will be covered by the established DESY structures, which ensure that DESY is a secure employer. They are also represented in the governance structure of the PETRA IV project (Figure 1.3), e.g. in the work packages WP 2.02 “Radiation Safety”, WP 2.03 “Interlock Systems” or WP 4.02 “Safety Management”. The sustainability issues mentioned above are only a first glance that needs further, more detailed development during the next phases of the project. In any case, structures are in place at DESY to ensure that sustainability aspects are comprehensively incorporated into the future thinking and development of the PETRA IV proposal (see Section 1.2).
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PETRA IV
Science and Innovation Case
3. Hard X-Rays for Understanding Complexity in Nature and Technology

Humanity is currently facing major global challenges in the fields of health, energy, environment, transport and information technology. Examples include the fight against cancer and infectious diseases, the supply of clean and sustainable energy as well as the reduction of greenhouse gases, to name a few. From a scientific point of view, solutions to these problems are closely related to our understanding of the structures and processes in matter on all length scales from atomic distances to macroscopic dimensions and of the underlying fundamental interactions.

A current lack of knowledge about the connection between the microscopic properties of matter on one side and the macroscopic behaviour of materials on the other side still prevents significant progress and further development in these areas. The scale-bridging mapping of structures and their dynamics under in-vivo and in-situ/operando conditions is therefore essential to decipher the processes and functionalities that occur in nature and thus to help solve important aspects of our grand challenges. PETRA IV will be a worldwide unique facility enabling scientists to gain insight into the structures and processes that are relevant to tackle these challenges.

The PETRA IV project at DESY aims to provide a unique X-ray light source that will yield 3D images of materials with over 100 times more detail than is achievable today. This will be made possible by upgrading the existing PETRA III facility on the basis of recent transformative developments in accelerator technology (Figure 3.2). As a result PETRA IV will generate X-rays with unprecedented brightness. They can be focused nearly without loss to nanometre spot sizes in order to achieve ultimate spatial resolution.

Figure 3.1.: Understanding the complexity in nature and technology requires a holistic view of structures and processes from the atomic/molecular level to macroscopic dimensions. Example: hierarchy of wood used with permission. Copyright University of Canterbury, 1996. Artwork by Mark Harrington.

This will allow for diffraction studies of highest resolving power and enable images with highest contrast to be obtained in order to reveal the faintest features of the materials under study – for the most detailed view on the structure and dynamics of matter ever (Chapter 4). With the conversion of the PETRA III storage ring into PETRA IV, the world’s most powerful synchrotron radiation source is planned to go into operation in 2027. The facility will be
the only synchrotron radiation source worldwide to reach the diffraction limit in the hard X-ray range (5 to 10 keV). As the ultimate 3D X-ray microscope, PETRA IV has the potential to make decisive, interdisciplinary contributions to today’s major challenges, e.g. by providing information on multifunctional hybrid materials and processes therein under in-vivo or operando conditions and with highest resolution and sensitivity. This will enable researchers and engineers to design and tailor the structure of complex materials down to the atomic level and thus provide solutions for novel materials in all research fields of the Helmholtz Association. In particular, PETRA IV will enable us to answer the following questions:

How can energy be harvested from sunlight and stored with highest efficiency?
This requires us to understand and control the interaction of atoms and molecules with light and the electronic and ionic transport in the complex structures of novel solar cells and batteries. PETRA IV will be able to visualise electronic transport phenomena in solar cells and electrochemical processes in batteries under working conditions and down to the atomic level, e.g. to understand the relevant ageing processes under operando conditions and on all relevant length scales (cf. Section 5.1).

How can the energy efficiency of engines and machinery be significantly improved to reduce harmful emissions?
This requires a fundamental understanding of tribological processes in order to be able to minimise frictional losses in a systematic manner. PETRA IV will be able to shed light on the physical and chemical processes at buried interfaces between moving parts in mechanical systems under working conditions, e.g. by means of X-ray microscopy with diffraction contrast at high X-ray energies (cf. Section 5.3).
How can we reduce greenhouse gas emissions, improve purification of exhaust gases and improve chemical production?

This requires chemical reactions in novel hierarchical catalyst materials to be monitored and controlled on all relevant length scales. PETRA IV will be able to image the chemical state of a catalyst material inside a reactor in three dimensions and under working conditions (cf. Section 5.1.4).

How can we stop or mitigate corrosion processes?

This requires a detailed understanding of surface (electro-)chemistry. PETRA IV will be able to image the local surface chemistry, in particular around defects, together with the dynamics of ions in aqueous solution (cf. Section 5.3).

How can we develop novel materials with exceptional properties?

This requires the understanding of the formation processes of novel materials, e.g. high-pressure synthesis of ultra-thin materials. Under extreme conditions of pressure and temperature, states of matter are created that not only help to explain geochemical, planetary and astrophysical processes, but can also produce revolutionary material properties. PETRA IV will be able to visualise the micro- and nanostructure in new materials during their production and under extreme conditions in order to correlate it with the materials' physical properties.

The central leitmotif of the questions mentioned above is to relate the structure and dynamics of materials on all length scales to the resulting macroscopic properties and functionalities. This can only be achieved with the highly brilliant X-rays of PETRA IV, whose large coherence length will enable high-resolution 3D images of materials in real time and under working conditions. The combination with complementary analytical methods, provided by other large-scale facilities and infrastructures available at DESY and on the Bahrenfeld campus¹ (FLASH, European XFEL, CSSB, CFEL, CXNS, CHyN), will offer a revolutionary cross-scale approach to solving critical questions in the natural and engineering sciences (cf. Chapter 2). When going into operation in 2027, PETRA IV will be able to provide a full coverage of all length scales to reveal the formation, structure and dynamics of complex systems in nature and technology.

With decreasing structural dimensions, the time scales for dynamical processes also decrease (cf. Figure 3.3). PETRA IV will be particularly suited to enter the temporal regime between nanoseconds and microseconds that is relevant for processes in the mesoscopic regime, thus shedding light on the dynamical origins of the formation of hierarchies and the emergence of function in nature and technology.

Figure 3.3.: Schematic view of the formation of complex systems. The key steps of structure formation and the emergence of functionalities take place on many length and time scales. With PETRA IV, scientists will be able to follow all these steps on all length scales and to understand and eventually design new functional materials and drugs.

¹To be developed into the Science City Bahrenfeld.
nology. Owing to its outstanding brightness, PETRA IV will in particular extend photon correlation techniques into the regime of nanoseconds and allow for low-dose correlation experiments by making use of the extended coherence volume at the larger photon energies. Complementary to the European XFEL that offers access to time scales from femtoseconds to nanoseconds, PETRA IV will provide access to longer time scales from nanoseconds up to hours. Making use of both the European XFEL and PETRA IV, scientist will be able study the dynamics in condensed-matter from femtoseconds to hours on the all relevant length scales (cf. Chapter 4).

These enhanced scientific capabilities of PETRA IV compared to existing sources are enabled by its outstanding X-ray beam properties. Thanks to its ultra-low emittance together with the implementation of new insertion devices, PETRA IV will exceed PETRA III by several orders of magnitude in the following performance parameters:

- The beams delivered by the PETRA IV undulators exhibit a more than 100-fold higher brightness and thus a more than 100-fold larger coherent flux (Figure 4.3).
- Up to an energy of 5 to 10 keV, the X-rays generated by PETRA IV will be diffraction-limited, i.e. laterally coherent, and can be focused almost free of loss. Smallest nanobeams with highest flux densities can therefore be generated. Moreover, the high coherent flux can also be used to study structure and dynamics of radiation-sensitive samples by coherent scattering with an extended beam.
- In the hard X-ray range well above 10 keV, the PETRA IV beam has an up to 1000 times higher brightness (Figure 4.3) and a much higher degree of lateral coherence than at PETRA III. For high-energy X-rays of 100 keV and beyond, the coherence will be comparable to that of present sources in the 10 keV range.

The following two chapters present the key enabling technologies of PETRA IV (Chapter 4) and the resulting science and innovation case (Chapter 5), respectively.

Jürgen Groß
Head of Central Division Research and Advance Engineering, Robert Bosch GmbH

“For a global technology company such as Bosch, PETRA IV as planned by DESY is extremely interesting, and we are looking forward to its implementation with excitement and great interest. Two aspects play an important role for us. On the one hand, such a project will bring basic research a long way forward and thus enable previously unknown insights into processes. These new findings are an important prerequisite for Germany’s future innovative strength in the global competition. New technical developments that go hand in hand with such a project are finding their way more and more quickly into industrial production. On the other hand, the possibilities offered by PETRA IV are very promising – especially for fuel cells: By studying these systems under operando conditions and improving our understanding of small-scale processes inside the cells, we can gain new insights and thus unlock potential for improvement that we want to fully exploit in terms of sustainability.”
4. Methods Enabling New Science with PETRA IV

Figure 4.1.: *With PETRA IV we will be able to image objects in-situ and operando from the nano to the macro scale and follow their dynamics from (sub-)nanoseconds to hours.*

PETRA IV will be the synchrotron radiation source with the highest spectral brightness worldwide, reaching the diffraction limit up to X-ray energies of about 10 keV (cf. Figure 2.4). This enables unique experiments to address the pressing societal challenges in fields such as energy, life and health, transport and technology, earth and environment, and information technology. This chapter describes the main experimental technologies that PETRA IV will enable and push to its limits thanks to its unique properties. A more technical description of the conceptual design of the storage ring and the beamlines is given in Part III in Chapter 6 and Chapter 7, respectively.
4.1. Generating Photons Made to Measure: Preparing X-Rays in a Well-Defined State

The key to enabling groundbreaking new experiments and improving most X-ray analytical techniques is to generate the X-rays already in the state needed for the experiment. Each electron in a storage ring emits X-rays in a certain cone around its direction of motion, as shown in Figure 4.2a. This defines the natural emission angle of the X-rays. To this natural emission cone corresponds a small effective diffraction-limited source size (cf. Figure 4.2a). The product of emission angle and diffraction-limited source size is called the natural emittance of synchrotron radiation for a single electron in the storage ring. Ideally, electrons in a storage ring would all radiate from the same source point into the same direction. In this case, the emission cones of all electrons would perfectly overlap and the radiation would be (spatially) as well defined as possible.

In a modern storage ring for synchrotron radiation generation, the horizontal electron beam emittance is much larger (typically by a factor 100 or more) than the natural emittance of synchrotron radiation for a single electron, as depicted in Figure 4.2b). Source size and beam divergence are large compared to the ideal case of perfect spatial and angular overlap mentioned above. The beam is thus less well defined, and the spectral brightness is reduced by roughly the same factor 100 or more compared to the ideal case. However, many experiments require the beam to be prepared in a much more defined state, in particular when investigating heterogeneous, hierarchically structured complex materials (cf. Chapter 3). This entails a filtering of the X-ray beam along the beamline, transmitting only the appropriate X-rays to the experiment and removing all others. For instance, to generate a small diffraction-limited beam for X-ray microscopy (cf. Section 4.2), only the coherent fraction of the beam can be focused. At the current synchrotron radiation sources (including PETRA III), for that purpose more than 99% of the radiation from the source has to be discarded.

PETRA IV will have a significantly reduced horizontal emittance, approaching the ideal overlap of emission cones for all electrons in a bunch for X-ray energies up to 10 keV. The X-ray source will therefore be much better de-
fined in size and divergence (cf. Figure 4.2c). Compared to present-day sources, the X-rays will be confined to a two to three orders of magnitude smaller phase space, resulting in a comparable increase in spectral brightness (cf. Figure 4.3) [1]. In addition, nearly the whole beam will be laterally coherent up to about 10 keV, which means that nearly the full beam can be efficiently focused for microscopy applications. For most experiments, the dramatic gain in spectral brightness translates directly into an improvement of the experimental conditions by many orders of magnitude. These large factors enable many new types of experiments and lead to significant improvements of existing techniques. The reduced emittance and improved spectral brightness of PETRA IV will push the following experimental fields:

**X-ray Microscopy**
The reduced horizontal emittance has the most prominent impact on X-ray microscopy, allowing all X-ray analytical techniques to be used as contrast mechanism in nanoprobe experiments. PETRA IV will thus be able to cover all length scales from nanometres to millimetres (cf. Chapter 3) and give a holistic view on hierarchical complex matter (cf. Section 4.2).

**Dynamics in Complex Materials**
The significantly increased coherent flux of PETRA IV has a strong impact on studies following the dynamics of complex materials (cf. Section 4.3). Because of the quadratic gain in signal-to-noise ratio as a function of brightness, huge improvements are expected for X-ray correlation spectroscopies (cf. Section 4.3). Other time-resolved techniques that depend linearly on the brightness will profit as well (cf. Section 4.2 and Section 4.3).

**Energy Resolution (Spectroscopy)**
Many high-resolution spectrometers select a tiny fraction of phase space, only. The high brightness helps to prepare a much larger fraction of photons in the desired phase space volume (cf. Section 4.4).
High-Energy X-rays
Today, the use of high-energy X-rays is strongly limited as a result of the comparatively low brightness at these energies. High-energy X-ray microscopy in particular is largely underdeveloped. Although high-energy X-ray beams at PETRA IV will not be diffraction-limited, the improvement in emittance directly translates into improved brightness and coherence properties. As a result, X-ray microscopy with high-energy X-rays will become highly efficient, making high-energy X-ray analytical techniques available as contrast in microscopy (cf. Section 4.5). PETRA IV will have coherence properties at 100 keV similar to those at 10 keV at PETRA III today, opening this X-ray energy range to coherence-based analytical and imaging techniques.

4.2. X-Ray Microscopy with Coherent Light: X-ray Analytical Measurements go Nano

X-ray microscopy techniques are those that will profit the most from the record emittance and spectral brightness of PETRA IV. At PETRA IV, all X-ray analytical techniques can in principle be combined with microscopy, allowing for quantitative X-ray analytical measurements of physical and chemical properties of spatially heterogeneous, complex specimens. The beam from a nearly diffraction-limited source can be focused to the Abbe limit nearly without losses, generating an ideal beam for all kinds of scanning probe techniques. In conventional scanning microscopy, the spatial resolution is limited by the lateral beam size. At the diffraction limit, the spatial resolution is given by Abbe’s resolution formula

\[ d_t = \frac{\alpha \lambda}{2NA}, \]

where \( \lambda \) is the X-ray wavelength, \( \alpha \) is a constant close to 1 given by the aperture function of the optics, and \( NA \) is the numerical aperture of the optics. All length scales \( l \geq d_t \) can be accessed directly in real space by imaging or scanning microscopy. This implies that the focal size does not depend on the demagnification ratio but solely on the numerical aperture of the optics. Therefore, large working distances can be combined with nanofocusing, allowing for more elaborate sample environments for in-situ and operando studies (cf. Section 4.7).

According to Equation (4.1), the key performance parameter of optics for diffraction-limited nanofocusing is their numerical aperture \( NA \). In the last decades, significant advances have been made in view of nanofocusing for various X-ray optics. Today, submicrometre beams are routinely generated using reflective, diffractive and refractive optics. Currently, almost all X-ray optics are limited by fabrication technology, and significant improvements are to be expected over the coming years. At least in principle, sub-nanometre focusing will be possible with diffractive optics [2–4]. Different nanofocusing schemes will be needed to address the full range of experimental requirements, e.g. in terms of focus size, beam shape and background, working distance and chromaticity.

To fully exploit PETRA IV for X-ray microscopy, efficient high-numerical-aperture optics will be needed. Currently, sub-10 nm beams are achieved with multilayer mirrors [5] and multilayer Laue lenses (MLLs) [6]. Single-digit nanofocusing is becoming more and more routine. For MLLs, numerical apertures corresponding to a diffraction limit of 3 nm have recently been achieved. By combining these optics with wavefront-corrective schemes [7], lower single-digit nanofocusing is expected to become routine by the time PETRA IV becomes available (cf. Section 7.3.2 for the design concept for nanofocusing optics).

In the case of diffraction-limited focusing, the flux of coherent photons in the focus is limited by

\[ F_c = Br \left( \frac{\lambda}{2} \right)^2 \frac{\Delta E}{E}, \]

where \( Br \) is the spectral brightness (cf. Figure 4.3) and \( \Delta E/E \) the spectral band width. For the presently brightest X-ray sources, such as PETRA III, the coherent flux is limited by the horizontal emittance of the storage ring and reaches about 0.1 to 1% of the total monochromatic radiation emitted by an undulator in the hard X-ray range (10 keV). With emittances
(both horizontal and vertical) in the range of 10 pm rad, X-ray beams at PETRA IV will be diffraction-limited at about 10 keV, i.e.

\[ \epsilon_{x,y} \leq \frac{\lambda}{4\pi}. \]  

This implies that (nearly) the full beam of an undulator is laterally coherent, i.e. the lateral coherence length is in the range of the beam size and can be focused to the diffraction limit [8]. At PETRA IV, scanning microscopy will therefore be more efficient by about two-to-three orders of magnitude, making novel applications in the nano cosmos possible.

Diffraction-limited focusing of the full undulator beam will have significant impact on all X-ray analytical techniques, as they can then all be efficiently used as contrast mechanisms in scanning microscopy. In this way, the “X-ray microscope” PETRA IV will give quantitative access on the nanometre scale to the local chemical distribution of (trace) elements by X-ray fluorescence (nanoXRF),

- (crystal) structure and mesoscopic order by X-ray scattering and diffraction (nanoXRD), both in the small-angle (nanoSAXS) and the wide-angle (nanoWAXS) regime,

- chemical state information and local chemical environment of an elemental species by X-ray absorption spectroscopy (nanoXAS) or inelastic X-ray scattering (nanoIXS),

- phononic and electronic excitations by inelastic X-ray scattering (nanoIXS),

- electronic properties and band structure by (angular-resolved) photoemission spectroscopy (AR)PES, also inside the bulk using hard X-ray photoemission (nanoHAXPES),

- fundamental excitations of complex materials with element selectivity and chemical state specificity by resonant inelastic scattering (nanoRIXS),

- magnetic properties and orbital ordering phenomena by resonant and non-resonant (magnetic) scattering, nuclear resonant scattering (nanoNRS) and X-ray magnetic circular dichroism (nanoXMCD),

- electronic transport properties by X-ray beam-induced current (nanoXBIC) and

- complex dynamics by correlation spectroscopies, i.e. photon and fluorescence correlation spectroscopy (nanoXPCS and nanoXFCS), including cross-correlation analysis (nanoXCCA).

These techniques can in many cases be combined to measure 3D maps of several chemical and physical properties simultaneously, an important prerequisite to understanding the structure and function of complex multifunctional materials.

The high flux in the focus makes 3D imaging by scanning microscopy with any of these contrasts feasible in short times. In addition, it is possible to study large samples with high resolution in a reasonable time, e.g. to find rare features in a complex surrounding (“needle in haystack” searches). Alternatively, the speed-up in data acquisition allows one to record movies of processes in-situ and operando (Section 4.7) with various X-ray analytical contrasts or under varying external parameters. Multi-parameter scans as needed in Small Angle X-ray Scattering (SAXS) and vector tomography [9, 10] for example will become routinely feasible (cf. Section 5.5.2).

So far, at current synchrotron radiation sources, photon-hungry techniques such as Inelastic X-Ray Scattering (IXS) and Nuclear Resonant Scattering (NRS) could not be combined with high-resolution microscopy. At a diffraction-limited source in the hard X-ray range, such techniques will be made available for nanoscopic investigations, giving for example access to local chemical information on low-Z elements in the bulk, such as the chemistry of lithium inside a battery (cf. Section 5.1) [11]. In addition, local electronic and magnetic properties that often vary on the nanometre scale [12, 13] will also become accessible with PETRA IV (cf. Section 5.5).

The spatial resolution in conventional microscopy depends on the quality of the X-ray optics, which is continuously being improved. When PETRA IV will start operation in the second half of the coming decade, single-digit nanometre focusing will be routine [5, 14]. To push the spatial resolution beyond the limits set by of X-ray optics and towards the atomic level, coherent X-ray diffraction techniques...
can be combined with scanning microscopy. This is possible because a diffraction-limited focused beam is laterally coherent [8]. At each scan point, a coherent diffraction pattern can be recorded. The speckle size (smallest resolvable unit) in reciprocal space is proportional to $NA/\alpha$. Thus, all lateral length scales

$$l = \frac{\pi}{q} = \frac{\pi}{2k\sin^{2}\theta} \leq \frac{\alpha}{kNA} = \frac{\lambda}{2NA} = d_t$$

smaller than the focus size $d_t$ can be accessed with a coherent beam in reciprocal space.

Here, $q$ is the momentum transfer of the scattered light, $k$ its wave number and $\theta$ the scattering angle. $\theta$ can significantly exceed the angle of numerical aperture. An example of a technique that takes advantage of this is ptychography [15–17], also known as scanning coherent diffraction microscopy. In ptychography, the sample is scanned across a confined coherent beam, and a far-field diffraction pattern is recorded at each scan position. From these data, the complex transmission pattern is recorded at each scan position. From these data, the complex transmission function, which quantitatively describes the attenuation and refraction inside the specimen, can be reconstructed with spatial resolutions well beyond the size of the beam [18]. Combined with tomography, ptychography yields the 3D distribution of the electron density. The spatial resolution in ptychography is limited by the coherent fluence on the sample and thus by the spectral brightness. Currently, the resolution limit lies around 10 nm [18, 19]. By focusing the PETRA IV beam to the (sub-)10 nm range, the spatial resolution can be pushed to the 1 nm level for radiation-hard samples.

The high brightness and coherence of PETRA IV will make local X-ray analytical measurements routinely feasible, and spatially resolved X-ray analytics are expected to become routine, turning PETRA IV into the ultimate X-ray analytical 3D microscope.

4.3. Time Scales:
Following Physical and Chemical Processes

The increased spectral brightness of PETRA IV significantly improves time-resolved studies. While it generally speeds up imaging experiments (cf. previous Section 4.2), it has a significant impact on correlation spectroscopies as discussed in this section and pump-probe studies in chemistry and biology (Section 4.6). Pump-probe experiments will mainly be carried out in timing mode (cf. Table 1.1 in Section 1.1.1) with 80 bunches in the storage ring separated by 96 ns. In the ultra-low-emittance ring, the bunch current is limited to 1 mA, leading to a ring current of 80 mA in timing mode. Compared to today, conventional pump-probe experiments will gain mainly through an increased flux due to optimised insertion devices. However, as soon as pump-probe experiments involve small objects for which focusing of the X-rays is needed, the full gain proportional to the brightness is expected. This is for example important for imaging magnetic dynamics in nanoscale spintronics (cf. Section 5.5.2). The largest gains, however, are expected for X-ray photon correlation spectroscopies. X-ray photon correlation spectroscopy (XPCS) permits the investigation of the dynamics of complex disordered systems, such as liquids and glasses [23, 24]. Today, XPCS is typically used to study slow dynamics (from milliseconds to hours) on (sub-)nanometre length scales [25]. On the same length scale, X-ray free-electron laser sources cover time scales from femtoseconds up to several nanoseconds [26, 27]. Thus, the time scales ranging from several nanoseconds to milliseconds are currently not accessible by any experimental technique. Covering this range, however, is crucial to fully understand processes in complex matter, for example diffusion processes in aqueous solutions (cf. Section 5.4.3). The method of X-ray cross-correlation analysis (XCCA) [28], which uses coherent synchrotron radiation, provides a novel approach to deciphering the local atomic symmetry of complex structures. XCCA enables access to the local structure of amorphous matter via bond order parameters, extending the conventional scattering methods that probe average order only. Both methods, XPCS and XCCA, are based on illuminating the sample with intense coherent X-rays and recording diffraction patterns in the far field (see scheme in Figure 4.4). The
diffraction patterns obtained by a 2D detector show a grainy structure, the speckle pattern, whose contrast is directly proportional to the coherent flux and thus to the brightness. In XPCS, series of speckle patterns are measured with a fixed delay time \( \tau \). The sample dynamics are obtained by calculating time correlations between the patterns. In contrast, in XCCA experiments spatial correlations are studied within single patterns, giving rise to higher-order structures.

The accessible time scales in XPCS experiments are limited by the signal-to-noise ratio \( R_{SN} \) of correlation functions retrieved from a series of coherent scattering patterns, given by [24, 29]

\[
R_{SN} \propto F_c \sqrt{T \tau_c n_{pix}},
\]

where \( F_c \) is the coherent flux [cf. Eq. (4.2)], \( T \) is the data acquisition time, \( \tau_c \) is the characteristic time scale to be studied in the system, and \( n_{pix} \) is the number of detector pixels. This means that for the same \( R_{SN} \), an increase of coherent flux by a factor \( K \) can be traded into a decrease of \( K^2 \) of the quantities under the square-root term. For a given number of detector pixels \( n_{pix} \) and data acquisition time \( T \), an increase in coherent flux by a factor 500 at PETRA IV compared to PETRA III (cf. Figure 4.3 at X-ray energies around 10 keV) allows the investigation of dynamical processes with a 500\(^2\)-fold shorter characteristic time \( \tau_c \).

Similarly, for a given system with characteristic time \( \tau_c \), the acquisition time can be 500\(^2\)-fold reduced, allowing the study of non-stationary and transient dynamics. In addition, most experiments performed today at third-generation synchrotron radiation sources can be carried out much faster (reduce \( T \) in Eq. (4.4)) and reach statistics far beyond what is possible today.

Nowadays, XPCS experiments on nanoscale materials are routinely performed on time scales of \( \tau_c \geq 0.1 \text{ ms} \) at PETRA III. Consequently, PETRA IV will enable experiments on time scales down to \( \tau_c \approx \text{ns} \), i.e. the funda-
Figure 4.5.: Map of spectroscopic techniques and their range in space and time. XPCS currently covers time scales down to the millisecond regime. At PETRA IV, the accessible time range will be extended down to the nanosecond regime.

Mental time scale of the pulse separation. In contrast, X-ray correlation methods at the European XFEL probe ultra-fast dynamics in the range of femtoseconds and nanoseconds using split-pulse devices. Thus, combining the XPCS studies at X-ray FELs and PETRA IV gives full access to all time scales for dynamical processes at nanometre length scales from femtoseconds to hours (cf. Figure 4.5). PETRA IV will thus enable several types of studies that are not possible with current sources:

- It will be possible to follow systems with fast dynamics down to nanoseconds. This will for example enable studies of diffusion dynamics in aqueous solutions, e.g. in biology and chemistry. In particular, the dynamics of radiation-sensitive biomolecules such as proteins will become accessible, probed at the relevant length scales for the first time (cf. Section 5.2).

- PETRA IV will enable studies of the unusual properties of water itself and as a solvent, whose dynamics lie in the range of nanoseconds to microseconds [30] (cf. Section 5.4.3). In particular, the glass transition of water and the dynamics of high- and low-density states of water [20], the structure and dynamics around ions in solution and the dynamics of biomolecules in aqueous environments will become accessible in this way.

- The increased coherent flux leads to an increased scattering signal at large $q$, thus providing access to the dynamics on much shorter length scales. In this way, atomic diffusion in metal alloys can eventually be followed [31].

- Likewise, the interplay of the structure (probed by XCCA) and dynamics (probed by XPCS) of supercooled liquids reaching the glass transition will be accessible for a broad range of systems, ranging from soft matter to metallic and network glasses [32].

- Studies will also be possible of non-equilibrium systems and transient behaviour, such as sliding or avalanche dynamics.
The superior coherent flux enables XPCS experiments at high X-ray energies for the first time. This will allow experiments using complex sample environments, such as high-pressure studies with diamond anvil cells, and help to reduce X-ray doses for radiation-sensitive samples.

XPCS experiments of radiation-sensitive samples strongly benefit from the increased brightness of PETRA IV. The combination of superior coherence volume, higher photon energy and increased coherent photon flux at PETRA IV yields an increase in signal-to-noise ratio of up to one order of magnitude for protein samples in solution compared to today’s sources (cf. Section 5.2). Long beamlines and large sample-detector distances are a prerequisite that can be accommodated at PETRA IV.

The coherent flux can be efficiently nanofocused so that inhomogeneous systems can be investigated, for example glasses, jammed granular materials and multiphase or soft materials. In addition, the dynamics of nanoobjects (for example, nanoparticles) or complex systems can be followed on the nanoscale (cf. also Section 4.2).

As this by no means exhaustive list of examples shows, PETRA IV will open up a multitude of new and unique experimental possibilities and thus pave the way towards new fields of science that were previously inconceivable. As PETRA IV will outperform all other currently planned sources by at least one order of magnitude in brightness, 100 times faster dynamics can be studied over all length scales. Together with the European XFEL, PETRA IV will enable XPCS experiments ranging from femtoseconds to hours, i.e. covering more than 18 orders of magnitude with one experimental technique.

4.4. Energy/Frequency/Polarisation Space: High-Resolution Spectroscopies

4.4.1. Nanoscale Spectroscopy

In many cases, materials consist of distinct phases that differ only marginally in their properties, yet are driving (or prohibiting) functionality. For example, in the whole class of phase-separated materials (encompassing giant-magneto-resistance materials and potentially also high-temperature superconductors), the chemical composition is homogeneous, while small details in the electronic structure (e.g. spin directions of valence electrons or small band gaps) are inhomogeneously ordered in nanometre-sized domains (cf. Section 5.5.1). Unfortunately, such domains are too similar to provide contrast for traditional X-ray microscopy, while at current sources X-ray spectroscopy does not achieve sufficient spatial resolution.

Angle-resolved photoemission spectroscopy (ARPES), on the one hand, provides a direct view of the full valence electronic band structure in the space of binding energy, 3D crystal momentum and electron spin direction. To map this large parameter space, high flux is required. On the other hand, resonant inelastic X-ray scattering (RIXS) gives direct access to the fundamental excitation spectrum of complex materials with element selectivity and chemical-state specificity and has helped to fully understand the dispersion behaviour of quantum correlated excitations such as phonons, (bi-)magnons, orbitons, or holons. This spectroscopic technique is also very photon-hungry and requires large photon flux with high monochromacity.

Limited by the 100 to 1000 times larger horizontal phase space of current storage rings compared to PETRA IV, the fields of microscopy and spectroscopy are currently fully disjoint: Small beams are available to provide sufficient spatial resolution for structures on the scale of tens of nanometres. Only the coherent fraction, i.e. 1% to 0.1% of the beam, can be focused today. This small fraction of the flux is insufficient to conduct high-resolution spectroscopy, especially when the beam needs to be highly monochromatic. On the other hand,
for spectroscopy, the highly monochromatic beams are typically sized on the order of tens of micrometres, thus intrinsically averaging over smaller structures, albeit with high information content.

PETRA IV now opens up the possibility to focus the full monochromatic beam down to spot sizes in the nanometre regime. For ARPES, this provides the ability to map in-homogeneities in the band structures at the Fourier limit between spatial and crystal momentum resolution. For RIXS, the benefits are even larger, when combined with unique instrumentation that is currently being explored.

Currently, state-of-the-art RIXS is conducted with gratings manufactured at the technological precision limit, requiring large spectrometer dimensions (often 10 m to 15 m) to compensate for limits in grating precision and beam size. These gratings disperse the beam in one dimension, while the other dimension of a 2D detector does not contain additional information. While PETRA IV clearly alleviates the source size limit to the resolution, the combination with 1D imaging spectroscopic elements opens up new possibilities: On one hand, one can image nanometre structures of the sample, and on the other hand, it enables the exit slit of a monochromator beamline to be kept open without affecting the energy resolution of the spectrometer. This provides orders of magnitude larger photon flux for use in the experiment, while not increasing the potentially damaging flux density on the sample.

Ideally, the monochromator beamline images the full bandwidth of the ultra-small photon source of PETRA IV onto a rainbow line on the sample, where different points contain different highly monochromatic photon energies. Imaging this line onto the detector while energetically dispersing the emitted photons in the orthogonal direction allows the measurement of a full RIXS map (a 2D range of emission spectra for different excitation energies) in parallel without moving anything and with the same signal level as usually for one single emission spectrum. At the same time, spatial information across the rainbow line is encoded in the measured data, and scanning the sample position allows separate RIXS maps to be recorded for every nano-sized point on the sample, thus providing sufficient spatial resolution and information to discern different domains in phase-separated samples.

This constitutes a new dimension in our ability to study complex materials, since for the first time with such a setup, relevant spatial resolution in the nanometre regime can be combined in reasonable time with highly specific and informative spectroscopic probes such as ARPES and RIXS to resolve nano-scaled differences in the electronic structure of complex materials that are presumably in general more inhomogeneous than currently discernible. The same arguments apply for the study of correlated materials using nuclear resonant scattering (NRS). These techniques offer the special feature to be sensitive to the Mössbauer isotope in the sample only. In combination with meV-bandwidth high-resolution monochromators, the elastic and inelastic nuclear resonant scattering processes can be monitored in the same experimental setup. While the elastic nuclear scattering reveals information about the hyperfine interactions of the nuclei in the sample and is thus a sensitive probe of electronic and magnetic properties, the inelastic nuclear scattering carries information about the vibrational excitations in the material. The combination of elastic and inelastic nuclear resonant scattering thus reveals unique information about the relation between electronic correlations and quasiparticle excitations such as phonons, which continues to be a critical aspect for fundamental phenomena such as superconductivity in materials that are already known and those that will be discovered in the future. For these techniques based on nuclear resonance excitation, it will also be indispensable to be able to efficiently focus the beam to dimensions of a few 10 nm in order to specifically select homogeneous regions in a phase-separated material.

The possibility of significantly enhanced focusing in the horizontal direction opens new perspectives to improve the performance of meV-resolution crystal optics and monochromators for hard X-rays. Beyond silicon as the established material for X-ray crystal optics, there are other promising materials such as sapphire and quartz that could be superior to Si due to their larger unit cell and the availability of high-order Bragg reflections in certain energy ranges. These materials, however, still lack the high degree of crystalline perfection that
is available for Si. Therefore, with efficiently focused beams (vertically and horizontally), homogeneous regions on crystals of these materials could be selected to construct novel types of high-resolution monochromators for applications in nuclear resonant scattering and inelastic X-ray scattering in general.

Efficiently collimated beams with small cross sections and thus a small footprint on the optical elements will also enable the construction of very compact high-resolution monochromators that are much less sensitive to vibrations and thus offer a much higher stability than present-day devices. This is particularly important in the case of high-order Bragg reflections, which require a high angular stability due to their very narrow angular acceptance. This opens new perspectives for realising high-resolution monochromators at very high X-ray energies, say, above 30 keV, where the Darwin width of Bragg reflections decreases significantly. This will enable inelastic X-ray scattering studies in absorbing sample environments and would allow high-energy nuclear resonances such as the 73 keV resonance of $^{193}$Ir [33] to be efficiently addressed.

4.4.2. High-Purity X-ray Polarimetry

The significantly reduced emittance of PETRA IV in the horizontal direction has immediate impact on X-ray optical schemes that include diffraction also in the horizontal plane. This applies in particular to X-ray polarimetry.

Polarimetry allows studies of electronic and magnetic anisotropies of materials and of dynamical processes that lead to polarisation changes in the X-ray scattering process. Applications range from resonant elastic X-ray scattering [34] (REXS) to nuclear resonant scattering (NRS) [35], X-ray quantum optics [36–38] and X-ray linear and circular dichroism (XMLD, XMCD) [39]. Thus, the development of high-purity X-ray polarimeters in recent years has improved and extended the spectrum of analytical methods at high-brightness X-ray sources. This development will continue with a further reduction of the emittance of these sources. PETRA IV in particular can significantly increase the efficiency and performance of high-precision X-ray polarimeters further (cf. Section 4.1), enabling new applications in fundamental and applied research in the future.

Precision X-ray polarimetry is based on Bragg diffraction at 45° on perfect crystals. The incident and reflected beam will then enclose 90°, which leads to a suppression of the polarisation component parallel to the diffraction.
plane. By increasing the number of reflections in channel-cut crystals (cf. Figure 4.6), a very high degree of linear polarisation purity $\delta_0$ can be reached. The use of perfect crystals provides a high reflectivity even for multiple reflections. Modern polarimeters reach a degree of linear polarisation purity of $\delta_0 = 2.4 \times 10^{-10}$ [40]. The parameters of the X-ray source are crucial for the performance of the X-ray polarimeter. The current limitation of the polarisation purity is determined by the divergence of the source at low X-ray energies. PETRA IV can overcome these limitations and reach polarisation purities in the range of $\delta_0 \approx 10^{-12}$ [41].

The enhanced spectral brightness and therefore increased photon flux transmitted by the polarimeter allow these extreme purities to be efficiently used in experiments. Exceeding even those purities that can be reached in the regime of visible optics, they will enable novel applications in fundamental physics. One of them is the verification of quantum electrodynamics through the observation of vacuum birefringence [42]. This effect could not yet be demonstrated because it is very weak. An improvement of the polarimeter by one order of magnitude will make the effect measurable.

Another application that will benefit from the increased degree of polarisation purity is nuclear resonant scattering. The higher polarisation purity increases the suppression of non-resonantly scattered photons and therefore significantly enhances the signal-to-noise ratio. This will open up new possibilities in materials science and quantum optics. Furthermore, the polarisation filtering of resonantly scattered photons will become more effective at PETRA IV because a smaller divergence matches better with the rocking-curve width of the channel-cut crystals at higher photon energies. Polarimetry becomes therefore more efficient at higher photon energies and enlarges the applicable energy range of this technique.

A recently developed method that will significantly benefit from the improvement of the polarimeter is spectropolarimetry. This technique is a combination of X-ray spectroscopy with X-ray polarimetry to reveal the spectral properties of tiny electronic anisotropies in correlated materials (cf. Section 5.5.1) and magnetic order at interfaces of functional heterostructures (cf. Section 5.5.2).

### 4.5. High-Energy X-Rays

High-energy X-rays are an important probe in many fields of science, mainly due to their large penetration depth, which makes them particularly suitable for in-situ and operando studies of samples inside special sample environments (Section 4.7), and to their short wavelength, which gives comfortable access to lengths scales down to the sub-atomic level.

As a high-energy storage ring with an electron energy of 6 GeV, PETRA IV will provide both high brightness and high flux for high X-ray energies above 30 keV. For high-energy X-rays, the beam will not be diffraction-limited (cf. Eq. (4.3)). However, the reduction in emittance translates nearly one-to-one into an increase in spectral brightness. In combination with new short-period undulators (cf. Section 7.2), two to three orders of magnitude in spectral brightness can be gained in the high-energy X-ray range (cf. Figure 4.3 for comparison with PETRA III).

This transformative improvement in spectral brightness opens up unparalleled possibilities for high-energy X-ray techniques, in particular for in-situ and operando experiments (cf. Section 4.7) that require complex sample environments, e.g. in solid-state physics, chemistry, biology, geoscience (cf. Section 5.4.2), nanotechnology and engineering materials science (cf. Section 5.3.2).

The spectacular gain in brightness in the high-energy X-ray range opens up the possibility to efficiently focus high-energy X-rays, making this powerful probe available for microscopy. This can, for example, be achieved using refractive X-ray lenses [43] and multilayer Laue lenses (MLLs) [6]. In this way, all high-energy X-ray techniques can be applied as local probes on the nanometre scale. As a result, the “high-energy X-ray microscope” PETRA IV will give access to the local structure of engineering materials [44] by high-energy X-ray
Two multilayer Laue lenses focusing the X-ray beam at approximately 16 keV to a spot size of $(8 \times 7) \text{nm}^2$ [6]. These optics can be adapted for high-energy X-rays (30 keV to 100 keV). The intrinsically larger focal length at these energies will facilitate the use of special sample environments.

4.6. Serial Crystallography

Serial crystallography is a disruptive new analysis method for macromolecular crystallography that allows structure determination at room temperature from crystals that would usually be considered too small for measurement. The technique was first introduced for diffraction measurements at X-ray free-electron lasers [49], but was quickly adopted for use at many synchrotron radiation facilities around the world [48, 50–54]. At PETRA IV, this method will receive an enormous boost from the possibility to efficiently focus the X-rays to spot sizes of 1 µm and below, thus tremendously enlarging the range of crystalline substances that can be studied.
In serial crystallography, a diffraction data set is built from many snapshot diffraction patterns from single crystals. This new strategy of distributing the measurement over many thousands (or even hundreds of thousands) of crystals allows the X-ray dose to be reduced to almost arbitrarily small amounts and thus the exposure time to be extremely brief — in fact, as short as single pulses from the synchrotron when using the unmonochromatised “pink” beam. It therefore opens up studies of the dynamics and kinematics of evolving or reacting macromolecular systems, large-scale screening and drug discovery studies with orders of magnitude higher efficiency than previously considered, and high-throughput screening of crystallisation conditions. Additionally, the method accommodates much smaller crystals than conventional crystallography, which enables measurements of a much greater range of protein systems and reduces the time and effort required to obtain crystals.

The approach has benefits for other fields besides structural biology: By carrying out powder diffraction one grain at a time, material phases can be numerically separated in a mixture and structural refinement can be improved.

The speed at which a serial crystallography data set can be acquired is directly proportional to the average source brightness, and the capabilities and opportunities of the technique scale with improvements in the photon flux density (photons per unit area and time) of the beam at the sample. This is unlike conventional crystallography, which cannot readily benefit from further source upgrades, since the data collection time is dominated by sample mounting and alignment. The method takes full advantage of improvements in the speed of detectors, and best performance will be achieved with high-frame-rate integrating detectors (cf. Section 7.6).

The requirement for serial crystallography measurements is that there is enough recorded diffraction signal in each pattern, relative to background scattering, to determine the crystal orientation, so that the diffraction information can be averaged and aggregated in a 3D reciprocal space. Thus, the method requires highest beam intensities at shortest possible exposure times to control radiation damage. These conditions can be met with the “pink” spectrum of an undulator harmonic. At PETRA IV, it should be possible to generate a pink beam that can be focused to micrometre dimensions with over $10^{15}$ photons per second, a hundred times increase over that of a monochromatic beam. This corresponds to about $10^8$ photons in an exposure from a single pulse, giving an exposure time of that of the electron bunch: about 100 ps. With this exposure, the radiation dose is about 30 kGy. This is tolerable for room-temperature measurements, but models predict that the short exposures out-run radiolysis processes mediated by the diffusion of solvated electrons and free radicals, causing
less radiation damage than for longer exposures.
A spectral bandwidth of 1 to 2% is beneficial for the analysis methodology. Since the crystal
diffraction disperses the light, this bandwidth provides complete Bragg reflections (known as Laue diffraction) instead of the partial reflections obtained with a monochromatic beam.
For data of high signal-to-background, this vastly reduces the number of patterns required to build a complete data set. In a demonstration carried out at APS with a bandwidth of 5%, less than 200 patterns were sufficient to obtain structures of several proteins ([48], cf. Figure 4.8), a 30 times reduction of the number of patterns needed with a monochromatic beam. It is estimated that with further reductions in background, crystals of 3 µm width can be measured with the pink-beam conditions of APS, and PETRA IV should enable a further reduction to about 1 µm. These sizes are well matched to optical laser extinction depths (for uniform photoexcitation) and can be used to provide diffusion times approaching 1 µs (for fast mixing experiments), enabling time-resolved measurements of a broad range of biological structural dynamics (cf. Section 4.3).

### 4.7. In-Situ and Operando Experiments

The *in-situ* and *operando* observation of processes and functional materials under industrially relevant conditions is at the heart of the heart of today’s and future research based on synchrotron radiation. X-rays allow observations under extremely harsh conditions, e.g. in extreme chemical environments, at high temperature and pressure, in extreme electromagnetic fields or including lasers. In this way, processes can often be followed in real time, such as the growth of nanoscale functional devices, the structure formation of nanoobjects from solution [55, 56], chemical vapour deposition including aggressive gas atmospheres or reactive sputtering and high temperatures [57], and corrosion processes [58].
The growth of nanostructures at solid-liquid or liquid-liquid interfaces can be monitored *in-situ*, helping to unravel fundamental building principles under such conditions [59].
High-pressure synthesis for the preparation of novel materials can be followed *in-situ* (cf. Section 5.3.1), and fundamental processes in solid-state physics and chemistry, including phase transitions, structural, electronic and magnetic excitations, can be investigated.
Various hard X-ray-based photon-in/photon-out techniques in particular can be applied. Synchrotron-radiation-based methods are especially suited for the *operando* investigation of working functional devices under realistic, industrially relevant conditions [60]. This comprises working heterogeneous catalysts or electrocatalysts involved in chemical production (Section 5.1.4), energy conversion and combustion as well as proton exchange membrane fuel cells or batteries (Section 5.1.3). The functioning and degradation of solar cells can be studied live [61]. In the field of microelectronics, single operating devices can be investigated. Today, due to a lack of sufficient brightness, most *in-situ* and *operando* experiments average over large sample volumes, while X-ray microscopy experiments are often performed under static or ex-situ conditions.
Hard X-ray imaging techniques will be strongly boosted by PETRA IV thanks to the extreme source brightness and will thus be available with enhanced resolution, sensitivity and data acquisition speed (cf. Section 4.2). Nanofoocusing can be achieved with large working distances due to the small source size. This is very favourable when using bulky sample environments. PETRA IV will thus pave the way for following natural and industrial processes *in-situ or operando* on the relevant length and time scales down to the microscopic level, thus taking into consideration the spatial heterogeneity of materials and processes, also in three dimensions. X-ray microscopes with large working distances will allow more genuine process conditions to be provided in combination with advanced analytical tools. In addition, *operando* X-ray investigations will be complemented by other analytical techniques, including pre- and post-experimental sample characterisation for example by means of scanning probe and electron microscopy at the DESY NanoLab.
References

5. Science and Technology Drivers

Figure 5.1.: PETRA IV will make major contributions to important societal challenges, like in the fields of Energy, Life and Health, Transport and Technology, Earth and Environment and Information Technology.

Today’s grand challenges require novel material solutions of highest complexity: multifunctional hybrid materials with tailored local structures ultimately designed atom by atom. PETRA IV provides the disruptive X-ray technologies that are able to access local molecular and electronic structures and processes in vivo, operando, in a non-destructive mode and with highest resolution and sensitivity. This chapter presents the science and technology case for PETRA IV in detail. It is organised along the grand societal challenges (Figure 5.1).
Figure 5.2.: PETRA IV will decrypt aging processes in novel batteries. In conventional lithium-ion batteries especially the smallest metallic deposits of lithium on the electrodes play an important role. The ultra-sharp X-ray view can scan the interior in operation of the battery and visualise how the battery components change over time, e.g. how during operation metallic lithium deposits on the electrodes forming needle-like outgrowths (dendrites). If the dendrites pass to both electrodes, this leads to short-circuits which can cause explosive reactions and dangerous battery fires.
5.1. Energy

Our society is challenged by an increase in energy consumption and the scarcity of natural energy resources. To meet this challenge and achieve a more sustainable use of energy in our society, fundamental changes at three stages are required that are in line with Germany moving from nuclear power and coal to renewable energies: (1) energy harvesting, (2) energy conversion and (3) energy storage, as depicted in Figure 5.3 for an artificial equivalent to photosynthesis. Materials that are critical at one of these stages are considered energy materials. Advances in these three fields are prompting the development of novel energy materials, and it is expected that advanced characterisation methods such as those provided by PETRA IV will greatly contribute to controlling and optimising their properties.

As examples for the broad range of energy materials, we focus here on photovoltaic, battery and catalytic materials for energy harvesting, storage and conversion. Similar research takes place in related fields, such as high-performance wind turbine blades, thermoelectric devices for the recovery of waste heat, hydrogen storage for mobile fuels, water-splitting devices or biomass conversion. The functionality of energy materials originates from chemical and physical effects at different length scales. Therefore, a fundamental understanding of their mechanism on different scales is necessary, as highlighted in Figure 5.9 using the example of a catalyst.

PETRA IV will be a game changer for research on energy materials. The increased coherent flux directly translates into higher flux after nanofocusing, which will be transformative at different levels (cf. Chapter 4). First, kinetics measurements will allow the assessment of orders of magnitude faster changes in local material properties. Second, the combined use of diffractive and spectroscopic techniques will provide access to the relation between structural and electronic material properties. Third, the higher throughput will yield an overall picture of large amounts of samples. Fourth, the high brightness at high photon energies will enable the use of photon-hungry techniques for the investigation of buried structures in complex systems such as batteries. Finally, the higher coherence will significantly increase the resolution in techniques such as ptychography and Bragg coherent diffraction imaging.

The unique possibility of merging high flux with high repetition frequency and rapid X-ray experiments with materials library synthesis triggers the development of highly efficient sample characterisation and sample selection schemes beyond laboratory approaches.

5.1.1. Energy Materials

Energy Harvesting

Enhancing both the conversion efficiency and the life span of solar cells is the largest leverage arm for lowering the levelised cost of electricity and the ecological footprint of photovoltaic energy conversion [63]. In recent years, solar cells with thin organometal halide perovskite absorbers have challenged traditional absorbers with the steepest efficiency increase in history [64]. In the field of organic solar cells,
solution-fabricated tandem solar cells achieved efficiencies that are comparable to devices based on solid-state semiconductors [65]. For next-generation photovoltaics, thin-film solar cells are promising thanks to their higher potential for further efficiency increase and cost reduction, as they can be produced in industry-friendly roll-to-roll and printing processes (cf. Figure 5.4) or in a wet green chemistry approach.

Figure 5.4: In-situ measurement during the printing of novel solar-cell layers. Reproduced with permission from [61]. © (2014) by WILEY-VCH Verlag GmbH & Co.

Thin-film solar cells have in common that their absorbers are polycrystalline semiconductors based on compound materials. Due to their small grain sizes, sophisticated measurement methods are needed to characterise them with high spatial resolution. Synchrotron-based X-ray beams are ideally suited for the in-situ tracking of solar-cell synthesis processes. However, the brightness available from modern synchrotron radiation sources still prevents sufficiently fast measurements to follow the synthesis of many materials. Today, the relevant questions in solar-cell research include: What do interfaces look like in solar-cell stacks? How can perovskite solar modules be manufactured without sacrificing efficiency due to lateral inhomogeneity? How can defects be engineered to be less detrimental? How can organic solar cells be fabricated using green chemistry approaches? Comprehensive answers to all these questions will only be possible through multimodal in-situ and operando measurements, as depicted in Figure 5.5. Unfortunately, such multimodal measurements are severely limited nowadays by the comparatively low nanofocused flux at nanoprobe beamlines of third-generation synchrotron radiation sources.

Energy Storage
Recent technical and economic developments have led to a dramatic change in societal energy concepts, including the internet of things, which enables smart electricity grids with distributed electricity generation. The energy cost structure has furthermore shifted from traditionally high running costs for power plants to high installation but low running costs. This paradigm change is expected to catch up speed with the continuous market share in-
crease of electric vehicles and heating with heat pumps. These developments shift weight towards electricity as an energy carrier with weather-dependent energy harvesting and underline the need for research into materials and systems for electricity storage. Current state-of-the-art batteries, for example based on Li-ion technology, have insufficient capacity, short life spans and long recharging times and are made of scarce and often poisonous elements. Therefore, the central goal of battery research is to enhance the energy density and lifetime of battery materials while keeping the CO₂ footprint low. High throughput in characterisation is a must to achieve a comprehensive understanding of multiscale heterogeneous materials, which form the backbone of many of today’s technologies. When the interplay between nanoscale and microscale features with different composition, surface characteristics, structural response, etc. comes to define the global properties and function of the material, these connected building blocks must be characterised in very large quantities in order to gain a complete picture of what are the enabling and limiting microelements of the system’s macroresponse. One example is reconciling phenomena such as stress-induced creep with collective grain motion in polygrained structural materials. Analogous cases can be made in many realms; they have in common that complex and hierarchical structures need to be controlled across different length and time scales. The degradation mechanisms of batteries are as manifold as their causes. Further complication is added by the non-trivial time structure of failure modes: Rather than continuous performance decrease, singular events such as short-circuiting due to Li-dendrite growth during charge/discharge cycling, overheating, mechanical deformation, or chemical reactions cause catastrophic failure. These aspects challenge characterisation approaches at different levels. Novel developments in coherent diffraction imaging have enabled 3D images with strain sensitivity well beyond what other methods can provide (cf. Figure 5.7).

However, the methods lack statistically meaningful numbers of images and are limited to proofs of concept. This is especially true when the structural outliers play an outsized role in defining global properties (cf. “finding the needle in the haystack” in Section 4.2). Large statistics are just as necessary as multiscale approaches that allow the investigation of the entire battery system and the tracking of failure modes from the macroscopic down to the chemical level.

![Figure 5.6: Development of the worldwide photovoltaic energy conversion and battery storage capacity (data from [67] and [68]).](image)

**Energy Conversion**

Heterogeneous catalysts are complex multicomponent systems, usually consisting of nanoparticles that are active in the catalytic reaction and anchored on a porous support. The reactants are typically supplied by the gas phase or through a liquid and penetrate the support. Heterogeneous catalysts play an eminent role for energy harvesting, conversion and storage and are involved in most technologies for the production of chemicals as well as in environmental preservation [70]. Specific challenges include the catalysis of CO₂ and hydrocarbons to enable a sustainable carbon cycle and the production of clean hydrogen for energy storage. There are several overarching goals for the development of future catalysts:

- Higher turnover, since an activity increase even on the percentage level has a huge impact on saving precious metals such as Pt, Rh or Pd. This includes the search for less precious catalysts or the development of new synthesis strategies, e.g. using bimetallic catalysts.
- Tuneable selectivity towards the desired product, since for many catalytic reac-
Catalysis research has greatly benefited from synchrotron facilities, using advanced scattering, spectroscopy and imaging techniques. These methods have allowed the elucidation of the geometrical and electronic structures of chemical species across different length and time scales and of their evolution under operando reaction conditions with varying parameters such as pressure, concentration, or temperature (cf. Figure 5.8 and Figure 5.9) [72, 73]. These studies have established structure-activity relations of catalysts under industrially relevant conditions [60, 74, 75]. Today, the main weakness of catalysis research is that the experiments are performed under far-from-realistic-reaction conditions, thus preventing direct correlations with industrial-scale heterogeneous catalysis [76]. In particular, atomic-scale information under true operando conditions involving high gas pressures and elevated temperatures is required, and measurements under realistic reaction conditions need to be performed. PETRA IV can provide fast and high-resolution imaging of catalyst chemistry at large working distances (cf. Section 4.2 and Section 4.7). In all energy aspects from harvesting to storage and conversion, research is currently limited by the brightness of hard X-rays. The following subsections therefore highlight examples that would greatly benefit from the boost in brightness offered by PETRA IV.
5.1.2. Benefit of PETRA IV for Energy Harvesting

PETRA IV overcomes the limitations of current X-ray nanoprobes: The higher nanofocused flux at PETRA IV will lead to transformative improvements for in-situ measurements during the synthesis of energy materials. Such measurements could be performed at least two orders of magnitude faster, giving direct insights into the synthesis and degradation processes of energy materials in real time. Moreover, rather than just enabling faster measurements, PETRA IV will enable new measurements that are not yet feasible today: A new type of correlative microscopy will be possible that is based on a multimodal combination of methods such as X-ray excited optical luminescence (XEOL) together with X-ray fluorescence (XRF), X-ray diffraction (XRD), ptychography and X-ray beam-induced current (XBIC), as suggested in Figure 5.5. Such measurements can yield for example the optical performance with bandgap and charge carrier lifetime, the composition, structure, electron density and electrical performance in buried semiconductors at unparalleled spatial resolution. PETRA IV will allow XBIC measurements of solar cells as a function of applied voltage, temperature and bias light to assess the full current-voltage dependence at nanoscale resolution under operando conditions.

Tomorrow’s questions in energy materials research will be different to those mentioned above. With multimodal measurement approaches involving an entire set of scanning nanoprobe techniques, PETRA IV will be ideally suited to tackle them. At the forefront of the discipline, this will enable the probing of inhomogeneities, defect chemistry, Fermi-level splitting and performance at a spatial resolution that no other probe can provide for complete devices. This is particularly important given that the structures in high-performance solar cells are becoming ever smaller. Ultimately, interfaces will govern the performance, and their defects will be of utmost importance. As the overall device performance is limited by the weakest spot, for the engineering of novel devices it is therefore mandatory to focus on nanoscopic approaches at highest sensitivity and spatial resolution in order to characterise defects at their length scale: As needle-in-a-haystack problem, macroscopic areas need to be mapped at highest resolution to track down defect mechanisms at the nanoscale.

Naively, it is expected that the net flux density increase at PETRA IV will increase X-ray beam-induced sample degradation. While this is true for many materials, it is particularly critical for energy materials that are measured in-situ or operando. However, the increased flux density will allow measurements to be performed faster at the same dose. Faster measurements will in turn allow higher doses due to dose rate effects: As defects are often only visible after a delay (e.g. ion movement after defect creation), the measurement approach “measure faster than the sample degrades” can mitigate beam degradation artefacts even

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**Figure 5.9.:** Hierarchical architecture of a real catalyst from the atomic to the macroscopic scale. Reproduced with permission from [77]. © (2016) by Royal Society of Chemistry.
at higher doses and measurement speeds than at present X-ray nanoprobes. As the source with the highest brightness at high photon energies, PETRA IV will open up new measurement windows: At high energies, the absorbed dose is reduced and damage is mitigated. At the same time, the penetration depth is enhanced, and the sensitivity increases for heavy elements that are of critical importance in many energy materials.

5.1.3. Benefit of PETRA IV for Energy Storage

**Figure 5.10.:** The higher nanofocused flux of PETRA IV both accelerates measurements and provides access to further dimensions, enabling microscopy even for photon-hungry techniques such as inelastic X-ray scattering to unveil the electronic properties of light elements inside batteries. Reproduced with permission from [66]. © (2019) by MultiMedia Pharma Sciences, LLC.

PETRA IV meets the characterisation challenge of battery systems with the bundled force of diffraction-limited high-energy X-ray beams. By providing highest sensitivity and spatial resolution in combination with a multitude of measurement techniques, hard X-ray synchrotron radiation is ideally suited to investigate battery materials and systems regarding structure, composition and functionality [78]. Thanks to the high resolution in real and reciprocal space that PETRA IV will achieve, it will be possible to raster scan battery samples in scattering and diffraction measurements. From these measurements, the structure and distribution of compounds in the sample material can be determined down to the nanoscale (e.g. by 3D diffraction tomography) [79]. The high X-ray energies delivered at PETRA IV will enable the penetration of just about any encapsulating material or environmental chamber. Suddenly, *in-situ* sample design, which often limits what we can imagine doing today, will no longer be a limiting issue (Section 4.7).

With PETRA IV, methods such as Bragg coherent diffraction imaging (BCDI) and X-ray photon correlation spectroscopy (XPCS) will be boosted in throughput, which also means that scanning tomography measurements, e.g. in ptychography mode, will become feasible for kinetics measurements. Such experiments will allow measurements of structural changes of polycrystalline or amorphous electrode materials on all relevant length scales during charge and discharge cycles in real battery cells as well as the high-resolution investigation of failure modes.

Beyond the improved throughput, the increased measurement speed translates into an increase in dimensionality, as depicted in Figure 5.10. Entirely new dimensions become reachable with PETRA IV, be it to systematically run X-ray absorption near edge structure (XANES) tomography or to vary external parameters such as temperature, stress, or atmosphere as further dimensions of parameter space. The boost in brightness is particularly important for photon-hungry techniques such as non-resonant inelastic X-ray scattering (IXS). With the highest brightness at hard X-rays, PETRA IV will be the worldwide unique instrument to probe the electronic structure of light elements that are buried in macroscopic structures made from heavier elements. This is precisely the case for batteries, where the state of Li and organic electrodes inside full devices cannot be probed directly today – but PETRA IV could shine light on the battery processes in multiple dimensions by means of IXS tomography.

The use of multimodal measurement approaches, *in-situ* environments and *operando* modes to study battery systems with PETRA IV will enable unique insights into charge and discharge cycles, failure modes and degradation...
mechanisms. This will ultimately lead to the advancement of current battery technologies and the development of novel material systems for economical, ecological and safe batteries.

5.1.4. Benefit of PETRA IV for Energy Conversion

The ambitious goals of developing novel catalysts with increased turnover, selectivity and lifetime can only be reached using a multi-technique strategy across different length scales. Today, however, such approaches are limited by methodology. On one hand, the link is missing between high-resolution momentum space and lower-resolution real-space information, which would enable atomic-structure information to be related to catalyst particles [81]. On the other hand, real-time methods yield information about transient states, but time-averaging methods are required for high spectral resolution [82].

With its ultra-high brightness, small source size and high coherent flux, PETRA IV will be the ultimate X-ray microscope to give a holistic picture and zoom into catalysts under operando conditions down to atomic length scales. This will yield structural and chemical information with unprecedented resolution, enabling researchers to address the most challenging open questions in the field of heterogeneous catalysis. The facility will enable the characterisation of all relevant building blocks that collectively control the overall functionality of catalytic systems on their natural length scales [83]. Moreover, PETRA IV complements the European XFEL and FLASH (cf. Section 2.3.1), such that eventually the kinetics of processes with time constants from femtoseconds to hours can be followed on one site.

A future key experiment at PETRA IV will be the imaging of such catalyst particles in operation to visualise their functioning and failure in real time with nanometre to atomic resolution. Advanced 3D X-ray tomographic microscopy under operando conditions will reveal the internal hierarchical 3D structure of working catalysts down to the atomic scale, as depicted in Figure 5.11. Nanometre-sized, intense X-ray beams will allow scientists to raster scan catalysts, thereby exploiting various contrast mechanisms: diffraction, fluorescence, absorption, phase contrast, photoemission and inelastic scattering (Section 4.2). Locally different structures, material phases, chemical composition, strain distribution and oxidation states of single catalyst nanoparticles will be resolved, which exhibit a complicated interplay and can undergo dynamical changes under working conditions [84]. This information is essential to understand the mechanisms controlling the activity, selectivity and deactivation of working catalysts, providing a foundation for the design and nanofabrication of revolutionary new industrial-scale catalysts with substantially improved properties.
Innovation Aspects

Green energy harvesting, storage and conversion are key challenges in the upcoming decades. This also holds for a large variety of industries and opens new and growing markets for companies to sell their innovative products. Companies will directly profit from access to an instrument that can measure the 3D structure, composition and strain distribution *operando*, *in-situ* and at the nanoscale in statistically significant numbers. These opportunities will have a tremendous impact on industry and society, ranging from the development of new solar cell types to next-generation batteries and catalysts – markets that are expected to continue to grow exponentially, as shown in Figure 5.6.

*Material usage, efficiency and degradation offer the largest leverage arms for reducing the levelised cost of energy (LCOE) from future solar cells.* The industry is therefore focusing heavily on replacing scarce, expensive and toxic elements, on achieving reproducibly high efficiencies on large areas and on increasing the solar-module life span. For example, the defect tolerance of perovskite solar cells predestines them for low-cost high-efficiency devices. However, these cells suffer from various degradation mechanisms, and upscaling the technology challenges current manufacturing schemes. PETRA IV will enable multimodal characterisation with flux-hungry techniques to correlate optical and electrical performance with structural and compositional 3D information down to the scale of defects. Hence, PETRA IV will substantially contribute to a better understanding of the impact of process parameters on performance and degradation, leading to increased efficiency and life span at reduced costs.

*The development of battery systems with enhanced energy density, longer live spans and shorter charging times will considerably change our technological environment in the future.* However, this requires sophisticated measurements of chemical processes at the nanometre scale in multiple dimensions during charge cycling. Only PETRA IV offers the necessary combination of penetration depth of hard X-rays with highest sensitivity and spatial resolution in a hierarchical approach (cf. Section 4.2). Using methods such as inelastic X-ray scattering tomography, this will allow for example the 3D imaging of defects during their evolution upon charging.

*In the energy-efficient production of basic chemicals with minimized waste, for clean processes with low emissions from households, industry and combustion engines and for sustainable energy conversion, there is a huge demand for improved catalysts.* From a commercial point of view, the main aspects are the activity, selectivity and lifetime of catalysts in technical applications. To understand catalytic processes, a comprehensive, holistic view across many length and time scales is required. Ammonia (\(\text{NH}_3\)), for example, is the basic chemical for the industrial production of fertilisers. Among the alternatives to the Haber-Bosch cycle, electrochemical synthesis of ammonia appears particularly attractive, since it can be driven by renewable electrical energy [85]. However, this requires a fundamental understanding of the electrocatalyst-driven nitrogen reduction mechanism on different length scales. *Operando* X-ray characterisation at PETRA IV can be expected to make a strong contribution to the development of such novel industrial catalysts.
Energy References

Figure 5.12.: Target point of modern dedicated treatments against cancer are cellular receptors which steer growth processes within the ill tissue, e. g. the growth of blood vessels towards the cancer nourishing it. New drug molecules (orange) can block receptor molecules (blue) on the surface of cells. These receptors can then not be activated by growth regulating molecules (red) and hence, e. g. the growth of the tumour is hampered. PETRA IV will provide photons with enough resolving power to image all involved processes from the molecular level up to the level of tissue.
5.2. Life and Health

Life science research is now in an era in which the application of different imaging technologies to related questions and systems has the potential to allow researchers to achieve a holistic and integrated view of organisms – in both healthy and diseased states – all the way from entire creatures to the biochemical basis of the underlying physiological processes (cf. Figure 5.13).

This will enable biologists, chemists, nanoscientists and engineers to tackle pressing societal challenges at the molecular and cellular level. Examples include antibiotic resistance, ageing (including neurodegenerative and cardiovascular disease) and cancer, as well as the greening of agrochemistry and fine-chemicals industries and the development of biotechnological tools to address the need for new, renewable energy sources and novel, biocompatible materials. Key to these endeavours is the availability of correlated multiscale and dynamic structural information from molecules and cells to tissues and organisms.

During recent decades, spectacular advances in terms of technologies and discoveries have already been made in crystallography (Nobel prizes in 1997, 2003, 2006, 2009 and 2012), superresolution light microscopy (Nobel prize in 2014) and electron microscopy (Nobel Prize in 2017). This is reflected in current international initiatives such as the Human Cell Atlas [86], the EU Human Brain project [87] and the CIFAR Molecular Architecture of Life project [88], which provide molecular structure information on length scales from 0.01 nm to hundreds of micrometres that can be combined into a single comprehensive model (cf. Figure 5.14 for an example of the current state of the art).

The next frontier is to add a dynamic dimension to these models. This will turn the models we can create today from simple hypothesis generators into interrogatable dynamic models that can be used to understand the effects of mutations, environmental stresses and signals, infection processes and drugs. A major dream of the life science community is to have a physically real, zoomable predictive model of living cells that captures both the structure and dynamics of the molecules, macromolecules, large assemblies, organelles and the cell itself. What is needed in order to create such a model are detailed, large-region-of-interest maps of cellular and subcellular architectures, the high-resolution structures of the component molecules and macromolecules, and information about their dynamic behaviour. Ultimately, we want to understand, for exam-
Figure 5.14.: An example of the potential of such a multiscale approach is the recent model of a synaptic bouton, the active player in neural transmission, which combines microscopy, structural and analytical data to produce the most accurate atomistic resolution model of a vital physiological unit to date. The figure shows a section through the synaptic bouton (A), together with high-zoom views of selected regions (B–D) to illustrate the hierarchical structure and the high degree of complexity of the system. Reproduced with permission from [62]. © (2014) by the American Association for the Advancement of Science.

Such a model will require a wide range of measurements on isolated components, complexes and cells. Some of these will be accessible in local laboratories, while others will depend on the availability of state-of-the-art research infrastructures at large-scale facilities. What is clear is that no one technique or experiment can provide all the answers – an integrated approach is required. This vision maps well onto the strategic priority areas for the life sciences identified during the recent Helmholtz Programme-oriented Funding (PoF) strategy process. The unique information that can be obtained from synchrotron-based experiments plays a vital role in delivering this vision. Key is our ability to harness X-rays to carry out a wide range of imaging experiments, employing different contrast mechanisms, that yield data at different length scales on systems as diverse as isolated molecules and entire living organisms. The high brightness of PETRA IV will allow us to extend our experimental portfolio in order to apply established methods more quickly and efficiently, and it will open the door to novel imaging modalities relying on coherence-based contrast and bright nanobeams, which will provide new information and insights that are difficult or impossible to obtain by other means.

5.2.1. Structure and Interaction of Subcellular and Molecular Components: Learning from the Building Blocks of Life

The field of structural biology has revealed insights into the molecular basis of living processes in great detail by taking a reductionist approach to examine purified macromolecules and metabolites as well as the molecular and cellular effects of signaling molecules, toxins and therapeutics. Macromolecular structural data had tremendous impact on most aspects of the modern life sciences, from agriculture, food science, infectious disease, oncology and ageing to biotechnology, drug discovery, diagnostics and green chemistry.

The well-established X-ray spectroscopic tools (i.e., EXAFS, XANES, XES, NRS) have allowed life science researchers to probe metal oxidation states and coordination, providing...
key insights into fundamental processes of life such as photosynthesis, respiration and biomineralisation, where transition metals play key roles. Such spectroscopic experiments provide insight into macromolecular folding, ligand binding and molecular reactions. The nascent field of micro/nanospectroscopy, which brings together nanoprobe spectroscopy and imaging experiments, has provoked particular excitement in the life science field, as it provides high-resolution chemical information in the context of an imaging experiment (Figure 5.15). The frontier challenge is now to add the time domain to these nanoprobe experiments. These photon-hungry experiments will greatly benefit from a higher sensitivity as a result of the increased brightness of PETRA IV, enhancing their applicability to studies involving difficult-to-prepare biological samples. Such measurements can also take advantage of the relatively strong signals (for both absorbance and fluorescence) from metal centres, which means that they can be detected at low concentrations and with low absorbed X-ray dose, raising the possibilities of making measurements on living systems [89]. The non-ionising spectroscopies [circular dichroism (CD), infrared (IR)] are also well suited to measurements on living systems and provide a valuable complement to imaging experiments. In particular, the ultra-bright nanobeams that will be available at PETRA IV will allow life science researchers to probe chemical reactions on the sub-micrometre scale in living cells or even tissues, using confocal or two-photon X-ray spectroscopy, which is not possible at PETRA III. Finally, the exceptional coherence properties and time structure of the synchrotron beam at PETRA IV will enable fast time-resolved correlation spectroscopy experiments (cf. Section 4.3) on transport processes at the nanoscale, in particular water transport and more generally biomolecular transport across biological and artificial nano-pores. This will provide new insights into the transport machinery of biomembranes and could reveal entirely new design principles for bio-inspired nano-fluidic devices.

While the “static” ensemble average structures obtained in standard macromolecular crystallography experiments have had a huge societal impact, attempts to rationally design both proteins and small molecule ligands (such as therapeutics) are still limited and mostly based on empirical approaches. This is largely because we are missing detailed information about the macromolecular dynamics.

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Managing Director of the Life Science Nord Management GmbH

“Companies in the biotech, pharmaceutical and medical-technology industries face many challenges and questions that can only be answered thanks to a detailed understanding of biological structures and materials. This ranges from the development of new active ingredients for the treatment of diseases to the improvement of materials for medical implants and the use of nanomaterials in the human body. We expect from PETRA IV that the member companies of the Life Science North cluster will be able to clarify many of these research questions better than before. The expected increase in efficiency for some experiments alone is very interesting. We as a cluster support PETRA IV since the upgrade will continue to strengthen the very well-developed life science sector in northern Germany, in particular in conjunction with DESY opening up to the increased use by industry. ”
5.2.2. Complexes and Intrinsically Disordered Macromolecules: Key Targets in Cancer and Diseases of Ageing

Much of life (and disease) relies on the formation of both transient and stable oligomeric macromolecular architectures within and outside cells. These are hierarchical structures, which can be as simple as a dimeric enzyme, ranging through more complex assemblies of diverse macromolecular components such as the ribosome, to macromolecular machines such as fatty acid synthases and polyketide synthases, as well as viruses. At the extreme, such architectures include for example the nuclear pore complex, flagella and muscle fibres, which are constructed from smaller building blocks that are themselves oligomeric complexes. Such hierarchical architectures also manifest in diseases, for example the fibrous depositions that are the hallmarks of degenerative diseases such as Alzheimer’s, Parkinson’s and amyotrophic lateral sclerosis (ALS).

A second class of macromolecules that are extremely challenging to study but whose biological relevance is becoming increasingly recognised are intrinsically disordered proteins (IDPs). These proteins have no single conformation in their unbound state and only order, or partially order, when in the presence of a cognate binding partner. IDPs are heavily implicated in a range of disorders including cancer, cardiovascular disease, amyloidoses, neurodegenerative diseases and diabetes, but our knowledge of their conformational space and dynamics remains limited. For large complexes, mobile molecular machines and IDPs, small-angle X-ray scattering (SAXS) measurements at synchrotrons have provided a wealth of information on stoichiometry, spatial arrangement, oligomerisation and aggregation. SAXS has also proven very useful for the study of the aggregation pathways associated with progressive, degenerative diseases and in the storage of protein-based pharmaceuticals. SAXS allows us to examine the conformational space sampled by a macromolecule. However, current experiments are predominantly carried out in dilute solutions that can be very far from the native physiological environment in which a macromolecule actually functions.

The highly coherent beam of PETRA IV offers the potential to combine SAXS measurements with X-ray photon correlation spectroscopies (cf. Section 4.3) [93], which is impossible at PETRA III. Such methods provide the exciting possibility of time-resolved imaging of functionally relevant processes such as aggregation (important in neurodegenerative disease), phase separations and partitioning (important for example in development and infection), and self-assembly (important in the development of tissues and organs, infection and the formation of bio-inspired materials). This combination of approaches, enabled by PETRA IV, will allow us to study crowded and dynamic biological systems and to provide extremely novel fundamental data describing interparticle interactions in the concentrated regime. This information would have a huge impact on specific questions, such as understanding how misfolding leads to aggregation and disease in pathologies as in the case of prion disease or Alzheimer’s. It would also help in the design and formulation of improved protein-based therapeutics that can be stored for longer, without the need for refrigeration, reducing their cost and easing their deployment within the developing world.

Protein aggregation and phase separation are dominated by both kinetic and dynamic effects in which the separation and role of the two is not always easy to distinguish – in fact, often they may be intimately intertwined. A typical example is the spinodal decomposition in protein-salt solutions approaching a liquid-liquid phase separation (LLPS). In systems dominated by short-ranged attraction, the
LLPS is often hindered by the formation of a highly dense phase cutting the gelation line. While the early phase of the LLPS is then dominated by a spatio-temporal evolution of the density $\rho(r,t)$ itself, the arrested state is dominated by the fluctuations of the two-point correlator $\rho(r,t)\rho(r,t+\tau)$. In many cases, the densities, volumes and volume fractions of the final states strongly depend on the actual dynamics of the system during the phase transition. However, despite the obvious importance of the dynamic properties in these systems, little is actually known about them. This is due to the experimental difficulty of measuring relatively slow dynamics on nanometre length scales. Light scattering misses the spatial resolution and is plagued by multiple scattering in dense and opaque solutions. XPCS at PETRA IV can fill this important time and length scale window (cf. Section 4.3). In particular, the facility will allow studies of jamming and stress formation, which are expected to be of high relevance for dense glass- and gel-like protein structures as well. The bottleneck of XPCS experiments on biological samples is the high dose accumulated when measuring long series of speckle patterns. SAXS experiments on proteins in solutions showed that the critical dose for aggregation at room temperature is on the level of kGy and below. The superior source parameters of PETRA IV will boost the signal-to-noise ratio $R_{SN}$ in XPCS experiments on protein samples by an order of magnitude, enabling studies of dynamics on the length scales of the hydrodynamic radius of a single protein molecule. Of decisive importance here is the large coherence volume of the X-ray beam of PETRA IV, which allows the energy density to be spread on a much larger volume, reducing the accumulated dose considerably. The large coherence volume of the X-ray beam in combination with higher coherent photon flux at larger photon energies yields an order of magnitude improvement in $R_{SN}$ for experiments with radiation-sensitive samples (cf. Section 4.3). The corresponding coherence beamlines need to be long, with hutch space for large sample-detector distances, which can also be ideally provided at PETRA IV.

Carsten Claussen  
**Head of the Fraunhofer Institute for Molecular Biology and Applied Ecology IME ScreeningPort**

“We are eagerly looking forward to PETRA IV because the investigations that can be carried out there offer enormous potential for biotechnology at the molecular level. In particular, our hits from screening of small molecules can be validated and evaluated at PETRA IV. Also for phenotypic screening new approaches can be found for target elucidation and the understanding of the mode of action. PETRA IV will undoubtedly provide new opportunities for analysing biological systems, understanding molecular relationships and thus contribute to the development of new drugs.”

### 5.2.3. Structure and Function of Biomaterials and Tissues: Tackling Challenges in Clinical Development

Imaging of the structures of organelles, cells, tissues and biomaterials has historically been the province of optical and electron microscopy techniques, in combination with fixing, staining and labelling approaches to provide additional contrast and stability during the imaging experiment. These methods have given us a detailed understanding of the architecture of living systems and, importantly, of how cells, tissues and organisms develop both normally, in disease states and under environmental stress. However, due to their density, biomaterials or in particular thick tissue samples such as brain sections are very difficult to image on the nanoscale and in the native environment using electrons or optical microscopy. Thanks to its increased penetration depth, X-ray imaging avoids the need for sectioning or milling and allows the imaging of entire cells or tissues to similar resolution in the absence of staining as well as the imaging of more dense materials such as bone (Figure 5.15). However, despite recent advances in the X-ray imaging of biological samples at synchrotron radiation sources, it is still not possible to analyse the large series of samples required for clinical studies with a sufficiently high spatial resolution in a reasonable amount of time. This becomes especially evident when aiming for the 3D characterisation of complex nanostructures such as bone or brain.
The weight-bearing human skeletal system is subject to ageing-related diseases, such as osteoporosis, and accidental bone fractures [98]. Bone diseases are often linked to alterations in bone mineralisation, i.e. in deviant mineral particle sizes and arrangements. Where broken or diseased bones are too damaged to heal naturally, a temporary or permanent metallic, ceramic, polymer or composite biomaterial support is often used. Biodegradable magnesium-based implants are a particularly exciting option, especially for children, where standard implants have to be removed as the bone grows, requiring additional surgical interventions. However, the use of magnesium alloy implant materials in clinical applications is currently limited by the need to better understand their complex interactions with biological tissue. A detailed understanding of the degradation process of magnesium alloys in physiological environments is necessary to tailor optimised magnesium-based biomaterials that avoid these drawbacks. Synchrotron wide- and small-angle X-ray scattering is an ideal tool to obtain this information [99], but to provide clinically relevant insight at all from this basic research we need to be able to rapidly screen many samples at high spatial resolution. PETRA IV’s increased brightness in a very small focus opens the door to such experiments as well as to extensions into imaging softer matter such as tendons and other tissues. One such softer tissue is the brain, where a major current challenge is to under-
stand brain anatomy and synaptic connectivity. While the human brain has always been a subject of scientific interest, gaining deeper knowledge about the function and dysfunction of the human brain is becoming ever more important with ageing populations in many societies and the concomitant increasing impact of neurodegenerative diseases. A key requirement is the ability to perform imaging experiments with sufficient spatial resolution in order to determine whether two adjacent neurons actually interact directly via a synaptic junction. While the recently reported BigBrain map [100] is based on classical histology techniques, in which 20 µm thin slices are X-ray analysed individually and the images then reassembled in three dimensions, PETRA IV has the potential to allow us to carry out synchrotron-based tomographic analyses of entire brains and/or regions of the brain, again with greatly increased throughput.

The recent advances in the X-ray imaging of biological samples, using spectroscopy, diffraction, scattering and microscopy, are hugely exciting. However, to achieve the dream of time-resolved imaging with a few-10 nm resolution in living organisms, the major challenge that remains – and that will be almost impossible to overcome – is radiation damage. For full-field applications, 10 nm resolution should be achievable under cryogenic conditions [101]. However, for living objects, 50 nm resolution seems to be the hard limit [102]. The total tolerable dose is on the order of kGy for single to few cells and on the order of Gy for multicellular organisms. These limits in total dose translate directly into achievable resolution (the resolution is proportional to the fourth power of the dose [8]).

While the absolute dose limits remain, the higher coherent fraction of PETRA IV will greatly increase the sensitivity of imaging modalities that rely on phase information (e.g. phase contrast full-field and ptychographic imaging).

For scanning applications, improved nanofo-cusing will translate into increased spatial resolution in all applications [87]. Ultimately, within tolerable dose constraints, the spatial resolution is limited by the size of the scanning beam only. This opens up the exciting possibility of using relatively low-dose micro-X-ray tomography to define the region of interest for a complementary high-resolution electron tomography imaging experiment, utilizing the benefits of each of both techniques. A complementary use of both synchrotron beamlines and local electron imaging resources will be crucial here (cf. Section 2.1).

PETRA IV will also allow us to make a huge leap in the investigation of bio- and bio-inspired materials thanks to the increase in brightness and in the flux of coherent photons at energies above 20 keV. With the availability of brighter nanofoocused beams, SAXS and XRD scanning experiments will be significantly sped up, allowing us to scan larger regions. In addition, the increase in coherent flux will be extremely beneficial for differential phase contrast (DPC) tomography experiments [92]. Finally, PETRA IV’s unique beam properties in combination with recent breakthroughs at DESY in multilayer Laue lens X-ray optics offer the tantalising possibility of atomic-resolution X-ray microscopy over large fields of view on bio- and bio-inspired materials.

An important final consideration for the impact of PETRA IV on life science research is that coherence-based sensitivity can be traded against flux in order to increase throughput. Choosing the right compromise between coherence and net photon flux will allow the users to increase the scan speeds for scanning applications, enabling them to image larger fields of view while maintaining a sufficiently high spatial resolution. Increased throughput is extremely desirable for imaging applications. At present, imaging studies using scanning modalities require hours to days of experiment time. This is not feasible for a routine user programme and limits uptake by industry (e.g. for imaging tumour vasculature), where many samples are needed for meaningful statistics.

In summary, the advanced imaging of soft matter and biological samples that will become available with PETRA IV represents an incredible opportunity for life science researchers to contribute to basic medical and biochemical research and to clinical and biotechnological applications of direct relevance to today’s societal challenges. In addition, users of PETRA IV will be able to take advantage of the physical proximity of a state-of-art hard X-ray free-electron laser (European XFEL), an increasing number of life-science-focused research institutes and other key complementary research infrastructures (cf. Section 2.1.1) in the Science City Bahrenfeld (cf. Section 2.1).
Innovation Aspects

The holistic view on physiological processes provided by PETRA IV will enable us to gain a deep understanding of the functions and interactions in organelles, cells and tissues. This will have a massive effect on companies from the pharmaceutical, bio- and medical-technology industries. The direct and easy access to PETRA IV will allow them to shorten their development of new and innovative drugs for these growing markets.

X-ray scanning microscopy with highest resolution combined with full-field X-ray microscopy will lead to the understanding of neurodegenerative diseases such as Alzheimer’s and Parkinson’s. This will allow new approaches to drugs and therapies that are fine-tuned or designed for a single person. In pharmacology, new imaging techniques will help to localise drugs in tumour cells. The combination of SAXS and imaging techniques will allow researchers for the first time to study the aggregation behaviour of insulin with high time resolution. Understanding the physics on the nanometre scale will also open up a vast range of industrial applications in the field of biomaterials. Nanoparticles will be used as carriers of active substances or drugs. One field of application in this context is the therapy for cancer. The release of the drug in the tumour cell can be controlled by the pH value, which is increased in cancer cells. This well-directed drug delivery and “targeted medication” will pave the way for new drugs or a smaller dose of known drugs with less side effects. All these aspects are of great importance for the pharmaceutical industry.

Biotechnological research utilising the new insights at PETRA IV will lead to novel products in a wide variety of markets. In the field of enzymology a much higher efficiency will lead to a significantly lower energy consumption in energy-intensive industries for example in the production of ethanol. Adapted and designed enzymatic processes for the decomposition of plastics to improve waste treatment procedures can be developed. High-resolution imaging in the field of bone and bone replacement materials (usually Mg, Ca, etc. or compounds) will help us to understand the degradation of bone substitute materials on the nanoscale. This will enable the industry to design new bone substitute materials. In addition, high brightness of PETRA IV will enhance the capabilities for automated and high sample throughput. With these increased statistics, preclinical study trials can be conducted faster and more cost-efficiently than today. Insights from research on the function of biomolecules in spatially restricted structures (such as pores) will have a significant effect on the efficiency of molecules in technical filter systems. Experiments that study the behaviour of water when passing through such a filter will strongly benefit from the high degree of coherence at PETRA IV. This will have a strong effect on the development of new dialysis filters. Next to that, the development of new bioactive films will enhance the capabilities of antimicrobial surfaces.
Life and Health References


[87] Human Brain Project, Online.
[88] CIFAR Molecular Architecture of Life project, Online.

Figure 5.16.: By performing friction experiments at PETRA IV, researchers can analyse how fine dust particles are released and distributed in the environment when a car tyre comes into contact with the road surface. In the future, innovative materials could reduce the production of nanoparticles from this abrasion and thus reduce the risk potential of fine dust.
5.3. Transport and Technology

The targeted synthesis of new materials is one of the grand challenges in the field of transport and technology in view of optimising processes and functionalities towards energy efficiency and reduction of emissions. This is particularly true in a world of limited resources, where the optimisation of materials towards enhanced durability will be crucial for the sustainable use of resources. At the same time, these materials have to fulfil demanding requirements regarding their functionality under extreme working conditions. It is clear that this requires advanced engineering efforts to control the structure and function of such materials on all length scales from atomic to macroscopic dimensions.

The research examples in this chapter represent key scientific areas that deal with these challenges and that can be uniquely addressed with the research opportunities unfolding at PETRA IV. These key areas are:

1. new materials and their properties emerging at ultra-high pressures,
2. the monitoring and control of the kinetics of processing materials and
3. the structural and dynamical origins of friction.

The overarching challenge that all materials research will face in the next decades is an increase in the complexity of material systems, which cover a wide range of length scales (from nanometres to millimetres) and time scales (from microseconds to years). In particular, the emerging field of computationally guided synthesis (“digital twin”) will only make significant progress when advanced characterisation tools to address all these scales simultaneously will be available. Ultra-low-emittance storage rings such as PETRA IV will fulfil these criteria and lead to a breakthrough in the targeted synthesis of materials. Applying the entire portfolio of coherent imaging techniques at high X-ray energies to complex sample environments that simulate materials working and processing conditions will profoundly enhance our ability to resolve increased hierarchical complexity across several length and time scales, laying the basis for studying real-life conditions in the fields of fundamental physics, physical chemistry and materials science.

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"The aviation industry continues to grow, and the demand for more efficient, resource- and environment-friendly aircraft and propulsion systems is increasing. To realise these, we are constantly working on the development of new products, materials and manufacturing processes. An X-ray source such as PETRA IV can make a significant contribution here. This is because it can be used to investigate important materials science issues with unprecedented depth of detail and outstanding efficiency. The development of both high-strength and lightweight materials, which are also exposed to the high thermal and corrosive stresses of flight operations, can be supported and accelerated with these new investigation methods. PETRA IV makes it possible to carry out material tests and characterisations under extreme conditions.”

5.3.1. Extreme-Conditions Science: Transforming Matter

A promising route towards new materials is the application of ultra-high pressures and temperatures to create compounds that would not form under conditions of conventional material synthesis and processing techniques and that will lead to synthesis of industrial relevant quantities of new materials, e.g. [103]. Extreme conditions of high pressures (1 GPa to 1000 GPa) at simultaneous low and high temperatures (4 K to 5000 K) play a crucial role in this field. These conditions can be created either in diamond anvil cells (DACs) or in large-volume press (LVP) devices. DACs can reach much higher pressures and extremely high or low temperatures, whereas LVP devices are used to synthesise larger quantities of a particular material. Together with the emergence of theoretical structure prediction tools...
such as \textit{ab-initio} quantum-mechanical calculations, evolutionary enthalpy minimisation algorithms and/or extensive data mining procedures, these activities have accelerated the field of materials discovery \cite{104}, as evidenced by several attempts to successfully synthesise previously predicted structures \cite{105–107}. For example, compounds that would violate chemical intuition but nevertheless were theoretically found to be stable, can indeed exist even in simple systems consisting of just Na and Cl in various stoichiometries at non-ambient conditions \cite{105} (cf. Figure 5.18). Another striking example is the observation of materials becoming superconducting under high pressures.

Research in the field of high-$T_c$ superconductivity has led to materials with transition temperatures far above the temperature of liquid nitrogen (cf. Figure 5.17). A very spectacular recent finding in this field is the observation of superconductivity in lanthanum hydride close to room temperature at pressures above 200 GPa \cite{109}. Even under these extreme conditions, a thorough investigation of such systems with advanced analytical tools will be an important step towards understanding superconductivity in general. This could eventually guide the synthesis of materials that are superconducting at room temperature under ambient pressures. It goes without saying that such a discovery would have a massive, productive impact on all branches of technology and society alike. Another very important endeavour for the years to come, relevant for immediate technological applications, will be the synthesis of materials by quenching from high pressures to ambient conditions. In sufficient quantities, these materials might be used either directly for industrial applications \cite{110} or as a seed for growing larger quantities with other synthesis techniques \cite{103}.

**Figure 5.17.**: Evolution of the superconducting transition temperature $T_c$. The champion today is lanthanum hydride with a step in $T_c$ up to 260 K at a pressure of 200 GPa, which is almost 60 K higher than the previous champion, sulphur hydride, with a $T_c$ of 203 K (Figure adopted from \cite{108}).

Research in the field of high-$T_c$ superconductivity will only be possible when combining high-energy X-ray diffraction and the portfolio of coherent X-ray diffraction and imaging techniques applied to samples in a large-volume press or a diamond anvil cell.”

**Figure 5.18.**: Electron localisation function in the cubic NaCl$_2$ structure that was theoretically predicted and found to be stable under pressures above 20 GPa \cite{105}. By courtesy of Artem Oganov, Stony Brook University.
For over a decade, theorists have predicted that at very high pressures above 4 Mbar to 5 Mbar and high temperatures, simple materials such as aluminium would transform into very complex structured polymorphs and not into simple closed-packed atomic arrangements. DAC experiments were unable to reach such pressures until five years ago, when the development of so-called double-stage DAC made it possible to achieve pressures as high as 10 Mbar [111]. Pioneering experiments in a double-stage DAC at pressures of up to 7.5 Mbar on osmium revealed unexpected changes in the hexagonal close-packed (hcp) cell parameter ratio $c/a$ at 4.4 Mbar [111]. The finding was attributed to pressure-induced interactions between core electrons of neighbouring atoms. Such an interaction would have a significant impact on the physical and chemical properties of compounds at very high pressures and requires further investigations to explore its general validity. Thus, the development of the double-stage or toroidal DAC technology has opened up a new field of research that will occupy high-pressure scientists for the next decades.

It is common to all of these studies that crucial information about the material transformation pathways and intermediate compounds very often remains elusive because the pressure cells contain only tiny amounts of confined samples under conditions that preclude access to the relevant length and time scales. The nanofocused beams of high-energy X-rays at PETRA IV will enable materials scientists to characterise the structural and dynamical properties during these synthesis processes under extreme conditions that are not accessible today (cf. Section 4.2 and Section 4.5).

Therefore, the biggest challenge in making significant progress in the pressure-induced synthesis of new materials with either fundamental or industrial relevance will be the increase in the complexity of the involved material systems, which span several length scales (from micrometres to millimetres) and time scales (from microseconds to seconds). The challenges of revealing the structure and dynamics over all these scales can only be tackled by developing new analytical techniques that enable imaging capabilities combined with X-ray diffraction (single-crystal and powder) and that provide information on the time-dependent processes during the synthesis. In particular, in combination with the unprecedented brightness of PETRA IV, the portfolio of coherent imaging techniques at high energies, which is essential for penetrating the complex sample environment of high-pressure devices, will significantly improve our ability to tailor synthesis processes across length and time scales.

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“Ultra-high-pressure physics in the area of materials science can only be conducted at a source such as PETRA IV that provides the brightest high-energy micrometre to sub-micrometre beams.”

5.3.2. Kinetics of Material Processing

Gaining control over the properties of advanced materials by adjusting and steering their processing conditions is one of the great challenges of modern materials science. Virtually all materials and manufacturing processes used today involve non-equilibrium conditions, either as an intermediate on the way to a final product or for the final product itself. This is not only a central aspect of materials science per se, but also the basis for manufacturing processes in all industrial materials. For example, microstructure modification and the controlled introduction of defects in the materials by rolling, extrusion, alloying, solute precipitation and thermal cycling are the key processes in the production of metal alloys. Traditionally, material processing involves conditions close to equilibrium, but processing far from equilibrium offers new opportunities for producing materials with new properties. In both cases, a thorough understanding of the dynamics of the underlying physical mechanisms has the potential for improving efficiency and achieving desired properties. The industry has been phenomenally successful in the (top-down) development and refinement of new materials and material-processing steps based on all of today’s material-processing technologies. Often, however, there is a lack of bottom-up ap-
approaches based on a fundamental understanding of the physical properties of materials, material microstructures and material-processing steps needed to develop materials and material properties outside known routes. When it comes to understanding the processing of engineering and energy materials, in-situ X-ray scattering and X-ray imaging investigations are mandatory to cover the full range from fundamental physical effects to complex industrial processes such as welding. The development of new materials requires the monitoring of structural changes as a result of indentation, bending, torsion, tensile and compressive deformation, heating and cooling, as well as electric-current applications.

One of the most important goals in the study and optimisation of industrial processes is to learn how to properly predict the lifetime of a component. The industry wants to avoid huge safety margins that are resource-consuming and create large costs. Simulation and modelling are required to understand materials and predict their behaviour under operating conditions. In-situ experiments with ultra-bright synchrotron radiation are an invaluable contribution to validating these results, yielding unique and complementary information about the kinetics of material processing. The elementary steps of a material reaction to an external stimulus occur on the level of single or few grains. Thus, the demand for modelling of material properties on all levels – from the local crystalline structure, individual defects and their interaction in sub-grains, single grains and their boundaries to the whole polycrystal – is growing significantly, supported by the continuously improving computational and modelling capabilities. Scanning X-ray microscopy with various contrasts and in particular with high-energy X-rays is crucial to develop a true digital twin of a material and follow processes within it (cf. in particular Section 4.2 and Section 4.5). Only at PETRA IV with its extreme brightness can the full hierarchical structure be followed in the required detail, in particular under process conditions with the required time resolution (cf. next section).

Time-Resolved Studies during Processing of Metallic Materials

A comprehensive understanding is presently lacking of microstructure-based heterogeneity and its consequences for materials damage and failure, as well as of phase transformation initiation during high-rate processing. Concentration and spatial variability in compositional and dissipative defects add to the difficulty of understanding dynamic effects in polycrystalline microstructures. Dislocations can be nucleated or activated and phase boundaries can be crossed during dynamic deformation. Many materials also produce twin-or slip-band structures with deformation that produce further heterogeneity within individual crystals. High-resolution X-ray techniques will be needed to probe the physics of dynamic solid-solid phase transformation and damage at length scales where these transformations nucleate. A detailed understanding of such processes is mandatory to relate the origin and dynamics of these processes to the microstructure of the materials. The extreme conditions encountered under dynamic loading provide the setting to explore the interplay between mechanical and thermal processes in these complex systems.

High heating and cooling rates and high deformation rates are frequently encountered during processing of advanced metallic and intermetallic alloys. For example, during welding, induction hardening or additive layer manufacturing (see below), heating/cooling rates higher than 1000 K/s occur, and hot rolling and forging are often performed with deformation rates higher than 1/s (this corresponds to e.g. a height reduction of 10% within 0.1 s). These fast processes can significantly influence the mechanical properties of materials. High deformation rates can generate strong textures, which result in unwanted mechanical anisotropy. High cooling rates can result in phase constitutions far away from thermodynamic equilibrium.

This especially concerns advanced metallic materials, e.g. TRIP steels, beta titanium alloys or TiAl-based alloys, which are usually complex multiphase alloys. The disequilibrium conditions can in turn be used to trigger the formation of novel microstructures, which change the materials’ mechanical properties, e.g. hardening by grain refinement. Modelling
of such disequilibrium conditions is still in its infancy, and in-situ experiments are thus indispensable to understand these fast processes. A gain in brightness at PETRA IV of about three orders of magnitude in the high-energy X-ray range compared to today (cf. Figure 4.3) will enable materials scientists to study such processes with a sufficiently high time resolution (>10 kHz).

Additive Manufacturing: Operando Imaging and High Position-Resolution Diffraction

During the last decade, different techniques of additive manufacturing (AM, also known as 3D printing) have become relevant for industrial-scale manufacturing processes [113]. This is most prominent in medical, aerospace and automotive industries [114], where the functionality of parts often relies on a high geometrical complexity, for which AM provides substantial benefits. Currently, most of the metal AM systems are of the laser powder bed fusion (LPBF) type, owing to its superior capability to make geometrically complex parts. In a typical LPBF process, a laser beam is scanned across a thin layer of metallic powders and locally melts the powders through to the layer below. However, the quality that is currently achievable in AM parts still puts heavy limitations on their applicability in many fields. Rough surfaces, significant porosities, residual stresses, unfavourable phase and grain structures – virtually any part produced by AM today suffers from at least one of these deficiencies, induced by the extremely high heating and cooling rates of about 10^6 K/s [115, 116] and their consequences, such as powder vaporisation, non-equilibrium phase transitions, uncontrolled melt flow and rapid solidification. In order to understand the mechanisms responsible for these processes, it is imperative to develop and apply in-situ characterisation techniques to study the dynamic microstructural evolution with highest spatial resolution. Unfortunately, it is extremely challenging to experimentally characterise the dynamics of the LPBF process due to the highly localised and very fast interaction of the laser beam with metal powders. To understand the formation of the aforementioned defects, the process of AM can for example be combined with in-situ X-ray diffraction and imaging, so that the dynamic microstructural evolution [112] can be investigated (cf. Figure 5.19). This conceptually simple idea is technologically very challenging because all the relevant processes, i.e. the interactions of the laser beam with the metal powder and the solidified part, are confined in space and time to a microscopic volume and a millisecond time frame.

The X-ray scattering and diffraction methods available at PETRA IV will allow an unprecedented combination of very high spatial and temporal resolution (i.e. small beam, high flux

Figure 5.19.: Dynamic X-ray images of laser powder bed fusion (LPBF) processes of a TiAlV alloy during an additive manufacturing procedure [112].
density, short exposure times), while providing a substantially increased coherent flux at higher energies, leading to an improved X-ray optical contrast in low density contrast systems. The elevated fraction of coherent flux at high energies will allow a more efficient focusing at these energies, thereby providing the prerequisite for high spatial resolution studies on high-Z material or very thick samples (cf. Section 4.5). In simple terms, both imaging and diffraction data (WAXS and SAXS from molten and solidified material fractions) will become more easily accessible, promoting investigations of the dynamics of solidification, grain and phase evolution and providing understanding of how these processes contribute to the stress build-up in the final part. This fundamental knowledge will be of essential value for developing pathways to avoid defects and specifically tailor grain/phase structure in order to locally customise the mechanical properties of an additively manufactured part.
Innovation Aspects

New and smart materials are among the most important requirement for innovative products in industry in the coming decades. Thanks to its unparalleled brightness, PETRA IV will provide an extremely high spatial resolution combined with a high temporal resolving power. This will allow scientists to study new phases of matter under extreme pressure and temperature conditions. Results and insights emerging from these experiments have the potential to significantly improve the physics models and simulation tools in these fields. The tools are of high interest to industry, as they will enable scientists and engineers to find new phases that are metastable at ambient conditions and that have special technical properties. One result could be novel nitrides and carbides that would provide innovative hard coatings for tools in milling, grinding and drilling applications. New types of perovskites have potential as semiconductor materials with outstanding properties, and the synthesis of new hydrate-bearing materials (e.g. iridium hydrates) will significantly improve storage technology for hydrogen. Next to that, a better understanding of storage behaviour in zeolith phases can be used to create new molecular sieves to improve processes for example in the petrochemical industry.

Additive manufacturing is a recent industrial development that has unprecedented power to shape and revolutionise the industrial chain and transform other industries as well. However, we need to understand more about the materials used and how they interact, especially when it comes to surfaces or the construction of layers. PETRA IV will bring great progress in this context, especially in scanning and imaging techniques with nanometre resolution. As a result, new materials optimised for the particular application will enhance our capabilities for lightweight and more durable constructions of vehicles and aircrafts. This will lead to less energy consumption and less emission of climate-critical gases.

Understanding materials on the nanometre scale is key to developing new and innovative products in the semiconductor, IT and medical-technology industry. The typical size of structures in integrated circuits has become smaller and smaller. With today’s technology, we are already reaching dimensions where mechanical stress between different semiconductor and metallic components becomes relevant. For example, the mechanical stress at the edges of conductor paths in integrated circuits currently prohibits the development of even smaller structures. Understanding these processes on the nanometre scale will enable the semiconductor industry to develop new generations of computer chips. In the field of medical engineering, stents for blood vessels will be a field of industrial research. The diameter of wires in these devices is approx. 200 μm. The typical grain size in such a wire is approx. 50 nm. Only with nanograin-mapping experiments and the beam quality of PETRA IV will it be possible to clearly understand the physics in these stents and thus to develop new and improved stent systems.
5.3.3. Structural and Dynamical Origins of Friction

Tribology is the science and engineering of interacting surfaces that are in sliding contact with each other. It covers the entire area of friction and wear including lubrication, comprising interactions between interfaces of solids with solids and liquids. The coupling of structural properties and chemical processes in the area of the sliding contact is commonly considered the key mechanism that results in the tribological properties of the system. This area of contact is buried, however, and thus not accessible to conventional imaging methods. Highly focused beams of high-energy X-rays are therefore the ideal tool for imaging, structural analysis and chemical identification of matter in the area of the buried contact. As illustrated in Figure 5.20, friction is a multidimensional problem, where structural entities ranging from single asperities on atomic scales to surface corrugation of millimetre dimensions determine what we experience as macroscopic friction. A thorough understanding of friction, lubrication and wear will thus only be possible if structure and dynamical properties can be revealed on all length scales.

Figure 5.20: Length scales in friction between two solid interfaces, encompassing entities ranging from single asperities on atomic scales to surface ripples of millimetre dimensions.

Energy dissipation due to friction and wear amounts to economic losses of more than 10% of the gross national product of industrialised nations. By conserving energy and reducing the environmental impact of fine dust resulting from abrasion and wear, the application of tribological knowledge leads to both economic assets and ecological advantages. Moreover, the minimisation of tribological losses leads to an increase in power, power density and efficiency. A fundamental understanding of the frictional processes, resulting in the synthesis of reduced-friction materials, would thus have an enormous economic impact. However, despite great advances in the measurement of frictional forces on the atomic scale, the mechanisms of frictional energy dissipation are not yet resolved.

Understanding the structure and dynamics of liquids confined in small volumes is important in many scientific fields, including for example lubricants between mating parts or biological interactions and adhesion. Tribology is of great importance in biology. Artificial joints, for example, are subject to constant friction and wear. Artificial hip replacement is most frequently performed. In Germany alone, 200,000 artificial hip joints are implanted every year. To improve the durability of artificial joints, it is important to understand tribosystems operating under...
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Figure 5.21.: Accessing the contact area between two materials in sliding friction with nano-focused hard X-rays to retrieve a coherent SAXS pattern from the contact area. By courtesy of Martin Dienwiebel, KIT.

ultra-mild wear conditions, i.e. at wear rates <1 nm/h. These systems are known to display various changes in the microstructure below the stressed surface. While plastic deformation of the grain structure can typically be observed at larger depth, recrystallisation and mechanical mixing with surrounding media or surface oxides takes place closer to the surface [117, 118]. The formation of such a compound layer ("tribomaterial") is assumed to be a prerequisite for very low wear rates.

In orthopaedic surgery, for example, self-mating couples from austenitic alloys are used for artificial hip joints. While in engineering applications such tribopairs typically lead to adhesion and seizure, the tribomaterial formed during articulation inside the body, consisting of nanometre-small metallic grains and organic substances, acts as a boundary lubricant [119]. Still, not all austenites show the high wear resistance required for implants, due to the type of wear particles formed. The suitable alloys eject nanometre-sized wear particles from the tribomaterial, while other, similar alloys produce micrometre-sized particles from the region below [120]. With the ongoing development and improvement of materials and tribosystems, ultra-mild wear conditions will become more and more relevant in the future. In these systems, the thin tribomaterial surface layer of 100 nm to 300 nm depth is decisive.

The small beam sizes at PETRA IV make it possible to investigate hard material contacts between metals, semiconductors and ceramics, which are interesting probe systems with high relevance in industrial applications. Non-compliant material contacts will generate only very small flat contact areas a few micrometres in size. A beam width significantly below 1 µm will therefore be mandatory to study realistic systems. In this field, cyclic friction experiments are performed to unravel wear mechanisms acting in bearings. Here, the structural evolution of surface and sub-surface regions, the development of tribofilms and the oxidation state of the surface are of particular interest. Examples for phenomena currently under discussion are the microstructural development at surfaces, such as the formation of nanocrystalline layers, rippling of the surface topography as well as oxidation and oxide removal, to name but a few.

Coherent SAXS is an ideal method to determine the structural changes of surfaces that are in sliding contact with each other, especially along those tracks where abrasion, wear and the formation of particulate matter occur (cf. Figure 5.21). High coherence allows structural correlations to be discovered within areas that extend beyond the contact itself, thus revealing mechanisms of ripple formation and correlated roughness over hundreds of micrometres, for example. The high intensity of the focused probing beam enables studies of structural features in regions buried deeply below the surface. In addition, X-ray spectro-
scopic techniques allow researchers to follow stoichiometric changes, the decomposition and inclusion of lubricant additives or the oxidation state of the surface. During sliding of a metallic contact, a mutated surface layer forms, which carries most of the plastic deformation occurring in the process and which largely determines friction and wear. The origin and evolution of this distinct subsurface layer remain elusive, since our knowledge of the elementary mechanisms promoting these changes is limited. On the other hand, however, only this knowledge will allow for a strategic tailoring of tribologically loaded metals. Already after only one sliding pass, atomic dislocations self-organise to form a distinct microstructural discontinuity down to a fraction of a micrometre below the sliding surface. This discontinuity introduces a weak interface into the material and later becomes the origin for the detachment of wear particles with a broad size distribution. Such particles make up a significant fraction of the particulate matter that is released into the environment and constitute a significant health risk if incorporated. Particularly dangerous are ultra-fine particles of a few 100 nm diameter, which could even pass the human blood-brain barrier. Innovative materials whose abrasion contains significantly smaller quantities of ultra-fine particles could therefore reduce the risk potential of particulate matter in the future. Friction experiments at PETRA IV can investigate the distribution of particle sizes and identify particulate matter contents that are hazardous to health. This will enable researchers and industrial users to understand in detail how fine dust particles are released from a car tyre when the tyre comes into contact with road surfaces, for example, and how the particles are distributed in the environment.
Innovation Aspects

Friction wastes a significant amount of resources in mechanical machinery and industrial production chains. Even small optimisation steps in this context will have a large impact on overall energy consumption and costs. Today, there is no clear understanding of friction on the nanometre scale. At PETRA IV, we will be able to improve it on all relevant length and time scales. In industrial applications, friction often occurs on the interfaces between metal workpieces and is difficult access with analytical techniques under working conditions. PETRA IV will deliver bright high-energy X-rays that have a high penetration power. This will enable studying friction processes at metal interfaces in-situ and operando and on the nanometre scale. Research in this field at PETRA IV will improve all kinds of technical devices, such as motors, drives, generators, gearboxes, etc., by optimising the losses due to friction and enhancing the devices’ overall energy efficiency. In addition, the reduction of friction will decrease wear and tear in mechanical systems, increasing their lifetime. In certain technical applications, however, the enhancement of friction is decisive. One example is brake systems, which can be found in many machines. An optimisation in this direction will lead to highly efficient brakes with less material budget cost and wear. In general, with the help of PETRA IV, friction processes can be optimised to the needs of specific technical applications in a great variety of technical settings. This is highly relevant in the automotive and aerospace industry, but also in all kinds of machine engineering industries. Research in this field also includes interactions of lubricant films between mechanical components, which are very interesting for lubricant manufacturers. Since friction is relevant in almost all technical systems, even small optimisations will lead to significant increases in overall energy efficiency, which will in turn result in reduced emissions. In the long run, this will help to improve public health.
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Figure 5.22.: Water shows characteristics like no other liquid. These anomalies make life on earth possible and are important for technical applications. Researchers are still searching for explanations to understand the unique behaviour of water. According to theory, in its liquid form it consists of two components. PETRA IV could for the first time differentiate these fluid states both structurally and dynamically.
5.4. Earth and Environment

In our global society, earth and environmental science should concentrate its efforts on the grand challenges facing humankind, with the goal of achieving sustainable growth while simultaneously preserving wildlife and habitat. The United Nations has defined Sustainable Development Goals\(^1\), many of which are of both environmental and geological relevance, e.g. Clean Water and Sanitation, Affordable and Clean Energy, Sustainable Cities and Communities, Responsible Consumption and Production, Climate Action, Life Below Water and Life on Land. Fundamental research will support industry in the development of innovative methods and materials.

Environmental science involves subjects such as the understanding of Earth processes, the evaluation of alternative energy systems, pollution control and mitigation, natural resource management and the effects of global climate change. The fate of trace metallic elements in aquatic media and soils – as contaminants or as essential elements for life – was and is still studied extensively. Determining the speciation of trace elements in natural systems and waste depositories to better control their mobility and bioaccumulation is a major goal of environmental science. In soils, surface and subsurface waters, and sediments, metallic elements will interact with different entities of relatively high chemical reactivity, including particles and colloids, made up of either mineral, organic or biological components. The concentration of metal solved in water is strongly influenced by the reactions occurring at the solid-liquid interface, such as natural colloids and particles constitute an almost infinite reservoir of reactive surface (cf. Figure 5.23) [121]. Low trace metal bioavailability in many soil types, including major areas of the world, causes a reduction in crop production and diminishes nutritional value. In other areas of the world, however, metal toxicity is a severe agricultural and environmental problem. For environmental risk assessment and remediation as well as improved agriculture (targeted fertilisation and breeding), the mechanisms of metal uptake, distribution, speciation, physiological use, deficiency, toxicity and detoxification need to be understood.

In general, many of the natural objects that are at the centre of environmental study are inherently heterogeneous. Therefore, the application of spatially resolved techniques, be it spectroscopic, imaging and/or structural characterisation, is paramount. Many environmental processes occur at interfaces, such as the water-rock interface, cell membrane or wall-water interface, as well as aerosol surface-air interface. There is a strong need to investigate the 3D structure of the interfaces by X-ray Fluorescence (XRF) and X-ray Absorption Near Edge Structure (XANES) nanotomography [122–124], providing key information in the nanometre range that cannot be accessed directly by any other in-situ experimental technique. The extreme brightness of PETRA IV will facilitate nanobeams with sufficient flux that will allow scientists for the first time to enter the relevant nanoscopic length scale with trace level sensitivity.

Water is undisputedly the most important liquid on Earth and omnipresent in our everyday life. It is therefore no surprise that water plays a major role in various scientific disciplines, such as chemistry, biology, physics and geoscience. Water owes its great importance to its many ways anomalous behaviour. Beside the well-known density anomalies, such as the density maximum of liquid water at 4°C or the increase in density upon melting, many macroscopic properties of water deviate from those of normal liquids. Based on our current understanding, life cannot evolve without water, likely also thanks to water’s anomalous behaviour. Although much effort has been undertaken during the last century, the local structure of water and its relation to microscopic and macroscopic properties remain a mystery and are still hot topics in research.

These topics will be part of the planned Centre for Molecular Water Science (CMWS) that will be founded at DESY (cf. Section 2.1). Research at CMWS will focus on the fundamental properties of water as well as on the role of water in geo- and astrophysical processes, nanoscience and technology, real-time chem-

\(^1\)https://www.un.org/sustainabledevelopment/
Figure 5.23.: Cycles of selective settling, weathering at the water-sediment interface, and remobilisation in contaminated river. The modification of suspended iron-rich particles provoke a modification of heavy metal (Zn) partitioning between water, suspended solids and sediments [121]. Modified version by courtesy of Emmanuelle Montarges-Pelletier, CNRS Université de Lorraine.

The unique properties of PETRA IV will allow us to answer many fundamental questions in water research. Besides enabling fundamental research on the structure and dynamics of water and ice, as outlined later, PETRA IV will provide a new level of understanding of structures, nucleation and growth at water interfaces with unprecedented spatial and temporal resolution. X-ray nanobeams at PETRA IV will offer unique new opportunities for electrochemistry and corrosion research. Furthermore, the novel experimental possibilities will facilitate the development and optimisation of green chemistry procedures and applications. In particular, ex-equilibrium characterisations of aqueous chemistry at PETRA IV will result in novel concepts of how water shapes chemistry.

The Sustainable Development Goals defined by the United Nations are equally dependent on the dynamic processes occurring in the Earth’s interior at different time and length scales and on their impact on the Earth’s surface environment. The reason is that likely all volatiles are recycled from the interior of the Earth to the surface (i.e. the atmosphere) through earthquakes and volcanic eruptions, for example, and back down via subduction of oceanic plates. Volcanic eruptions and earthquakes have an influence on the composition of the Earth’s atmosphere, since these processes can suddenly release substantial amounts of greenhouse gases (CO$_2$ and methane). Forecasting the location of the next big earthquake or volcanic eruption is furthermore essential and requires an integral knowledge of the underlying processes responsible for their genesis. In particular, understanding the H$_2$O-bearing mineral cycle and the release of H$_2$O in the Earth’s interior is still one of the major unknowns that need to be clarified if forecasting of earthquakes and volcanism is to improve.

None of the processes responsible for the occurrence of earthquakes or volcanism can be studied directly. They need to be simulated in high-pressure devices such as large-volume presses (LVPs) or diamond anvil cells (DACs). Probing the crystallographic and spectroscopic properties at simultaneous high pressures and temperatures to determine the stability and
physical properties of deep-Earth materials can only be achieved through photon-based investigations. The nano-sized, high-brightness, high-energy X-ray beam of PETRA IV will enable the study of tiny (sub-millimetre to micrometre) samples under extreme conditions of high pressures and temperatures, providing superior spatial resolution to resolve sample inhomogeneities. Far- and near-field imaging combined with X-ray scanning diffraction microscopy will provide the most powerful tools to resolve crystallographic structures and processes in geologically relevant materials and elucidate the hierarchical complexity across several length scales. Research at PETRA IV will for example enable high-resolution visualisation of the onset of cracking, of the stress distribution and of the formation of melting, which on large scale can cause earthquakes and volcanism due to e.g. the breakdown of water-bearing Earth materials.

The high gain in spectral brightness in the high-energy X-ray range (> 40 keV, cf. Figure 4.3 and Section 4.5) will be transformative for studying the states of matter under extreme pressures and temperatures. Making use of efficient nanofocusing with low background, crystallographic diffraction studies of single crystals at pressures up to 1 TPa will become possible at PETRA IV. This development will open up new research opportunities for investigating processes in the deepest part of the Earth and enable studies of the interiors of massive super-Earth exoplanets by delivering highest-quality crystallographic data from minute sample volumes. PETRA IV might even open up the possibility to study warm dense matter (WDM) under constrained states like those encountered in astrophysical environments, such as the interior of large gas giants (e.g. Jupiter and Saturn), white dwarfs or even on the surface of neutron stars. In contrast to traditional laser or gas gun shock compression, creating WDM in a diamond anvil cell would take away the transient state of the systems and for the first time enable studies of WDM under equilibrium conditions. Probing this state without additional heating at PETRA IV would be unique and open up a complete new field of studies not possible today.

5.4.1. Environmental Science

Imaging Metal Metabolism in Plants

Many metals, such as copper, are essential for all organisms as active centres of enzymes – about one third of all proteins are metalloproteins. In higher concentrations, however, many essential trace metals are highly toxic. Both deficiency and toxicity occur in many parts of the world and affect natural environments as well as agricultural production. In agriculture, not only the growth of plants is compromised on deficient or toxic soil, but these stress conditions furthermore affect the nutritional value and success of the harvested crops. In order to cope better with deficiency or toxic conditions through risk assessment, remediation and in agriculture also breeding, it is therefore decisive to understand the mechanisms of metal metabolism in plants, i.e. (1) uptake into the plant, (2) long-distance translocation to different organs, (3) sequestration to specific cells and subcellular compartments, (4) metabolic use, (5) deficiency and toxicity stress and (6) tolerance to deficient or toxic concentrations. These processes are therefore highly relevant research themes in basic and applied sciences (cf. [125, 126] for reviews). Synchrotron radiation X-ray fluorescence microscopy (\(\mu\)XRF) and microscopic X-ray Absorption Spectroscopy (\(\mu\)XAS) play a crucial role, because they combine high spatial resolution with high sensitivity for trace metals and sample preparation close to the native state (cf. Figure 5.24).
The high brightness of PETRA IV will allow for easy focusing of the beam into the few-nanometre range (cf. Section 4.2), enabling subcellular details to be resolved down to the level of membranes or the location of viruses [127]. This is decisive for the mechanistic interpretation because each subcellular compartment has a different physiological function. The two to three orders of magnitude higher flux in the nanofocused beam will allow for measuring µXRF tomograms of biological samples not only of one slice, but in 3D. Currently, this is only possible at low (tissue-level) resolution and with relatively high metal concentrations (e.g. hyperaccumulator plants). With PETRA IV, µXANES tomography will become possible in tissue at subcellular resolution and for regular metal concentrations in non-accumulator plants.

Figure 5.24.: Current state-of-the-art µXRF and µXANES tomography at PETRA III, showing tissue-specific spectroscopic information around the Zn Kα edge of a virtual cross section through a virus-infected model plant leaf in a frozen hydrated state [127]. (a) submicrometer resolution µXRF tomogram; (b) XANES spectra representing the average of the pixels of the labelled objects in the tomogram shown below. (c) single XRF tomogram of the XANES stack of tomograms collected at lower resolution.

5.4.2. Earth Science and Extreme-Conditions Research

Volatile and Melt Cycles in the Earth and their Relevance for the Dynamics of the Earth’s Surface

Volatile species (e.g. nitrogen, H2O, carbon dioxide, ammonia, hydrogen, methane and sulphur dioxide) play a key role in a wide range of dynamic processes at the Earth’s surface. Volcanic eruptions, earthquake generation and rupture propagation are for example connected to the breakdown of H2O- or CO2-bearing Earth materials resulting in the release of H2O- or CO2-dominated fluids and melts. Furthermore, recent studies indicate that Earth’s interior might be a major reservoir not only for CO2 (crust 1.5 wt %, about 6.5 × 10⁸ Gt carbon and mantle and core 98 wt %, about 7 × 10¹⁹ Gt carbon [128]), but also for H2O (more than 50 wt %, 4.5 × 10²¹ kg [129]). Thus, the transfer, storage, recycling and release mechanisms in the interior of the Earth are crucial to understand the dynamics of the crust and mantle of our planet as well as the long-term evolution of the CO2 and H2O budget in the biosphere, hydrosphere and atmosphere of the Earth.

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“The superb coherence of PETRA IV will open up new fields of research through imaging at high energies, revolutionising the emerging field of impact and earthquake simulation science and providing unprecedented insights into the structural processes underlying these dynamic processes.”

New mineral phases are routinely being discovered, which can carry hydrogen, carbon and other volatiles into the Earth’s interior via subduction of oceanic plates. It has been found that various physical and chemical processes...
subsequently release volatiles at much greater depth than previously known [130–133]. Thus, the total budget and the actual storage of H₂O and carbon may be much greater than previously assumed, with significant consequences for the understanding of plate tectonic convection in the Earth. Photon-based crystallographic and spectroscopic studies are the only way to study the stability, physical properties and formation of volatile-bearing minerals and melts in different pressure- and temperature-generating devices in order to provide accurate data at extreme conditions. Such studies are thus key to understanding processes in the Earth’s interior today as well as in the past.

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“The brightness of PETRA IV at high energies will enable high-resolution kinetic studies of H₂O and CO₂ release in the Earth’s interior. Melt studies become possible, explaining the recycling of tectonic plates and ultimately the formation of the Earth’s atmosphere, which is crucial for the evolution of life itself. The enhanced coherence at high X-ray energies opens a wealth of opportunities for sub-micrometre imaging in deep-Earth geosciences.”

The high-brightness, high-energy X-ray nanobeams of PETRA IV will enable photon-based studies that are impossible today (cf. Section 4.5). For example, pinpointing the microscopic location of a dehydration reaction and at the same time the mechanisms that lead to the breakdown and consequently formation of ruptures or melts requires a clean high-energy X-ray nanobeam (>40 keV). PETRA IV will provide the necessary photon characteristics to conduct X-ray diffraction imaging up to an order of magnitude faster than at any other future synchrotron radiation source. This is crucial, since the extreme states of matter involved can only be prepared for short times.

PETRA IV will thus offer the unique opportunity to spatially resolve the formation and progress of solid-solid and solid-liquid reactions on an intermediate time scale, providing essential insights into the genesis of earthquakes and volcanism. The ability to resolve hierarchical complexity across several length scales with a “medium” time resolution of milliseconds to microseconds will be one of the most outstanding properties of PETRA IV for solving today’s problems in the Earth sciences.

5.4.3. Water Science and Corrosion

Supercooled Water and Amorphous Ice

Knowledge of the structure and dynamics of water is believed to be key to understanding the unusual properties of water, such as density anomalies, high surface tension and the polymorphism of ice. Furthermore, water is special in that it exists in at least two different amorphous solid forms, low-density amorphous (LDA) and high-density amorphous (HDA) ice, with a density difference of 20%. Debate is ongoing on the nature of the glass transitions of water, which occur at low temperatures and may indicate the existence of two different liquid forms, the low-density liquid (LDL) and the high-density liquid (HDL) form [135, 136]. However, crystallisation prevents measurements on the bulk liquid phase below ≈227 K and above ≈160 K, which represents the “no-man’s land” of liquid water. Recently, studies at PETRA III on the transition of HDA to LDA revealed that the dynamics become diffusive on length scales of 100 nm, indicating the appearance of HDL and LDL close to the glass transition temperature [20]. These studies were complemented by small-angle X-ray scattering experiments at free-electron lasers (FELs), where a maximum isothermal compressibility of water at 229 K was reported [138], suggesting a liquid-liquid transition in water. Complementary to storage rings, experiments at FEL sources enable access to the dynamics of liquid water in the femtosecond to nanosecond regime by means of single- or split-pulse X-ray speckle visibility techniques [26, 27]. Ultimately, dynamics ranging from
femtoseconds to several seconds have to be revealed to understand the phase behaviour of water and the relation between its structure and its anomalous behaviour. Furthermore, the hydrogen bond network of water is believed to be influenced, both structurally and dynamically, by the presence of dissolved ions. In the proximity of ions, water can be either more locally coordinated or more disordered, i.e. different ions can act either as “structure-makers” or “structure-breakers”, although the microscopic origins of these features remain elusive. Likewise, the dynamics of water molecules around ions can also be dramatically affected.

PETRA IV will enable scientists to reveal the structure and dynamics of liquid water and amorphous ice over the whole phase diagram. Thanks to the superior coherent flux of PETRA IV, the complex dynamics of water can be studied in the currently inaccessible range between nanoseconds and milliseconds (cf. Section 4.3). Access to nanosecond and microsecond dynamics is crucial to understand the glass transition of water and gain insight into the properties of low- and high-density states. One aim is to extend previous X-ray photon correlation spectroscopy (XPCS) investigations [20] to measure dynamics on molecular length scales, which will become feasible with the high coherent flux of PETRA IV (cf. Figure 4.4 in Section 4.3). This approach allows the investigation of time scales below microseconds and thus provides insights for the controversial question of whether water consists of two liquids or not and the relationship between the structure of water and its anomalies. [135, 136, 139].

Anders Nilsson
Stockholm Universitet

“Water is not yet understood in detail. The revolutionary capabilities of PETRA IV make it possible to study water with unprecedented resolution to understand biological and chemical processes.”

Moreover, PETRA IV will facilitate the investigation of ion-ion correlated dynamics in the deeply supercooled regime of aqueous solutions with variable “structure-making” ability, ranging from high concentrations to physiological conditions.

With PETRA IV, high coherent flux will be available even at high X-ray energies (>30 keV), enabling the use of high-pressure sample environments in coherent X-ray scattering experiments (cf. Section 4.5). XPCS at elevated pressures would provide a unique tool to elucidate the pressure dependence of the hypothesised glass-to-liquid transition in amorphous ices.
Electrochemically Driven Wet Corrosion

Wet electrochemical corrosion involving water as active transport medium is a major threat to the stability of most metallic materials, often causing catastrophic failure and immense costs to society. The benefits of improved corrosion knowledge and control are significant in many industrial applications. Advances in surface science have revealed detailed insights in the homogeneous modes of corrosion on well-defined, flat surfaces. Mostly averaging over larger areas, the surface-science approach has provided understanding of the development and stability of the rather smooth layers, passive films, and interfaces involved in corrosion, and have very successfully addressed simplified model systems [58, 140, 141]. Corrosion engineering of typically complex, commercial materials and the modern design of alloys and steels is based on a huge body of materials testing. Today’s understanding of corrosion is severely limited when it comes to truly three-dimensional heterogeneity in materials such as precipitations, elemental variations (eventually caused by oxide or hydroxide scale growth itself), or the origin of detrimental localised corrosion and treacherous pitting [142]. In the context of wet corrosion, in-situ characterisation is of particular importance. It allows to follow the formation and dissolution of nanometre thick passive films. Very often lateral heterogeneities in the sub-micrometer range control the corrosion process [143]. Often, wet chemical corrosion is accompanied by mechanical stress leading to stress corrosion cracking, a mechanical failure mechanism which is promoted by corrosion [144]. A further challenge is that localised corrosion events occur stochastically, preventing observation. Apart from the detrimental action of wet chemical corrosion it can also be utilised for a tailored fabrication of materials with novel properties. Controlled corrosive dealloying may lead to 3D nanoporous materials with variable architecture and hierarchical levels for novel applications [145] or 2D nanoporous arrays, which can be used as templates for nanoscale electrochemical deposition [146]. Corrosion often depends on single-digit nanometre-sized, even atomic-scale lateral
heterogeneities. This is particularly true for corrosion-resistant passive metals, steels, or new high-strength alloys, needed for many modern applications from electromobility to wind power. The strong dependence on the actual environment during the corrosion process or on the applied conditions such as load or pre-damage also renders in-situ characterisation with ultimate spatial resolution very important. In particular, in-situ experiments to reveal the correlation of corrosion triggering parameters and the actual corrosion event are becoming important. Major opportunities in corrosion research are thus based on combining controlled local corrosion scenarios with in-situ characterisation of initiation or initial stages of degradation. Such initial knowledge needs to lead into better models, predicting long-time degradation behaviour where complex and coupled processes often blur any meaningful insight.

The vision of X-ray nanobeams at PETRA IV offers excellent unique new opportunities for corrosion research. High-energy beams will allow to access absorptive sample environments for in-situ studies under relevant conditions. Small nano-sized beams will be able to probe ever smaller regions with PETRA IV targeting the 10 nm range ultimately relevant for localised corrosion. In combination with new approaches to trigger corrosion locally in a controlled way, new opportunities will be created to locally observe corrosion at work. The synchrotron light of PETRA IV will offer a plethora of new X-ray based methods for corrosion insight with unprecedented ability to interrogate materials with high spatial resolution, improved data acquisition schemes, and higher analytical throughput and efficiency.
Innovation Aspects

Environment protection is one of the key challenges that society is facing in the 21st century. Research in this field will widely benefit from the capabilities of PETRA IV, and the research results will strongly support industrial companies in developing new machines, devices and methods.

Cleaning our environment from heavy metals is one of the key problems that we need to address. The difficulty is that heavy metals are dispersed in the whole ecosystem. We find them in plants and animals, in water and sediments. Apart from their location in the environment, their transport pathways are not well understood. The superior brightness of PETRA IV will allow nanofocus imaging experiments on cells, cell membranes, single plants and minerals in sediments. The sedimentation of heavy metals for example in river beds can thus be investigated. PETRA IV is the ideal tool for these studies because the spatial resolution it will reach fits the typical range of composites in sediments. On the one hand, understanding these processes will help us to reduce the introduction of heavy metals into our environment. On the other hand, this know-how will be utilised by innovative companies to effectively clean our environment.

A secure, long-term, underground disposal site for nuclear waste has not yet been found. Locating one is difficult, because we need to be sure that no radioactive particles will ever reach the surface or – even worse – the ground water. In this context, geologists and mineralogist are interested in transport phenomena of radioactive particles on long time scales. Mineral grains and grain interfaces have a typical diameter of a couple of nanometres to several ten micrometres, a regime that is not covered with today's synchrotron radiation sources. PETRA IV will be the ideal tool to study these transport processes. Research results in this field will enable the nuclear industry to find and operate reliable sites for nuclear waste.

Water is the most important substance in our lives. Water is key not only in biology, but also in a number of industries. Whether in corrosion processes, as a solvent, in suspensions of nanoparticles and in nanopores – understanding the dynamics of water is paramount. The production of hydrogen by hydrolysis is not understood well enough on the nanometre scale. PETRA IV will be able to provide deep insights into this process and thus help to optimise the production process of hydrogen for technical applications, in particular for energy storage solutions, thereby opening up new markets for green-energy industries. The consumer goods industry will also greatly benefit from an enhanced understanding of nanoparticles in water, which will lead to the improvement of cosmetics, detergents and cleaning agents, among others. A detailed understanding of the physics of water in nanopores will help to improve water filters, which is crucial for the supply of clean drinking water and for wastewater treatment. In addition, water embedded in nanopores is important for water deposits in rock material. Industrial companies will benefit from detailed insights and be able to explore new water deposits. Improved knowledge of the water cycle in the geosphere is also crucial for understanding ore deposit formation of economically relevant metals, such as aluminium and copper, and of the rare earth elements. This will strongly improve exploration efforts of the mining industry, enabling it to better predict locations of new deposits and establish new mines.

Corrosion processes start out from inhomogeneities and defects on the nanometre or atomic scale. With PETRA IV, it will be possible to image corrosion processes from the very beginning to the formation of cracks and pores under realistic ambient conditions (chemical properties of the surrounding atmosphere, humidity, pressure and temperature). In addition, the time resolution that will be accessible with PETRA IV will allow the evolution of corrosion processes to be studied on all relevant scales. One example is industrial research in the field of duplex steel materials. Depth-resolved imaging of chemical changes in the natural corrosion steps will help to optimise materials and hence to increase the life span of machines and reduce production costs. It will reveal how corrosion processes are related to the morphology and composition of technical materials and how those can be optimised to the needs of the industrial application.

As soon as the physics and chemistry of corrosion are better understood, the process itself can be utilised to modify or structure materials on the nanometre scale. This could open up new approaches to building devices with a large surface or high volume density of pores. Such materials are very good candidates for substrates in technical catalysts. Materials with a high volume density of nanopores have different electromechanical and chemomechanical properties. The thermal expansion coefficient for example can be much larger compared to classical, homogenous materials of the same kind. This behaviour will lead to new classes of sensors and actuators that have a wide field of application in many different industrial disciplines.
Earth and Environment References


Figure 5.27.: Latest research on new classes of high-temperature superconductors hints in the direction that not order but disorder on the nano-scale enhances the non-resistive flow of electrons through the material. PETRA IV will provide the spatial resolution to image these disordered structures in detail to be able to tailor the electronic and crystallographic structure accordingly. This will open up new paths for the development of electronic devices for the digital world of tomorrow.
The omnipresence of information technology is drastically changing our society. Our economy exhibits a digital revolution as it approaches Industry 4.0 and the internet of everything. Gigantic data centres and billions of stand-alone devices consume vast amounts of energy of hundreds of terawatt hours per year [151]. This causes an immense ecological impact. While the semiconductor industry strives for low power consumption and increased performance in terms of computation and data storage, today’s information technologies will soon reach their physical limits. Power handling and the 2D topology on chips are becoming serious challenges [152]. Already now, devices are beginning to run into fundamental thermal limits.

The current concepts of performance and functionality increase have been based mainly on the downscaling of transistors and storage elements. This trend – known as Moore’s law – will face disruption within the next five years. The smallest features of transistors on processor and memory chips have already reached the scale of just a few atomic layers and, accordingly, further downscaling will not be applicable any more. Therefore, information technology as we know it today faces a paradigm shift. In view of the societal impact and economics of information technologies (e.g. aspects concerning the internet of things, big data, artificial intelligence, autonomous systems and mobility, intelligent networks for power handling and distribution, etc.), many

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**Figure 5.28.** Exploring novel nano and quantum materials with the ultra-high-brightness X-ray source PETRA IV.

- **High-Temperature Superconductivity:** Reproduced with permission from [147]. © (2016) by Springer Nature Limited.
- **Topological Spin Textures:** Reproduced from [148], with the permission of AIP Publishing.
- **Morphology and Growth of Semiconductor Structures:** By courtesy of Marcel Verheijen, Eindhoven University of Technology.
- **Spin Waves and Spin Currents:** Taken from [149].
- **Fundamental Atomic and Molecular Processes:** By courtesy of Till Jahnke, Universität Frankfurt am Main.
efforts are being undertaken to plan for the future. A thorough incorporation of improved materials into existing technologies is required and logic and memory devices based on new physical effects are inevitable. These devices will be not only faster or non-volatile but more efficient regarding energy consumption.

The future of electronics will be based on 3D device architectures and equivalent scaling, which means that technologies based on new physical effects will replace the traditional technologies in order to increase performance at lower cost and with lowest energy consumption [152]. This development will rely on new complex materials and nanostructures that have to be well understood to be tailored and controlled in their specific properties. The characterisation of these novel materials and structures on the nanoscale is absolutely necessary in order to introduce them into industry, where precise fabrication processes with great reliability are indispensable requirements.

Novel and better crystalline substrate materials are needed for electronics in power markets, such as for electromobility. Next-generation crystals for photonics, such as lasers and frequency modulators, will enable optoelectronic integrated circuits. Synthesis of new materials, driven by band gap and strain engineering, requires an in-depth structural analysis. The grand challenge is to harness the material properties at the nanoscale. Because of the reduced dimensions, surfaces and interfaces increasingly determine the physical properties. Defects and the atomic-scale structure become crucial, not only for future semiconductors, but also for other highly functionalised materials, such as novel ferroelectrics and ferromagnets.

Already today, transistors are approaching dimensions of a few nanometres, and quantum effects start to play a decisive role. Now that “nano” meets “quantum”, the realm of quantum materials emerges. Such materials are “solids with exotic physical properties, arising from the quantum mechanical properties of their constituent electrons” [153]. This class of materials includes strongly correlated, topological, spin and 2D materials, but also oxide and van der Waals heterostructures. Classical manifestations of electronic quantum effects in these materials are ferromagnetism, ferroelectricity and superconductivity. More “exotic” manifestations of quantum effects include quantum Hall effects, high-temperature superconductivity, tunnel or colossal magnetoresistance, metal-to-insulator transitions, topological states, spin liquids and ices, as well as emergent electronic and spin properties at interfaces. A common characteristic is that collective excitations of quantum materials are very different from elementary excitations of the individual electrons and atoms that constitute the material. Quantum materials are often characterised by a delicate balance between coexisting, competing or cooperating phases. Thus, their properties are highly tuneable, for example by strain, doping or electrostatic gating. Importantly, in quantum materials on the brink of instability, weak stimuli can cause anomalously strong responses. The intrinsic interactions in quantum materials can lead to new physical states in nanostructures and at interfaces, thus providing new functionalities from their quantum interactions.

One of the most intriguing questions is how the complex mesoscopic behaviour found in nano- and heterostructures emerges from quantum interactions.

To ensure the technological advance over the next decades, new technologies based on quantum interactions have to be explored and understood. Instead of only indirectly exploiting quantum effects, they will distinctly control modes of operation. Innovative future applications range from quantum communications over quantum sensors to quantum computing. Within the High-Tech Strategy 2025 of the German Federal Ministry of Education and Research (BMBF), quantum technologies are expected to be one of the future key technologies with a considerable added value for our society and economy [154].

For practical applications of quantum technologies, major obstacles have to be solved. Quantum states are prone to noise and are likely to lose their well-prepared properties in rugged environments. Cryogenic temperatures and appropriate shielding are needed to eliminate such noise sources. Topological quantum materials are prime candidates to solve this problem. The quantum states in these materials are topologically protected, making them robust against intrinsic or extrinsic perturbations. Transistors based on topological materials would not be perturbed by material defects, thus enabling ultra-fast, dissipation-free de-
Quantum devices and computers based on topological matter could stabilise fragile quantum states possibly even up to room temperature. Research on such quantum materials is just about to start, and the future impact is expected to be immense. Thus, quantum materials provide one of the most productive platforms for discovering fundamentally new physical phenomena and phases of matter, solving fundamental problems in physics and realising entirely new concepts and devices in energy and quantum information technologies. Another, bottom-up approach to understand and develop novel quantum materials lies within the profound knowledge of the quantum world as such. Atoms and molecules are inherently quantum systems, and basic research addresses the fundamental quantum interactions responsible, for example, for chemistry in general or, more specifically, for the aforementioned features vital to quantum information technology. Investigations are necessary on the electronic structure of atoms and molecules, unveiling the microscopic composition of electronic orbitals and the ultra-fast dynamics within atoms, molecules or clusters. The electrons emitted during a photon-triggered removal from an atom can be employed to reconstruct molecular geometries and to provide in-depth information from within the molecule or on solute-solvent interactions. Even information from the atomic time domain can be extracted, yielding comprehensive understanding of the features and properties of the microscopic quantum world.

The development of future devices used for electronics with unprecedented functionality and performance, which are based on quantum interactions, complex materials, and their mutually integrated interfaces, will need detailed nanometre-scale X-ray characterisation as will be provided by PETRA IV. Furthermore, this precise experimental view in both space and time is necessary to bridge the gap between the mesoscopic behaviours and the microscopic quantum interactions as well as to understand the correlations in such new classes of nano and quantum materials. PETRA IV will address these questions raised by new physical effects and new materials for future technologies. The following examples highlight experiments that will be possible only at existing light sources. PETRA IV will provide an unprecedented insight into the complex nature of nano and quantum materials, thus laying the foundation for future technology applications.

5.5.1. Turning Quantum Effects into Function

The quantum correlation interaction of electrons in complex materials is at the heart of their functionality. A precise understanding of the electron interactions holds promise that these functionalities can be tailored to specific demands. One of the big challenges however, is to resolve the role of nano-sized structures that arise as a direct consequence of the co-existing, competing, or cooperating phases that exist in many quantum materials despite of chemical and structural homogeneity.

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"The advances in energy-resolved spectroscopies over the past couple of decades have been astonishing. If they can be combined with nanometre-scale spatial resolution, whole new fields of research will open up. This is particularly important because of parallel advances in techniques for preparing microstructures of complex quantum materials."

One iconic example is nanoscale granular superconductivity in the high-temperature superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$, where oxygen-rich puddles alternate with superconductive channels in an intricate, potentially stabilising way [155]. The exceptional electronic properties of correlated materials are also highlighted in topological quantum materials. They display a spatial segregation between the interior of the material and its boundaries. According to the fundamental bulk-edge correspondence principle and even for a bulk insulator, topologically non-trivial electronic states in the bulk must lead to robust gap-less, i.e., metallic states at the edges. Remarkably, these edge states can behave as dissipation-free transport channels.
Figure 5.29.: The unique source properties of PETRA IV will transform soft X-ray microspectroscopy into highly-efficient soft X-ray nanospectroscopy.

Moreover, in any real material, the most common source of heterogeneity is disorder. This disorder, which is often introduced by chemical doping, is instrumental for inducing a specific electronic phase. A detailed understanding of the local electronic structure, excitation spectrum and spin polarisation is required in order to get access to the seemingly ambiguous correlation of various emerging phenomena in these materials and their intrinsic nanoscopic heterogeneity. “Embracing disorder” in a controlled way is thus a tool for discovering and understanding quantum materials [153].

PETRA IV transforms current X-ray spectrosocopies limited to micrometre spatial resolutions into powerful, efficient nanospectroscopies down to below 10 nm spatial resolution (see Figure 5.29). As a consequence, nanoARPES, nanoRIXS, and nanoXMCD will enable researchers to map charge, orbital and spin heterogeneity as well as variations of local electronic structure and excitations on their intrinsic nanoscopic length scale (cf. Section 4.2 and Section 4.4). For the first time, electronic heterogeneity in quantum materials can be directly seen, quantified and ultimately controlled [156].

In addition, device-like structures and real devices made from quantum materials can be investigated operando, probing local electronic structure changes under gate bias and mapping the accumulation of spins at sample edges, surfaces and interfaces. Furthermore, using position-dependent electrical and optical pump/soft X-ray probe schemes at PETRA IV, we will be able to track ballistic and drift-diffusion charge currents along conducting channels, across interfaces and in topologically protected edge channels, map spin-polarised currents, including the direct observa-

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“Performing advanced soft X-ray spectroscopies with combined high energy and spatial resolutions at PETRA IV will revolutionise our understanding of quantum materials by allowing us to probe them embedded in functional devices under working conditions.”
Figure 5.30.: Left: Schematic representation of a racetrack wire. Skyrmions (shown in blue) are generated in this particular material system behind the constriction formed by the small notches, as soon as strong current pulses are sent through the wire. The presence or absence of a skyrmion encodes the bits “1” or “0”. The background shows part of an X-ray hologram as used by researchers to image the skyrmions. By courtesy of Stefan Eisebitt. Right: Spin structure of a skyrmion (a, c, e). Reproduced from [157].

5.5.2. Nanoscale Spintronics

Quantum materials based on spin interactions are one of the future key technologies for energy-efficient and non-volatile computation with additional high speed. The main problem in the investigation of these materials is a lacking direct view of the magnetic states and spin interactions at their corresponding intrinsic nanometre dimensions. Knowledge of the structure and dynamics of spin textures and of their magnetic moment distribution on nanometre length and sub-nanosecond time scales is required for a fundamental understanding of these spintronic effects. Magnetic skyrmions are topologically protected spin states on nanometre length scales (cf. Figure 5.30). They can be sensitively and efficiently manipulated by external magnetic fields or electrical currents, which is of particular interest due to their application potential as information bits in high-density, non-volatile memory devices.

A concept that has been particularly brought forward is the skyrmion racetrack memory [158], where the digital information is encoded by the presence or absence of a skyrmion. An electrical current pulse is used to shift the skyrmion along the track. Imaging of magnetic skyrmions requires both nanometre spatial and sub-nanosecond temporal resolution. Experiments combining real-space imaging at sub-50 nm resolution, magnetic sensitivity to a monolayer of material, and nanosecond temporal resolution are state of the art and have pushed the understanding of the basic mechanisms at work, even allowing researchers to test first model devices for applications.

Sub-10 nm skyrmions as well as the internal spin structure of skyrmions are currently not resolvable with X-ray methods. However, this information is indispensable to obtain an element-specific picture in these complex materials. The most crucial limitation for investigating magnetic skyrmions at the nanoscale is the lack of sufficient coherent photon flux at present synchrotron radiation.
sources. PETRA IV will provide sufficient X-ray brightness and coherent flux for improving the spatial resolution well below today’s limit (cf. Section 4.2). Coherence-based imaging techniques such as ptychography, holography, scanning transmission X-ray microscopy or tomography with additional use of magnetic dichroism (XMCD or XMLD) will directly profit from the brightness increase.

Axel Müller-Groeling  
Managing Director, Fraunhofer Institut für Siliziumtechnologie (ISIT)

“The new possibilities for analytical investigations and the enormous brightness and coherence that the new beam will offer are interesting for us as a research institute. We also welcome that PETRA IV will finally be able to image more length and time scales under real conditions. These possibilities will advance the investigation of micromechanical and microelectronic systems, in particular regarding interfaces and transitions of functional layers, to such an extent that we expect great potential for further developments and improvements. We can benefit greatly from a project such as PETRA IV, which can contribute to our highly specialised technology developments in the long term.”

As a result, the measurement time will be drastically reduced by at least an order of magnitude, enabling magnetic 3D imaging while providing nanometre precision X-ray beams. Targeting a sub-10 nm 3D spatial resolution in order to also resolve the smallest magnetic texture will only be possible at the ultra-high brightness X-ray source PETRA IV.

Nanobeams with high coherent flux together with a bunch length of about 100 ps provided by PETRA IV will enable imaging of sub-10 nm magnetic features and additionally of sub-nanosecond spin dynamics. Thus, experimental access to the nanoscale spin dynamics in real nanostructures will be possible and generate important insights into the mechanisms of creation, propagation and manipulation of skyrmions in novel spin materials. The ability to resolve these topological spin structures in detail, follow their excitation dynamics and obtain information in more complex systems is required to optimise the materials for applications and will transform this area of research. It will enable researchers to study most fundamental phenomena, e.g. interaction of spin structures with spin-polarised electrons, light or magnons on intrinsic excitation length and time scales. Given the large application potential of such systems, time-resolved operando studies of devices can be envisioned as well. PETRA IV will thus generate the opportunity to gain important new insight both into the fundamental physical mechanisms at work and into device operation and optimisation questions.

### 5.5.3. Fundamental Atomic and Molecular Processes and Properties

Studies on atoms and molecules in the gas phase have covered a breadth of fundamental quantum mechanical processes in the past, and the development and understanding of novel quantum materials is based on new scientific findings from this discipline. Electron (or in general many-particle) correlation effects, initial state entanglement, molecular structure and rearrangement are a few examples of fundamental subjects. A revolutionary new era of studies on fundamental atomic and molecular quantum processes will emerge once orbital angular momentum (OAM) photon beams become available. By manipulating the wavefront of a photon field, a phase modulation is created that carries orbital angular momentum in addition to the spin of the photon (cf. Section 7.3.2). OAM photon beams (or “vortex beams”) are routinely generated in the visible light range using table-top laser sources for various applications. They have also been demonstrated in the X-ray range [159–161]. However, so far, these beams are laterally macroscopic, and their interaction with matter is largely dominated by conventional interactions. The high brightness and lateral coherence of PETRA IV may allow scientists for the first time to generate these novel photon beams at nanometre dimensions (cf. Section 4.2), which match the size of extended electronic states in molecules and solids, and may enable them to probe unusual electronic transitions.
The enhanced transverse coherence of the PETRA IV photon beam also has the potential to trigger a further new class of related experiments at the foundation of quantum physics. By using appropriate optics to generate a coherent double focus (with a distance of a few nanometres), a future tool for a novel quantum-technology-inspired few-particle spectroscopy can be developed (see Figure 5.31): Corresponding studies will extract information from the coherent emission of an electron wave emitted from two spatially separated sites, exploring for example fundamental questions on the quantum entanglement properties of photoelectrons and their parent ions [162]. The photon-matter interaction using OAM photons or novel coherent focal schemes is a completely untouched area of fundamental research on basic quantum processes, and the properties of PETRA IV will allow us to enter this frontier for the first time.

PETRA IV can provide important insight into the fundamental scientific questions and industrial challenges associated with the technological demand for ever increasing computation power and automatisation of our modern society and industry. New nano or quantum materials, new physical effects and new quantum manipulation schemes have to be explored to ensure the future ecological balance and exploit the economic potential of information technology for our society. The ultimate X-ray microscope PETRA IV will enable researchers and engineers to unravel the nano and quantum cosmos. The main ingredients are the nanobeams and the unrivalled degree of beam coherence that PETRA IV will deliver. The former will open the realm of nano-objects to typical spectroscopic techniques matching the intrinsic sizes of the new nano and quantum materials. The latter will pave the way for unique imaging techniques, such as nanoptychography, nanotomography or even more advanced coherent spectroscopic techniques currently not feasible at any other X-ray source. These techniques provide the opportunity to gain a thorough understanding of the interactions of the material constituents at the atomic level and to decipher their mesoscopic features, which are responsible for new functionalities in these materials.
Innovation Aspects

The rising demand of information storage capacity, computing speed, new sensors, and the more and more important need of energy efficient IT solutions (green IT) are key challenges in the upcoming decades. New technology solutions are needed. Future technologies will incorporate new materials and physical concepts with properties that are based on the intriguing atomic and electronic interactions. Semiconductor industry has a long tradition of collaborating closely with academia in order to improve and develop new technologies. The grand challenge for the successful introduction of new material systems and concepts into industry, the so-called lab-to-fab stage, is to completely understand the physical processes to facilitate and to exploit new device technologies.

PETRA IV will take the leading role in deciphering the complex material behaviour on the atomic- and nanoscale. With its unique beam properties and achievable resolution, PETRA IV has an enormous potential to contribute to industrial device development, especially in operando, nanoscale or atomic scale structure imaging. Harnessing the wealth of properties displayed by nanostructures, quantum materials, and 2D materials is the precondition to revolutionise the future development of smart devices and solve challenges that have been raised by big data, artificial intelligence, quantum computing, and the internet of everything.

More Moore: Improved Semiconductor Technologies. To advance semiconductor technology, problems arising with existing materials have to be solved. These problems deal with residual stress at the edges of the conductor paths limiting the design of smaller structure sizes, the growth of new crystal materials and the three dimensional integration of devices. PETRA IV will host the analytical tools to advance existing technologies and to study the challenges the semiconductor industry faces. Owing to the penetrating power of X-rays, all characterisation can be performed under realistic and operating conditions on real devices in various environments. For example, in-situ studies for strain control are key for controlling electron and hole mobilities. The spatial resolution at PETRA IV will reach the typical dimension of structures in electronic and opto-electronic devices allowing in-situ and operando high resolution imaging to analyse future electronics during development. Each of these issues will require a detailed atom-resolved characterisation at the nanometre scale. The typical features, which are responsible for the materials properties and the resulting device performances, are small, dilute and possibly short-lived and can only be studied at PETRA IV.

Emerging research materials for electronics. One main goal of industrial research and development is targeted at novel materials to replace existing ones or integrate them in existing technologies, in order to take the performance of ICs and electronic devices to the next level. Such novel materials are correlated or complex magnetic materials. However, tremendous hurdles are still to be overcome in understanding the interactions governing these materials properties and to take advantage in a real device. Prevention or specific control of nanoscale heterogeneities that occur during growth are crucial for the materials quality and functionality. Results from magnetic skyrmion research at PETRA IV can lead to new data storage technologies that offer a much larger storage density compared to current memories. Correlated systems could provide new ultra-fast electronic switches or high-temperature superconductors enabling lossless energy transport. With its exceptional spectral and spatial resolution, PETRA IV will image these materials quality and functionality contributing to the success of research and development of industrial applications.

Beyond Near-Future Technologies: Quantum Information Technologies. In addition to rather concrete demands for industrial applications in the near future to improve or replace existing materials, fundamentally new physical effects of quantum materials or quantum manipulation revealed and studied at PETRA IV can have substantial impact. The realisation of innovative quantum technologies requires a basic understanding of the novel solid state physics and material control on all synthesis and processing levels beyond today’s state of the art. The required analytical tools will be offered by the unique X-ray beams of PETRA IV.
Nano and Quantum Materials for Information Technology References


Conceptual Design of PETRA IV
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6. Accelerators

In the framework of the PETRA IV project, it is foreseen to upgrade the existing synchrotron radiation source PETRA III at DESY to a synchrotron radiation source with an ultra-low emittance. Unique new experiments and scientific opportunities will be made possible in this way. The scientific potential of PETRA IV is presented in Chapter 5. The project includes:

- Upgrade of the storage ring PETRA III to a storage ring with ultra-low emittance,
- Upgrade and refurbishment of the pre-accelerators,
- Relocation, refurbishment/upgrade and in part new construction of photon beamlines,
- Construction of a new experimental building in the west of the PETRA ring.

The upgrade of the storage ring is the most expensive part and needs the greatest share of the investment. Since 2009, the PETRA storage ring has been operated as a synchrotron radiation source, named PETRA III [1]. Fifteen experimental stations working in parallel are installed in the Max von Laue hall. In 2014, the Paul P. Ewald and Ada Yonath experimental halls were built in the context of the PETRA III extension project so that ultimately up to 12 additional beamlines will be available. Presently, 22 undulator beamlines are in operation at PETRA III. The number of beamlines at PETRA IV will exceed the number of beamlines at PETRA III to allow a relocation of all PETRA III beamlines to the new storage ring and provide space for additional beamlines. For details see Section 7.1.

Originally, the PETRA storage ring was built as an accelerator for high-energy physics in 1976. From 1978 to 1986, it delivered collisions of electrons with positrons for high-energy physics experiments. PETRA was then used from 1988 to 2007 as a pre-accelerator for HERA, the hadron-electron ring accelerator, for the acceleration of protons, electrons and positrons. Figure 6.1 shows the PETRA storage ring, the experimental buildings of the PETRA III synchrotron radiation source and the additional experimental hall proposed for PETRA IV.

The PETRA storage ring consists of eight arcs with a total length of 1612.8 m as well as eight straight sections with a length of 64.8 m and 108 m. This geometric arrangement was originally designed in view of the requirements of high-energy physics experiments, but was also very beneficial for the synchrotron radiation source PETRA III, since the straight sections could be used to install damping wigglers and thus improve the beam quality. The large circumference and large bending radius \( R = 256.68 \text{ m} \) is very beneficial for PETRA IV, as the beam emittance scales with the bending angle per arc cell cubed. The long straight sections provide space for the 10 m long insertion devices for the so-called flagship beamlines (cf. Section 7.1.2), ease the layout of injection and extraction sections and provide more than sufficient space for the radio frequency (RF) system and other subsystems. These advantages, together with the considerable cost saving related to reusing most of the existing ring tunnel and the existing experimental hall, outweigh potential advantages of a fully symmetric ring that would be constructed entirely from identical arc cells. The beam dynamics of such a symmetric ring would be somewhat relaxed, with a momentum acceptance and dynamic acceptance possibly a factor of 1.5 – 2 higher. However, as we show in the following section, the properties of the PETRA IV ring in the geometric configuration of the present ring are such that the beam dynamics can be kept safely under control and that stable and efficient operation will be guaranteed.

The major challenge for the reconstruction lies in the modification of the magnet arrangement and therefore of the beam optics in the arcs of the PETRA ring, so that a horizontal emittance is obtained that is almost two orders of
magnitude smaller than the emittance of the PETRA III storage ring operated today. The emittance of the beam together with the beam optical functions determines the beam size and the beam divergence and therefore also the properties of the X-rays.

6.1. Storage Ring

First ideas concerning the possibility of upgrading PETRA were put forward in 2015, and the (initially small) PETRA IV design group was formed and started to meet regularly in February 2016. It was found that moderate modifications of the PETRA lattice would not be sufficient to maintain its competitive edge as a world-leading hard X-ray facility and that an upgrade to a lattice with an emittance of at least 30 pm rad would be required. A more relaxed lattice with an emittance on the order of 60 pm rad was ruled out on grounds of insufficient brightness and increasing demand for experimental techniques that require very coherent X-rays, such as X-ray microscopy and X-ray correlation spectroscopy.

Extremely coherent X-rays at the diffraction limit are obtained if the size of the electron beam and its divergence can be brought to the same order of magnitude as exhibited by the natural divergence of X-rays from an undulator source. The following relation exists between the wavelength of the X-rays ($\lambda$) and the natural beam size ($\sigma_r$) and divergence ($\sigma_{r'}$) of the radiation:

$$\epsilon_r = \frac{\sigma_r \sigma_{r'}}{4\pi} = \frac{\lambda}{4\pi},$$

which is a consequence of the wave nature of light. The quantity $\epsilon_r$ describes the smallest transversal phase space volume of the photons. In order to optimise the coherent fraction of the X-rays compared to the entire photon flux from the X-ray source, it is essential to bring the corresponding quantities of the electron beam, namely the horizontal and vertical emittance, to the same order of magnitude:

$$\epsilon_y \leq \epsilon_x \leq \frac{\lambda}{4\pi}.$$

With emittances $\epsilon_{x,y}$ (both horizontal and vertical) in the range of 10 pm rad, X-ray beams will be diffraction-limited at about 10 keV. This implies that (nearly) the full beam of an undulator is laterally coherent – i.e., the lateral coherence length is in the range of the beam size – and can be focused to the diffraction limit [2]. With this and some improvements in X-ray optics, X-ray microscopy techniques at PETRA IV can cover all length scales down to the atomic level (cf. Section 4.2).

Initially, a beam energy of 5 GeV was considered, but soon it became apparent that a 5 GeV storage ring has a limited reach into the high-energy X-ray part of the spectrum and that the combined effect of a reduced photon flux and intra-beam scattering offsets gains from the emittance reduction due to the lower beam energy. Therefore, a beam energy of 6 GeV was chosen as the design goal. Studies have shown that, for a momentum acceptance of 2% (a typical value for PETRA IV candidate lattices), an emittance below 10 pm rad is beneficial for Touschek lifetime, which first decreases with emittance but then starts to increase again due to reduced transverse temperature of the beam. However, the influence of intra-beam scattering on equilibrium emittance is always detrimental, and ultra-low emittances below 10 pm rad cannot be reached with reasonable bunch currents in a machine such as PETRA with a circumference of 2.3 km. These considerations set the target horizontal emittance in the range between 10 pm rad and 30 pm rad.

Ultra-low emittance and a reduced number of electron bunches with similar total current for timing experiments are conflicting design goals that cannot be met with a single mode of operation of PETRA IV. Therefore, it is planned to provide two operation modes for PETRA IV, the high-brightness, high-coherence continuous mode and a timing mode with fewer bunches with increased bunch charge but with larger emittance and thus slightly reduced brightness.

At an early stage of the lattice design, it became clear that a design based on multibend achronomats (MBA) [3] is a preferable approach to achieve extremely low natural emittances. A MAX IV-type MBA lattice [4] was considered, similar to PEP-X design approaches [5], but it was found to exhibit a rather small dynamic acceptance (DA). Several options with a more favourable ratio of DA to emittance were inves-
tigated in more detail: an option based on the ESRF-upgrade-type hybrid 7BA cell approach [6] as well as lattices with distributed chromaticity correction [7] and two types of ring cells, suitable for the PETRA geometry where only part of the ring is occupied by insertion devices. A distributed chromaticity correction approach was already chosen for PETRA III, where the double-bend achromat (DBA) cells in the experimental Max von Laue hall do not have sextupoles and the chromaticity correction is done in the FODO arcs. An advantage of this approach is that different lattice optimisations can be applied for octants with undulators and those without. Several options of such non-locally correcting lattices were studied and found to be feasible (round beam [7], double-$I$-transform cells DMI [8]), but in the end, the design constraints favoured a solution, where a larger portion of the ring than initially foreseen could be equipped with insertion devices and the possibility to even further expand the number of insertion devices was kept open. For these reasons, the hybrid 7BA approach was chosen. Investigations of integrating the reverse bend concept [9, 10] into this lattice type showed that a noticeable but not drastic improvement in magnet strength, emittance and tuneability of the beta function at the insertion device can be achieved. However, mainly driven by time constraints, we decided to follow the design through without the reverse bends in the CDR phase and resume the implementation of the reverse bend into the lattice design at a later stage.

The dependence of brightness on beta functions in the IDs was investigated. The optimum beta function at the centre of the ID straight sections corresponds to approximately $L/\pi$ [11], where $L$ is the length of the undulator, and cannot be reached for the 5 m long IDs in our design. The loss in brightness for the PETRA IV 7BA design compared to an optimum horizontal beta function is approx. 60%. At the same time, pushing the beta functions to the optimum values requires increased focusing and comes at the price of substantially worse non-linear dynamics. Additional special, up to 10 m long IDs in the long straight sections of the PETRA ring, with a better beta function matching the optimal conditions, are included in the design for high-end applications.

Damping wigglers reduce the emittance and help to mitigate the effect of intra-beam scattering and were therefore also considered during the lattice design process. However, high-field wigglers can increase the energy spread of the beam. There is no consensus yet on the influence of energy spread on the performance of the ultra-low-emittance storage ring [12]. PETRA IV will already require...
Accelerators | Storage Ring

A substantial RF system, and damping wigglers would make it even more demanding. Strong damping wigglers were therefore excluded from the baseline accelerator design. However, the possibility of installing a certain number of moderate-field “damping undulators” is still considered, which could be operationally beneficial by maintaining a constant emittance when user beamline undulators are opened or closed.

A common request in the upgrade of radiation facilities from the third to the fourth generation is to preserve the beamlines and the source point locations. Effort was invested in understanding the significance of this constraint in the case of PETRA IV. The PETRA III DBA cells in the Max von Laue hall are only 23 m long, and in five of the nine ID straight sections, canting dipoles with a deflection angle of 5 mrad are installed. In the Ada Yonath and Paul P. Ewald halls, canting dipoles with an even larger deflection angle of 20 mrad are installed in all DBA cells. A 7BA optics with a cell length of 23 m (original PETRA III cell length) was investigated, resulting in very aggressive magnet strength. Additionally, it was found that preserving the existing canting configuration is incompatible with an ultra-low emittance. Based on these findings, we concluded that preservation of source point locations should not be constraining our design. Nevertheless, effort will be invested during the technical design phase in further investigating the possibility of preserving at least a subset of beamline locations.

Finally, the geometry of PETRA is not only a complication preventing an optics design with a high degree of symmetry that would be beneficial for non-linear dynamics, but also an asset for several aspects of design optimisation. The long straight sections can be used for the up to 10 m long IDs with optimised beta functions and potentially in the future for hosting advanced radiation generation setups (such as the XFELO [13]). Furthermore, they provide space for injection and extraction elements and subsystems such as RF.

Given time and resource constraints, the approach taken was to first come up with a feasible high-performance design that addresses all critical issues and enables the science and industrial case and to concentrate on further lattice optimisation in the next stage, when more time and resources are made available. The design that emerged from the considerations and constraints discussed in this section is presented in the next sections.

Table 6.1 summarises the parameters targeted for PETRA IV. For comparison, the table also lists the parameters of the existing synchrotron radiation source PETRA III.

### 6.1.1. Lattice Design

#### Design Overview

The design of the lattice of PETRA IV has to consider boundary conditions from the current layout of PETRA III. The machine consists of eight arcs with a length of 201.6 m, which are connected by eight straight sections with two different lengths of 108 m and 64.8 m. Five arcs use a FODO-type lattice with a cell length of 23 m, and the cell contains no sextupoles. Due to their weaker strength, all sextupoles are installed in the FODO arcs at locations of large dispersion function. Two other arcs were modified in 2014. They were partly replaced by two DBA cells, while the rest of the arc uses the same FODO lattice as in the other five arcs.

The lattice of PETRA IV has to fit into the existing tunnel and experimental halls, with enough space for the installation of components on girders. Due to the fixed tunnel radius of 256 m, the geometry of PETRA IV has to closely match that of PETRA III. An additional goal is to provide enough user beamlines. Space for 25 insertion devices (IDs) with a length of 5 m and additional IDs with 10 m has to be provided. The lattice version in this section takes four 10 m long IDs into account. During the refinement of the lattice design in the technical design phase further IDs can be added.

Although it would be very desirable to keep the PETRA III cell length of 23 m, it is difficult to achieve a natural emittance in the range of 10–20 pm rad with such a short achromat. For space reasons, the magnets would accordingly have to be shorter and stronger. Therefore, a larger cell length of 26.2 m was chosen, and
Table 6.1.: Design parameters of PETRA III and PETRA IV.

<table>
<thead>
<tr>
<th>Design parameter</th>
<th>PETRA III</th>
<th>PETRA IV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy / GeV</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>Circumference / m</td>
<td>2304</td>
<td>2304</td>
</tr>
<tr>
<td>Operation mode</td>
<td>Continuous</td>
<td>Timing</td>
</tr>
<tr>
<td>Emittance (horiz. / vert.) / pm rad</td>
<td>1300 / 10</td>
<td>&lt; 20 / 4</td>
</tr>
<tr>
<td>Total current / mA</td>
<td>100</td>
<td>200</td>
</tr>
<tr>
<td>Number of bunches</td>
<td>960</td>
<td>1600</td>
</tr>
<tr>
<td>Bunch population / 1010</td>
<td>0.5</td>
<td>0.6</td>
</tr>
<tr>
<td>Bunch current / mA</td>
<td>0.1</td>
<td>0.125</td>
</tr>
<tr>
<td>Bunch separation / ns</td>
<td>8</td>
<td>4 / 20 (gaps)</td>
</tr>
</tbody>
</table>

* 80 × 20 bunches

the number of cells per arc was reduced from nine to eight to keep the radius of curvature fixed.

With an achromat length of 26.2 m, all the beamlines in the Max von Laue hall and in the two extension halls Ada Yonath (PXE) and Paul P. Ewald (PXN) have to be rearranged. However, most of the beamlines in PETRA III are installed in canted ID straight sections with canting angles of 5 mrad and even 20 mrad in the two extension halls using IDs with 2 m length. Calculations have shown that even small canting angles will increase the emittance significantly. Although a small number of canted beamlines with reduced canting angle would be acceptable, four canted straight section with a canting angle of 4 mrad would already increase the emittance by a factor of 2 with the relatively large horizontal beta function of the chosen lattice.

For this reason, canting was abandoned as an option in the current design of PETRA IV.

To accommodate a large enough number of beamlines, an additional large experimental hall West is planned for PETRA IV (cf. Figure 6.1). Not using canting also has the advantage that longer undulators with 5 m length are possible, enhancing the brightness compared to canted beamlines with undulators of only 2 m length.

Nevertheless, a shorter cell length of 23 m with nine cells per arc will be investigated again during the technical design phase. This shorter cell length would allow most of the current beamlines in the Max von Laue hall to remain in their present location. This would represent a significant saving of resources (both funding and time). Stronger magnets would be required, which can be achieved by reducing the aperture radius from 13 mm to a smaller value around 8 mm to 10 mm. A decrease of the dynamic aperture due to the stronger sextupole magnets and a stronger sensitivity to mechanical errors of the yokes and alignment errors are expected, and these challenges will be weighed against the benefit of maintaining some of the beamlines.

Design Considerations for Achromat

The natural emittance of PETRA IV should be two orders of magnitude smaller than that of PETRA III, which has an emittance of 1.3 nm rad. This cannot be achieved with the current magnetic structure of PETRA III.

In the last years, several projects have been proposed that make use of multibend achromats (MBA) [3] to achieve extremely low natural emittances. Pioneering work has been done at the MAX IV Laboratory to use the MBA concept for the storage ring MAX IV [4]. Upgrade or green-field construction projects using MBA exist for the ESRF-EBS [6, 14], APS-U [10], HEPS [15], SIRIUS [16] and other sources. All of them have in common that strong focusing is necessary to achieve the small emittances. As a consequence, a large negative chromaticity has to be compensated. The strong sextupoles have a negative impact on the non-linear dynamics of the lattice and lead to a strong decrease of the dynamic aperture of the ring.

The MBA of MAX IV uses a magnet configuration with distributed sextupoles in five unit cells and two end cells [4]. The chromaticity is corrected locally where it is generated. This
The MBA lattice has a large momentum acceptance and results in an acceptable Touschek lifetime required for lower-energy rings. The sextupole strengths needed for chromaticity correction are high but technically feasible. However, for larger rings with a similar MBA cell length, the bending magnet angles and the amplitude of the dispersion function are accordingly smaller. In addition, higher-energy rings like PETRA IV need stronger gradients compared to lower-energy ring like MAX IV. The sextupole strengths would then become too large with distributed sextupoles.

To reduce the problem of strong sextupoles, ESRF has developed the hybrid multibend achromat (HMBA) for the ESRF-EBS upgrade [6]. It uses a seven-bend achromat with additional space between the outer two dipole magnets on both sides of the achromat. In this region, three families of chromatic sextupoles are installed. The additional space between the outer dipoles creates two bumps of the dispersion function. In addition, the phase advance between the two horizontally focusing sextupoles is chosen to be $\Delta \mu_x \approx 3\pi$ (and $\Delta \mu_y \approx \pi$ in the vertical plane) to compensate much of the non-linearities of the sextupole magnets. Even not fully cancelling the geometric aberrations due to the interleaved scheme with vertically focusing sextupoles in between the arrangement of the sextupoles within the dispersion bumps is beneficial to reduce their strength. In addition, the HMBA lattice has a smaller emittance compared to the MAX IV MBA.

**Achromat**

For these reasons mentioned before, the HMBA of the ESRF-EBS was chosen for the achromat cell of PETRA IV. Compared with the length of 26.37 m of the ESRF-EBS achromat, the achromat length of 26.2 m of PETRA IV is nearly equal. The dispersion in the ID straights was matched to zero, as the effective emittance of PETRA IV is increased for a non-zero dispersion in the ID straights when undulators are closed. In addition, this simplifies the matching to the dispersion-free long and short straight sections. The optical functions of the achromat are shown in Figure 6.2. The parameters of the magnetic elements of the PETRA IV achromat are described in Section 6.3.1 in more detail.

The HMBA lattice uses a number of uncommon magnets not found in third-generation light sources [14]. The outer two magnets at both ends are longitudinal-gradient magnets with a variable dipole field in five steps of equal length. The bending angle is adapted to the dispersion function $D_y(s)$ to minimise the contribution to the dispersion invariant $H(s)$ of these magnets. The central part of the achromat is a FODO-like structure with focusing quadrupoles and combined function magnets in between. The combined function magnets have an integrated defocusing field to shift the
horizontal damping partition number in order to decrease the emittance further. The amplitude of the dispersion function peak in the two outer dipole magnets is a factor of 2 smaller compared to the ESRF-EBS due to a smaller bending angle of the PETRA IV cell of 5.625°, which is only half of the value of the ESRF-EBS with 11.25°. For a slightly positive chromaticity, the sextupoles installed in these regions have to be a factor of ≈2 stronger compared to the ESRF-EBS. In addition, they have to compensate the contribution to the natural chromaticity of the eight straight sections of PETRA IV.

As a consequence, the amplitude-dependent tune shifts are considerably larger compared to the ESRF-EBS cell, as they scale with the squared sextupole strength and the squared number of sextupoles [17]. In contrast to this, the increase in the second-order chromaticities is due to the fact that there are twice as many sextupoles compared to the ESRF-EBS lattice and due to the contributions of the straight sections.

In the achromat, linear optics and non-linear dynamics are strongly coupled. The linear optics was changed together with the three sextupole families, the octupoles and the harmonic sextupoles to optimise the dynamic aperture and momentum aperture of the lattice for PETRA IV.

### Other Achromat Options

The emittance could be somewhat reduced using reverse-bend magnets in the achromat, which better decouples the beta function and dispersion function and allows for a smaller $\beta^*$ at the ID location. The upgrade projects of SLS II [9], APS-U [10] and ALS-U make use of this method. Nevertheless, the additional bending using off-centred quadrupoles increases the energy spread and complicates the beam-based alignment measurement in these magnets.

Whether reverse bends are advantageous in terms of increased brightness will be carefully analysed later once the parameters of the undulators are fixed. The integration of the reverse-bend option in a later stage is relatively easy, as the only change would be the off-centre installation of some of the quadrupoles by some millimetres. Nevertheless, a complete optimisation of the lattice would then be necessary.

### Arc Sections

The phase advance of $3\pi$ resp. $\pi$ between the sextupoles cancels already most of the non-linearities generated by them. Due to the interleaved sextupole arrangement, the cancellation is not perfect, however. The non-linearities are further reduced by building the arc as a higher-order geometric achromat. With a phase advance of an achromat of $\mu_x = 2\pi(2 + 3/8)$ and $\mu_y = 2\pi(1 - 1/8)$, the arc is a quasi forth-order geometric achromat with a transport matrix of $+I$ [5, 18]. All of the third-order geometric resonances and most of the fourth-order geometric resonances are cancelled. The uncompensated terms in fourth order are three amplitude-dependent tune shifts and the $2Q_x - 2Q_y$ resonance, which is systematically driven by the phase advance condition between the sextupoles. The latter is compensated by an appropriate phase advance in the straight sections.

### Straight Sections

The eight arcs of the PETRA IV lattice are connected by four long and four short straight sections with a length of 100 m and 56.8 m, respectively. The lengths of these straight sections are slightly shorter than the geometrical length of the straight sections. Different designs are necessary, as some of the straights use a modified optics for the installation of 10 m long undulators with optimised beta functions. In all the straights, the dispersion function is zero.

The regular long and short straight sections (LSS and SSS) consist of matching triplets at both ends and periodic FODO cells with a length of 14.4 m in the central part. The FODO cells have a phase advance of less than 90° to reduce the contribution of the chromaticity of the straights to the total chromaticity. The optical functions of SSS and LSS are shown in Figure 6.3.

The short straight section in the south-east can be used for on-axis swap-out injection, as there are suitable locations for septa and stripline kickers with high beta functions and enough phase advance in between. The injection elements can be installed downstream of...
the centre of this short straight section and the extraction elements in the section upstream of the centre. The injection is discussed in more detail in Section 6.1.4.

In between the long straight section in the south, the RF system of PETRA III is currently installed, with nearby buildings for the transmitters. In a similar way, the 500 MHz RF system of PETRA IV could also be installed in the LSS south together with the 1.5 GHz higher-harmonic cavity system. The layout of the RF system in the LSS south is described in Section 6.3.8.

Short and long straight sections with space for a 10 m long undulator and optimised beta functions (SSSU and LSSU) are planned in the straights in the north, northeast, east and south-west. For the beta functions at the centre of the undulator, \( \beta^* = 4 \text{ m} \) was chosen as a compromise between optimum matching of electron and photon beams and the generation of additional local chromaticity, which scales as \( 1 / \beta^* \). The optical functions are shown in Figure 6.4. The straight sections are initially matched to approximately \( 2\pi \) resp. \( 4\pi \) phase advance in both planes to make them transparent for on-momentum particles. Due to the integer phase advance of the arcs, the fractional part of the tune has to be set by the straight sections. It is equally distributed to all eight straights. In addition, the short straights SSS and SSSU are used to compensate the driving term of the \( 2Q_x - 2Q_y \) resonance by an constraint of the phase advance of \( \Delta \mu_x - \Delta \mu_y = \pm 1/4 \cdot 2\pi \) and a mirror symmetric design of two arcs.

### Parameters of the Ring

The optical functions of PETRA IV are shown in Figure 6.5. The start of the lattice is in the centre of the LSS south. The ring consists in total of 64 HMBA cells in eight arcs. Note that due to the non-symmetric positions of the straights with space for long undulators (SSSU
and LSSU) in the lattice, the super periodicity of PETRA IV is reduced to 1. Without these straight sections, it would be 4 instead. The additional chromaticity contribution of all straight sections is approximately 9%.

The parameters of PETRA IV are listed in Table 6.2 and computed for zero single-bunch current without the effect of intra-beam scattering (IBS). The values in the left column are calculated for the case of open gaps of all undulators with an RF voltage of 6 MV. The values in the right column are for the case that all 29 undulators – in the three existing halls (Max von Laue, PXN and PXE), in the new hall West and the IDs in the straight sections – are closed. In this case, an RF voltage of 8 MV was assumed.

As the parameters of the IDs are not fixed yet, an U32 undulator with a length of 5 m, a period length of 32 mm and a peak field of 0.91 T was assumed for the calculations.

No damping wigglers are used in the lattice design of PETRA IV, since the undulators of the user beamlines already have a damping effect if they are closed. This damping effect will decrease the emittance by a factor of 2 and increase the energy spread and the energy loss per turn. Nevertheless, some additional damping undulators in one of the arcs are necessary to keep the emittance constant during gap changes of the undulators.

**Dynamic Aperture**

For an efficient injection during top-up operation of PETRA IV, the dynamic aperture (DA) has to be at least 0.8 mm mrad assuming an emittance of 19 nm rad for the injected beam. In a lattice version assuming off-axis injection in the horizontal plane with an injection point at the centre of the LSS south with $\beta_x = 100$ m, an acceptance slightly above 1.0 mm mrad...
Table 6.2.: Lattice parameters of PETRA IV with open and closed gaps of all 29 undulators without IBS for zero beam current.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value (IDs open)</th>
<th>Value (all IDs closed)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy $E$</td>
<td>6 GeV</td>
<td>6 GeV</td>
</tr>
<tr>
<td>Circumference $C$</td>
<td>2304 m</td>
<td>2304 m</td>
</tr>
<tr>
<td>Natural emittance $\epsilon_0$</td>
<td>17.4 pm rad</td>
<td>7.6 pm rad</td>
</tr>
<tr>
<td>Tunes $Q_x, Q_y$</td>
<td>164.18, 68.27</td>
<td>164.18, 68.27</td>
</tr>
<tr>
<td>Momentum compaction factor $\alpha_p$</td>
<td>$1.485 \times 10^{-5}$</td>
<td>$1.485 \times 10^{-5}$</td>
</tr>
<tr>
<td>Natural chromaticities $\xi_{x0}, \xi_{y0}$</td>
<td>$-229.9, -185.1$</td>
<td>$-229.9, -185.1$</td>
</tr>
<tr>
<td>Chromaticities $\xi_x, \xi_y$</td>
<td>$+5, +5$</td>
<td>$+5, +5$</td>
</tr>
<tr>
<td>Damping partition number $J_x$</td>
<td>1.536</td>
<td>1.175</td>
</tr>
<tr>
<td>Damping times $\tau_x, \tau_y, \tau_s$</td>
<td>45.6 ms, 70.0 ms, 47.8 ms</td>
<td>19.5 ms, 22.9 ms, 12.6 ms</td>
</tr>
<tr>
<td>Rel. energy spread $\sigma_E$</td>
<td>$0.678 \times 10^{-3}$</td>
<td>$0.903 \times 10^{-3}$</td>
</tr>
<tr>
<td>Bunch length $\sigma_s$</td>
<td>1.24 mm</td>
<td>1.52 mm</td>
</tr>
<tr>
<td>Bunch length $\sigma_t$</td>
<td>4.14 ps</td>
<td>5.07 ps</td>
</tr>
<tr>
<td>Energy loss per turn $U_0$</td>
<td>1.317 MeV</td>
<td>4.024 MeV</td>
</tr>
<tr>
<td>RF voltage $V_{RF}$</td>
<td>6 MV</td>
<td>8 MV</td>
</tr>
<tr>
<td>Bucket half height $\Delta p/p$</td>
<td>8.7%</td>
<td>7.1%</td>
</tr>
<tr>
<td>Synchrotron frequency $f_s$</td>
<td>387 Hz</td>
<td>421 Hz</td>
</tr>
<tr>
<td>Hor. beta function $\beta_x$ at ID</td>
<td>6.86 m</td>
<td>6.86 m</td>
</tr>
<tr>
<td>Ver. beta function $\beta_y$ at ID</td>
<td>2.36 m</td>
<td>2.36 m</td>
</tr>
<tr>
<td>Hor. dispersion function $D_x$ at ID</td>
<td>0 m</td>
<td>0 m</td>
</tr>
<tr>
<td>Space $L$ for ID</td>
<td>5 m</td>
<td>5 m</td>
</tr>
</tbody>
</table>

1 For the insertion devices, a 5 m long U32 undulator with a peak field of 0.91 T was assumed.

could be achieved without misalignments and other imperfections. Nevertheless, computations with realistic errors indicated that off-axis injection appears to be risky. The conceptual design is therefore based on the on-axis injection scheme.

The on-axis injection is planned for PETRA IV in the SSS south-east in the horizontal plane (see Section 6.1.4). The dynamic aperture at the injection point is shown in Figure 6.9.

For an injection in the horizontal plane, the acceptance in 6D tracking would be approx. $A_x = 1.1$ mm mrad and large enough to accept more than $7\sigma$ of the injected bunch of a 19 nm rad beam from the booster synchrotron DESY IV. The vertical acceptance has a similar value of $A_y = 1.1$ mm mrad. The dynamic aperture is significantly reduced by alignment and field errors of the magnets. The impact of errors on the dynamic aperture is discussed in Section 6.1.2.

The non-linear dynamics of PETRA IV for on-momentum particles is dominated by large amplitude-dependent tune shift (ADTS) terms. They are caused by the strong sextupole magnets in the achromats. For small actions $J_x$ and $J_y$, the amplitude-dependent tune shift is linear in $J_x$ and $J_y$ and has a large cross-term. For larger actions, the higher-order terms of the ADTS dominate the tune shifts, leading to a reversal of the direction of the tune shift. This can be seen in the 4D frequency map shown in Figure 6.6. The limit of the dynamic aperture is reached when the tune shift is so large that the particle is lost at the nearby integer or half-integer resonance.

Local Momentum Aperture

Due to the extremely small emittance of PETRA IV, the lifetime will be dominated by Touschek scattering. It depends mostly on the single-bunch current, the bunch volume and the local momentum aperture (LMA). The LMA of PETRA IV is shown in Figure 6.7 for the two cases when all IDs are open or closed. The RF bucket momentum height of 7% to 8% is not limiting the LMA and is larger than the limitation by the non-linear dynamics of the lattice. The LMA reaches 2.4% in the straight sections, but is the smallest in the arc sections.
near the dispersion bumps of the achromats where the $H$-function is maximum. In these regions, Touschek-scattered particles at a position $s^*$ start with the largest induced betatron oscillation amplitudes of $\sqrt{\beta(s)H(s^*)}\delta$ relative to the chromatic closed orbit of $D_x(s)\delta$. However, the relevant locations for the LMA are the regions with high Touschek scattering rates. They are in the ID straights and the central FODO part of the achromat, where the beta functions and dispersion function are smallest.

### Optimisation of DA and LMA

The dynamic aperture and the local momentum aperture were optimised by scanning the multipole strength of the non-linear elements (three sextupole families and an octupole family) of the achromat [19]. Furthermore, the linear optics and the non-linear optimisation cannot be separated for the HMBA cell. With parameters such as the phase advance between the sextupoles, the phase advance of the achromat and the optical functions near the sextupole magnets, the amplitude-dependent tune shift and the non-linear chromaticites can be changed. In addition, a multiobjective genetic algorithm (MOGA) [20] has been explored and will be further used to enhance the dynamic aperture and momentum aperture of PETRA IV.

### 6.1.2. Tolerances

At PETRA III, the vertical emittance of below 10 pm rad already requires sub-micrometre orbit stabilisation in the vertical direction. The difference of the PETRA IV lattice compared to PETRA III or other third-generation light sources that are already diffraction-limited in the vertical direction due to extremely low achievable coupling is not in the increased level of orbital stability, but in the fact that the sensitivity of the beam dynamics to alignment errors is dramatically increased. In this section, requirements on alignment, optics correction and orbit feedback are discussed.

#### Requirements on Alignment and Field Tolerances for Machine Start-Up and Operation

A preliminary study of the influence of alignment and field errors on the storage ring performance was conducted. To safely guarantee beam accumulation, we require the dynamic aperture after threading, trajectory correction and tune correction to be on average larger than $5\sigma$ and in no case worse than $3\sigma$ of the injected beam. With the booster beam of 20 nm rad natural emittance and 20% coupling, the $5\sigma$ beam would require approx. 4 mm of horizontal and approx. 0.7 mm of vertical dynamic aperture at the injection point location with $\beta_x = 21.7$ m, $\beta_y = 3.7$ m. Establishing the circulating beam and recovering the dynamic aperture require an iterative

---

**Figure 6.7:** Local momentum aperture of an octant of PETRA IV with (a) open gaps with 6 MV and (b) closed gaps with 8 MV of all undulators. The computation was done with 6D tracking (1024 turns) and synchrotron radiation on.
procedure that involves correcting the open trajectory, ramping up the sextupoles and octupoles and correcting the closed orbit, the tune and the chromaticity, a procedure similar to that performed during the APS-U [21] or the ESRF-EBS [22] studies. Simulations of this procedure were performed with elegant [23] based on a statistical model of alignment errors that generates random seeds representative of possible alignment scenarios in the PETRA tunnel. The simulations demonstrate that this goal can be achieved. For more details on the assumed alignment model and the start-up procedure, see [24].

The estimates of alignment and field tolerances resulting from simulations are shown in Table 6.3. Here $\Delta x$, $\Delta y$ and $\Delta \phi$ are the horizontal and vertical offsets and the roll angle with respect to the survey coordinates for the individual elements on the girder. For the girder, the number corresponds to the deviation from each of the neighboring girders. For magnets, $\Delta k/k$ is the relative error of the primary multipole component. Higher-order multipole components of the magnets will be carefully investigated during the technical design phase. Nevertheless, the strong sextupole magnets are dominating the nonlinear dynamics of PETRA IV. The maximum deviation of the element alignment with respect to the survey coordinates within one octant should be limited to 250 µm in both the horizontal and the vertical plane. The alignment values in Table 6.3 refer to the standard deviation of an assumed Gaussian distribution. For the simulation, a 3σ cut-off was used, showing acceptable performance. For the engineering specification, we set the tolerance to 2σ, i.e. 60 µm maximum deviation in the most demanding case. This would allow us to have contingency and potentially reduce the number of correctors. Note that the alignment requirements could be relaxed for some elements such as the quadrupoles in the long straight sections to speed up installation.

Figure 6.8 shows a typical alignment scenario generated by the statistical model. Figure 6.9 depicts the dynamic aperture calculated for 20 random seeds.

![Figure 6.8: One of the realisations of the misalignment.](image)

**Figure 6.8:** One of the realisations of the misalignment.

![Figure 6.9: Dynamic aperture (6D tracking) without errors (blue curve) and with errors (dots), with the orange line representing the average. Tracking point with $\beta_x = 21.7$ m, $\beta_y = 3.7$ m. Aperture requirements for 3σ and 5σ incoming beam with $\kappa = 20$ % coupling are also shown.](image)

**Figure 6.9:** Dynamic aperture (6D tracking) without errors (blue curve) and with errors (dots), with the orange line representing the average. Tracking point with $\beta_x = 21.7$ m, $\beta_y = 3.7$ m. Aperture requirements for 3σ and 5σ incoming beam with $\kappa = 20$ % coupling are also shown.

Figure 6.10 shows the local momentum acceptance with errors prior to optics correction. After the machine start-up procedure, the beam lifetime is estimated to be at least 30 min for 0.1 mA bunch current (cf. Figure 6.11), enough to perform optics measurement and correction, which is required to recover the dynamic aperture and momentum acceptance to 80 – 90 % or more of the original value, the goal of the operation. Preliminary studies suggest that the optics correction will require the sextupoles to be placed on movable supports. Note that, in the third-generation facilities, particular attention is payed to coupling correction to achieve ultra-low vertical emittances. This is not so in PETRA IV and other fourth-generation machines, where a large coupling ratio is required to mitigate the effect of IBS. Studies with round
beams have been performed at PETRA III, and it is assumed that this mode of operation will be available at PETRA IV [25].

**Table 6.3.: Summary of allowed alignment and field integral errors.**

<table>
<thead>
<tr>
<th>Element</th>
<th>$\sigma_{\Delta x}$</th>
<th>$\sigma_{\Delta y}$</th>
<th>$\sigma_{\Delta \phi}$</th>
<th>$\Delta k/k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dipole</td>
<td>50 µm</td>
<td>50 µm</td>
<td>200 µrad</td>
<td>$1 \times 10^{-3}$</td>
</tr>
<tr>
<td>Combined-function dipole</td>
<td>30 µm</td>
<td>30 µm</td>
<td>200 µrad</td>
<td>$0.5 \times 10^{-3}$</td>
</tr>
<tr>
<td>Quadrupole</td>
<td>30 µm</td>
<td>30 µm</td>
<td>200 µrad</td>
<td>$0.5 \times 10^{-3}$</td>
</tr>
<tr>
<td>Sextupole</td>
<td>30 µm</td>
<td>30 µm</td>
<td>200 µrad</td>
<td>$1 \times 10^{-3}$</td>
</tr>
<tr>
<td>Octupole</td>
<td>30 µm</td>
<td>30 µm</td>
<td>200 µrad</td>
<td>$1 \times 10^{-3}$</td>
</tr>
<tr>
<td>BPM</td>
<td>30 µm</td>
<td>30 µm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Girder</td>
<td>50 µm</td>
<td>50 µm</td>
<td>200 µrad</td>
<td></td>
</tr>
</tbody>
</table>

In the TDR phase, more detailed studies of algorithms for beam threading, fast optics correction and beam-based tuning will be undertaken to understand best strategies and develop online software for achieving the design beam parameters. Online beam control and optimisation tools available through the well-established frameworks MML [26] and OCELOT [27] will be accessible. MML is currently in use at PETRA III, and it is foreseen to further employ it at facilities such as MAX IV and ALS. OCELOT has enjoyed rapid development in the past. It has been widely used at DESY for the commissioning of the European XFEL [28] and has been ported to the PETRA III control system [29]. Furthermore, due to the potential need to repeatedly benchmark the optics performance and control the energy deposition, an online model will be implemented, an approach taken at the LHC that is instrumental during commissioning [30]. Although the alignment goals are ambitious, similar values have been reported at other facilities [31], and for the installation of the new PETRA III octants, values not too far from those required for PETRA IV have partially been achieved [1]. A more technical discussion of the alignment issues is presented in Section 6.3.2.

**Figure 6.10.: Local momentum acceptance with errors prior to optics correction (undulators open).**

**Figure 6.11.: Touschek lifetime vs. bunch current prior to optics correction for error seeds used in the start-up simulations.**

**Orbit, Spurious Dispersion and Optics Correction Requirements**

The residual orbit, dispersion and beta beating have two effects on the machine performance: The effective beam size is increased, and the beam dynamics characteristics, such as dynamic aperture and momentum acceptance, are suffering. The effective electron beam size is a convolution of the unperturbed beam size, orbit fluctuations, beta beating and residual dispersion. The beam size including emittance degradation and beta beating is
Table 6.4.: Summary of requirements on beam stabilisation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam size variation at ID, ( x, y )</td>
<td>less than 10 %</td>
</tr>
<tr>
<td>Spurious dispersion at ID BPMs, ( x )</td>
<td>less than 700 µm</td>
</tr>
<tr>
<td>Spurious dispersion at ID BPMs, ( y )</td>
<td>less than 180 µm</td>
</tr>
<tr>
<td>Orbit stability at ID BPMs, ( x )</td>
<td>less than 800 nm</td>
</tr>
<tr>
<td>Orbit stability at ID BPMs, ( y )</td>
<td>less than 160 nm</td>
</tr>
<tr>
<td>( \Delta \beta/\beta ) correction, rms, ( x ) and ( y )</td>
<td>2 %</td>
</tr>
<tr>
<td>( \Delta \epsilon/\epsilon ) max., ( x ) and ( y )</td>
<td>10 %</td>
</tr>
</tbody>
</table>

| BPM resolution | 140 nm at 600 Hz |
| BPM vibration amplitude | 50 nm above 10 Hz |
| Compensation bandwidth | at least 600 Hz |
| Corrector strength DC | at least 1 mrad |
| Corrector strength AC | at least 100 µrad |

\[
\sigma_{u,\beta} = \sqrt{\left( \epsilon_{u0} + \Delta \epsilon_u \right) \left( \beta_{u0} + \Delta \beta_u \right)}
\]

where \( u \) can stand for either \( x \) or \( y \). The beam size growth is to the first order

\[
\frac{(\sigma_{u,\beta} - \sigma_{u,0})}{\sigma_{u,0}} = \frac{\Delta \beta_u}{2\beta_{u0}} + \frac{\Delta \epsilon_u}{2\epsilon_{u0}}
\]

The rms fluctuation of the beam size due to emittance growth and beta beating together with the orbit fluctuation and the residual dispersion is

\[
\Sigma_u^2 = \frac{1}{4} \Sigma_{\Delta \beta/\beta}^2 + \frac{1}{4} \Sigma_{\Delta \epsilon/\epsilon}^2 + \Sigma_{r/\sigma_{u0}}^2 + \Sigma_{\delta E/\eta/\sigma_{u0}}^2
\]

where \( \delta E/\eta/\sigma_{u0} \) is the relative beam size variation due to dispersion, \( r/\sigma_{u0} \) is the relative orbit jitter, and \( \Sigma \)'s are the variations of those values. Assuming an emittance of 17 pm and a coupling of 20 %, beam sizes at the ID are approx. 10 µm horizontally and 2.6 µm vertically. The beta beating correction level is set to 2 % and below from beam dynamics considerations as described later. This contributes up to 1 % increase in the beam size.

Residual dispersion in undulators can lead to emittance growth when IDs are closed. So a canting angle of 2 mrad at all IDs (introducing 5 mm dispersion at the ID BPMs) would lead to a 100 % emittance increase. Following similar logic, the average residual dispersion at the ID BPM locations of approx. 1 mm will result in approx. 4 % emittance growth, due to quadratic dependency on the dispersion. This requirement sets the limit on the dispersion correction in case the beam size smearing due to the energy spread is irrelevant. Otherwise, the dispersion correction should be done with a higher precision. The specification on the residual dispersion (see Table 6.4) is particularly challenging in the vertical plane. It is about a factor two lower than the residual dispersion of 500 µm, which is regularly achieved in the wiggler sections of PETRA III.

The influence of IDs on beam emittance in PETRA IV is strong, with one ID contributing on average 7 % emittance damping (cf. Table 6.2). Thus, while small gap changes in several IDs or opening and closing up to two IDs would not lead to more than 10 % change in the beam size, the need to stabilise more severe gaps changes might require the installation of additional emittance feedback IDs.

The requirements on beta beating, dispersion correction, orbit and emittance stability to reach 10 % beam size stability are summarised in Table 6.4.

The dynamical influence of optics correction is such that for the uncorrected lattice harmful resonances are excited, the most prominent being the half-integer resonance crossed by particles with large momentum deviation. This resonance is not excited when the optics is corrected sufficiently well [32, 33], which in the case of PETRA IV corresponds to 2 – 3 % beta beating, a precision that is achievable e. g. with the LOCO algorithm [34]. Multiturn-based optics measurement is an attractive alternative to LOCO. Tests at PETRA III have been performed, showing inferior precision to LOCO [35]. The approach will however be
helpful during initial stages of machine setup when the beam lifetime might be low and a quick measurement with moderate precision is required. Appropriate software will be prepared for commissioning.

**Orbit Feedback**

The orbit stability requirements for the beam size fluctuation to not exceed 10% is 800 nm in the horizontal and 160 nm in the vertical direction, as discussed in the previous section. The orbit response for the PETRA IV lattice to dipole kicks $\theta$ is to good approximation

$$\Delta r_{\text{beam},i} = \theta_j \sqrt{\beta_i \beta_j} \frac{2}{\sin \pi Q} \cos(2\pi |\mu_i - \mu_j| - \pi Q).$$

(6.2)

Beta functions in MBA lattices are typically smaller than in DBA lattices, and thus the corrector strength required to achieve the same orbit precision is also smaller. The orbit distortion is however dominated by feed-down from the quadrupole movement. The rms closed-orbit distortion from quadrupole support movement is

$$\Delta r_{\text{beam}} \propto \langle \beta \rangle \sqrt{N_{\text{mag}} \left( \frac{L_{\text{mag}} g}{3.33E} \right)} \Delta r_{\text{sup}}$$

(6.3)

where $N_{\text{mag}}$ is the number of quadrupoles in the lattice, $\Delta r_{\text{sup}}$ is the rms displacement of magnet support (girder), $E$ is the energy in GeV and $L_{\text{mag}} g$ is the integrated magnet strength in $m \cdot T/m$.

Magnet support-to-orbit amplification factors at the BPM locations next to the IDs are 90 in the horizontal and 125 in the vertical direction when defined as rms orbit deviation value, and 300 and 380, respectively, when defined as the maximum deviation value. The amplification factors scale with the square root of the beta function and could vary by approx. a factor of 2 in other locations of the lattice.

For the PETRA site, the ground vibrations integrated down to 1 Hz lie in the 0.1 $\mu$m range (cf. Figure 6.53). Due to the approximately fourth inverse power dependency of the ground motion spectrum on frequency [36], ground vibrations above 100 Hz can be neglected. For the PETRA site, the ground vibrations integrated above 100 Hz lie below $1 \times 10^{-10}$ m. On the other hand, vibrations at low frequencies have long coherence length: All accelerator components and the photon beam transport line will move as a whole, and no impact on the experiment will be seen. For the APS-U site, the coherence length was estimated as $L_x \approx \frac{100}{f^{3/2}}$ and $L_y \approx \sqrt{\frac{100}{f}}$ [37]. Below 1 Hz, the coherence length is larger than 100 m in both planes, and a length of 30 m (what might be a short photon transport line) corresponds to 3 Hz highest coherent frequency. Coherence length measurements will be performed at the DESY site during further design work, but the estimates indicate that the lower frequency cut-off of the feedback system should lie in the range of 1 – 3 Hz.

**Figure 6.12.:** Maximum and rms corrector strength depending on alignment error. All 800 orbit correctors are used.

With the given lattice amplification factors and realistic support design, the beam cannot be stabilised to the desired precision without fast orbit feedback. If all orbit correctors are used simultaneously for slow and fast feedback, the AC part of the correction required to stabilise 0.1 $\mu$m vibrations will be below 1 $\mu$rad (cf. Figure 6.12). Some headroom is left to optimise the corrector configuration by having only a subset of correctors run in AC and DC mode simultaneously, an approach taken in the ESRF-EBS design [38]. A similar concept can be used at PETRA IV. With three correctors per cell, rms magnet vibrations up to 1 $\mu$m can be compensated with a maximum corrector strength below 10 $\mu$rad (cf. Figure 6.13). The skin depth of metals $\delta_{\text{skin}}$ is proportional to $f^{-1/2}$, and for the typical beam pipe materials Cu and Al, it reaches 1 mm, the typical beam pipe thickness, at about 4 kHz. Above 10 kHz, the magnetic field does not noticeably
penetrate the beam pipe, and magnet vibration is not influencing the beam. Care should however be taken in the frequency range between 1 kHz and 10 kHz not to introduce more ambient noise through pumps, water cooling etc.

Figure 6.13.: Residual closed orbit at ID BPMs after correction with 192 fast correctors (three per cell). The distortion is 1 µm rms.

The compensation cut-off frequency of 600 Hz or more appears to be safe from the mechanical point of view, while for the electrical disturbances a frequency of 1 kHz and above is desirable.

The use of photon BPMs would be beneficial to stabilise the electron beam with a very high (below 100 nm) precision with respect to the X-ray optics. These BPMs may be included in the system to set the reference ("golden orbit") for the fast orbit feedback based on the photon beam, which would reduce the sensitivity to thermal drifts during the process of machine start-up.

Based on the previously introduced coherence length estimate, BPMs located 5 m apart will vibrate incoherently at 10 Hz and above when attached firmly to the ground or to the girder. The ground motion above this frequency is 50 nm for the PETRA site. Adding 50 nm of mechanical vibration to 140 nm resolution in quadrature results in approx. 150 nm combined resolution, which is still within the requirements but with little safety margin.

6.1.3. Collective Effects

The collective effects depend on the charges of the beam, since a beam circulating in a storage ring interacts with its vacuum chamber surroundings via electromagnetic fields. These wakefields, in turn, act back on the beam and can lead to instabilities, which limit either the achievable current per bunch or the total current or even both. In PETRA IV, we expect the space charge effects to be small because of the high energy, and effects due to electron cloud are unlikely to be observed in an electron storage ring. But, since ion instabilities were observed in the early days of PETRA III under a poor vacuum, we need to know the stability condition. Without a clearing gap, the trapping condition for the ion is expressed as [39]

$$A \geq A_{\text{crit}} = \frac{QN_BR_p L_{\text{sep}}}{2\sigma_y(\sigma_x + \sigma_y)}.$$  (6.4)

where $A$ is the ion mass, $Q$ is the ion charge, $N_B$ is the number of electrons in a bunch, $r_p$ is the classical radius of the proton, $L_{\text{sep}}$ is the bunch separation, and $\sigma_x$ and $\sigma_y$ are the horizontal and vertical beam sizes. Ions with a mass number larger than $A_{\text{crit}}$ will be trapped. We applied this formula to PETRA III and PETRA IV, assuming a continuous mode of filling 100 mA in 960 bunches for the comparison. The critical mass $A_{\text{crit}}$ is shown in Figure 6.14 in comparison with the mass number of the CO$_2$ molecule. It becomes clear that trapping occurs in the multiple sections in PETRA III more than in PETRA IV. However, ion instability has not been a critical issue for user operation at PETRA III as long as the chamber is under a good vacuum and the spurious beam motion is controlled by the feedback system. Since the stored beam of PETRA IV will be distributed in 80 bunch trains with gaps (cf. Section 6.1.4), lowering the probability of ion accumulation in the brightness mode, we do not expect ions to be a critical issue in the PETRA IV storage ring.

Figure 6.14.: Critical mass for PETRA III and PETRA IV, compared with the mass number of CO$_2$. 154
Figure 6.15.: Plots of long-range wake of the proposed HOM-damped EU cavity and its corresponding HOMs. (a) Longitudinal Wake. (b) HOMs.

The wakefield excited by the beam is unavoidable and, as the radius of the vacuum chamber gets smaller, its effect will increase. In the following, we assume that the radius of the chamber is 10 mm and the undulator chamber’s full gap is 6 mm. A longitudinal coupled-bunch instability was observed in PETRA III, caused by the higher-order modes (HOMs) of the 500 MHz cavities. In order to mitigate the unwanted beam motion, a feedback system was installed, which has been operated successfully for 100 mA operations [40]. New cavities for PETRA IV have been proposed based on the HOM-damped EU cavity [41]. Its long-range wake was computed up to 400 m using the program GdfidL [42]. The simulation result is shown in Figure 6.15 together with the corresponding HOMs. The stability condition indicated in Figure 6.15 corresponds to 200 mA. Hence, the proposed cavity satisfies the stability requirement. A comprehensive analysis based on the recent measurement is presented in Section 6.3.8.

In transverse planes, the dominant long-range wake is produced by the resistive wall. Due to the $1/b^3$ scaling, its impedance will increase significantly with smaller radius $b$ of the vacuum chamber compared with PETRA III. But the small-gap chambers still dominate the impedance as 130 MΩ/m vs. the remaining 40 MΩ/m from the arc (note that the impedance was evaluated at the revolution frequency of 130.1 kHz assuming an aluminium chamber with NEG coating). This is comparable to other light sources in development, and the magnitude is not extreme. The preliminary analysis showed that the fastest grow rate is no greater than 4700/s at a chromaticity equal to zero. If we compare this with the damping rate tuned to 10 000/s of the feedback system currently used in PETRA III [40], the same class of feedback system will be sufficient to stabilise the coupled-bunch instability driven by the resistive wall.

The short-range wakefield causes a sudden beam losses where the feedback is too slow to counteract the unstable motion. This limits the single-bunch current, and its threshold can be estimated by the transverse mode-coupling instability (TMCI) which is [39]:

$$I_{th} = \frac{4\sqrt{\pi}(E/e)\sigma_p\alpha_c^\beta}{RZ_{t,eff}F}$$

(6.5)

where $R$ is the radius of the ring, $\nu_0$ is the betatron tune, $\sigma_p$ is the energy spread, $\alpha_c$ is the momentum compaction factor, and the parameter $F = \sigma_z/\sigma_{20}$ reflects the bunch lengthening by the impedance and/or by the harmonic cavity.

In order to evaluate the threshold current, we need to estimate the impedance of the ring. Even if a small aperture increases the impedance, in general, a comparative study of two chambers with different apertures [43] showed that the impedances of both chambers were similar to each other. Using this study as a guidance, we estimate the impedance of PETRA IV to be $Z_p= 1.1$ MΩ/m [44].

Substituting the lattice parameters in Table 6.2 (IDs closed) into Eq. (6.5), we computed the threshold current $I_{th} = 0.1$ mA$\times F$. To achieve a single-bunch current of 1 mA for the timing mode, we need to lengthen the bunch by a factor of 10. We may expect a factor of 2 longer due to impedance effects of the ring. The ad-
additional factor should then be achieved with a bunch-lengthening cavity.
In addition to the bunch-lengthening effect, we have an option to operate the machine at high chromaticities (e.g. $+5/5$) in PETRA IV to further increase the instability threshold [45, 46].

Even if the theoretical analysis of Eq. (6.5) can be useful to predict the single-bunch current limit, we have developed a detailed impedance model, which can be used to study beam physics with wakefield effects included. In this way, we can quantify the complex phenomena occurring within the RF bucket formed by the fundamental and the higher-harmonic cavity (HHC). The study's main results with the collective effects taken into account are presented in the following.

**Impedance Model**

Since the engineering design of the accelerator components is not yet available and since the question of how many of those components will be installed in the ring is not firmly decided, we have to establish the working assumptions for the impedance model. These are in compliance with the ongoing design and based on the assumption that the new design will not be much different than a scaled-down version of PETRA III. The main assumptions used in the impedance model are:

- The beam chamber is circular with a radius of 10 mm, and the ID chamber is elliptical with a full gap of 6 mm. For the calculation of the impedance 29 ID chambers have been taken into account.
- The beam chambers will be made of aluminium with non-evaporable getter (NEG) coating on the inner surface of the chamber around the ring.
- The accelerating voltage will be produced by 24 500 MHz cavities and 24 1500 MHz cavities.
- The beam will be injected into PETRA IV on-axis by stripline kickers with a full gap of 20 mm.
- Regular BPMs are located next to the quadrupoles, and ID BPMs are placed at the ends of the small-gap chambers.
- Radiation absorbers are located in the arcs.
- Bellows are placed in the arcs and in both the long straight sections (LSSs) and the short straight sections (SSSs).
- RF cavities (500 MHz and 1500 MHz) are in the LSSs.
- Feedback systems are in the LSSs (longitudinal) and SSSs (transverse).
- Scrapers and collimators are in the SSSs.

Using the aforementioned working assumptions and the lattice function, we established a list of the impedance elements. For all components in Table 6.5 the wake potential excited by a 1 mm long Gaussian bunch has been computed. For the case of a transverse wake, the dipolar and quadrupolar wakes are computed separately. All computations were carried out.
using the software GdfidL [42]. The salient points of the modelling are described in [47]. The total wake potential of the ring is then obtained by summing the wake potentials in Table 6.5 as

$$ W_{x,y,z} = \sum_{\text{Elements}} \left( N_j \times \beta_{x,y,z} \times W_{x,y,z} \right)_j \langle < \beta_{x,y,z} > \rangle, \tag{6.6} $$

where $ N_j $ is the number of each element in the ring, $ \beta_{x,y,z} $ is the lattice function at the location of the wake $ W_j $, and $ \langle ... \rangle $ is the average over the ring. The longitudinal wake potential of the ring and its corresponding impedance are shown in Figure 6.17. Separate from the geometric wake we used the program Impedance-Wake2D [48] to compute the resistive-wall impedance of a round chamber with three layers, i.e. vacuum, 2 mm thick aluminium and NEG coating inside. The resistive-wall impedance of a 10 mm round chamber with a range of NEG coatings is shown in Figure 6.18, where a resistivity $ \rho = 1 \times 10^{-6} \Omega \text{m} $ is used for the NEG coatings.

The thinner the coating, the less impedance there is at high frequency. We assumed a 1 $ \mu $m thick coating to be applied to the surface. Then the total transverse impedance of PETRA IV, which is the lattice-function-weighted sum of the geometric and resistive-wall impedance, is shown in Figure 6.19. Only the imaginary part of transverse impedance is displayed. The impedance function presented here is used to compute the wake potential of an arbitrary charge distribution, which will produce the charge-dependent kicks along the bunch at every turn as the bunch passes the impedance element.

**Beam Parameters with Collective Effects**

Due to the extremely small emittance, intra-beam scattering (IBS) at PETRA IV will be significant unless it is reduced by bunch lengthening. The single-bunch current will also be lower than the required 1 mA with the funda-
Table 6.5.: Impedance elements.

<table>
<thead>
<tr>
<th>Impedance element</th>
<th>Number</th>
<th>(\beta_x)</th>
<th>(\beta_y)</th>
<th>(\beta_z)</th>
<th>Remark</th>
</tr>
</thead>
<tbody>
<tr>
<td>BPM</td>
<td>1190</td>
<td>6.0</td>
<td>8.8</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Bellow</td>
<td>375</td>
<td>2.23</td>
<td>5.37</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Flange</td>
<td>375</td>
<td>2.23</td>
<td>5.37</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Absorber</td>
<td>375</td>
<td>2.23</td>
<td>5.37</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>ID arcs (25 \times 5,\text{m} + 4 \times 10,\text{m})</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ID6mm</td>
<td>25</td>
<td>7.8</td>
<td>5.0</td>
<td>1</td>
<td>5 m ID</td>
</tr>
<tr>
<td>P06mmR</td>
<td>50</td>
<td>7.8</td>
<td>5.0</td>
<td>1</td>
<td>ID BPM</td>
</tr>
<tr>
<td>ID6mm</td>
<td>4</td>
<td>10.3</td>
<td>10.3</td>
<td>1</td>
<td>10 m ID</td>
</tr>
<tr>
<td>P06mmR</td>
<td>8</td>
<td>10.3</td>
<td>10.3</td>
<td>1</td>
<td>ID BPM</td>
</tr>
<tr>
<td>Bellow</td>
<td>125</td>
<td>2.23</td>
<td>5.37</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Flange</td>
<td>125</td>
<td>2.23</td>
<td>5.37</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Absorber</td>
<td>125</td>
<td>2.23</td>
<td>5.37</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

Long straight section (LSS)

<table>
<thead>
<tr>
<th>Impedance element</th>
<th>Number</th>
<th>(\beta_x)</th>
<th>(\beta_y)</th>
<th>(\beta_z)</th>
<th>Remark</th>
</tr>
</thead>
<tbody>
<tr>
<td>RF1</td>
<td>24</td>
<td>7.9</td>
<td>7.8</td>
<td>1</td>
<td>Fundamental RF</td>
</tr>
<tr>
<td>RF3</td>
<td>24</td>
<td>7.9</td>
<td>7.8</td>
<td>1</td>
<td>Harmonic RF</td>
</tr>
<tr>
<td>LFB</td>
<td>8</td>
<td>7.9</td>
<td>7.8</td>
<td>1</td>
<td>Longitudinal feedback</td>
</tr>
<tr>
<td>FCT</td>
<td>4</td>
<td>7.9</td>
<td>7.8</td>
<td>1</td>
<td>Fast current monitor</td>
</tr>
</tbody>
</table>

Short straight section (SSS)

<table>
<thead>
<tr>
<th>Impedance element</th>
<th>Number</th>
<th>(\beta_x)</th>
<th>(\beta_y)</th>
<th>(\beta_z)</th>
<th>Remark</th>
</tr>
</thead>
<tbody>
<tr>
<td>TFBV</td>
<td>2</td>
<td>11.0</td>
<td>8.4</td>
<td>1</td>
<td>Transverse feedback (vert.)</td>
</tr>
<tr>
<td>TFBH</td>
<td>2</td>
<td>11.0</td>
<td>8.4</td>
<td>1</td>
<td>Transverse feedback (hroz.)</td>
</tr>
<tr>
<td>HSCR</td>
<td>1</td>
<td>7.4</td>
<td>9.3</td>
<td>1</td>
<td>Scrapper (horz.)</td>
</tr>
<tr>
<td>VSCR</td>
<td>1</td>
<td>7.4</td>
<td>9.3</td>
<td>1</td>
<td>Scrapper (vert.)</td>
</tr>
<tr>
<td>VCOL</td>
<td>4</td>
<td>7.4</td>
<td>9.3</td>
<td>1</td>
<td>Collimators</td>
</tr>
</tbody>
</table>

Injection straight

<table>
<thead>
<tr>
<th>Impedance element</th>
<th>Number</th>
<th>(\beta_x)</th>
<th>(\beta_y)</th>
<th>(\beta_z)</th>
<th>Remark</th>
</tr>
</thead>
<tbody>
<tr>
<td>InjKicker</td>
<td>4</td>
<td>11.0</td>
<td>8.4</td>
<td>1</td>
<td>Injection kicker</td>
</tr>
<tr>
<td>ExtKicker</td>
<td>4</td>
<td>11.0</td>
<td>8.4</td>
<td>1</td>
<td>Extraction kicker</td>
</tr>
</tbody>
</table>

mental RF system alone. Hence, we plan to use bunch-lengthening cavities as described in Section 6.3.8. Assuming an ideal higher-harmonic cavity (HHC), the RF voltage produced is then

\[
V(\tau) = V_{rf} \left[ \sin(\omega_{rf}\tau + \phi_s) + k \sin(n\omega_{rf}\tau + \phi_n) \right],
\]

where \(\omega_{rf}\) is the fundamental frequency, \(\phi_s\) is the synchronous phase, \(k\) is the voltage ratio, and \(n\) is the harmonic number.

For optimum bunch lengthening, we require not only \(V(0) = U_0/e\) to compensate the radiation loss \(U_0\) per turn, but also \(V'(0) = V''(0) = 0\) for a flat RF potential.

The harmonic voltage and phase are then given by

\[
k = \sqrt{\frac{1}{n^2} - \frac{(U_0/eV_{rf})^2}{n^2 - 1}} \tag{6.8}
\]

and

\[
\tan \phi_n = \frac{-nU_0/eV_{rf}}{\sqrt{(n^2 - 1)^2 - (n^2U_0/eV_{rf})^2}} \tag{6.9}
\]

The synchronous phase angle of the beam with respect to the main RF voltage \(\phi_s\) is changed to the new value given by

\[
\sin \phi_s = \frac{n^2 U_0}{n^2 - 1/eV_{rf}} \tag{6.10}
\]

With all IDs closed, the energy loss is \(U_0 = 4.0\,\text{MeV}\). If we use the fundamental RF voltage
$V_{rf} = 8$ MV, which provides 7.1% of the momentum acceptance, the optimum harmonic voltage and phase for $n = 3$ are $V_3 = kV_{rf} = 2.26$ MV and $\phi_3 = -12.8^\circ$, respectively. The equilibrium bunch length at the ideal quartic potential is estimated to be $\sigma_z = 9.8$ mm. With the active cavity system, we can control the RF amplitude and phase independently to reach the optimum condition. However, for the passive cavity system, the amplitude and phase cannot be adjusted independently because of the fixed $Q$ and the shunt impedance of $R_s$. So we adopted the active system for bunch-lengthening, and the ideal voltage in Eq. (6.7) is used in the following beam physics simulations.

Apart from the optimum condition, we need a numerical program to compute the bunch length in the combined RF system. We used the program *elegant* for this. Two methods are available to compute the bunch length; one is using the matrix method and the other is by tracking many particles. The former is fast but valid for zero current only, and the latter is slow but its result can be extended to the finite-current case including impedance effect. An initial 2D search was carried out using the matrix method, from which we found that a pair of voltages of 8.0 MV and $\sim 2.3$ MV are optimum for lengthening the bunch when the harmonic phase is set to zero.

\[ V_3 = kV_{rf} = 2.26 \text{ MV and } \phi_3 = -12.8^\circ \]

\[ \sigma_z = 9.8 \text{ mm} \]

\[ 2.3 \text{ MV} \]

\[ \phi_3 = -12.8^\circ \]

Figure 6.20 shows the bunch length as a function of the harmonic voltage. Figure 6.20 shows the bunch length as a function of the harmonic voltage, with the fundamental cavity voltage at 8.0 MV. The line graph represents the moment output of *elegant*. This is used to benchmark the results independently obtained by tracking 200 000 particles without impedance effect (black symbols). The agreement in bunch lengths computed by two different methods is good, giving some confidence in the following simulations. With the impedance effects included, we found their impact on the 1 mA beam is doubling the length (red symbols). From this, we conclude that the required bunch lengthening by a factor of 10 is feasible.

Not shown in Figure 6.20 are the phenomena caused by the microwave instability. At zero current, the beam is Gaussian in time and momentum space, as shown in the top of Figure 6.21. With the bunch-lengthening cavity, the distribution becomes flat, as shown in the middle. At a current of 1 mA, the impedance effect is in full display in the bottom, showing the dynamic microbunching around the edge of the distribution as well as the stationary potential-well distortion (PWD) at the core.

We tracked 200 000 particles over 50 000 turns for a range of initial currents. The longitudinal predictions are made by averaging the last 20 000 turns once equilibrium has been reached. The results from this study are summarised in Figure 6.22. Error bars in the plot show $\pm \sigma$ levels of fluctuation in the bunch length and the energy spread, the latter of which becomes rather significant above the microwave instability threshold at 0.3 mA.

Final beam parameters including IBS, harmonic cavities and impedance effects were calculated using *ibsEmittance* [49]. For a coupling ratio of 20%, the transverse and longitudinal bunch parameters were computed, and the results are shown in Figure 6.16.
These beam parameters were used to compute the Touschek lifetime for a given local momentum acceptance (LMA) of the ring whose results are shown in Figure 6.23. The data can be approximated as 

\[ \tau = 0.77 + \frac{0.49}{I_b} \]  

where \( \tau \) is the lifetime in hours, and \( I_b \) is the bunch current in mA.

Finally, the beam parameters are summarised in Table 6.6. Without a higher-harmonic RF system, the lifetime would be below one hour in timing mode.

**Single-Bunch Intensity Limit**

For PETRA IV, we envision full-intensity injection. How much charge we can store is the subject of research. A first estimate based on the TMCI threshold Eq. (6.5) was too low. In order to raise the intensity limit, we suggested to use the bunch-lengthening cavity. Since the high-current phase space exhibits such a complex distribution in the combined RF system, an accurate prediction of the intensity limit must be established through multiparticle simulations. Previous experience has shown that the accuracy in the transverse instability critically depends on the longitudinal beam distribution; hence, determining the single-bunch current limit requires the full 6D tracking.

In an idealised injection scheme where the offset is zero, no wakefields will be excited. However, there are always injection errors, which we assume to be 200 µm in the horizontal and the vertical plane, respectively.

In the simulation, we lumped all impedance elements at one location and modelled the ring as a one-turn map. Following the initial beam offset, we tracked over 40 000 turns, which is longer than ten radiation-damping times. The long-term tracking was necessary in order not to miss the lethargic start of instability if it occurs. At high current, we observed beam loss in both planes, but the vertical plane exhibited stronger instability. The vertical beam position and size during the first 20 000 turns are shown in Figure 6.24, which shows that increasing the chromaticity stabilised the beam motion resulting in the high injection efficiency.

Finally, the single-bunch intensity limits for a range of chromaticity values are summarised in Figure 6.25. At a chromaticity of 1, we can store up to 0.3 mA, which is acceptable for the
brightness mode but not acceptable for the timing mode. In order to ensure that we can store sufficient charge in a single bunch in timing mode, we need to operate the ring with a chromaticity greater than 3.

6.1.4. Injection Scheme

On-Axis Injection Scheme

The dynamic aperture of PETRA IV (cf. Figure 6.9) is on average approx. 5σ and in no case less than 3σ of the injected beam, when alignment and field errors are taken into account. This is sufficient for a horizontal on-axis injection, but considered risky for off-axis accumulation when a septum blade of 3 mm or thicker has to be additionally cleared, even if the beta function at the injection location is increased to about 100 m. For this reason, a swap-out on-axis injection is foreseen.

The short straight section (SSS) on the southeast of the PETRA IV storage ring downstream of the Ada Yonath Hall (cf. Figure 6.1) is chosen as the injection and extraction section. It provides sufficient space to accommodate both the injection and the extraction at the same straight section. The optical functions of the section are shown in Figure 6.27.

Table 6.6: Final beam parameters including effects of IBS, higher-harmonic RF system and impedance.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Reference</th>
<th>Brightness mode</th>
<th>Timing mode</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bunch current ( I_b ) (mA)</td>
<td>0.01</td>
<td>0.125</td>
<td>1.0</td>
</tr>
<tr>
<td>Hor. emittance ( \epsilon_x ) (pm rad)</td>
<td>7.37</td>
<td>11.60</td>
<td>19.21</td>
</tr>
<tr>
<td>Ver. emittance ( \epsilon_y ) (pm rad)</td>
<td>1.47</td>
<td>2.32</td>
<td>3.84</td>
</tr>
<tr>
<td>Bunch length ( \sigma_z ) (mm)</td>
<td>11.7</td>
<td>13.7</td>
<td>19.3</td>
</tr>
<tr>
<td>Bunch length ( \sigma_t ) (ps)</td>
<td>39.1</td>
<td>45.7</td>
<td>64.3</td>
</tr>
<tr>
<td>Energy spread ( \sigma_p ) ((10^{-3}))</td>
<td>0.914</td>
<td>0.963</td>
<td>1.562</td>
</tr>
<tr>
<td>Touschek lifetime ( \tau ) (h)</td>
<td>49.4</td>
<td>4.7</td>
<td>1.2</td>
</tr>
</tbody>
</table>

Figure 6.23.: Local momentum acceptance (left) used to compute the Touschek lifetime (right) with a higher-harmonic RF system and impedance effects included. A coupling of 20% and closed undulators are assumed.

Figure 6.27.: Beta functions of the short straight section (SSS).

Figure 6.26 shows a schematic of the injection and extraction section. The incoming beam is positioned on-axis with a septum
and two stripline kickers (cf. Figure 6.28). A septum similar to the existing pulsed septum of PETRA III operated with a half-sine pulse is considered as the baseline. To reduce the stray field effect of the pulsed septum, a DC Lambertson septum is under consideration. Other injection options such as vertical on-axis injection will be studied in the next phase of the project.

The beam will be extracted by a combination of kickers and a septum, as shown in Figure 6.26. For the extracted beam, two options are possible. The baseline is to dump the beam immediately after the extraction. Due to the low natural emittance of PETRA IV, the transverse beam size of the electron bunch is extremely small. To dump the beam safely, it is necessary to increase the beam size before extraction. This swap-out dump procedure is studied in Section 6.3.12. The other option is to re-inject the beam from the storage ring into the booster and accumulate there. For this option, a transfer line to the booster will be required, and the dump can be placed in the booster tunnel.

Separation Distance and Kicker Strength

At the septum end, the separation distance between the injected beam and the stored beam is considered to be

$$\Delta x_{\text{sep}} = 3\sigma_{\text{inj}} + x_{\text{err}} + s_d + s_a$$  \hspace{1cm} (6.12)

where $\sigma_{\text{inj}}$ is the injected-beam size, $x_{\text{err}} = 1$ mm is the orbit error, $s_d = 5$ mm is the septum thickness including vacuum chamber, and $s_a$ is the aperture required for the stored beam. Assuming a booster emittance of 19.3 nm rad, an energy spread of $1.12 \times 10^{-3}$, a beta function at the septum location $\beta_x = 31.17$ m and a dispersion $D_x = 0.02$ m, the injected-beam size is $\sigma_{\text{inj}} = 0.78$ mm. The minimum required aperture for the stored beam $s_a$ can be set to $5\sigma$ of the injected beam plus the orbit error, which would be sufficient for capturing 99% of the injected beam, resulting in approx. 5 mm stored-beam aperture. We conservatively choose a larger aperture $s_a = 10$ mm, however, which is a typical beam pipe radius in the storage ring. In total, the separation distance is $\Delta x_{\text{sep}} = 18.4$ mm. To provide this separation, two kickers need a deflection angle of 0.67 mrad each. The injected-beam trajectory is shown in Figure 6.28.

Injection Fill Pattern

PETRA IV will be operated in two modes: the brightness mode and the timing mode, as shown in Table 6.1. For the timing mode, a single bunch will be injected at each injection, while for the brightness mode, a bunch train of 20 bunches will be injected each time. The injection fill pattern is shown in Figure 6.29. For each bunch train, a flat-top of at least 76 ns is required. Between each train, a gap of 20 ns will accommodate kicker rise and fall times. The details of the kickers and the septa are discussed in Section 6.3.9.
When the charge variation in the fill pattern is dominated by the charge decay rather than the fluctuation of the injected-beam intensity, the maximum variation is given by \( 1 - \exp\left(-\frac{\tau}{T_{\text{inj}}}\right) \), where \( T_{\text{inj}} \) is the time required for the full injection cycle, and \( \tau \) is the beam lifetime. In the worst-case scenario, with 30 minutes lifetime and 80 bunches in the timing mode, an injection frequency of 0.41 Hz and higher (192 second injection cycle) would guarantee a maximum charge variation below 10\%. An injection rate of 0.5 Hz is planned, resulting in a maximum intensity variation of 8.4\%.

The charge of the injected bunch in every transfer step is shown in Table 6.7. Here, we assume roughly 90\% transmission in every transfer step and use 80 mA in the timing mode and 200 mA in the brightness mode. The new transfer line from the DESY IV synchrotron to PETRA IV will be at the position of the current positron transfer line to PETRA (P-Weg), and the extraction line will be at the position of the present injection line (E-Weg). In addition, the injection/extraction kickers will be used for beam dilution for the beam dump, as discussed in Section 6.3.12.

### Table 6.7: Charge (and number of particles) of the injected bunch in every transfer step.

<table>
<thead>
<tr>
<th>Transfer Line</th>
<th>Charge (nC)</th>
<th>Timing mode bunch train</th>
<th>Brightness mode single bunch</th>
</tr>
</thead>
<tbody>
<tr>
<td>PETRA IV stored ((10^{10}))</td>
<td>4.80</td>
<td>12.0</td>
<td>0.600</td>
</tr>
<tr>
<td>PETRA IV injection ((10^{10}))</td>
<td>7.69</td>
<td>19.2</td>
<td>0.961</td>
</tr>
<tr>
<td>DESY IV extraction ((10^{10}))</td>
<td>5.75</td>
<td>13.9</td>
<td>0.696</td>
</tr>
<tr>
<td>Electron Gun and LINAC II ((10^{10}))</td>
<td>6.87</td>
<td>17.2</td>
<td>0.859</td>
</tr>
<tr>
<td>Electron Gun and LINAC II ((10^{10}))^1</td>
<td>11.0</td>
<td>27.5</td>
<td>1.38</td>
</tr>
</tbody>
</table>

^1 The frequency of the S-band linac is 3 GHz, six times that of the booster (500 MHz). We assume that three bunches from the linac could be captured by the booster as one bunch. The charge intensity of one bunch from the linac is 1/3 of what is shown in the table.
6.2. Injector Complex

To meet the requirements for the PETRA IV injection (Section 6.1.4), the transverse emittance of the delivered beam at the injection energy of 6 GeV has to be sufficiently small, well below 30 nm rad.

As described in Section 6.1.4, the injection into PETRA IV could only be done with an on-axis scheme. In top-up operation, this means that bunches are not filled up by an accumulation process, but can only be exchanged completely. As a consequence, the injector complex always has to deliver the full beam (bunch) intensity. In addition, during top-up operation of PETRA IV, the delivered intensity at every single injection has to be close to the requested intensity (within about 1%).

Independently of the intensity requirements, the existing PETRA III injector complex – consisting of a 450 MeV S-band linac (LINAC II), a small 450 MeV accumulator ring (PIA) and a fast-cycling booster synchrotron (DESY II) for acceleration to 6 GeV – cannot be used for PETRA IV, since the emittance of DESY II is by far too large and significant improvements are impossible. A new injector complex will be constructed to fulfil all requirements: single-bunch intensities up to $5.57 \times 10^{10}$ electrons, bunch train intensities up to $13.9 \times 10^{10}$ electrons (cf. Table 6.7), both with an intensity precision of better than 3% and a horizontal emittance of better than 20 nm rad at 6 GeV.

For this new complex, it is foreseen to prepare the required beam intensities and time structures directly at the particle source, followed by the existing, but significantly refurbished LINAC II. The acceleration to the final beam energy will take place in a new low-emittance booster ring (DESY IV). Since the existing LINAC II would be able to deliver electrons up to 700 MeV without losing all existing redundancy and reliability, the booster injection energy will be increased from the current 450 MeV to 700 MeV, relaxing intensity limitations at the on-axis booster injection. As specified in Section 6.1.4, PETRA IV requires injection every two seconds in timing mode. It is foreseen to operate the gun and the linac at 10 Hz; thus, the full intensity could be delivered with 10 Hz. To be able to make some use of this ability while avoiding a fast-cycling booster based on a White circuit, we chose 2 Hz as the repetition rate of the new booster, instead of the minimal required 0.41 Hz.

Injector Options

As an option, the booster will also allow an off-axis injection. By exploiting the booster repetition rate, which is significantly higher than required by PETRA IV, this would allow an intensity accumulation using more than one booster magnet cycle. As another option, it is foreseen to integrate a 6 GeV injection into the booster layout, allowing, in principle, to reinject the beam extracted from PETRA IV at every injection into the booster. Since the transport of such a high energy density beam is connected to serious risks (cf. Section 6.3.12) and since a reinjection would require perfectly adjusted path lengths of the transport lines, at this stage of the project this option is not part of the baseline operation concept.

Since PETRA IV will be a user facility whose availability will be a very important key performance indicator, the injector complex has to be highly available as well and has to operate very reproducibly. This is an argument for choosing an injector design that is as robust as possible; the overall number of active components has to be as low as possible; redundancy will be included where reasonably possible.

Recently, significant progress has been achieved with respect to laser plasma acceleration of electrons [50]. At the BELLA facility at Berkeley Lab, electrons with an energy of up to 7.8 GeV and a charge of 5 pC were obtained from a 20 cm long plasma cell. In the future, laser plasma accelerators could become a suitable complement to conventional accelerator-based injection systems. During the technical design phase of PETRA IV, the status and maturity of these new technologies will be further analysed. We plan to design the injector complex in a way that enables the integration of these new technologies in the future.

Test Beams at the PETRA IV Complex

Due to their central role for detector development in particle physics, nuclear physics, photon science and beyond, the availability of electron/positron test beams is essential.
Currently, test beams are generated at DESY in Hamburg at the synchrotron DESY II by inserting thin carbon fibre targets into the primary beam, generating bremsstrahlung photons and converting these photons back into electrons or positrons at a secondary target station. The current operation mode of this DESY Test Beam Facility [51] provides a constant flux of particles with rates up to several 10 kHz without any disturbance of PETRA III operation. At each of the three existing beamlines, the particle energy can be varied individually between 1 GeV to 6 GeV, as can the particle flux. Important for almost all users is a low particle multiplicity.

The future PETRA IV complex should be able to provide test beams in a similar fashion to DESY II today. While parts of the user community require larger rates at the highest possible beam energy, other groups need a wide range of particle energies, e.g. to calibrate their detector response [52]. All groups, however, prefer a particle multiplicity maintained at a maximum of a few particles per event.

To fulfil the given test beam requirements even after converting PETRA III into PETRA IV, it is foreseen to use DESY IV as the test beam source. As in the present scheme, internal targets will be used. To completely decouple the test beam production from the operation for PETRA IV, we plan to use independent DESY IV magnet cycles and produce test beams either by moving the beam orbit to fixed targets or by moving the targets, synchronised with the magnet cycle, into the beam orbit.

### 6.2.1. Injector Linac

**Current Source (Gun)**

The concept of on-axis injection into the main storage ring necessitates that the total charge is either produced directly at the gun or accumulated in an intermediate ring. Depending on the filling scheme, 1.4 nC to 11 nC have to be produced per bunch (cf. Table 6.7). The maximum charge per bunch train is 27.5 nC.

To fill a 500 MHz bucket of the storage ring, the charge can be distributed over three bunches in the 3 GHz RF of the linac [53], i.e. the maximum charge to be produced per bunch is 3.7 nC. While this charge is difficult to impossible to achieve with a thermionic DC gun, it is readily available from photocathode RF guns with emittances far better than required for injection into a synchrotron [54]. Scaling up the results from the S-band gun of LCLS [55] to the higher charge, one can expect normalised emittances in the range of 18 mm mrad. A common problem for photocathode guns is the achievable charge stability. As an example of the state of the art, Figure 6.30 shows a typical measurement from the European XFEL.

In a typical run with 250 pC bunch charge, an rms jitter of 2 pC is observed, corresponding to a relative jitter of 0.8 %. The jitter within the pulse is of the same order of magnitude. In section 6.1.4, the expected charge spread of bunches in the main accelerator is estimated to be close to 8 %. Hence, a charge jitter of 0.8 % appears tolerable. Unlike the L-band guns used for the European XFEL or FLASH, the gun for LINAC II would be operated with short pulses of a few microseconds only, which should not cause any serious reliability issues. Nevertheless, a redundant gun and photocathode laser would be recommended. The RF feed of the guns could be shared with two of the downstream accelerating sections. The required pulse structure would have to be produced by the cathode laser. It is assumed that this pulse structure can be achieved with splitters and delay stages from a single UV pulse, easing the requirements for the laser oscillator.

![Figure 6.30: Charge stability measured in the European XFEL. The overlaid Gaussian curve corresponds to a mean value of 0.25 nC and an rms value of 2 pC, i.e. 0.8 %.](image)

To achieve easier operation and maintenance as well as higher reliability, it is desirable to further reduce the complexity of the electron source and the sensitivity of the cathode material. To this end, a thermionic RF gun is envisaged, as developed at MAX IV Laboratory [53]. A gun of that type was tested at DESY...
in 2008. At pulse lengths of 50 ns, a current limit of 1 A was determined, corresponding to a bunch charge of 330 pC. The limit was due to self-heating of the cathode, probably caused by back-bombardment. It will be investigated if this limit can be overcome by increasing the cathode area or laser-enhancing the emission. A conventional approach to the latter can be found in [56]. A very interesting and promising alternative approach is described in [57]. By using femtosecond laser pulses, effectively only the electron gas gets heated, allowing for very high temperatures that result in very strong thermionic emission while keeping the energy deposited in the material low.

**Linac**

The current LINAC II consists of ten full acceleration sections with a 24 MW klystron and SLED system, each capable of an acceleration voltage up to 90 MV. Two shorter sections serve as capture sections for one injector each and deliver 5 MV. When upgrading the electron sources to RF guns, these stations would instead feed the guns, delivering approximately the same beam energy. With two sections reserve, 700 MeV beam energy can currently be achieved. To accommodate bunch trains of 100 ns and 200 mA, a slight change of the operation point would be necessary, resulting in a reduction of the acceleration voltage of approximately 6 MV per acceleration section. In detail, the beam needs to be injected before the structure is completely filled, thus compensating the beam loading. Adding two RF stations and acceleration sections and taking into account the beam loading, 800 MeV can be reached while keeping a safe reserve of two stations. Currently, the RF stations consist of thyatron-switched PFN-type modulators. The stability of the RF is approximately $1 \times 10^{-3}$. To increase the stability and availability and to reduce long-term maintenance costs, it is advisable to change to semiconductor switches. Currently, a one-to-one replacement for the thyatrons is being developed. Should this development fail, then the modulators could be replaced by inductively adding devices. A few of these already operate at DESY very satisfactorily. In the latter case, it would also be possible to change to bigger klystrons (45 MW) with the capability to feed two RF sections in parallel. In that way, only half the number of klystrons would be necessary. The voltage stability of these devices is considerably better, with values approaching $1 \times 10^{-5}$. The increased voltage stability especially benefit the guns, resulting in much improved charge stability compared to what is achieved nowadays. In addition, the energy stability of the beam injected into DESY IV would be improved, and the injection efficiency would be better and more stable.

### 6.2.2. New Booster Synchrotron DESY IV

The injector chain upgrade requires a new booster, DESY IV. The main challenge of the new injector is the delivery of up to $5.6 \times 10^{10}$ particles (9 nC) per bunch with a beam emittance less than 30 nm rad. Important factors to be taken into account include the stability of the bunch intensity and energy, good injection efficiency, cost and throughput. Beamlines for the DESY Test Beam Facility must be taken into account as well. The capability to reinject the swapped-out beam from PETRA IV into DESY IV is optional, but included in the design phase.

**Figure 6.31.: Layout of the electron optical elements of DESY II and DESY IV.**

**Lattice**

The present PETRA III booster synchrotron DESY II shares a tunnel with the decommissioned proton synchrotron DESY III, which was used as a preinjector for the HERA hadron–electron ring accelerator. For the upgrade,
DESY III will be removed to install DESY IV. The layout of DESY IV within the currently existing infrastructure is shown in Figure 6.31. Unlike DESY II, the orientation of DESY IV will be counter-clockwise.

Unlike DESY II, the orientation of DESY IV will be counter-clockwise.
Table 6.8: Booster parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Periodicity</td>
<td>6</td>
</tr>
<tr>
<td>Circumference</td>
<td>316.8 m</td>
</tr>
<tr>
<td>Harmonic number</td>
<td>528</td>
</tr>
<tr>
<td>Repetition rate</td>
<td>2 Hz to 5 Hz</td>
</tr>
<tr>
<td>Straight length</td>
<td>2.745 / 0.935 / 1.165 m</td>
</tr>
<tr>
<td>Working tune</td>
<td>18.25 / 10.37</td>
</tr>
<tr>
<td>Natural chromaticity</td>
<td>-22.16 / -19.40</td>
</tr>
<tr>
<td>Damping partition</td>
<td>-0.36</td>
</tr>
<tr>
<td>Momentum compaction</td>
<td>$3.30 \times 10^{-3}$</td>
</tr>
<tr>
<td>Beam energy at 6 GeV</td>
<td>700 MeV</td>
</tr>
<tr>
<td>Energy loss per turn</td>
<td>4.04 MeV / 0.748 keV</td>
</tr>
<tr>
<td>Equilibrium emittance</td>
<td>19.3 nm rad / 0.261 nm rad</td>
</tr>
<tr>
<td>Equilibrium energy spread</td>
<td>$1.12 \times 10^{-3} / 1.23 \times 10^{-4}$</td>
</tr>
<tr>
<td>Horizontal damping time</td>
<td>2.29 ms / 1.44 s</td>
</tr>
<tr>
<td>Vertical damping time</td>
<td>3.14 ms / 1.98 s</td>
</tr>
<tr>
<td>Longitudinal damping time</td>
<td>1.92 ms / 1.21 s</td>
</tr>
</tbody>
</table>

Table 6.9: DESY IV magnet specification.

<table>
<thead>
<tr>
<th>Magnet</th>
<th>BD</th>
<th>BF</th>
<th>BM</th>
<th>Q1</th>
<th>Q2</th>
<th>S1</th>
<th>S2</th>
</tr>
</thead>
<tbody>
<tr>
<td>L (m)</td>
<td>1.75</td>
<td>1.85</td>
<td>1.00</td>
<td>0.3</td>
<td>0.3</td>
<td>0.2</td>
<td>0.2</td>
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<tr>
<td>$B_0$ (T)</td>
<td>0.86</td>
<td>0.35</td>
<td>0.90</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>$K_0$ (m$^{-1}$)</td>
<td>0.043</td>
<td>0.0175</td>
<td>0.045</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$K_1$ (m$^{-2}$)</td>
<td>-0.44</td>
<td>0.49</td>
<td>-1.84</td>
<td>1.66</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$K_2$ (m$^{-3}$)</td>
<td>-4.78</td>
<td>2.89</td>
<td>3.0$^c$</td>
<td>3.0$^c$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td># Element</td>
<td>54</td>
<td>60</td>
<td>6</td>
<td>12</td>
<td>12</td>
<td>12</td>
<td>12</td>
</tr>
</tbody>
</table>

$^a$ The dipole fields are estimated at 6 GeV.
$^b$ $K_0 \equiv 1/\rho$, $K_1 \equiv (\partial B_y/\partial x) B_\rho$ and $K_2 \equiv (\partial^2 B_y/\partial x^2) B_\rho$.
$^c$ Maximal strength normalised at 6 GeV.

Figure 6.34: (a) Dynamic aperture with tune diffusion. (b) Tune dependency on momentum deviation and amplitude.

Magnets
There are two kinds of combined-function magnets, each comprising dipole, quadrupole and sextupole components. The quadrupole components repartition the damping coefficients in order to achieve a small emittance, while the sextupole components correct the chromaticities to slightly positive. The magnet type with focusing gradient is named BF, the other BD. The magnet strengths of DESY IV are listed in Table 6.9. Programmable independent power supplies should be included for sextupoles and trim coils in quadrupoles in order to gain finer dynamic control of tunes and chromaticities. The scalar potential of 2D magnetic fields in a combined-function magnets is $\Phi(x, y) = K_0 y + K_1 xy + \frac{A_2}{2}(3x^2 y - y^3)$. The ideal pole faces can be found using the equipotential-line equations $\Phi(x, y) = \Phi(0, \pm h)$, where $h$ is
Figure 6.35.: Ideal pole face of combined-function magnets (a) BD and (b) BF.

the half gap. Defining $p \equiv \frac{2K_0}{K_2} + \frac{2K_1}{K_2}x + x^2$ and $q \equiv \frac{h^3}{2} - \frac{3K_2}{K_2}h$, the analytical solutions around $x = 0$ follow the curves $y = \pm 2\sqrt{p} \cos \left(\frac{1}{3} \cos^{-1} \left(\frac{1}{2} \sinh^{-1} \left(|p|^{-3/2}q\right)\right) - \frac{2\pi}{3}\right)$ for BF and $y = \pm 2\sqrt{|p|} \sinh \left(\frac{1}{3} \sinh^{-1} \left(|p|^{-3/2}q\right)\right)$ for BD. As an example, the ideal pole faces of BD and BF are shown in Figure 6.35 assuming $h = 0.018$ m. The magnets are made of pieces of laminated iron to reduce eddy currents. To design the magnets in 3D finite element codes, the actual pole faces need to be tweaked. In general, H-type magnets are preferred over C-type magnets. In principle, one can change the gap and the winding number in order to match the driving currents of BD and BF so that they can be connected in series and powered by a single power supply.

Closed Orbits with Errors
The following errors are assumed. The rms misalignment errors of bending magnets and quadrupoles are $\Delta x = 0.1$ mm, $\Delta y = 0.1$ mm and $\Delta \theta = 0.2$ mrad, where $\theta$ is the roll angle about the longitudinal axis. The relative field errors are 0.02% and 0.2% for dipole and quadrupole fields, respectively. Errors more than three times the standard deviations are truncated. Of 100 random machines, all have stable closed orbits. The ensembles of closed orbits and beta beatings of 50 random machines are shown in Figure 6.36a. The closed-orbit deviation peak is located in the insertion sections. The histogram of the horizontal orbit at the injection point is shown in Figure 6.36b. The “beam stay clear” (BSC) is defined by $BSC = 3\sigma$ beam size + max closed orbit. Without orbit corrections, the horizontal BSC is estimated to be $<13$ mm in insertion sections and $<10$ mm in FODO arcs. This also determines the inner radii of the beam pipes, as shown by the circles in Figure 6.35.

RF
The total RF cavity voltage has to compensate the energy loss per revolution and sustain enough energy acceptance throughout the whole ramping process. The required voltage is essentially determined by the longitudinal quantum lifetime. The longitudinal quantum lifetime as a function of the cavity voltage is shown in Figure 6.37. At extraction energy, a total RF voltage of more than 5.5 MV provides sufficient longitudinal quantum lifetime. At injection energy, the total RF voltage has to be larger than 1.8 MV to have enough energy acceptance to accommodate three successive bunches ($\sigma_\delta = 0.27\%$) from LINAC II.

Figure 6.37.: Longitudinal quantum lifetime vs. cavity voltage.

The RF modules are 500 MHz five-cell PETRA cavities. Four cavities supply a total of 6 MV voltage, with each of them providing a nominal voltage of 1.5 MV. An additional cavity will be added as a spare. The beam loading effect has not been considered yet.
Eddy Current Effect

Assuming a repetition rate of 2 Hz, one cycle duration is 500 ms. The changing magnetic fluxes induce eddy currents in the beam pipe, which lead to small deviations of the dipole and sextupole fields. The induced fields depend on the bending radii and gaps of the magnets as well as on the form factor and the material of the beam pipes. Time-wise, they are proportional to the ratio of the field change rate to the field itself, $\Delta B / B$ or $\Delta E / E$. The effects from other pulsed magnets are ignored. The sextupole components induced in the bending magnets and the chromaticity changes are shown in Figure 6.38a. To maintain the chromaticities at the initial level, the additional sextupoles need to oscillate with their phase shifted by $-\pi/2$ compared to the other magnets. The energy ramping curve and the required sextupole strengths scaled by the beam rigidity are shown in Figure 6.38b. The parameters used to calculate the eddy current effect are listed in Table 6.10.

<table>
<thead>
<tr>
<th>Table 6.10: Parameters used to estimate the eddy current effect.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Repetition rate</td>
</tr>
<tr>
<td>Injection energy</td>
</tr>
<tr>
<td>Extraction energy</td>
</tr>
<tr>
<td>Magnet half-gap</td>
</tr>
<tr>
<td>Beam pipe radius</td>
</tr>
<tr>
<td>Beam pipe thickness</td>
</tr>
<tr>
<td>Beam pipe resistivity</td>
</tr>
</tbody>
</table>
6.3. Technical Subsystems

6.3.1. Magnets

Magnets for the Achromats of PETRA IV
For the layout of the magnetic structure of the hybrid multibend achromat of PETRA IV, the ESRF-EBS achromat [6] was used as a guideline. As described in Section 6.1.1, an achromat length of 26.2 m was chosen, which is similar to the length of the ESRF-EBS achromat with 26.37 m. The layout of the achromat is shown in Figure 6.39. Due to the limited dynamic aperture, an on-axis swap-out injection is required for PETRA IV. This allows the use of magnets with small aperture radius, which greatly helps to reduce high pole tip fields and saturation in the yokes of the magnets. A value of 13 mm for the aperture radius was chosen for all the magnets in the achromat.

The parameters of the main magnets of the achromat of PETRA IV, according to the optics shown in Figure 6.2, are listed in Table 6.11. As a naming convention, we adopted the element names of the ESRF-EBS magnets. The total number of main magnets can be found in Table 6.15, the number of corrector magnets in Table 6.16. The magnets of the achromat are described in the following section.

Dipole Magnets
The magnets DQ1 and DQ2 in the central part of the achromat are combined-function (CF) magnets with a dipole and a quadrupole field component. A possible way to realise these magnets is using a half-quadrupole design. Using off-centred quadrupoles would require an offset of ≈7 mm of the quadrupole centre relative to the closed orbit. The magnets DL1 and DL2 are longitudinal-gradient dipole magnets consisting of five parts with equal length and different magnetic fields. The five pieces have magnetic fields between 0.34 T and 0.09 T for the DL1 dipole magnet and between 0.09 T and 0.27 T for the DL2 dipole magnet. Due to differences of the dispersion function in the longitudinal-gradient dipole magnets, the fields in the five pieces of the DL1 and DL2 magnets are different. At the ESRF-EBS, permanent magnets are used to achieve the longitudinal variation of the vertical magnetic field in the five segments [6].

While this is advantageous in terms of compactness and power saving, there is a potential risk of demagnetisation due to radiation damage. Such effects have been observed for some of the undulators of PETRA III. To avoid any such risk, an electromagnet will be used for the longitudinal dipoles of PETRA IV. Such magnets will also be used for APS-U [10].

Quadrupole Magnets
The quadrupole magnets QF1, QD2, QD3, QF4A/B and QD5 are medium-gradient magnets with gradients between 45 T/m and 64 T/m. The magnets QF6 and QF8 are high-gradient quadrupole magnets. The necessary gradients are $g = 87.9$ T/m and 92.4 T/m, respectively.

To reach such high gradients, especially for the QF6 and QF8 quadrupole magnets, is very challenging. Quadrupole magnets have been designed and built for the ESRF-EBS [58], APS-U [59] and HEPS [60], and gradients up to 100 T/m turned out to be achievable. To explore the technical limits for the field gradients, simulations have been carried out for different magnetic materials for PETRA IV, and a high-field quadrupole prototype has been built. The results are described later in this chapter.

Chromatic Sextupole Magnets
Three families of sextupole magnets are installed in the lattice (SD1A, SF2A and SD1B), which are used to set the linear chromaticities to a slightly positive value. SF2A is used to change mainly the horizontal chromaticity, while the families SD1A and SD1B change mainly the vertical chromaticity. The ratio of the sextupole strengths of SD1A and SD1B is used to optimise the amplitude-dependent tune shifts.

Sextupole gradients up to $g_s = B'/2 \approx 4300$ T/m$^2$ are required for a chromaticity correction of $+5/+5$ in both planes. The sextupole magnets of PETRA IV are a factor of ≈2 stronger than the sextupoles of the ESRF-EBS for a chromaticity corrected to a slightly positive value (cf. Section 6.1.1).
Harmonic Sextupole Magnets
The achromat contains four harmonic sextupoles. Two of them (SH1 and SH3) are installed in dispersion-free sections at the entrance and exit of the achromat near the ID straight and another two (SH2A/B) at the centre of the achromat, where the dispersion function is very small. The sextupoles SH2A and SH2B share the same power supply. It has been observed that, for a lattice without alignment and field errors, the harmonic sextupoles have only a weak influence on the non-linear properties of the lattice. Whether these sextupoles are really necessary, has to be decided later. This requires the simulation of the full correction of the optics, including errors.

Corrector Magnets
Because of the strong multipole magnets, a good orbit correction is necessary in the achromat. In total, 10 corrector magnets are foreseen for the two planes. In addition, skew quadrupole correctors are needed in the achromat for coupling and dispersion correction, and at least two fast corrector coils in both planes for the fast-orbit feedback to independently correct the beam position and the angle at the IDs.

Magnets for the Straight Sections of PETRA IV
For the eight straight sections LSS, SSS, LSSU and SSS, only quadrupole magnets and corrector magnets are needed. The number of main magnets is shown in Table 6.15, the number of corrector magnets in Table 6.16.

Quadrupole Magnets
The quadrupole magnets for the straight sections are low-gradient magnets with a gradient $g$ of typically 4 T/m to 8 T/m and a length of 0.5 m. The strongest quadrupoles are the two doublets up- and downstream of the location of the 10 m IDs. The maximum gradient of these quadrupoles is 26 T/m.

Corrector Magnets
In the eight straight sections, only orbit corrector magnets are foreseen. In the four straight sections with the 10 m IDs, some more correctors have to be installed for local steering of the beam inside the undulator. In addition, four fast correctors for the local stabilisation of the position and angle for each long ID are needed. Because of the great length of the long and short straight sections, problems due to limited space are not expected.
Investigation of Field Gradient Limits

For the PETRA IV hybrid multibend achromat with a cell length of 26.2 m, quadrupole gradients up to 100 T/m and sextupole gradients up to 4500 T/m² are necessary. Due to the limited space between the magnets, which is needed for coils, BPMs and vacuum components, increasing the length of the magnets is not an option.

A reduction of the aperture radius \( r \) of the magnets is very advantageous to reduce the pole tip field \( B_p \) of the magnets. The pole tip field of a multipole \( b_n \) scales with \( B_p \propto b_n r^{n-1} \).

The strength of higher-order multipoles can be effectively reduced by choosing a smaller aperture radius \( r \). However, this increases the sensitivity of the field harmonics to mechanical errors of the yoke (pole contour errors and assembly errors).

Using a different material for the yoke is also an option to increase the field gradient. For the PETRA IV lattice cell, different yoke materials were investigated to reach high magnetic field gradients in short quadrupole and sextupole magnets. This work was done by the Efremov Institute together with DESY. The technical parameters for the simulations of high-gradient magnets are given in Table 6.12.

For calculations of these magnets, grain-oriented, non-grain-oriented and developed steel (produced by ThyssenKrupp Steel) were used. Three aperture bore diameters were taken into account: 20 mm, 26 mm and 33 mm. The sextupole magnet calculations were only made with non-grain-oriented steel.

The results of the simulations are shown in Table 6.13. The sextupole magnet was also simulated with integrated correction coils, which generate the vertical and horizontal field and a gradient of a skew quadrupole corrector (these coils change the gradient of the sextupole magnet by up to 15%).
Table 6.11.: Parameters of the main magnets of the hybrid multibend achromat of PETRA IV. The parameters are the number of magnets $N$ in the achromat, the length $L$ in m, the bending radius $\rho$ in m, the focusing strength $k_i = 1/(B\rho) \cdot \partial^2 B_y/\partial x^2$ in $1/m^{i+1}$, the bending angle $\alpha$ in degrees, the field gradient $1/i \partial^2 B_y/\partial x^2$ in T/m, the half gap $h$ in mm, the bore radius $r$ in mm, the pole tip field $B_p$ in T, and the type of the magnet.

### Dipole Magnets

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<thead>
<tr>
<th>Name</th>
<th>$N$</th>
<th>$L$ / m</th>
<th>$1/\rho$ / m$^{-1}$</th>
<th>$\alpha$ / °</th>
<th>$h$ / mm</th>
<th>$B_p$ / T</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>DQ1</td>
<td>2</td>
<td>1.021</td>
<td>0.0143</td>
<td>0.837</td>
<td>13</td>
<td>0.29</td>
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<tr>
<td>DQ2</td>
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<td>0.795</td>
<td>0.0099</td>
<td>0.450</td>
<td>13</td>
<td>0.20</td>
<td>CF magnet</td>
</tr>
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<td>DL1</td>
<td>2</td>
<td>1.776</td>
<td>0.0089</td>
<td>0.908</td>
<td>13</td>
<td>0.34–0.09</td>
<td>Long. gradient</td>
</tr>
<tr>
<td>DL2</td>
<td>2</td>
<td>1.776</td>
<td>0.0083</td>
<td>0.843</td>
<td>13</td>
<td>0.09–0.27</td>
<td>Long. gradient</td>
</tr>
</tbody>
</table>

### Quadrupole Magnets

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<thead>
<tr>
<th>Name</th>
<th>$N$</th>
<th>$L$ / m</th>
<th>$k_1$ / m$^{-2}$</th>
<th>$B'$ / T m$^{-1}$</th>
<th>$r$ / mm</th>
<th>$B_p$ / T</th>
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<td>2</td>
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<td>0.59</td>
<td>Medium gradient</td>
</tr>
<tr>
<td>QF4A</td>
<td>2</td>
<td>0.211</td>
<td>+2.62</td>
<td>+52.5</td>
<td>13</td>
<td>0.68</td>
<td>Medium gradient</td>
</tr>
<tr>
<td>QF4B</td>
<td>2</td>
<td>0.211</td>
<td>+2.62</td>
<td>+52.5</td>
<td>13</td>
<td>0.68</td>
<td>Medium gradient</td>
</tr>
<tr>
<td>QD5</td>
<td>2</td>
<td>0.211</td>
<td>-2.97</td>
<td>-59.4</td>
<td>13</td>
<td>0.77</td>
<td>Medium gradient</td>
</tr>
<tr>
<td>QF6</td>
<td>2</td>
<td>0.385</td>
<td>+4.62</td>
<td>+92.4</td>
<td>13</td>
<td>1.20</td>
<td>High gradient</td>
</tr>
<tr>
<td>QF8</td>
<td>2</td>
<td>0.481</td>
<td>+4.39</td>
<td>+87.9</td>
<td>13</td>
<td>1.14</td>
<td>High gradient</td>
</tr>
<tr>
<td>DQ1</td>
<td>2</td>
<td>1.021</td>
<td>-1.92</td>
<td>-38.4</td>
<td>13</td>
<td>variable</td>
<td>CF magnet</td>
</tr>
<tr>
<td>DQ2</td>
<td>1</td>
<td>0.795</td>
<td>-1.37</td>
<td>-27.4</td>
<td>13</td>
<td>variable</td>
<td>CF magnet</td>
</tr>
</tbody>
</table>

### Sextupole Magnets

<table>
<thead>
<tr>
<th>Name</th>
<th>$N$</th>
<th>$L$ / m</th>
<th>$k_2$ / m$^{-3}$</th>
<th>$\frac{1}{2}B''$ / T m$^{-2}$</th>
<th>$r$ / mm</th>
<th>$B_p$ / T</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>SD1A</td>
<td>2</td>
<td>0.165</td>
<td>-427</td>
<td>-4277</td>
<td>13</td>
<td>0.72</td>
<td>Chrom. Sextupole</td>
</tr>
<tr>
<td>SF2A</td>
<td>2</td>
<td>0.199</td>
<td>+379</td>
<td>3790</td>
<td>13</td>
<td>0.64</td>
<td>Chrom. Sextupole</td>
</tr>
<tr>
<td>SD1B</td>
<td>2</td>
<td>0.165</td>
<td>-368</td>
<td>-3680</td>
<td>13</td>
<td>0.62</td>
<td>Chrom. Sextupole</td>
</tr>
<tr>
<td>SH1</td>
<td>1</td>
<td>0.099</td>
<td>tbd</td>
<td>tbd</td>
<td>13</td>
<td>tbd</td>
<td>Harm. Sextupole</td>
</tr>
<tr>
<td>SH2</td>
<td>1</td>
<td>0.099</td>
<td>tbd</td>
<td>tbd</td>
<td>13</td>
<td>tbd</td>
<td>Harm. Sextupole</td>
</tr>
<tr>
<td>SH3</td>
<td>1</td>
<td>0.099</td>
<td>tbd</td>
<td>tbd</td>
<td>13</td>
<td>tbd</td>
<td>Harm. Sextupole</td>
</tr>
</tbody>
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### Octupole Magnets

<table>
<thead>
<tr>
<th>Name</th>
<th>$N$</th>
<th>$L$ / m</th>
<th>$k_3$ / m$^{-4}$</th>
<th>$\frac{1}{6}B'''$ / T m$^{-3}$</th>
<th>$r$ / mm</th>
<th>$B_p$ / T</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>OF1</td>
<td>2</td>
<td>0.089</td>
<td>-85 230</td>
<td>-284 297</td>
<td>13</td>
<td>0.62</td>
<td>Octupole</td>
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</table>
Table 6.12.: Technical parameters for the simulations of high-gradient magnets.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Quadrupole</th>
<th>Sextupole</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aperture diameter $d$ / mm</td>
<td>20</td>
<td>26</td>
</tr>
<tr>
<td>Yoke length $L$ / m</td>
<td>0.2</td>
<td>0.1</td>
</tr>
<tr>
<td>Gradient $g$ in T/m and $g_s$ in T/m$^2$</td>
<td>120–160</td>
<td>4500</td>
</tr>
<tr>
<td>Good field region (GFR) / mm</td>
<td>6</td>
<td>8</td>
</tr>
<tr>
<td>Field quality at GFR</td>
<td>$5 \times 10^{-4}$</td>
<td>$1 \times 10^{-3}$</td>
</tr>
<tr>
<td>Nominal current $I$ / A</td>
<td>to be defined in the course of the design</td>
<td></td>
</tr>
<tr>
<td>Nominal voltage $U$ / V</td>
<td>$\leq 250$</td>
<td>$\leq 250$</td>
</tr>
<tr>
<td>Pressure of cooling water $p$ / bar</td>
<td>$\leq 10$</td>
<td>$\leq 10$</td>
</tr>
<tr>
<td>Max. pressure of cooling water $p_{\text{max}}$ / bar</td>
<td>15</td>
<td>15</td>
</tr>
</tbody>
</table>

Table 6.13.: Dependence of the maximum value of the quadrupole gradient $g$ and the sextupole gradient $g_s$ on the yoke material and the aperture diameter $d$.

<table>
<thead>
<tr>
<th>Iron material</th>
<th>$d$ / mm</th>
<th>$g$ / T m$^{-1}$</th>
<th>$g_s$ / T m$^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grain-oriented steel</td>
<td>33</td>
<td>76.6</td>
<td></td>
</tr>
<tr>
<td></td>
<td>26</td>
<td>97.2</td>
<td></td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>126.4</td>
<td></td>
</tr>
<tr>
<td>Non-grain-oriented steel</td>
<td>33</td>
<td>84.6</td>
<td>3365</td>
</tr>
<tr>
<td></td>
<td>26</td>
<td>107.3</td>
<td>4600</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>139.5</td>
<td>9379</td>
</tr>
<tr>
<td>Developed steel</td>
<td>33</td>
<td>81.0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>26</td>
<td>102.8</td>
<td></td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>133.6</td>
<td></td>
</tr>
</tbody>
</table>

Results
Following the high-gradient calculations, a prototype quadrupole magnet with an aperture diameter of 20 mm and a yoke length of 200 mm was built from non-grain-oriented steel (Figure 6.40). Magnetic measurements with a Hall sensor were carried out for this prototype. The excitation curve is shown in Figure 6.43. The gradient value at the onset of iron saturation is 120 T/m.

For a larger aperture diameter of 26 mm, saturation starts at a lower gradient. For the proposed high-gradient quadrupole magnets QF6 and QF8 (cf. Table 6.11), this is just sufficient. Nevertheless, using different materials for the yoke pole allows the quadrupole saturation to be increased to a slightly higher value. This has been proposed for some of the magnets of the APS-U and the ALS-U upgrade.

Figure 6.43.: Measured excitation curve of the prototype quadrupole with an aperture diameter of 20 mm.

Due to the good agreement between calculations and measurements, we only continued with calculations for the sextupole magnet. The calculated excitation curve of the sex-
tupole with an aperture diameter of 26 mm is shown in Figure 6.44. It confirms that a gradient up to 4000 T/m is below the saturated region. This sextupole magnet design could be used for the SD1A magnet (cf. Table 6.11). Saturation of such a sextupole magnet would start above 60 A and reach nearly 30 % for a current of 100 A. Using cobalt–iron alloys such as Vacoflux 50 or Vacoflux 27 (produced by VAC Vacuumschmelze) for the yoke pole allows for a reduction of the saturation effect by up to 7 %. However, these materials are very expensive.

Magnetic Measurements
Several different measurement techniques will be used to ensure the magnet quality and to align the magnets. The former will be done with Hall sensors to map the field of the longitudinal-gradient dipoles and with a conventional rotating-coil setup to measure the field quality of the different magnet types. These techniques are well established at DESY.

In the past years, new magnetic measurements systems were developed to meet the alignment requirements of fourth-generation light sources [61, 62]. A vibrating-wire test bench is under construction at DESY. This technique is well suited to measure the magnetic axis of magnets with $n > 2$. However, it is very challenging to determine the wire position. We are developing a new indirect measurement technique to reduce this error by several micrometres. To align the combined-function dipole–quadrupole magnets, APS developed a loop wire measurement technique, which will be adapted.

Magnets for the Booster Synchrotron DESY IV
For the design of the booster synchrotron DESY IV, a compact lattice with combined-function magnets was chosen. Details of the lattice design can be found in Section 6.2.2. Due to the shape of the pole face of these magnets, a vertical field with a combined dipole, quadrupole and sextupole field is produced. Similar designs for booster synchrotron magnets have been used in the past for other booster synchrotrons, e.g. SLS and NSLS II. However, at 6 GeV, the extraction energy of the booster DESY IV is a factor of two higher than that of the NSLS II booster, and higher field gradients especially of the multipoles are needed. The necessary fields of the different multipoles of the BF and BD magnets are given in Table 6.9.

Figure 6.44: Simulated excitation curve of the sextupole with an aperture diameter of 26 mm. By courtesy of the Efremov Institute, St. Petersburg, Russia.

Preliminary magnetic-field calculations using a 2D model in OPERA were performed by the Efremov Institute to investigate whether such a magnet design is feasible for the booster DESY IV. Parameters similar to the values of Table 6.9 were used for the calculations. For the shape of these magnets, an H-type profile instead of a C-type profile was chosen to reduce the saturation in the yoke and achieve a better mechanical stability. The cross section of the magnets is shown in Figure 6.45 together with lines of constant magnetic field $|B|$. In this calculation, it was assumed that a full gap height of 30 mm is necessary at the horizontal position of the design orbit for the vacuum chamber.

By using pole face curves similar to the ones described in Section 6.2.2, the desired multipole components of the field can be achieved at the extraction energy of 6 GeV for the BF and BD magnets. The distribution of the vertical component of the magnetic field is shown in Figure 6.46. The design orbit of the BF and BD magnets would be at 0 mm. Due to the fixed shape of the pole face, the multipoles can only be optimised for one energy. Further investigations are needed to compute multipole coefficients at an injection energy of 700 MeV.
To reduce eddy currents in the magnets, they have to be produced from steel laminations. In addition, 24 quadrupole and 24 sextupole magnets (each of them grouped in two families) are needed to compensate for tune and chromaticity changes due to eddy currents induced in the vacuum chamber. To correct tune and chromaticity during the fast ramping between the injection energy of 700 MeV and the extraction energy of 6 GeV, they have to be ramped. Although the quadrupole magnets have relative large gradients, they lie within the technical limits. The additional sextupole magnets are relatively weak.

6.3.2. Alignment

Various effects determine the accuracy of the alignment of accelerator components. The most important factors are instrument accuracy, arrangement of the reference point grid inside the accelerator tunnel, temperature gradient during surveys, accuracy and conditions of the fiducialisation measurements, and arrangement (placement) and geometry of the survey instruments during the survey tasks. The survey tasks range from network measurement, network adjustment and alignment of components in the tunnel to alignment of components on girders, fiducialisation measurements of single components, precise determination of the magnetic axis of the magnets and simultaneous fiducialisation measurements with respect to the magnetic axis.

PETRA III Experience

For the setup of PETRA III, the accuracy demands were 50 µm magnet-to-magnet, 100 µm girder-to-girder and an overall placement accuracy of the components of 300 µm along any 100 m long section of the accelerator. These accuracy demands were only met with the help to the following setup: an equispaced reference point grid with rings of seven reference points on the floor, wall and ceiling every 10 m; survey instruments with a maximum permissible error (MPE) of ±15 µm + 6 µm/m; fine adjustment of components on the girder with two simultaneously measuring laser trackers (one on each side of the girder), precisely stationed by means of a dense reference point grid in a climatic room with a temperature stability of 1.0 K; and fiducialisation measurements of every single component in a climatic room with
a temperature stability of 1.0 K. Quadrupoles were referenced directly to the magnetic axis. The temperature within each climatic room was adapted to the design data of the accelerator tunnel. Each component had to be acclimatized to the room temperature for 48 hours prior to the fiducialisation measurements and to the alignment on the girder. Each component on the girder was rigidly fixed to the girder with epoxy glue after final precise alignment. Each girder was placed in the tunnel directly after assembly in the climatic room. Table 6.14 gives an overview of the accuracies (standard deviation) reached for PETRA III.

### Alignment Concept

The demands on magnet alignment for the operation of PETRA IV are given in Section 6.1.2 as rms values (1σ) of 30 µm for the transverse magnet offsets Δx and Δy and of 200 µrad for the roll angle Δϕ for selected and/or the most delicate magnets.

The alignment precision achieved at PETRA III nearly reaches the range of the PETRA IV demands, cf. [63]. Simulating the measurement procedure showed that an enhancement of the magnet alignment on the girders can be achieved by changing the geometry of the survey instrument stands and doubling the number of simultaneously employed instruments. This simulated setup achieves an accuracy that corresponds to the one mentioned in [31]. The overall alignment accuracy of the girders produced for installation will then be about 20 µm rms for the transverse magnet-to-magnet offsets Δx and Δy (compared to 30 µm for PETRA III) and better than 100 µrad for Δϕ when leaving the production lab. In addition, the simultaneous application of different measurement methods for magnetic axis determination in direct combination with the alignment of all the magnets on the girder is conceivable and will be investigated.

Several activities and factors, including transport, disassembly of magnets for vacuum chamber installation, bake-out of the vacuum chambers, mechanical tunnel stability, stability of tunnel temperature control etc., contribute to the final alignment accuracy of the components installed in the tunnel. These factors can contribute additional risk that needs to be addressed. Survey and alignment are essential during all steps of the storage ring assembly and installation. Several approaches for enhancing the precision of the installation should be explored during the future technical design work, such as using additional survey methods on short sections in addition to laser trackers and making the reference point grid in the accelerator tunnel denser in order to achieve
6.3.3. Buildings for the Accelerator

The buildings for the PETRA III accelerator originate from different construction periods. Many sections of the storage ring are still located in the original tunnel sections from 1976, which were built in open cut construction with a 30 cm thick foundation. During the conversion of the storage ring into a synchrotron light source, the Max von Laue hall was constructed from 2007 to 2009. In 2014, two extension halls, the Paul P. Ewald and Ada Yonath halls, were built to house ten additional beamlines. An aerial view of the DESY site with the existing PETRA III experimental halls is shown in Figure 6.47. The new hall for PETRA IV in the west of the DESY site is also indicated, as well as a new building for the RF systems.

The thick blue line marks the original tunnel sections from 1976.

Figure 6.48a shows a cross section of the original accelerator tunnel. The accelerator tunnel in the Max von Laue hall was built from concrete blocks (cf. Figure 6.48b). The layout of the tunnel in the more recent Paul P. Ewald and Ada Yonath halls is similar to the tunnel in the Max von Laue hall, but the walls were constructed as a cast concrete structure rather than from concrete blocks. The new experimental hall for PETRA IV will differ in several aspects from the Max von Laue hall, as several parts will not be located above ground. However, the accelerator tunnel in the new hall will also be built from concrete blocks in a similar way to the tunnel in the Max von Laue hall.

6.3.4. Tunnel Stabilisation

Ultra-precise positioning is only possible in temperature-controlled environments. A certain complication is presented by the existing PETRA tunnel infrastructure. About half of the PETRA IV accelerator will be placed in the tunnel segments inherited from the original
PETRA collider. In the existing tunnel, temperature changes of 12 K between shutdown and user operation lead to movements at joints between different segments of the tunnel. Gradients of this local movements are on the order of 50 µm/K in the transverse directions and 300 µm/K in the longitudinal direction. In addition, movements of the different tunnel segments are caused by settlements and changes within a seasonal cycle. Figure 6.49 shows the air temperature in the PETRA III tunnel and the relative movement between the Paul P. Ewald experimental hall and the tunnel. Data are displayed over one year.

For PETRA IV, it is foreseen to heat the tunnel during breaks in beam operation. The goal is to stabilise the tunnel temperature to 1 K and thereby limit the movement of the tunnel segments to a tolerable rate. In the parts of the old tunnel that will be used for PETRA IV, a massive concrete ring girder will be installed in pieces of up to 350 m length. This ring girder will be mechanically decoupled from the old tunnel and will thus balance out the local movements of the tunnel segments. The ring girder will consist of six pieces, which will not be connected to each other or to the base plates of the experimental halls. Ten of the 12 gaps between the pieces of the girders and the experimental floors will be in straight sections of the ring. Here, in a relaxed magnet lattice, orbit correction magnets can be installed near the gaps. Measurements of the relative girder movements are shown in Figure 6.50.

**Figure 6.49.:** *Air temperature in the PETRA III tunnel and relative tunnel movement vs. time in days between the Paul P. Ewald experimental hall (PXN) and the tunnel during the seasonal cycle.*

**Figure 6.50.:** *Air temperature in the PETRA III tunnel and relative tunnel movement vs. time in days between the Paul P. Ewald (PXN) and Ada Yonath (PXE) halls and the tunnel during the start-up of PETRA III in March 2019.*
movement at the gaps can be used as input for a local slow orbit feedback, which can be improved by using BPM data. This feedback will run through breaks in beam operation and ensure a good injection orbit after the break. Figure 6.50 shows the air temperature in the tunnel vs. vertical movements between the Paul P. Ewald and Ada Yonath halls and the adjacent tunnel segments during the start-up of PETRA III in March 2019. All mechanical movements are slower than 10 µm per day and therefore well within the reach of a slow orbit feedback.

6.3.5. Magnet Supports

The magnets supports (girders) are essential for efficient pre-assembly, for precise alignment, and for reducing the coupling of ground motion to the magnets. The design of the PETRA IV girders will be based on the PETRA III design (cf. Figure 6.51) with some possible improvements, which will be described later in this section. The influence of relative magnet-to-magnet alignment errors (cf. Table 6.3 and Table 6.14) is most noticeable on distances shorter than the betatron wavelength. Therefore, in the preliminary design, the neighboring high-gradient quadrupole and sextupole magnets are mounted on the same girder. This results in one girder of about 6 m length, two of about 3 m length and two of about 1 m length inside the 26.2 m long cell (cf. Figure 6.52). Alignment of dipoles located between girders is not critical, and they can be placed on separate supports. Other configurations that might prove more beneficial from a logistics perspective, such as having one type of girder for all components, will also be investigated in the technical design phase.

The PETRA IV site is located in the western part of the city of Hamburg, with two main roads close by. The integrated ground vibration level (cf. Figure 6.53) is about 80 nm at noon and about 40 nm at midnight. These values are larger than at quiet sites such as SPring-8 (Harima, Japan) or APS (Argonne, USA) and smaller than at ESRF (Grenoble, France), BNL (Upton, USA) or SSRF (Shanghai, China) (cf. Figure 6.54) [65]. Fast orbit feedback will be implemented for electron beam stabilisation, as discussed in Section 6.1.2. In addition to this, ground motion amplification is to be avoided, and the target value for the first eigenfrequency of support structures for machine components is of at least 50 Hz or more.

Figure 6.53.: Vertical power spectral density measured in the Paul P. Ewald hall (PXN), which is closest to the road “Luruper Chaussee”, on November 14th, 2016. Ground motion at frequencies below 1 Hz is coherent at the length scales of interest.
To address the eigenfrequency issue, novel magnet supports are being developed in collaboration with the Alfred Wegener Institute, Helmholtz Centre for Polar and Marine Research (Bremerhaven, Germany). The goal is to design stiff girders that exhibit high eigenfrequencies. To this end, structural optimisation combining biologically inspired structures and optimisation techniques is being performed. Moreover, topology optimisation is carried out to determine the optimal material distribution in order to reach high eigenfrequencies, a high stiffness and a low mass.

The studies have produced first promising results (cf. Figure 6.55 and Figure 6.56), achieving first eigenfrequencies up to 120% higher than the reference (PETRA III) gider, depending on the strategy (cf. Figure 6.57) [66]. A critical point yet to be addressed for this novel design is the integration of the adjustment units, which may significantly reduce the overall eigenfrequency and the stiffness. Fabrication of first prototypes is expected soon.

### 6.3.6. Power Supplies and Utilities

DESY has a long experience in building highly reliable power supplies for large facilities, such as HERA, PETRA III and the European XFEL. For PETRA IV, new challenges arise due to the great number of magnets. PETRA IV contains 64 achromats and eight straight sections. The numbers add up to 2562 main magnets and nearly 700 corrector magnets. The values of current, voltage and power can be handled very well. However, due to the large number of power supplies, the system has to be extremely reliable. To decrease investment cost and increase reliability, as many magnets as possible will be combined into series circuits.
Table 6.15.: Number of magnets $N_{mag}$ and number of power supplies $N_{PS}$ for the main magnets.

<table>
<thead>
<tr>
<th>Location</th>
<th>Magnet type</th>
<th>$N_{mag}$</th>
<th>$N_{PS}$</th>
<th>Factor</th>
<th>$N_{mag\ total}$</th>
<th>$N_{PS\ total}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Achromat</td>
<td>Longitudinal-gradient dipole</td>
<td>4</td>
<td>2</td>
<td>64</td>
<td>256</td>
<td>128</td>
</tr>
<tr>
<td>Achromat</td>
<td>Dipole/quadrupole</td>
<td>3</td>
<td>1</td>
<td>64</td>
<td>192</td>
<td>64</td>
</tr>
<tr>
<td>Achromat</td>
<td>Quadrupole (medium-gradient)</td>
<td>12</td>
<td>12</td>
<td>64</td>
<td>768</td>
<td>768</td>
</tr>
<tr>
<td>Achromat</td>
<td>Quadrupole (high-gradient)</td>
<td>4</td>
<td>4</td>
<td>64</td>
<td>256</td>
<td>256</td>
</tr>
<tr>
<td>Achromat</td>
<td>Chromatic sextupole</td>
<td>6</td>
<td>6</td>
<td>64</td>
<td>384</td>
<td>384</td>
</tr>
<tr>
<td>Achromat</td>
<td>Harmonic sextupole</td>
<td>4</td>
<td>3</td>
<td>64</td>
<td>256</td>
<td>192</td>
</tr>
<tr>
<td>Achromat</td>
<td>Octupole</td>
<td>2</td>
<td>1</td>
<td>64</td>
<td>128</td>
<td>64</td>
</tr>
<tr>
<td>Achromat</td>
<td>Skew quadrupole</td>
<td>4</td>
<td>4</td>
<td>64</td>
<td>256</td>
<td>256</td>
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<tr>
<td>SSS</td>
<td>Quadrupole</td>
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<td>6</td>
<td>2</td>
<td>22</td>
<td>12</td>
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<td>LSS</td>
<td>Quadrupole</td>
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<td>10</td>
</tr>
<tr>
<td>SSSU</td>
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<td>14</td>
<td>2</td>
<td>28</td>
<td>28</td>
</tr>
<tr>
<td>LSSU</td>
<td>Quadrupole</td>
<td>20</td>
<td>13</td>
<td>2</td>
<td>40</td>
<td>26</td>
</tr>
<tr>
<td>SSS</td>
<td>Skew quadrupole</td>
<td>4</td>
<td>4</td>
<td>2</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>LSS</td>
<td>Skew quadrupole</td>
<td>4</td>
<td>4</td>
<td>2</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>SSSU</td>
<td>Skew quadrupole</td>
<td>4</td>
<td>4</td>
<td>2</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>LSSU</td>
<td>Skew quadrupole</td>
<td>4</td>
<td>4</td>
<td>2</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
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<td></td>
<td></td>
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<td>2220</td>
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</tbody>
</table>

On the other hand, single power supplies are necessary to ensure the flexibility to cope with unavoidable field and alignment errors. For the arc sections, a design was chosen that supports the use of serial connection as much as possible. Using the same layout for all 64 achromats and taking advantage of the mirror symmetry of the cell gives the possibility to reduce the number of power supplies. The list of main magnets in the achromat can be found in Section 6.3.1. Since the magnets are still being investigated, final values are not fixed. In accordance with [6] and internal discussions with magnet designers, it was agreed that the nominal currents of the major part of the magnet types will be kept below 100 A. For dipoles and combined-function magnets, the current is assumed to be below 200 A. With max. inner resistances of 100 mΩ to 200 mΩ, the power per magnet can be kept well below 2 kW. For the corrector magnets, the final specification is less important. The corrector power supplies of PETRA III provide a wide range of current and voltage that should be sufficient to cope with future demands.

Number of Power Supplies
The numbers of magnets and power supplies needed for the main magnets and for the orbit corrector magnets are listed in Table 6.15 and Table 6.16. The tables include the number of components for the eight arcs and the straight sections SSS, LSS, SSSU and LSSU. An achromat comprises seven dipole magnets. By making use of the symmetry and powering equal magnets in series, the number of required power supplies can be reduced to three. The five steps of the magnetic field of the four longitudinal-gradient dipole magnets can be realised by means of a special coil design powered by one power supply. In the central part of the achromat, three power supplies are required for the combined-function magnets. In total, an achromat includes 19 quadrupole magnets. The three combined-function magnets in the central part need no additional power supply due to the interdependence of the dipole and quadrupole fields. The split quadrupoles QF4A/QF4B in the two dispersion bumps can both be connected in series because of the small phase advance. Altogether, 14 power supplies for quadrupoles are needed per achromat.
Table 6.16.: Number of magnets $N_{mag}$ and number of power supplies $N_{PS}$ for the orbit corrector magnets.

<table>
<thead>
<tr>
<th>Location</th>
<th>Magnet type</th>
<th>$N_{mag}$</th>
<th>$N_{PS}$</th>
<th>Factor</th>
<th>$N_{mag}$ total</th>
<th>$N_{PS}$ total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Achromat</td>
<td>Hor. corrector magnet</td>
<td>5</td>
<td>5</td>
<td>64</td>
<td>320</td>
<td>320</td>
</tr>
<tr>
<td>Achromat</td>
<td>Ver. corrector magnet</td>
<td>4</td>
<td>4</td>
<td>64</td>
<td>256</td>
<td>256</td>
</tr>
<tr>
<td>SSS</td>
<td>Hor. corrector magnet</td>
<td>4</td>
<td>4</td>
<td>2</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>SSS</td>
<td>Ver. corrector magnet</td>
<td>3</td>
<td>3</td>
<td>2</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>LSS</td>
<td>Hor. corrector magnet</td>
<td>7</td>
<td>7</td>
<td>2</td>
<td>14</td>
<td>14</td>
</tr>
<tr>
<td>LSS</td>
<td>Ver. corrector magnet</td>
<td>6</td>
<td>6</td>
<td>2</td>
<td>12</td>
<td>12</td>
</tr>
<tr>
<td>SSSU</td>
<td>Hor. corrector magnet</td>
<td>4</td>
<td>4</td>
<td>2</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>SSSU</td>
<td>Ver. corrector magnet</td>
<td>4</td>
<td>4</td>
<td>2</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>LSSU</td>
<td>Hor. corrector magnet</td>
<td>7</td>
<td>7</td>
<td>2</td>
<td>14</td>
<td>14</td>
</tr>
<tr>
<td>LSSU</td>
<td>Ver. corrector magnet</td>
<td>6</td>
<td>6</td>
<td>2</td>
<td>12</td>
<td>12</td>
</tr>
<tr>
<td>Sum</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>658</td>
<td>658</td>
</tr>
</tbody>
</table>

Due to the need for optic corrections, a further reduction of the number of quadrupole power supplies by making use of the mirror symmetry is not advisable. In addition, beam-based alignment (BBA) has to be possible. Current changes of the quadrupole near the BPM are necessary to determine the BPM offset relative to the magnetic axis of this quadrupole. As an alternative, the possibility to do BBA could also be realised with an additional power supply, which can be connected to the magnet near the BPM. Both methods are currently used at PETRA III.

An achromat has six chromatic sextupole magnets: four harmonic sextupole magnets and two octupole magnets. For the chromatic sextupoles and the octupoles, the symmetry of the achromat can be used to reduce the number of power supplies by a factor of two. Whether harmonic sextupoles are actually necessary has to be decided later. Optimisation of the dynamic aperture using these magnets for the bare lattice had only a small effect until now, but could be important if magnet and alignment errors break the symmetry of the achromats and have to be corrected.

The straight sections of PETRA IV have two different lengths and two different designs, as discussed in Section 6.1.1. Beside quadrupoles and orbit corrector magnets, some skew quadrupoles are foreseen in the straight sections.

Design of the Power Supplies
The DESY philosophy is to buy most of the necessary components, when available, from industry. Only the components that require special expert knowledge are designed by DESY, including the control electronics as accuracy-defining component and all components that are safety elements. DESY staff will be responsible for the installation of the power supplies to guarantee a high-level quality. The system integration and the responsibility for the system performance are therefore in the hands of DESY.

Specification
The power supply specifications are:

- **Resolution**: 20 bit
- **Accuracy**: $10^{-4}$ long-term, $10^{-5}$ short-term (24 h)
- **Linearity**: 10 ppm
- **Repeatability**: 10 ppm short-term
- **Power parts**: Switched-mode power supplies, high switching frequency for small ripple
- **EMI**: According to standards

The power supplies have to be remote controlled i.e. via Ethernet. This includes remote analysis, commissioning of large number of power supplies and scanning of parameters over all power supplies including fast Fourier transform. In case of system failure the alarm message system has to be able to send emails and SMS to reach all experts and the alarm system has to be remote controlled as well.
Main Magnet Power Supplies
The power supply topology for the main magnets will be built according to the standard DESY design. A diode rectifier converts the 400 V AC to the required voltage of the DC link in the range of 48 V to 60 V. Depending on the nominal power, the converter will be either in 6-pulse or 12-pulse topology.

Figure 6.58.: Schematic of the power supply topology.

DC/DC converters in buck converter topology will deliver the required voltage level at the magnets. The fully digital control electronics will be developed by DESY. High-accuracy direct-current current transformers (DCCTs) are available from industry. Figure 6.58 shows a schematic of the used topology, Figure 6.59 a view of the power supply assembly. A further size reduction might be possible and is the goal of further R&D.

Corrector Power Supplies
DC correctors:
As design baseline, the corrector power supply can be built in the technology of the PETRA III correctors. Although the final values are not fixed yet, currents up to 10 A and voltages up to 60 V can readily be built. The power part is internally redundant. As a possibility for further price reductions, a solution with different power parts in the same crates will be investigated.

DC and AC correctors:
Due to the limited space in the cell, it might be necessary to combine the DC and AC corrector function in one power supply. The DC component of the current will be in charge of the slow orbit feedback. For the fast orbit feedback, an AC part with a frequency up to 1 kHz is required. These frequencies can be generated by the semiconductor and controller. However, the overall design of the supplies including filters still has to be drawn up. To suppress subharmonics caused by interferences, the switching frequencies of all power supplies have to be synchronised. This demands an adequate timing system available around the PETRA IV ring.

Location of the Power Supplies
The power supplies will be distributed around the accelerator ring, mainly in the existing PETRA halls. Because of the high number of supplies, they will have a large footprint. In general, sufficient space is available in the halls, but further planning is required in close coordination with the other groups involved. It might be possible that additional levels have to be constructed inside the halls. This has been done before, e.g. in the Max von Laue hall, to achieve more installation space. For the new PETRA IV experimental hall, a concept for the location of the technical infrastructure is necessary. The existing Max von Laue hall is situated above ground. Air conditioning and power supplies are located on the inner side of the ring at ground level. Since the new hall will be situated well below ground, constructing a large underground surface for the infrastructure will be quite costly, and an additional building might be more cost-efficient.
Cabling
The cabling between the power supplies and the magnets involves several optimisation aspects. A cost optimum has to be found taking into account the price, efficiency and sustainability of the power supply system. In addition, the cabling has a large impact on the power losses inside the tunnel. The effects of power distribution and losses on the temperature stability have to be investigated. Different solutions such as cable routing outside the tunnel are possible and have to be investigated more deeply.

Utilities
AC distribution
For PETRA III, a new 10 kV ring with distributed substations was built in 2006 to supply power to the PETRA halls. This ring will also be used for PETRA IV. However, the structure of the main distributions (switchboards) does not fit the new local demands of the power supplies. A new main distribution will have to be installed near the locations of the power supplies.

Air conditioning
Although the power supplies do not have high demands for temperature stability, air conditioning units will be installed in the power supply halls to absorb the heat losses and keep the temperature in the room at a level of ±3 K.

Water cooling
The power electronics of the power supply will be water-cooled. In this way, the supplies can be built more compact, allowing for a higher density of the installation. The cooling-water temperature will correspond to the nominal temperature of the water-cooling system. For PETRA III, this was 30 °C. For PETRA IV, the optimal temperature of the plant has yet to be determined. The temperature difference between inlet and outlet temperature of the deionised water will be around 10 K.

Reliability/hot swap
The existing PETRA III power supplies are a good source for failure analysis. The 600 power supplies have a mean time between failures (MTB) of 280 h on average over the last four years. For a single power supply, this corresponds to app. 165 000 h. Applying these numbers to PETRA IV, a power supply failure every 43 h has to be assumed. Since the MTBF of a single PETRA III power supply corresponds to the high level at other accelerators all over the world, no significant increase in the MTBF of the power supplies can be expected and another solution, the “hot swap system”, has to be introduced.

The hot swap system consists of a spare power supply for a group of power supplies, freewheeling/reverse blocking devices and a semiconductor switch matrix, as shown in Figure 6.60. In case of a power supply one trip, the load will be disconnected from the tripped supply and reconnected to the spare waiting in stand-by. This supply will continue to feed the current of the magnet without or with only very small delays. This switching action has to be performed so quickly that the beam will stay in the accelerator.

![Figure 6.60: Overview of the hot swap system.](image)

Alternative Solution for Power Supply and Magnet System
The above-mentioned solution with a single power supply for each magnet or for a group of magnets has the advantage that it has a very simple and forward design. The disadvantages are the cost of the power parts, cabling and permanent losses due to the high current. Therefore, a second option, called the “add-on coil” design, will be mentioned here and investigated further.

In this design, the magnets will be fitted with additional “add-on” windings to enhance the magnetic field. This topology is similar to the corrector coils added on magnets, e.g. back-leg windings in the existing PETRA III dipoles or the corrector coils on sextupole magnets. The difference is that the add-on coils have no
steering function, but will increase the main field of the magnet. This will allow a further grouping of magnets into series connection. Only a small number of large power supplies will then be necessary. Corrector-magnet-type power supplies (CMPS) will be installed to feed the add-on coils. The schematic is shown in Figure 6.61.

The advantages are:

- The CMPS have a much lower price.
- The MTBF of the CMPS is much better than the MTBF of large power supplies.
- The hot swap components can be chosen smaller.
- The cable cross sections can be significantly smaller.
- The losses in the tunnel are much lower.

The disadvantages are:

- The magnets have to be designed with the additional windings.
- There is a possibility of crosstalk of the power supplies due to the transformer behaviour of the magnets with additional coils.
- The controls of the power supplies get more complicated due to the crosstalk.

**Power Supplies for the Pre-Accelerators**

The power supplies for LINAC II and for the transport beamlines including cabling and infrastructure will have to be replaced. Due to their function as pure DC power supplies, no special problems are assumed. For DESY IV, a ramping design is foreseen.

Although the current DESY II accelerator is driven with a White circuit in resonant mode, no problems for the power supply are assumed. Since DESY III served as a pre-accelerator for the former HERA proton ring, knowledge of this technology exists at DESY.

### 6.3.7. Vacuum System

The vacuum system for PETRA IV has a wholly different set of challenges compared to the one in use for PETRA III [1]. A significantly tighter longitudinal spacing of magnets and diagnostics combined with small apertures limited by the magnetic elements necessitate new design approaches. Other diffraction-limited storage ring projects have been facing similar issues, which have already led to a wide range of developments [68].

A summary of various vacuum system design parameters for PETRA IV is given in Table 6.17. As a key parameter for the evaluation of pressure profiles, the vacuum-related beam lifetime is currently expected to be $\geq 10\ h$, which is higher than for other limiting effects (cf. Section 6.1.3).

**Vacuum System Simulations: Vacuum Lifetime, Pressure Profiles and Synchrotron Radiation Load**

In total, the vacuum-related beam lifetime $\tau_v$ is estimated by

$$
\tau_v(p) = \left( \sum_i h_i \cdot \left( \frac{1}{\tau_{B,i}(p)} + \frac{1}{\tau_{el,i}(p)} \right) \right)^{-1}
$$

(6.13)

where each gas and atomic component with a relative quantity $h$ contributes individually via bremsstrahlung ($\tau_B$) and elastic scattering ($\tau_{el}$). By numerically inverting Eq. (6.13), the average pressure can be estimated cf. (Table 6.18).

Pressure calculations that consider simple, round chamber profiles and activated non-evaporable getter (NEG [69]) coating show that $10^{-8}$ mbar can be quickly achieved even
Table 6.17.: Design parameters for the PETRA IV vacuum system.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vacuum lifetime</td>
<td>h</td>
<td>$\geq 10$</td>
</tr>
<tr>
<td>Average pressure</td>
<td>mbar</td>
<td>$&lt; 1 \times 10^{-8}$</td>
</tr>
<tr>
<td>Typical chamber aperture</td>
<td>mm</td>
<td>20</td>
</tr>
<tr>
<td>SR power</td>
<td>W mA/cm</td>
<td>$&lt; 3 \times 10^{-2}$</td>
</tr>
<tr>
<td></td>
<td>W mA/cm$^2$</td>
<td>$&lt; 1.8 \times 10^{-2}$</td>
</tr>
<tr>
<td></td>
<td>W/cm$^2$</td>
<td>$&lt; 36$</td>
</tr>
<tr>
<td></td>
<td>W</td>
<td>$&lt; 620$</td>
</tr>
</tbody>
</table>

Table 6.18.: Maximum average pressures for a vacuum lifetime of 10 h and various gas compositions (cf. Table 6.19) depending on the momentum acceptance ($\delta_{acc}$), the transverse beta function ($\beta_\perp$) and the inner diameter of the vacuum chamber ($d$).

<table>
<thead>
<tr>
<th>$\delta_{acc}$</th>
<th>$\beta_\perp$</th>
<th>$d$</th>
<th>Maximum mean pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>in %</td>
<td>in m</td>
<td>in m</td>
<td>in $10^{-8}$ mbar</td>
</tr>
<tr>
<td>2</td>
<td>5</td>
<td>0.02</td>
<td>4.5 0.93 1.5 0.38 1.4</td>
</tr>
<tr>
<td>1.5</td>
<td>5</td>
<td>0.015</td>
<td>4.1 0.85 1.4 0.34 1.3</td>
</tr>
<tr>
<td>1</td>
<td>2.5</td>
<td>0.015</td>
<td>3.7 0.78 1.3 0.32 1.2</td>
</tr>
</tbody>
</table>

Table 6.19.: Gas compositions used in Table 6.18.

<table>
<thead>
<tr>
<th>No.</th>
<th>Relative abundance</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>H$_2$</td>
</tr>
<tr>
<td>1</td>
<td>0.96</td>
</tr>
<tr>
<td>2</td>
<td>0.1</td>
</tr>
<tr>
<td>3</td>
<td>0.5</td>
</tr>
<tr>
<td>4</td>
<td>0.22</td>
</tr>
<tr>
<td>5</td>
<td>0.75</td>
</tr>
</tbody>
</table>

shortly after commissioning and for several mA beam current (cf. Figure 6.62 and Table 6.20) [71]. Two sputter ion pumps (SIP) are at least necessary in order to assist with pumping of methane. An alternative approach that uses antechambers in dipoles with additional SIPs may significantly reduce contributions from methane, whereby the total pressure further decreases. However, the NEG saturation due to uncoated surfaces becomes less predictable [71].

Initial estimations of synchrotron radiation power loads have been done by geometrical ray-tracing in Mathematica. Further 3D Monte Carlo simulations were performed in SynRad+ [72]. The results show up to 620 W of dipole radiation at crotch absorber positions with a maximum power density of $< 36$ W/mm$^2$. In addition, BPMs need to be shadowed by absorbers, as the power densities would be up to 3 W/mm$^2$.

Figure 6.62.: Layout of the magnetic lattice (top) and dynamic pressure rise per mA beam current for various gas species and after different conditioning steps (bottom) [71].
An overview of vacuum-related simulations and corresponding methods, which also contains the aforementioned results, was published as an internal report [71].

**Table 6.20.: Dynamic pressure rise per mA beam current either with (+) or without (-) methane (CH\(_4\)), whose probability to be pumped may vary during operation depending on the current.**

<table>
<thead>
<tr>
<th>CH(_4)</th>
<th>(\int \frac{I_b}{dt}) in A h</th>
<th>Pressure rise in (1 \times 10^{-10}) mbar/mA</th>
</tr>
</thead>
<tbody>
<tr>
<td>+</td>
<td>0.001</td>
<td>Mean 11, Max 26</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>Mean 0.32, Max 0.67</td>
</tr>
<tr>
<td>-</td>
<td>0.001</td>
<td>Mean 0.30, Max 0.72</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>Mean 0.065, Max 0.14</td>
</tr>
</tbody>
</table>

**Layout of the Vacuum System**

The successful commissioning of the MAX IV facility [73] proves the applicability of a compact storage ring vacuum system design using NEG-coated chambers without antechambers. For the conceptual design of PETRA IV, a comparable approach is considered as the baseline choice. An alternative, specific use of coated aluminium chambers and antechambers is investigated in parallel. Vacuum chamber connections are generally considered to be made with stainless steel ConFlat flanges. The vacuum segmentation is preliminarily based on the level of one achromat. A further segmentation may be considered for specific insertion devices and RF cavity sectors.

Most of the synchrotron radiation load in the PETRA IV machine is expected to be absorbed in the copper beam pipes, which thus need to be water-cooled. Specific wedge or crotch absorbers and tapered absorber faces are furthermore necessary at the separations towards front-end beamlines and around BPMs, respectively. In order to protect NEG-coated surfaces from saturation, SIPs are especially needed at corresponding highly out-gassing regions.

Vibrational stability will be a major challenge for PETRA IV (cf. Section 6.1.2 and Section 6.3.10), which is why a mechanical decoupling of the BPMs from the vacuum chambers is mandatory. While BPMs are regarded as mechanically fixed points, surrounding vacuum chambers will be connected via RF-shielded bellows.

**NEG Coating**

Apart from their composition, NEG coatings can generally be classified according to their microscopic structure into columnar and dense films [74]. While columnar NEG films typically provide good pumping properties, dense films primarily act as a barrier for out-gassing from the substrate material. The NEG coating applied at MAX IV shows the typical columnar structure [75].

At DESY, tests on the internal fabrication of NEG-coated copper chambers are ongoing. A setup for magnetron sputtering deposition was already built in the framework of the PETRA III project. After being primarily used to coat aluminium undulator chambers for PETRA III [76], it is currently being adapted to the prototyping for the PETRA IV chambers. Subsequent tests will involve detailed investigations in terms of pumping speeds, activation temperature and saturation of columnar and dense NEG films. A corresponding measurement setup for these parameters has recently been developed.

NEG films need to be activated at high temperatures > 180 °C in order to initiate pumping. A suitable baking system that can be applied in-situ will be investigated, involving the use of specific heater elements. This issue is not trivial due to space constraints and potential mechanical stresses on magnets and beamline components, which need to be kept aligned with high precision.

While the baseline is the development of an active heater system, a study is currently being prepared to understand whether in-situ activation with synchrotron radiation can suffice to achieve reasonable pumping speeds. For this, a set of 10 standard PETRA III dipole chambers has been replaced with chambers where most of the surface is NEG-coated. The corresponding sector is also instrumented with additional pressure gauges and a residual gas analyser. In 2019, measurements of the pressure in this sector will be compared to the initial conditioning in 2009. They will further be compared to ex-situ measurements of the pumping speed.
Pressure Measurement and Technical Interlock
While the pressure measurement of PETRA III relied on the use of the SIPs as pressure sensors, for PETRA IV additional pressure gauges will be introduced to make sure that the properties of the NEG films are monitored properly. Apart from at least one extractor-type hot cathode gauge per achromat, these also comprise residual gas analysers in several sectors, which should facilitate a faster online diagnosis of potential problems.
A study of the possible electronic layout of the vacuum interlock system has been launched. The programmable logic controller (PLC)-based systems of the European XFEL and FLASH have shown very good reliability and flexibility. A system based on microcontrollers as used for PETRA III will be compared in terms of reliability and cost.
The experience with the operation of the three large accelerator facilities PETRA III [77], FLASH and European XFEL will be used to design a technical interlock that both ensures technical safety and maintains a high availability.

Installation
Installation of sensitive vacuum equipment needs to be done in a controlled environment. In particular, the areas connecting to the photon beamlines and the RF cavities must be assembled under controlled conditions to avoid migration of particulates towards them and maintain the high quality of the cleaned surfaces. We are currently evaluating whether a room cleaned according to “VDA 19 Teil 2 SaS2” is sufficient or whether a cleanroom with defined ISO class needs to be established for the assembly of the vacuum system of PETRA IV. For comparison, MAX IV has been using flow boxes to implement a clean environment at flange connection.

Vacuum Systems for the Pre-Accelerators
The vacuum system for LINAC II may remain essentially in the same configuration as today for the operation for PETRA III. Nonetheless, all vacuum parts will be thoroughly refurbished. In addition, a reliability review will be conducted and redundancy will be added where appropriate.
The vacuum system layout for DESY IV is still at a very early stage. However, as the machine is probably less spatially restricted as PETRA III, a classical layout using lumped pumps is considered. If the spacing becomes too tight, a vacuum system layout analogous to the one for PETRA IV needs to be investigated.

6.3.8. Radio Frequency System
The role of an RF acceleration system of a storage ring is to generate a sufficient beam-accelerating voltage to compensate beam energy losses caused by synchrotron radiation in bending magnets and in insertion devices. Since 2009, the RF system of the PETRA III storage ring has been generating a voltage of 20 MV at a frequency of 499.665 MHz and accelerating an electron beam with a current of 100 mA for synchrotron radiation users. The required RF power is generated by klystrons in two RF stations and supplied to 12 seven-cell cavities in a straight section of the PETRA III storage ring.
When upgrading the storage ring for PETRA IV, the nearly two orders of magnitude smaller momentum compaction factor gives sufficient RF-acceptance already with 8 MV RF voltage. This lower RF voltage makes it reasonable to replace the more than 35 year old seven-cell cavities by state-of-the-art single-cell ones. If the 12 seven-cell cavities were replaced by the same amount of single-cell cavities, each would have to supply a critically high voltage of 667 kV. To reduce the risk of cavity vacuum arcs and as a consequence the impact on the beam, the installation of 24 single-cell cavities is planned.
The lifetime and emittance of PETRA IV will be negatively affected by Touschek and intra-beam scattering. As a countermeasure, harmonic cavities will be installed to lengthen the bunches and thus lower their charge densities.

Fundamental RF System
Cavities
In order to suppress coupled-bunch instabilities arising from the impedances of parasitic resonant cavity modes, a single-cell cavity with
A broadband higher-order-mode (HOM) damping scheme was designed for third-generation synchrotron radiation sources [41]. Single-cell cavities using this HOM damping scheme are foreseen to provide the RF voltage for PETRA IV.

The relevance of a given cavity impedance spectrum for the excitation of multibunch instabilities in a storage ring is best described by the threshold impedance [78]. The threshold impedance $Z_{\text{thresh}}$ can be obtained by equating the radiation damping time with the respective multibunch instability rise time. The equations for the longitudinal and transverse case are:

\[
Z_{\text{thresh}}^\parallel = \frac{1}{N_C} \frac{1}{f_{\parallel \text{HOM}}} \frac{2E}{Q_s} \frac{I_B}{\alpha \tau_s},
\]

\[
Z_{\text{thresh}}^\perp = \frac{1}{N_C} \frac{1}{f_{\text{rev}}} \frac{2E}{I_B \beta_{x,y} \tau_{x,y}},
\]

where $N_C$ is the number of cavities, $f_{\parallel \text{HOM}}$ is the longitudinal HOM frequency, $E$ is the beam energy, $I_B$ is the average beam current, $Q_s$ is the synchrotron tune, $\alpha$ is the momentum compaction factor, $f_{\text{rev}}$ is the revolution frequency, $\tau_{x,y}$ are the damping times and $\beta_{x,y}$ are the beta functions at the cavities.

In this consideration, the conservative assumption has been made that every HOM coincides with an instability-driving beam frequency and that all cavities have identical impedances. With these expressions, the threshold impedances were calculated already some time ago for PETRA IV and for two other synchrotron radiation sources using the “BESSY HOM-damped cavity”. In Figure 6.63, the threshold impedances are plotted together with the HOM impedances of the prototype cavity [79]. The large space between HOM impedance and stability threshold of about a factor of 8 in longitudinal direction and a factor of 2 in transverse direction guarantees a low tendency to coupled-bunch instabilities in PETRA IV and offers space for the not yet considered impedance contribution of the harmonic cavities.

BESSY HOM-damped cavities operate at gradients up to 1.7 MV/m at ALBA and at BESSY II. In order to reduce the risk of cavity vacuum arcs, a cavity voltage gradient of about 1 MV/m has been chosen for PETRA IV (at PETRA III, the cavity voltage gradient is 0.79 MV/m). The less challenging gradient requires the installation of 24 cavities. The large number of cavities has the additional advantage that a single cavity fault has only little impact on the beam. The required power to generate the accelerating voltage is 16.3 kW per cavity. The beam loading power at 200 mA beam current is 33.3 kW per cavity. Taking 5% transmission loss into account, the power required to supply one cavity is 52.1 kW. Each
transmitters, each equipped with two 800 kW klystrons. If a fault occurs in this structure, at least one transmitter will be switched off. This means that half of the accelerating voltage will be missing and the beam will be lost. To minimise the influence of RF faults on the beam, it is reasonable to assign a dedicated transmitter to each cavity. Instead of klystron or inductive output tube (IOT) transmitters, solid-state amplifier (SSA) transmitters are preferred for the PETRA IV RF systems. Today, SSAs for the required RF power range are available from various manufacturers [80, 81]. Key benefits of SSAs are:

- Easy maintenance because of elimination of high-voltage handling.
- No experienced and – nowadays rare – tube specialists are required for fault diagnosis and repair.

Harmonic RF System

The negative effects on both lifetime and emittance of PETRA IV caused by Touschek and intra-beam scattering can be reduced by using higher-harmonic cavities (HHCs). These cavities lengthen the bunches and thereby reduce their charge density [82]. If another voltage is added to the main RF voltage with an amplitude and phase such that the slope at the bunch centre is zero, the bunch will lengthen and the peak charge density will decrease. Higher-harmonic cavities have been used successfully for many years in second- and third-generation light sources in both active and passive configurations. The frequency ratio between the harmonic and the fundamental RF is basically freely selectable in a wider range. A large frequency ratio will result in a lower voltage of the harmonic cavities. However, the flat bottom of the potential well will shrink as well. For practical reasons, one usually chooses frequency ratios in the range of two to four between the harmonic and the fundamental RF.
When using a passive harmonic system, the transient beam-loading effects along the fundamental RF system. For PETRA IV, \( n = 3 \) was chosen. The energy loss per turn is \( U_0 = 4.0 \text{ MeV} \) and the RF voltage \( V_{rf} = 8.0 \text{ MV} \). This gives an optimum value for the harmonic voltage of \( V_{HHC,opt.} = 2.26 \text{ MV} \). With some safety margin, the system is designed for \( V_{HHC} = 2.4 \text{ MV} \). The number of harmonic cavities required is scaled from the fundamental RF system. A three times higher frequency leads to three times shorter cavities. If one allows the same gradient as for the fundamental cavities of about 1 MV/m, 24 harmonic cavity cells are required. The shunt impedance \( R_s \) of a single-cell harmonic cavity such as the down-scaled BESSY HOM-damped cavity is \( R_s = 1.5 \text{ M} \Omega \) [83]. The dissipated power \( P_{HHC} \) of such a single-cell harmonic cavity is

\[
P_{HHC} = \frac{(V_{HHC}/24)^2}{2 \cdot R_s} = \frac{(100 \text{ kV})^2}{2 \cdot 1.5 \text{ M} \Omega} = 3.33 \text{ kW}.
\]

When using a passive harmonic system, the cavity power is generated by the beam itself, but for several reasons (different beam currents for brightness and timing mode, uneven bunch pattern with gaps during filling), an active harmonic system is be essential for PETRA IV.

Transient beam-loading effects along the bunch train could significantly degrade the total amount of bunch lengthening, and thus the lifetime improvement will be degraded [84]. Transient beam loading could probably be counteracted by a feed-forward beam-loading compensation using the harmonic power transmitter. Due to the large circumference of the PETRA IV ring, the revolution harmonics are just 130.12 kHz apart in the case of an uneven bunch pattern. The unloaded bandwidth of the harmonic cavities is about 90 kHz and thus in the same range. In consequence, not only the harmonic component \( n f_{rf} \) but also a couple of neighbouring revolution harmonics induce a significant voltage in the harmonic cavities. Because the harmonic cavities have to be detuned according to the beam current with

\[
\Delta f_{HHC} = \frac{R_s \cdot n \cdot f_{rf} \cdot I_B}{V_{HHC} \cdot Q_0}
\]

by several 100 kHz with respect to \( n f_{rf} \), the amplitudes of the higher neighbouring revolution harmonics may even be dominant. For PETRA IV, an extremely uneven bunch pattern with just half of the ring filled with 40 times 20 bunches has been simulated [85]. The simulation included the beam spectrum from the first revolution harmonic below \( n f_{rf} \) to the fifth revolution harmonic above \( n f_{rf} \). It turned out that under these conditions, the first revolution harmonic above \( n f_{rf} \) is 20 % stronger than \( n f_{rf} \) and the potential well is deformed accordingly. The potential well can be flatten again by increasing the harmonic transmitter power from \( P_{HHG} = 3.11 \text{ kW} \) to \( P_{HHG} = 28.4 \text{ kW} \) per harmonic cavity and introducing an additional phase shift of \( \phi_{HHG} = -32^{\circ} \). A more elegant solution would be a stronger coupling of the harmonic cavities. Calculations with different coupling factors for the harmonic cavities show an optimum coupling factor of \( \beta = 5.3 \) with respect to the required harmonic transmitter power for the simulated uneven bunch pattern with just half the ring filled. Choosing \( \beta = 5.3 \), the potential well can be flattened again by increasing the harmonic transmitter power from \( P_{HHG} = 3.11 \text{ kW} \) to \( P_{HHG} = 10.5 \text{ kW} \) per harmonic cavity and introducing an additional phase shift of \( \phi_{HHG} = -27^{\circ} \).

Technical Layout of the RF System

To avoid a single point of failure, the PETRA IV RF is going to be divided into six independent and uniform RF systems with four fundamental cavities and four higher-harmonic cavities each. Each cavity is supplied by its own SSA transmitter, as shown in Figure 6.65. In case of a fundamental-cavity or transmitter fault, the missing accelerating voltage can be compensated by the remaining three cavities of this RF system by raising the cavity supply power from \( P_{HHG} = 3.11 \text{ kW} \) to \( P_{HHG} = 76 \text{ kW} \). Even if one of the six RF systems is already out of service and a fundamental-cavity or transmitter fault occurs in one of the remaining five RF systems, the trip can be compensated by raising the cavity supply power from 67 kW to about 105 kW. The cavity voltage of the remaining three cavities of the affected system must then
be increases to 533 kV. However, even with well-conditioned cavities at good vacuum conditions, this voltage includes a high arcing risk. In addition to the correction of the missing accelerating voltage, transient phase correction will also be required to counteract the excitation of synchrotron oscillations [86, 87].

In nominal beam operation, each cavity delivers 1/24 of the required RF voltage. The needed RF power is

\[ P_{\text{Cin}} = P_{\text{Cdiss}} + P_B, \]

with

\[ P_{\text{Cdiss}} = \frac{(V_{rf}/24)^2}{2 \cdot R_S} = 16.3 \text{ kW} \quad \text{and} \]

\[ P_B = I_B \frac{U_0}{e_0} \cdot \frac{1}{24} = 33.3 \text{ kW}, \]

where \( P_{\text{Cin}} \) is the cavity coupler input power, \( P_{\text{Cdiss}} \) is the copper loss of the cavity, and \( P_B \) is the beam loading power. In nominal beam operation, the cavity is matched to the generator. Therefore, no reflected power will appear. The required coupling factor for a matched cavity operation is

\[ \beta_{\text{match}} = 1 + \frac{P_B}{P_{\text{Cdiss}}} = 3.04. \]

To calculate the transmitter power \( P_{\text{trans}} \) in nominal beam operation, 5% transmission losses still have to be considered.

\[ P_{\text{trans}} = (P_{\text{Cdiss}} + P_B) \cdot 1.05 = 52.1 \text{ kW} \]

The transmitter power in nominal beam operation is \( P_{\text{trans}} = 52.1 \text{ kW} \) per cavity.

In order to achieve high reliability and availability, some extra power is needed. In case of a cavity or transmitter failure, the missing accelerating voltage will be compensated by the remaining three cavities of the RF system by raising the cavity supply power. This trip compensation should still work even if another RF system is already out of service.

**Fault Mode Operation of the Fundamental RF**

Assumptions for beam operation in fault mode are:

- One of the six RF systems is already out of service.
- In addition, a trip of a component of a remaining RF system occurs.

The RF system with the tripped cavity or transmitter has to deliver 1/5 of the total RF voltage and a corresponding percentage of the power extracted from the beam by the tripped cavity. The needed transmitter power in fault beam operation for each remaining cavity of the RF system affected by the tripped component is \( P_{\text{trans}} = 104.1 \text{ kW} \) [85].

**Figure 6.65:** One out of six independent and uniform RF systems with four fundamental cavities and four harmonic cavities each, plus the related transmitters and the common low-level RF system.

**Figure 6.66:** Fault mode beam operation of the fundamental RF. One of the six RF systems is already out of service and, additionally, a cavity or transmitter of a remaining RF system trips.
### Table 6.21: Essential PETRA IV parameters for the RF system design.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Brightness mode</th>
<th>Timing mode</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam energy</td>
<td>6 GeV</td>
<td></td>
</tr>
<tr>
<td>Beam current</td>
<td>200 mA</td>
<td>80 mA</td>
</tr>
<tr>
<td>Number of bunches</td>
<td>1600 (=80 x 20)</td>
<td>80 (=80 x 1)</td>
</tr>
<tr>
<td>Bunch spacing</td>
<td>4 ns</td>
<td>96 ns</td>
</tr>
<tr>
<td>Bunch filling gap</td>
<td>20 ns</td>
<td>96 ns</td>
</tr>
<tr>
<td>Harmonic number</td>
<td>3840</td>
<td></td>
</tr>
<tr>
<td>Revolution frequency</td>
<td>130.121 kHz</td>
<td></td>
</tr>
<tr>
<td>Energy loss per turn</td>
<td>4.02 MeV</td>
<td></td>
</tr>
<tr>
<td>in bending magnets</td>
<td>1.32 MeV</td>
<td></td>
</tr>
<tr>
<td>in insertion devices</td>
<td>2.70 MeV</td>
<td></td>
</tr>
<tr>
<td>Momentum compaction factor</td>
<td>$1.485 \times 10^{-5}$</td>
<td></td>
</tr>
</tbody>
</table>

### Table 6.22: Parameters for the PETRA IV fundamental RF system.

- RF frequency (fundamental RF system): 499.665 MHz
- RF voltage (fundamental RF system): 8 MV
- Synchronous phase: 30.2°
- Synchrotron frequency: 421 Hz
- Number of RF single-cell cavities: 24
- RF voltage per cavity: 333 kV
- Shunt impedance per cavity: 3.4 MΩ
- Unloaded quality factor: 29 000
- Loaded quality factor: 7400
- Total wall loss in cavities: 392 kW
- Total beam loading power: 800 kW
- Cavity coupling factor: 3.0
- Number of RF stations: 24
- Nominal transmitter power per RF station: 110 kW

### Table 6.23: Parameters for the PETRA IV third-harmonic RF system.

- RF frequency: 1498.995 MHz
- RF voltage: 2.26 MV
- Number of single-cell cavities: 24
- RF voltage per cavity: 94 kV
- Shunt impedance per cavity: 1.5 MΩ
- Unloaded quality factor: 17 000
- Loaded quality factor: 2700
- Total wall loss in cavities: 71 kW
- Cavity coupling factor: 5.3
- Number of RF stations: 24
- Nominal transmitter power per RF station: 10 kW

### Installation Site and Visualisation of the RF System

The RF system is to be built in the south of the PETRA ring. The cavities are to be installed at approximately the same location as the current PETRA III cavities. To connect the 24 fundamental and 24 harmonic cavities in the shortest way to their transmitters, a new hall above the tunnel and between the existing PETRA III transmitter halls has to be built, as shown in Figure 6.67. Figure 6.68 depicts how the 24 transmitter systems could be arranged in the new hall and how the power could be
transmitted via waveguides into the tunnel. Figure 6.69 shows the arrangement of the fundamental and harmonic cavities in the tunnel.

**Figure 6.67:** New transmitter hall above the tunnel and between the existing PETRA III transmitter halls.

**Figure 6.68:** Visualisation of the six PETRA IV RF systems.

**Figure 6.69:** Detailed visualisation of one cavity system.

### 6.3.9. Septa and Kicker

In order to convert PETRA into a fourth-generation synchrotron light source, both kicker magnets and driving pulsers have to be studied with respect to reliability, availability and specification. For PETRA IV, we need an on-axis injection with a fast rise and fall time and high pulse repetition stability. Two stripline kicker magnets and one DC septum magnet are included in the PETRA IV storage ring to provide an on-axis injection of the beam from the DESY IV transfer line into PETRA IV. The kickers are designed to work with identical currents and waveforms with an amplitude stability of $3 \times 10^{-4}$. The data of the stripline kicker magnet and the pulser are shown in Table 6.24. The details are described in the following.

#### Concept of the Kicker Magnet

We can adopt the present European XFEL dump kicker design (cf. Figure 6.70), but the geometry has to be adapted to the conditions of the PETRA IV vacuum system, i.e. the distance between the electrodes has to be reduced from 30 mm to 20 mm. In addition, the high-voltage feedthroughs have to be replaced, since the current dielectric strength of 7 kV is not sufficient. The baseline design calls for a voltage of up to 11 kV at the feedthrough. Should this voltage not be reached, then it might be necessary to increase the length of the kicker or decrease the distance between the electrodes.

The stripline kicker is inside the vacuum and has an impedance of 50 Ω. In order to obtain a small reflection factor, it is important to take into account the dimensions of the kicker on parallelism, separation and concentricity of the striplines (Item 5 in Figure 6.70) to each other and the location of the striplines within the vessel. The striplines are mounted to half-shells with ceramic spacers. After assembling the striplines, the half-shells of the vacuum tank are welded together with a 2 m weld. Ceramic spacers allow for mechanical expansion of the striplines relative to the vessel and vice versa, e.g. during vacuum bake-out. The centre spacer is fixed, while the end spacers allow for longitudinal movement (sliding). Bellows (Item 13) are installed for decoupling so that the forces of the length change (thermal expansion) of the conductor (Item 5) do not damage the insulating ceramics of the high-voltage feedthroughs (Item 17).

For single-bunch injection, short kicker pulses with rise and fall times in the range of 1 ns or below are needed so that neighbouring bunches are not disturbed. Currently, such pulses are hard to obtain, and the achievable amplitude stability is approximately 1%. Injection of bunch trains using flat-top pulses has been chosen instead, as shown in Figure 6.29. To accommodate the rise and fall times, the fill pattern will have to have gaps of 20 ns.
Figure 6.70.: European XFEL dump kicker cross section (a) and 3D image. (b) The corresponding beamline of the European XFEL is suspended from the ceiling, therefore the adjustment elements are on top.

Table 6.24.: Data of the stripline kicker for PETRA IV injection.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Kicker magnet</th>
<th>Pulser</th>
</tr>
</thead>
<tbody>
<tr>
<td>Impedance</td>
<td>50 Ω</td>
<td>50 Ω</td>
</tr>
<tr>
<td>Free aperture</td>
<td>20 mm</td>
<td></td>
</tr>
<tr>
<td>Kicker length</td>
<td>2000 mm</td>
<td></td>
</tr>
<tr>
<td>Deflection</td>
<td>63 μrad/kV</td>
<td></td>
</tr>
<tr>
<td>Pulse waveform</td>
<td>80 ns rectangular</td>
<td></td>
</tr>
<tr>
<td>Repetition rate</td>
<td>1 Hz</td>
<td></td>
</tr>
<tr>
<td>Rise and fall time</td>
<td>&lt;4 ns</td>
<td></td>
</tr>
</tbody>
</table>

Concept of the Pulser
The future pulser for PETRA IV is designed to have a rectangular pulse with very high amplitude stability and with rise and fall times in the nanosecond range. The pulser is divided into three sections (cf. Figure 6.71): one for the rising edge (blue), one for the amplitude control (green), and one for the trailing edge (red). For the rising edge, we aim to use GaN MOSFET technology. The lower gate and output capacitance of GaN allows for operation at several hundred MHz switching frequencies while reducing gate and switching losses to increase efficiency. Since these MOSFETs have an operating voltage in the range of several 100 V, the modules have to be connected in series. In order to provide the current, several modules must also be connected in parallel. For the amplitude control, we aim to use LD-MOS semiconductors that can be used in the microwave range up to several GHz, and for the pulse flatness, we intend to implement a feed-forward control. For the trailing edge, we aim to use an active snubber to minimise the after-pulse ripple.

Figure 6.71.: Pulser scheme.
Accelerators | Technical Subsystems

Figure 6.72: (a) PETRA III septum (b) European XFEL Lambertson septum.

Septum
The preliminary design of the septum is based on the existing PETRA III septum (cf. Figure 6.72a), which is operated by a half-sine pulse of 170 µs. To suppress the effects of stray fields due to eddy currents, substantial shielding is necessary, which increases the size of the septum bar to 5 mm. However, the stored beam is still affected by the stray field. Some oscillation of the stored beam is observed.

Another option is a DC Lambertson septum, as shown in Figure 6.72b, which reaches distinctly better amplitude stability values compared to a pulsed septum. The septum bar thickness is 5 mm. One example of a DC septum is the Lambertson septum operated at the European XFEL. The data of the septum is shown in Table 6.25. At the European XFEL, the iron yoke of the septum is outside the vacuum, adding the walls of the vacuum chamber to the effective thickness of the septum bar. We will investigate whether the yoke can be incorporated into the vacuum chamber.

6.3.10. Diagnostics
The upgrade of the PETRA IV storage ring will require diagnostic systems similar to those already successfully installed in PETRA III. They have to provide all the information that is needed in order to accurately characterise the electron beam in dedicated beam studies and to guarantee stable beam operation for users. However, the new design of the storage ring requires a larger number of diagnostic devices with partially tighter specifications. In addition, their technical realisations have to be adapted to the specific needs of PETRA IV. In the following, the beam position and emittance monitor systems will be considered because their design considerations will have the biggest impact on the performance of the new storage ring from the diagnostic point of view. In addition, the remaining diagnostic systems will briefly be described.

Beam Position Monitors
The beam position monitors (BPMs) are by far the largest diagnostic system in PETRA IV. A total of 10 BPMs per MBA sector cell is needed, and with 64 cells in the arcs and eight straight sections, about 700 BPMs are required in order to operate the new storage ring. As for PETRA III, all BPMs will be used by the fast orbit feedback (FOFB) system. For the commissioning of the machine, a single-bunch single-turn BPM resolution of \( \leq 20 \mu m \) (assuming 0.5 mA bunch current) is required, while the closed-orbit resolution should amount to 100 nm (rms, for 200 mA beam current in 1600 bunches) at a bandwidth of 300 Hz.

The PETRA IV BPM system will be based on button pickup electrodes, as is common practice in circular synchrotron light sources and as has been done for PETRA III [88]. The BPM vacuum chambers (inner beam pipe diameter of 20 mm in regular sections) will feature shielded bellows on both flanges in order to allow the vacuum chamber to move (e.g. due to thermal stress), while keeping the BPM chamber itself in a fixed position with respect to the
Table 6.25.: European XFEL Lambertson septum data.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air gap</td>
<td>50 mm</td>
</tr>
<tr>
<td>Magnetic field $B_0$</td>
<td>0.42 T</td>
</tr>
<tr>
<td>Core length</td>
<td>1000 mm</td>
</tr>
<tr>
<td>$\Delta B / B_0$ at R=40 mm</td>
<td>0.15</td>
</tr>
<tr>
<td>Number of magnets</td>
<td>4</td>
</tr>
<tr>
<td>Number of winding turns</td>
<td>120</td>
</tr>
<tr>
<td>Nominal current</td>
<td>155 A</td>
</tr>
<tr>
<td>Conductor with dimensions</td>
<td>6x6 - diameter 3 mm</td>
</tr>
<tr>
<td>Resistance</td>
<td>0.183 $\Omega$</td>
</tr>
<tr>
<td>Voltage drop</td>
<td>32 V</td>
</tr>
<tr>
<td>Power loss</td>
<td>5 kW</td>
</tr>
<tr>
<td>Total weight</td>
<td>560 kg</td>
</tr>
<tr>
<td>Water flow</td>
<td>2.3 l/min</td>
</tr>
<tr>
<td>Temperature overheating</td>
<td>30 °C</td>
</tr>
</tbody>
</table>

adjacent quadrupole or girder. To minimise the excitation of trapped RF modes and the overall power dissipation, design studies of both pickup and bellow-isolated BPM assembly are under way using CST Microwave Studio. First calculations indicate that the power loss in a pickup electrode is well below 1 W and therefore seems not to be critical [89].

In order to achieve the beam stability goals, low-noise BPM electronics are essential. Nowadays, digital processing electronics are widely used [90], and like most of the present third-generation light sources, PETRA III is equipped with the Libera Brilliance electronics of commercial supplier Instrumentation Technologies [91]. It enables good long-term stability in addition to low-noise fast data acquisition for orbit feedback. Turn-by-turn and analog-to-digital buffered data are available on demand for machine studies. Figure 6.73 shows the performance of the present PETRA III BPM system. Scaling the measured closed-orbit data with the bandwidth to the required 300 Hz according to the specification results in a (rms) resolution of about 430 nm. Therefore, both the closed-orbit and the single-bunch single-turn resolution have to be improved by a factor of 2–4 for PETRA IV. Recent studies with the follow-up device Libera Brilliance+ [92] indicate that the resolution requirements can be met with these electronics [93]. Thus, for PETRA IV, we envisage to set up the system based on this commercial BPM processor. A Libera Brilliance+ unit has already been procured to test its performance, first studies with beam are under way. As a backup, in order to gain independence from commercial suppliers, an in-house development of BPM electronics is also being discussed.

Beam Profile and Emittance Monitors

The longitudinal bunch profile and the transverse emittances in a storage ring can be determined by measuring the beam profiles using synchrotron radiation (SR) from a bending magnet or a short three-pole wiggler. For this purpose, it is planned to set up three diagnostic beamlines, as was the case for PETRA III. Synchrotron radiation in the visible and the X-ray region will be deflected out of the accelerator tunnel and guided to experimental hutch where the corresponding monitors will be located.

The dual-sweep synchro-scan streak camera Hamamatsu C5680, which is presently in use at PETRA III [94], will be sufficient also for longitudinal diagnostics in PETRA IV and, consequently, it will be reused. The 2 ps time resolution of the fast 250 MHz synchro-scan unit together with the sweep time range from 100 ns up to 100 ms of the dual time base extender unit allows all kind of bunch length studies to be performed at different time scales. The streak camera will be set up behind one of the visible SR light diagnostic beamlines.
The second beamline for visible SR will host a Mitsuhashi-type double-slit interferometer [95, 96] to probe the spatial coherence of the beam and derive its beam size resp. emittance from a measurement of the interferograms. At PETRA III, an emittance monitor based on a two-dimensional interferometer is in operation, performing online transverse emittance measurements for daily use in the accelerator control room [97, 98], and a similar monitor will be set up at PETRA IV. According to the experience with PETRA III, the minimum resolvable beam size is on the order of about 5 µm. In principle, this value could be slightly reduced using imbalance techniques as proposed and tested in [99], and as were tested also with the PETRA III setup. However, a drawback of this technique is the reduced SR light intensity, which may cause stability problems, as observed at PETRA III.

In order to resolve the ultra-low transverse beam emittances resp. beam sizes with high precision, a third diagnostic beamline for beam imaging via SR in the X-ray region will be installed. Compared to imaging with visible light, X-ray imaging has the advantage of minimising the diffraction limit imposed by the uncertainty principle. As imaging optics, an X-ray pinhole will be used. While X-ray pinhole cameras with a resolution on the order of 10 µm are widely used at third-generation light sources [100, 101], the planned PETRA IV beam size monitor will be operated as a Fresnel diffractometer [102, 103], i.e. the pinhole size is slightly larger than the one of a conventional pinhole camera, so that diffraction effects take place in the Fresnel rather than the Fraunhofer regime. With proper design of the setup (pinhole size, distance from source point to pinhole, distance from pinhole to observation point, photon energy), the diffraction pattern will exhibit a double-lobed structure. The depth of the central dip in the double-lobed diffraction pattern correlates with the transverse beam size, i.e. the dip will become shallower with increasing beam size. A similar monitor is planned e.g. at the APS [10]. A drawback of a Fresnel diffractometer is the limited sensitivity range for beam size variations, i.e. if the beam size is too large, the central dip will be completely smeared out and the monitor will be insensitive to a change in beam size. In order to overcome this limitation, the PETRA IV X-ray imaging monitor will be equipped with a second but smaller pinhole, so that it can be operated as a conventional pinhole camera in case the beam size is too large for the Fresnel diffractometer.

Furthermore, by combining the beam size measurements from both transverse beam profile monitors (Fresnel diffractometer and Mitsuhashi-type double-slit interferometer), we will be able to extract information about the beam energy spread.
Other Diagnostic Devices
Position stability is crucial for the successful operation of a facility like PETRA IV. Therefore, position and movement of each BPM pickup have to be monitored with respect to either the ground floor or the girder. For this purpose, each pickup will be attached to a movement sensor that measures the actual position with respect to a reference one. At PETRA III, a high-frequency movement monitor system determines pickup movements with a resolution of $< 1 \mu m$ based on the measurement of the distance between four terminated ($50 \Omega$) striplines and a stiff solid wire. For PETRA IV, this system will be overhauled and adapted to the needs of the new accelerator.

The design strategy for beam current measurements in PETRA IV is based on the experience with the instrumentation currently deployed in PETRA III. Three parametrical current transformers for DC current measurements are foreseen: one as main source for DC measurements, one acting as spare, and one independent monitor as integrated part of the machine protection system. In addition, three fast passive beam transformers will be used for single-bunch current measurements: one to measure the single-bunch intensity of the incoming beam right after injection, one to do so before closure of the first turn, and a third monitor to measure the single-bunch currents of the stored beam for swap-out operation. For PETRA IV, we plan to purchase the beam current monitors from a commercial vendor [104].

In collaboration with this vendor, design studies of ceramic gap vacuum chambers and their associated RF shielding and cooling components are under way based on CST Microwave Studio simulations. First calculations indicate that power losses in the transformers might heat up the devices up to $300 \, ^\circ C$, which is well above the damage threshold [89]. Therefore, active cooling of the critical monitor components based on compressed air in combination with water will be essential. In order to circumvent this problem, visible SR detected by a fast avalanche photodiode might be used as an alternative, as is done resp. proposed for the SLS and its upgrade SLS-2 [9, 105].

6.3.11. Machine Protection System
Both the electron and photon beam of a synchrotron light source like PETRA IV have the potential to damage technical components of the accelerator itself. Therefore, a number of different monitors, which will be discussed in the following, is required in order to operate the machine under safe conditions.

The machine protection system (MPS) is the central part of the accelerator safety system aimed at preventing critical beam-induced damage of technical components. It collects the information from different subsystems and reacts by switching off or dumping the electron beam in case of an ambiguous machine operation state. For PETRA III, the MPS successfully supported smooth beam operation right from the start-up of the accelerator [106, 107]. Several fast alarms, generated by beam position monitors, beam loss monitors, experiments, vacuum systems, magnets and further sub-systems are collected and processed in a fast manner. Additionally, postmortem triggers are generated to trigger ring buffers of external systems. Automated alarm cause studies support the operators in understanding situations right after the beam has been lost. The MPS for PETRA IV will be based on the successful design strategy of the present system. We plan to revise the PETRA III system in view of an updated technical platform and to integrate additional alarms, e.g. from the swap-in/out injection and extraction elements.

The beam loss monitor (BLM) system is one of the main subsystems of the MPS. For PETRA IV, we plan to build the BLM system based on the one used at the European XFEL [108]. This strategy will save significant engineering time and costs, and only the necessary adaption of the requirements in view of a circular machine will entail modifications in the firmware.

Similar to the system used at the European XFEL [109] to monitor the radiation dose at the undulators and at sensitive electronic equipment, an online dosimetry system will be designed for the specific needs of a circular machine. Both BLM and dosimetry system are important to keep the radiation damage of the undulators as small as possible. Furthermore, the temperature system of PETRA III, which is monitoring the temperature at critical loca-
6.3.12. Beam Dumps

The 6 GeV electron beam in a 200 mA (~1500 nC) fill (brightness mode) of PETRA IV corresponds to a stored energy of about 9.2 kJ. That amount is able to increase the temperature of a 100 cm³ water volume by ~22 K, which does not seem alarming at first. But due to the very small beam size of a few micrometres (1 µm to 10 µm), the beam will dissipate its energy in a tiny volume only. As a consequence, one has to expect very high local energy densities on the order of 500 kJ/g, more than 50 times the specific evaporation heat of aluminium. Thus, if lost in the vacuum chamber, the beam will immediately burn a tiny hole into the material. For that reason, a concept for a safe abort of the total fill is required in an emergency situation, such as too large orbit deviations, or magnet or RF trips. Unlike PETRA III, PETRA IV also requires a so-called swap-out dump in addition to the emergency dump system. Due to the small dynamic aperture, an on-axis injection is foreseen for PETRA IV. The beam will be continuously exchanged in portions of 1/80 of the total fill in order to keep the stored current constant within the desired range. In brightness mode, a “fresh” train of 20 bunches with about ~20 nC is injected every 2 s to replace the “old” train, which is extracted and guided to the swap-out dump.

Finding an appropriate dump concept is strongly connected to the requirements for both the emergency case and the swap-out case, which are discussed here shortly in a very general classification. As a consequence of tiny beam spots, the design of the emergency dump in particular is dominated by dealing with high local energy densities. These cause a high instantaneous local temperature rise, which might translate into severe mechanical stress in the absorber material. But compared to regular swap-out, the emergency case happens rarely, so the absorber material is exposed neither to long-term cyclic load nor to significant average power. Therefore, the emergency dump must be capable of “digesting” single beam shots every once in a while, but average heating, activation, shielding and even full energy capture are not key issues here. In addition to the absorber layout, the whole concept has to guarantee that the beam arrives at the dump without being lost before. Especially for the emergency case, where the beam is typically not in a well-defined state, this has to be thoroughly investigated.

Compared to the emergency case, the swap-out absorber is hit by beam pulses with a charge of only 1/80 of the total charge. Nevertheless, the challenge of instantaneous local heating and induced stress still remains, because a reduction by two orders of magnitude is not enough when looking at the destruction potential, as mentioned at the beginning of this section. Furthermore, these pulses arrive in a regular cyclic manner every ~2 s. On the one hand, this requires a layout for long-term operation with a large number of about $1 \times 10^8$ stress cycles within 20 years of beam operation, where material fatigue must be strictly considered. On the other hand, the average power on the dump is on the order of ~100 W ($\frac{20\text{nC}}{2\text{s}} \cdot 6 \text{ GeV} = 60 \text{ W}$). Therefore, the dump layout has to take cooling, ~100 % energy capture and proper shielding into account. For a better understanding of both dump concepts as later described, please refer to [110], which gives a short review of the energy deposition and heating in materials caused by an electromagnetic shower process. The main results are summarised in the next paragraph.

**Energy Deposition in Matter by High-Energy Electron Beams**

We consider a pulsed high-energy electron beam, in which a limited number of bunches, evenly separated in time by $T_{\text{bunch}}$, form a train. The train itself carries a total charge $q_t$, has a temporal length $T_i$ and repeats with a rate $\nu_i$. When the electron beam hits matter, the primary energy is spatially deposited in the material according to the shower process. In each mass element $dm$, a certain amount of energy $dQ$ is deposited by the total primary electron charge $q_t$ at position $(x, y, z)$ and time $t$. This energy is mainly transformed into heat, and for short bunch trains, it will not spread out by thermal diffusion during the time $T_i$. Thus, the deposited energy density $\frac{dQ}{dm}(x, y, z, t)$ translates via the specific heat capacity $c$ of the material into an instantaneous temperature rise $\Delta T_{\text{inst}}$. 

In the time between subsequent trains, the temperature decreases due to thermal diffusion, before the next pulse adds again a temperature jump of $\Delta T_{\text{inst}}$. This process is sketched in Figure 6.74. It has a saw-tooth appearance, in which the average temperature level slowly increases after starting beam operation and reaches a quasi-steady state when the average temperature rise $\Delta T_{\text{eq}}$ reaches equilibrium.

Average heating is determined by the average beam power deposition and the heat flow towards the heat sink of the material. The instantaneous cyclic heat component decreases with transverse distance from the shower axis at $r = 0$, where it has its maximum $\max\left(\frac{dQ}{dm}\right)_{z = t_E} = \frac{dQ}{dm}(r = 0, z = t_E)$ somewhere between the surface ($z = 0$) and the shower maximum ($z = t_{\text{max}}$) of the material.

Energy deposition from electrons, whose energy $E_0$ is large compared to the critical energy $E_c$, is dominated by ionisation loss, with an almost material-independent value of $\frac{1}{\rho} \left(\frac{dE}{dz}\right)_{\text{min}} \approx 2 \text{MeVcm}^2/\text{g}$ for one minimum ionising particle.

For a transversely Gaussian distributed bunch train of $N_t$ minimum ionising electrons with a size $\sigma_x$ and $\sigma_y$ at the surface ($z = 0$) of the material, the maximum deposited energy at the beam axis ($x = y = 0$) is [110]:

$$\max\left(\frac{dQ}{dm}(z = 0)\right) \approx 0.032 \text{J/g} \cdot \frac{[\text{MeV}]}{\sigma_x \sigma_y} \cdot \frac{q_t}{[\text{nC}]} \quad (6.14)$$

Eq. (6.14) is valid as long as the broadening of the transverse energy density profile by heat diffusion during the time $t$ of the energy deposition, which is characterised by the thermal diffusion length $\Lambda(t)$, is negligible compared to the beam spot size, i.e. $\sigma_x, \sigma_y \gg \Lambda(t)$. $\Lambda(t)$ is defined as:

$$\Lambda(t) = \sqrt{\frac{\lambda}{\rho c \cdot \sqrt{t}}} \quad (6.15)$$

Here, $\lambda$ is the thermal conductivity, $c$ the specific heat capacity and $\rho$ the mass density of the material. For example, within the PETRA revolution time of 7.68 µs, the diffusion length in aluminium is more than 20 µm and thus comparable to the size of the stored beam.

Going deeper into the material, there are two counteracting processes, which determine the local energy density: particle production and shower broadening.

On the one hand, particle multiplication increases up to the so-called shower maximum at a depth of $t_{\text{max}}$, where the energy of all secondary particles is too low for a continuation of the two essential shower processes, bremsstrahlung and pair production. Thus, the transversely integrated energy deposition per unit of length and per primary beam electron $\frac{dE}{dz}$ increases from the surface ($z = 0$) of the absorbing material towards the shower maximum at $z = t_{\text{max}}$, after which it decreases again.

On the other hand, the transverse distribution of this energy deposition widens with increasing depth. Its width is a superposition of the incoming beam spot size and the width of the energy profile due to the shower of a single primary electron. As a consequence, the value and the position $t_E$ of the maximum energy
density $\max \left( \frac{dQ}{dm} \right)$ are determined by both the shower process and the incoming beam size. If the beam size is small enough that the increasing energy loss due to shower development cannot compensate the widening of the transverse energy deposition profile, the maximum energy density $\max \left( \frac{dQ}{dm} \right)$ will be located at the absorber front and has a value given by Eq. (6.14). This applies especially for tiny beams and for a small multiplicity (cf. Eq. (6.17)) due to low beam energy.

In the opposite case when the beam has a very large size compared to the intrinsic shower width at the shower maximum, the maximum energy density is located at the shower maximum. In all other cases, the position $t_E$ of $\max \left( \frac{dQ}{dm} \right)$ is located somewhere on the shower axis between the absorber face and the shower maximum. Unfortunately, an analytical description of the shower profile along its axis in the absorbing material is not trivial. Thus, if $\max \left( \frac{dQ}{dm} \right)$ is not located at the entrance of the absorber, its position and quantity can be derived by Monte Carlo codes only. Much easier is an estimate of transversely integrated figures, such as the average power $dP$, which is dissipated in a longitudinal slice $dz$ of the absorbing material at the beginning and at the shower maximum of the absorber. For a given average beam current $I_{ave} = N_t \cdot e \cdot \nu_t$ directed on an absorber, the following Eq. (6.16) can be used to estimate these values:

$$
\frac{dP}{dz}(z) = \left( \frac{1}{\rho} \frac{dE}{dz} \right)_{min} \cdot \rho \cdot \frac{t_{max}}{E} \cdot M(z) \approx \begin{cases} 
2 \text{W/cm} \cdot \frac{\rho}{[g/cm^3]} \cdot \frac{t_{max}}{[\muA]} & \text{at } z = 0 \\
2 \text{W/cm} \cdot \frac{\rho}{[g/cm^3]} \cdot \frac{t_{max}}{[\muA]} \cdot M(t_{max}) & \text{at } z = t_{max} 
\end{cases}
$$

(6.16)

At the absorber face, each electron deposits a quantum of energy, as every minimum ionising particle does. At the shower maximum, each primary electron has produced a factor of $M(t_{max})$ more minimum ionising particles, where $M(z)$ denotes the multiplicity of the shower process. The multiplicity goes up with increasing beam energy $E_0$ and decreasing critical energy $E_c$ of the absorbing material. The depth of the shower maximum as well as the multiplicity there are estimated by Eq. (6.17):

$$
t_{max} = X_0 \cdot 1.01 \cdot \left[ \ln \left( \frac{E_0}{0.21 \text{MeV}} \right) - 1 \right] \quad \text{and} \quad M(t_{max}) = 0.31 \cdot \frac{E_0}{E_c} \cdot \left[ \ln \left( \frac{E_0}{0.37 \text{MeV}} \right) - 0.37 \right]^{-\frac{1}{2}}
$$

(6.17)

Basic estimates of the instantaneous and average beam load on a dump can already be done with the instructions given above in order to select the appropriate material for the given case. For a given material, the size of the dump will be determined by its energy capability. An estimate of the length $L_{99\%}$ and the radius $R_{99\%}$ of a homogeneous cylindrical absorber, which captures about 99% of the primary beam energy, is given by the radiation length $X_0$ and the critical energy $E_c$ of the absorbing material as, Eq. (6.18):

$$
R_{99\%} \approx 5 \cdot R_M \approx 5 \cdot \frac{212 \text{MeV}}{E_c} \cdot X_0 \\
L_{99\%} \approx \left[ 1.52 \cdot \ln \left( \frac{E_0}{1 \text{MeV}} \right) - 4.1 \cdot \ln \left( \frac{E_c}{1 \text{MeV}} \right) + 17.6 \right] \cdot X_0
$$

(6.18)

$R_M$ is the so called Molière radius, which characterises the radial shower extension and is independent of the beam energy $E_0$.

**PETRA IV Constraints and Absorber Materials**

The information above in combination with the PETRA IV parameters specifies the main points in the layout of a suitable absorber. The average load on the dump is low. For the swap-out case, not more than 100 W of average beam power is expected, as described above. Even for a heat source with small transverse dimensions, this can be extracted in a good thermal conductor without a large temperature gradient. For an average power dissipation $\frac{dP}{dz}$ with a radial round Gaussian distri-
The temperature drop \( \Delta T_{eq} \) between the axis of a cylindrical absorber and its circumference at \( r = R \) can be approximated as:

\[
\Delta T_{eq} = \frac{4P}{\pi \cdot \sigma} \cdot \frac{1}{\ln(1 + \frac{R^2}{2\sigma^2})} \tag{6.19}
\]

This analytical result is obtained when the transverse Gaussian is approximated by a so-called Grindhammer distribution. According to Eq. (6.16), the power density at the shower maximum in aluminium is about 1.6 W/cm² for \( E_0 = 6 \text{ GeV} \) and \( P_{\text{ave}} = 100 \text{ W} \), respectively.

The corresponding tolerable energy density will be named \( \Delta T_{\text{tol}} \). The tolerable temperature rise can be estimated from the cyclic strength limit \( \sigma_{\text{cycl}} \), and \( \Delta T_{\text{tol}} \) is derived via the specific heat of the material as, Eq. (6.20):

\[
tol(\Delta T_{\text{inst}}) = (1 - \nu) \cdot \frac{\sigma_{\text{cycl}}}{\alpha \cdot \beta \cdot \epsilon} \implies tol\left(\frac{dQ}{dm}\right) = \frac{\Delta T_{\text{inst}}}{T_{i} + tol(\Delta T_{\text{inst}})} \cdot c(T) \cdot dT \tag{6.20}
\]

Thus, the dump design is heavily dominated by an extremely high local instantaneous load, which can be reduced to tolerable levels by making the beam spot larger (optics, fast sweeping, etc.). Simply looking at the thermal consequences, the tolerable limit of the deposited energy density should not heat the material up to its melting point \( T_{\text{melt}} \), i.e.,

\[
\max \left(\frac{dQ}{dm}\right) \leq \int_{T=T_{melt}}^{T=T_{i}} c(T) \cdot dT,
\]

where a temperature-dependent specific heat is taken into account. Since average heating does not contribute, the temperature of the material before the beam pulse enters \( T_i \) is close to the ambient temperature, namely \( \sim 30 \text{ °C} \) in our considerations. Inhomogeneous heating is always accompanied by mechanical stress due to thermal expansion. This may lead to irreversible deformation, cracks and microfissures especially when applied cyclically, in which case an originally ductile material tends to get brittle due to long-term fatigue effects. We define \( tol(\Delta T_{\text{inst}}) \) as the tolerable instantaneous local temperature rise, which a material can withstand in a repetitive way without damage. The corresponding tolerable energy density will be

\[
tol(\Delta T_{\text{inst}}) = (1 - \nu) \cdot \frac{\sigma_{\text{cycl}}}{\alpha \cdot \beta \cdot \epsilon} \implies tol\left(\frac{dQ}{dm}\right) = \frac{\Delta T_{\text{inst}}}{T_{i} + tol(\Delta T_{\text{inst}})} \cdot c(T) \cdot dT \tag{6.20}
\]

In contrast to the negligible average issues, instantaneous cyclic load is the key problem. For a \( \beta_x(\text{ID}) \) = 6.9 m and \( \beta_y(\text{ID}) \) = 2.3 m, the PETRA IV emittance of \( \epsilon_x = 20 \text{ pm} \) and \( \epsilon_y = 4 \text{ pm} \) gives a beam size of \( \sigma_x = 12 \mu\text{m} \) and \( \sigma_y = 3 \mu\text{m} \). According to Eq. (6.14), the total fill of 1500 nC would create an absolutely intolerable energy density of \( \sim 1.3 \text{ MJ/g} \) at the surface of any absorber material. This is more than two orders of magnitude larger than the evaporation heat of aluminium, for example.

Absorbers, collimators or beam windows. The values of \( \sigma_{\text{cycl}} \) are valid for the pure material. Of course, some alloys might have larger values, but in the presence of neutrons and heat diffusion processes lead to new inter-metallic zones and grain boundaries, by which the properties degrade to those of the pure material just in the region around the highest beam impact.

A reasonable material selection follows from the last four rows in Table 6.26. The first of these demonstrates that even for a very dense material like tungsten, average load is not an issue, as was already emphasised...
Accelerators | Technical Subsystems

<table>
<thead>
<tr>
<th>Property</th>
<th>C</th>
<th>Al</th>
<th>Ti</th>
<th>Cu</th>
<th>Fe</th>
<th>W</th>
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<tbody>
<tr>
<td>$\rho$ (g/cm$^3$)</td>
<td>1.9</td>
<td>2.7</td>
<td>4.54</td>
<td>8.96</td>
<td>7.87</td>
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<td>$X_0$ (cm)</td>
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<td>3.6</td>
<td>1.44</td>
<td>1.76</td>
<td>0.35</td>
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<td>$E_c$ (MeV)</td>
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<td>40</td>
<td>24</td>
<td>19</td>
<td>21</td>
<td>8.2</td>
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<td>$T_{melt}$ (°C)</td>
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<td>660</td>
<td>1670</td>
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<td>1536</td>
<td>3380</td>
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<tr>
<td>c (J/(g K))</td>
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<td>0.9</td>
<td>0.55</td>
<td>0.4</td>
<td>0.47</td>
<td>0.13</td>
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<tr>
<td>$c_{melting}$ (J/g)</td>
<td>—</td>
<td>398</td>
<td>323</td>
<td>205</td>
<td>268</td>
<td>193</td>
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<tr>
<td>$c_{evaporation}$ (kJ/g)</td>
<td>—</td>
<td>10.9</td>
<td>8.8</td>
<td>4.8</td>
<td>6.3</td>
<td>4.4</td>
</tr>
<tr>
<td>$\lambda$ (W/(cm K))</td>
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<td>1.7</td>
<td>0.17</td>
<td>3.9</td>
<td>0.81</td>
<td>1.5</td>
</tr>
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<td>$\Lambda(t=10 \mu s)$ (µm)</td>
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<td>26</td>
<td>8.3</td>
<td>33</td>
<td>15</td>
<td>28</td>
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<tr>
<td>$E$ (GPa)</td>
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<td>70</td>
<td>100</td>
<td>120</td>
<td>175</td>
<td>350</td>
</tr>
<tr>
<td>$\alpha$ ($1 \times 10^{-6}$ K)</td>
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<td>26</td>
<td>8.2</td>
<td>17</td>
<td>12</td>
<td>4.5</td>
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<td>0.38</td>
<td>0.26</td>
<td>0.3</td>
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<td>3.9</td>
<td>9.3</td>
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<tr>
<td>$tol(\Delta T_{inst})$ (K)</td>
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<td>15</td>
<td>120</td>
<td>15</td>
<td>53</td>
<td>130</td>
</tr>
</tbody>
</table>

$\int_{30^\circ C}^{T_{melt}} c(T) \, dT$ (J/g) = 7300 J/g 570 J/g 900 J/g 420 J/g 700 J/g 430 J/g
$tol\left(\frac{dQ}{dm}\right)$, at $T_i = 30^\circ C$ (Eq. (6.20)) = 240 J/g 13 J/g 65 J/g 6 J/g 25 J/g 17 J/g

1 Sublimation, 2 compressive load, 3 tensile load

Table 6.26.: Comparison of dump-related material properties.

above. The last two rows give operation limits for pulsed energy impact. Here, graphite and titanium are excellent candidates, which is why they have been used for the exit window and the high-power beam dumps at the European XFEL [112], where average load ($\frac{dP}{dz}(t_{max}) \approx 2 \text{ kW/cm}$) is significant too. But if not necessary, one should avoid these materials and use more standard ones. As amongst the remaining metals none is very predominant, one should also take technological and radiological aspects into account. From this point of view, aluminium is a good choice. Especially for small beam spots, its non-negligible thermal diffusion helps if the beam abort is stretched over several revolution times. There are well-known aluminium jointing techniques with stainless-steel (flanges) available, and aluminium is used in vacuum systems and easy to machine. In addition, it still has a rather low atomic mass, which, especially compared to copper, leads to less total and less long-lived radioactivity.

Therefore, the conceptual design of the required PETRA IV dumps is based on aluminium as absorbing material. The 6 GeV shower in aluminium has a multiplicity of 22 at its maximum, which is located in a depth of 36 cm. A 99% shower capture requires a 1.4 m long cylindrical aluminium absorber with a diameter of 47 cm, since the Molière radius is 4.7 cm.

Emergency Dump

Figure 6.75.: Horizontal cut of the PETRA III dump chamber. Dimensions in mm.

Getting rid of the total fill safely before a significant beam loss might damage machine components is not a new challenge at PETRA IV. At PETRA III, the total fill has a factor of two less intensity and the beam size is a little
larger than in PETRA IV, but the destruction potential is still immense. When the machine protection system detects a critical situation (magnet trip, orbit deviation in the undulator, etc.), it triggers the RF to be switched off. At the place where the PETRA III optics offers a dispersion of \( D_x = 0.8 \text{ m} \), a special aluminium vacuum chamber with a reduced horizontal aperture is installed (cf. Figure 6.75).

The beam size is about \( \sigma_x \approx 1.2 \text{ mm} \) due to an energy spread of \( 1.5 \times 10^{-3} \) and \( \sigma_y = 10 \mu\text{m} \) as a result of \( \beta_y \) and \( \epsilon_y \). According to Eq. (6.14), such a spot size would lead to an instantaneous energy deposition at the surface of roughly 2 kJ/g, which is sufficient to heat the chamber material up to the melting point and still has overhead for the phase transition rigid→liquid. However, two major effects have to be considered in addition: heat diffusion and energy capture.

**Figure 6.76.: Temporal development of RF voltage and beam current during an emergency beam dump in PETRA III.**

Fortunately, the beam is not lost in one turn, because the relative energy loss per turn is about \( 1 \times 10^{-3} \), which is comparable to the energy spread of the beam. The bunch, which just passed the dump chamber already very close but without touching it, arrives there in the next turn with a horizontal displacement of \( \Delta x \approx 0.8 \text{ mm} \). Thus, the beam is not scraped continuously, but each single bunch hits the dump chamber successively in vertical slices of horizontal width \( \Delta x \). This means that, within three to four turns (~30 \( \mu \text{s} \)), the major part (FWHM) of the Gaussian beam profile has been lost. This is confirmed by Figure 6.76, where the transient signals of the cavity voltage and the beam current are recorded, as done regularly for every alarm event. After the RF is switched off, the beam current still remains completely in the machine until it has reached the edge of the chamber. From then on, the beam is completely lost within ~50 \( \mu \text{s} \), which accounts for the total beam width and not just the major fraction as estimated above. The small vertical energy deposition profile in particular widens significantly by heat diffusion during the 30 \( \mu \text{s} \) period of substantial energy impact. This effect corresponds to an effective vertical beam size for instantaneous impact of \( \sigma_y,\ eff \approx 35 \mu\text{m} \) and reduces the energy density by a factor of 3.5 to about 570 J/g.

The PETRA III dump chamber is not a real dump, it should more correctly be called collimator or even spoiler. First, its length is far too short compared with the longitudinal shower size. A 30 cm long aluminium absorber captures no more than 35% of the primary 6 GeV electrons. In addition, a lot of energy escapes laterally, and overall, something like 10% is deposited in the dump chamber only. Thus, the maximum energy density stays below 100 J/g and the dump chamber survives. The major fraction of the whole fill is lost somewhere else in the machine, however, and because the escaping or strayed particles have a wide angular distribution, these losses do no harm. Since the PETRA III RF is switched off in case of a severe alarm, a failure of the fastest system in the machine, namely the RF, is covered intrinsically. In addition, the concept of an internal “dump” is the most reasonable strategy for an emergency abort system. Otherwise, the transfer line to the external dump must allow beam acceptance for all variants and combinations of failure modes, which seems fairly difficult to realise. Furthermore, pulsed systems, which may fail just when required, have to be introduced. Still the question of how to blow up the beam size remains and can hardly be solved by a huge betatron function. The well-proven PETRA III concept should thus be adapted for PETRA IV as well. Fortunately, although not foreseen originally, a dispersive section can be introduced in one of the straight sections of PETRA IV. Its layout will be described in more detail at the end of this section, but a dispersion of \( D_x = 0.22 \text{ m} \) can be achieved with tolerable effect on the key performance – the emittance.

For a PETRA IV energy spread of \( 0.7 \times 10^{-3} \) (all IDs open), one gets \( \sigma_x = 150 \mu\text{m} \), while the vertical size is still tiny (\( \sigma_y \approx 3 \mu\text{m} \)). The resulting energy density from Eq. (6.14) is
~107 kJ/g, which is far from being a satisfying solution. Hence, a fast vertical sweep should be introduced to decrease the impinging particle density. This can be realised using a closed vertical kicker bump, e.g. with a full sine pulse shape that fits to the time period over which the beam is lost at the corresponding dump chamber edge. By that means, the beam will be distributed almost linearly in the vertical direction within the sweep length $L_{\text{sweep}}$. The vacuum system of PETRA IV is proposed to have a round aperture with a diameter of 20 mm. The horizontal edge should be positioned as far as possible towards the beam axis, but without any conflict in terms of aperture required for machine operation. In the process of the technical design, more detailed simulations have to be carried out to check whether the beam can be safely stored within the time between RF off and beam arrival at the chamber edge. If necessary, a horizontal kicker bump has to be introduced to shorten this period. The aperture of the dedicated dump chamber could be of rectangular shape with a height of 20 mm. This is why a vertical sweep of ±10 mm, i.e. $L_{\text{sweep}} = 20$ mm, is assumed here. Applying a linear vertical sweep to a transverse Gaussian distributed beam leads to a new distribution function $f_{\text{sweep}}$ (normalised particle distribution per unit of area), which has its maximum in the central part of the sweep axis. For the case $\sigma_y \ll L_{\text{sweep}}$, the maximum of $f_{\text{sweep}}$ can be analytically estimated as, Eq. (6.21):

$$
\max(f_{\text{sweep}}) = \frac{1}{\sqrt{2\pi} L_{\text{sweep}} \sigma_x} \Rightarrow \max\left(\frac{d^2 q}{dz^2}(z = 0)\right)_{\text{sweep}} \approx 0.08 \text{ J/g} \cdot \frac{|mn^2|}{\sigma_y L_{\text{sweep}}} \cdot \frac{\sigma_y}{\sigma_x} \quad (6.21)
$$

As a result, the maximum energy density at the surface of an aluminium dump chamber at a dispersive position with $D_x = 0.22$ m and a 20 mm linear sweep has a safe value of 40 J/g when hit by the total fill of 1500 nC. This is equivalent to the load of a non-swept round Gaussian beam with $\sigma = 1.1$ mm. This spot is not small any more compared to the transverse shower profile, and therefore, the position $t_E$ of the maximum energy deposition will develop deeper in the material.

From existing 4 GeV shower simulations [113] with the Monte Carlo code MARS [114] for aluminium-based beam absorbers in the context of the European XFEL dump layout, we know that $t_E(4 \text{ GeV}, \sigma = 1.1 \text{ mm}) \approx 13 \text{ cm}$ and $\frac{d^2 q}{dz^2}(t_E) = 103 \text{ J/g}$. In a rough approximation, the situation for a 6 GeV electron beam is stretched in length by a factor of $\frac{t_E(6 \text{ GeV})}{t_E(4 \text{ GeV})} \approx 1.13$, and the particle density scales with $\frac{\mathcal{L}(t_{\text{max}}, E_0 = 6 \text{ GeV})}{\mathcal{L}(t_{\text{max}}, E_0 = 4 \text{ GeV})} \approx 1.45$. Therefore, the maximum load in the emergency dump is located at a depth of $t_E \approx 15$ cm and has a value of about 150 J/g. This is a conservative estimate because the effect of poor shower capture is not included. Dilution contributed by thermal diffusion is negligible due to a comparatively large beam size in both planes. Without taking the non-captured energy effect into account, a value of 570 J/g at the existing and reliably working PETRA III dump chamber has to be compared with a much safer amount of 150 J/g as derived for the PETRA IV case. Therefore, the presented concept for an emergency abort system at PETRA IV is regarded as well feasible. For a more clean dump, a round-aperture collimator can be installed downstream in the long drift behind the dump chamber in order to catch stray and secondary particles, which would not make another turn.

**Beam Preparation for the Emergency Beam Dump**

The emergency beam dump scheme of PETRA IV will be based on the dump concept of PETRA III, i.e. a combination of turning off the RF voltage and locating the beam absorber in a high-dispersion point to increase the horizontal amplitude at the absorber face. But due to the dimensions of the beam stored in PETRA IV, additional modifications have been made to ensure the feasibility of such a scenario. First of all, a dispersion bump of 0.22 m has been introduced in one short straight section to increase the horizontal beam size (cf. Figure 6.77). Such dispersive section is produced by a chicane composed by four soft bending magnets of 20 mrad of bending angle each one and 600 m of bending radius. The aluminium
A detailed description of that scheme is given. Extrapolating from 4 GeV shower calculations by a 6 GeV beam pulse of 20 nC with a size ing Eq. (6.20), which is function or non-function must either stop the correct functioning can be monitored. Any malfunction or non-function must either stop the train is ejected towards the swap-out dump, its stored in citation has to start several 10 turns before the end of this section. Since the kicker extraction is required. Such a blow-up can be achieved by means of a kicker-induced emittance growth of the bunch train that is going to be extracted. A detailed description of that scheme is given at the end of this section. Since the kicker excitation has to start several 10 turns before the train is ejected towards the swap-out dump, its correct functioning can be monitored. Any malfunction or non-function must either stop the ejection or trigger the emergency dump system. Otherwise, the swap-out dump is at risk of being hit by a too tiny and thus destructive beam. However, with the correct preparation, the beam can be directed onto an aluminium-based dump, which may be located in a dedicated extraction line. A detailed layout will be done in the scope of a technical design report, but the dump in the so-called bunch compressor section 2 (BC2) at the European XFEL serves as a very good reference of what such a device would look like. It is designed for a ~600 µs long pulse train of up to 3000 nC at 4 GeV and sketched in Figure 6.78. From the thermal point of view alone, this dump can withstand up to 10 kW of average beam power, but because of limited space in the European XFEL tunnel, the heavy-concrete shielding is poor, and thus air activation determines the upper beam power limit for long-term operation of the dump.

The absorber itself consists of a sub-assembly unit that can be manufactured to fulfill the vacuum specifications of a Class 100 system. It combines the aluminium beam pipe with the first part of the aluminium core, which can be regarded as a thick exit window. The stainless steel (sS) vacuum flange is attached to this chamber via an explosion-bonded sS–Al bimetal. The length of the first aluminium core segment guarantees that one single shot with a pencil-sized but fully charged train creates a very safe energy density of $\leq tol \left( \frac{dQ}{dm} \right)$ at the end of this segment. Thus, one single train with a too tiny spot size will not burn a hole through the thick “window” and hence does not create a vacuum leak. This is important, e. g. when a non-blown-up bunch train is ejected due to spontaneous firing or wrong timing of the extraction kicker. The length of this first aluminium core segment may also be shortened by about 20 cm for the 6 GeV / 20 nC case. Some other modifications for PETRA IV use are advisable. Due to the relatively low average power, water cooling might be obsolete, which makes the system more passive and thus more reliable. The outer copper surface has an area of at least $ACu \geq 0.6 m^2$. For unforced convective air cooling, the heat transfer coefficient at smooth surfaces is about $\alpha \approx 5.6 W/(m^2K)$, resulting in a temperature drop of 35 K between surface and ambient air if 100 W
have to be dissipated. In principle, this looks promising, but has to be discussed in detail in light of the shielding constraints at the final location. The overall length of the swap-out dump will not differ much from the BC2 layout. The radial layout is independent of the energy and might shrink only if the required vacuum pipe aperture is less than in the BC2 design.

Beam Preparation for the Swap-out Beam Dump

As shown in Figure 6.26, a swap-out beam dump scenario is proposed to extract and dump the PETRA IV beam. Before the extraction, the transverse beam size of the stored beam can be increased by applying a kick in both planes. After the kick, the transverse beam size blows up quickly during the following turns, which can greatly dilute the energy density of the beam before the swap-out extraction. According to the Eq. (6.14), the deposited energy density for a Gaussian beam distribution is inversely proportional to the transverse beam size. Figure 6.79 shows the transverse beam size normalised with the initial beam sizes of the stored beam for different values of kicks (0.04 mrad, 0.08 mrad and 0.1 mrad) as a function of the number of turns. The initial beam sizes considered are $\sigma_x^0 = 19.4 \mu m$ for the horizontal plane ($\beta_x = 21.6 m$) and $\sigma_y^0 = 3.8 \mu m$ for the vertical plane ($\beta_y = 3.7 m$). The simulations take into account 1000 particles, 4 pm rad vertical emittance and the other values from Table 6.2. A kick of 0.1 mrad in both planes is sufficient to increase the transverse beam size by more than three orders of magnitude, as required for the operation of the dump.

6.3.13. Timing System

The timing system of the future PETRA IV accelerator and its pre-accelerator chain will be implemented in MTCA.4 technology. The main capabilities of the envisaged timing system will include
• Distributing a continuous reference RF signal generated by a unique, stable master oscillator to drive local, low-noise oscillators

• Deducing continuous timing signals (e.g. synchronous to PETRA IV revolution frequency or bunch repetition) for synchronisation purposes (e.g. available at the backplane of the MTCA.4 crate to trigger ADC boards)

• Providing trigger events (e.g. beam injection, beam ejection, beam swap-in/out, beam dump, LINAC II pulse, start/stop of DESY IV ramp-up) according to the designated beam mode if applicable

• Providing beam-synchronous data such as
  – Unique time stamp (with microsecond accuracy),
  – Unique beam pulse or beam revolution counter numbers, respectively,
  – Designated beam mode,
  – Designated bunch pattern,
  – Most-recently measured bunch currents,
  – Number of bunch train to be replaced by the next swap-in/out action.

The timing system will come with the following features, including

• Integration into the accelerator control system,

• Dynamically configurable,

• Flexible and fast pulse-synchronous beam mode switching,

• Embedded simulation or test mode,

• Low-jitter RF and timing references,

• Path length compensation algorithm for reference RF signals (e.g. to compensate for local temperature changes),

• Dedicated fibre network,

• Common timing interface for both accelerator (e.g. beam position monitors) and beamline components (e.g. photon detectors).


As at PETRA III, beam-stabilising systems will also have to be installed at PETRA IV in order to achieve the desired beam currents and the required orbit stability. Active damping of coupled mode oscillations will be achieved by multibunch feedback systems that operate in the longitudinal and transverse directions. A fast orbit feedback system will be installed in order to stabilise the beam trajectory in the transverse planes against perturbations in the range of 1 kHz down to daily drifts. The structure and principle operation of the PETRA IV beam stabilisation systems are based on many years of experience with PETRA III operation. What is new at PETRA IV is mainly a more advanced technology with increased processing bandwidth and expanded capabilities for real-time analysis of the running processes.

Multibunch Feedback Systems – MBFB.4

The high availability and robustness of the systems for PETRA III show that the basic signal processing and the mechanisms for achieving long-term stability should also be used for PETRA IV. Phase drifting of the reference frequencies, for example due to temperature influences, are locally compensated by means of beam signal coupling with phase-locked loop (PLL) techniques. The challenge consists mainly of porting the systems to the modern and commonly used MTCA.4 platform. In addition, the required processing bandwidth is doubled compared to the previous versions.

Transverse MBFB

The intended minimum bunch spacing in PETRA IV is 4 ns, resulting in a minimum required system bandwidth of 125 MHz. Automatic beam offset compensation and suppression of revolution harmonics using 180° hybrids are used for analogue pre-processing of the BPM signals. The beam oscillation detector will be realised as a MTCA.4-compatible device. Its two-stage automatic gain control optimises the input level for direct to baseband mixing. Digital signal conversion and processing are then performed using another MTCA.4 module. Its functionality includes all functions such as phase and delay adjustments, signal analysis, mode damping and tune measure-
ment etc. PCIe bus and direct memory access (DMA) technology enables fast data transfers within the MTCA.4 crate. The CPU module, running a Linux operating system, provides further functional analysis and connection to the control system.

**Longitudinal MBFB**

Multibunch phase oscillation detection is done by baseband mixing with the machine RF. Unlike the signal processing for the transverse planes, due to the small momentum compaction factor in PETRA IV, down-sampling methods must be implemented to process the longitudinal multibunch modes. The eight feedback cavities used for PETRA III with a resonant frequency of 1375 MHz can be reused in PETRA IV. However, they must be adjusted according to the modulation method, either double-sideband (DSB) or single-sideband (SSB) modulation.

**Fast Orbit Feedback - FOFB.4**

Fast orbit feedback systems are essential for fourth-generation light sources. In the case of PETRA IV, over 700 BPMs will generate twice as many position data streams. About 200 fast corrector coils are required to stabilise the beam at all photon beamlines. All digital data transfers will be synchronous to the machine's revolution frequency to provide shortest latency and best signal purity. The topology of the FOFB will again be a star structure. Thanks to the centralisation, minimal processing latency and maximum flexibility in terms of the modifiability and adaptability of the algorithm can be provided. Compared to PETRA III, the expected input spectrum of position perturbations remains almost unchanged. Influences synchronous to the mains frequency and its harmonics will be compensated up to 600 Hz. This will require vacuum pipe material with $\mu_r < 1.05$ at the corrector coil positions.

Position detector electronics will be realised as MTCA.4 boards. The goal is to create an ultra-compact design with fast interfaces (PCIe and DMA), such that eight detector modules will fit into one MTCA.4 crate. Three of these per rack would result in about 30 monitor racks, which seems feasible. At the location of central processing, a further reduction and conversion of optical data lines is carried out by means of a separate MTCA.4 crate. By this, high-speed serial electrical data links with a total of approximately 8 Gbit/s, suitable to feed into the processing unit, will be produced. Reversely, after processing, serial data streams are generated, to be distributed to digital current source amplifiers that will finally feed fast corrector coils.

**6.3.15. Accelerator Controls**

DESY has long-time experience in operating control systems for large-scale accelerators (synchrotrons, linear accelerators). The development and implementation of the future PETRA IV accelerator control system will be embedded in a long-term process to consolidate the whole accelerator control system landscape at DESY and to take advantage of...
synergies between the accelerator facilities operated by DESY.

The features of the control system envisaged for PETRA IV can be derived from functional requirements (e.g. turn-by-turn data acquisition capability, use of the high-end hardware interface standard MTCA.4) and non-functional requirements (e.g. operation experience gained at PETRA III, general fast and dramatic technological changes with respect to hardware and software). Prominent features include

- Use of up-to-date software technologies,
- Extensible and scalable architecture,
- High performance and reactivity,
- Thorough and consistent status monitoring and error handling capability,
- Up-to-date IT security level,
- Use of common open standards and technologies as far as possible or applicable.

Past experience shows that exchanging relevant data concerning e.g. undulator control or beam diagnostic between accelerator and beamlines is essential for both accelerator and photon detector operation. The envisaged accelerator control system of PETRA IV will be capable of interfacing the beamline control system appropriately.

**Quality Management**

The constantly increasing and demanding requirements concerning availability and maintainability will necessitate the establishment, revision, strengthening and optimisation of workflows at various levels, including

- Software development, e.g. unit testing, continuous integration and deployment, code review,
- Simulation (Virtual PETRA IV), e.g. integration tests, exploring dependencies and scalability,
- Operations, e.g. remote inspection, debugging and monitoring, data-based performance evaluation, preventive maintenance and failure analysis.

**Configuration Management**

In order to ensure reproducibility and consistency, a central repository will be established, holding a comprehensive set of configuration data including

- Device-specific data (e.g. hardware addresses, calibration data, limits),
- Data related to accelerator operations (e.g. set-up files, measured references),
- Data generated by the software development and release workflow (e.g. software versions, application building and deployment details).

**Hardware Interfaces**

In general, the hardware interfaces for triggered, high-performance applications (e.g. beam diagnostics, injection/ejection system, feedback systems, timing/synchronisation system, machine protection system, RF control) will be compliant with the high-end MTCA.4 technology. MTCA.4 has been the long-term standard for the DESY accelerators and is enjoying growing popularity within the accelerator community and the related industry. The operating system for server hosts running within the MTCA.4 platform will be Linux.
Likewise, the hardware interfaces for conventional slow-control applications (e.g. magnet power supplies, vacuum system) will be compliant with industrial process control standards, preferably providing a well-established and widely used industrial application programming interface (API).

**Data Acquisition and Data Warehouse Service**

A data acquisition and data warehouse (data storage, online/offline data processing) service will be implemented with domain-specific interface standards and technologies. The time resolution capability of the data acquisition service will cover a wide range, being able to handle static data (e.g. calibration data), less-frequently varying data (e.g. vacuum pressure values) as well as clock-synchronised bunch-by-bunch (single-turn) and turn-by-turn data (e.g. beam positions) to serve the initial use cases of the users of the PETRA IV facility. Train-by-train or full bunch-by-bunch time resolution might be requested by future users and implemented at a later stage.

The data warehouse service will be organised according to the needs of the data acquisition applications, i.e. snapshot archive, slow archive and fast archive, and will provide the appropriate API. Particular emphasis will be placed on the capability to support data science applications operated in either online (e.g. learning feedbacks, learning tuning procedures) or offline (e.g. failure prediction, predictive maintenance forecast) mode.

**High-Level Control Applications**

Based on encouraging experience at DESY with the commissioning and operation of the European XFEL, a team of control experts and accelerator physicists will be established to

- Interface specific needs of beam commissioning and operations,
- Collect, assort and manage requirements,
- Implement corresponding tools and applications.

Up-to-date languages for fast prototyping and scripting (e.g. Python, MATLAB) will be supported. Resulting applications intended afterwards for regular standard operations will be transformed into well-behaved operator panels or server applications.

**6.3.16. Radiation Safety and Interlock Systems**

**Radiation Safety**

The shielding of the PETRA IV storage ring is built in such a way as to ensure total containment of the primary electrons in the storage ring tunnel. The storage ring shielding is designed to absorb both primary electrons and their secondary radiation. The optics hutch shielding in turn will block bremsstrahlung and its secondary radiation only. The schematic layout of the tunnel cross section in the Max von Laue hall is shown in Figure 6.82. The details for the shielding calculations can be found in [1]. Any loss of primary electrons in the optics hutch must be safely prevented. The relevant technical components are several dipole magnets located in the photon beamline downstream of the insertion device (cf. Figure 6.83). A failure of one or several dipole magnets in the electron storage ring will cause a loss of the stored beam. To ensure that a further injection into the storage ring cannot lead to a loss of primary electrons in the optics hutch either, a permanent dipole magnet is located in the photon beamline, deflecting all primary particles. The permanent magnet fields will be measured once a year to ensure their integrity.

![Figure 6.82: Cross section of the tunnel in the Max von Laue hall and the optics hutch.](image)

The main parameters relevant for radiation protection are the electron energy of 6 GeV, the maximum beam current, corresponding to the maximum number of circulating electrons, and the beam lifetime. The parameters for the
different operation modes of PETRA III and PETRA IV are summarised in Table 6.27. The total number of electrons $N$ in the storage ring is decaying according to:

$$N = N_0 \exp(-t/\tau),$$

where $N_0$ is the initial number of electrons and $\tau$ the beam lifetime. The corresponding loss rate is:

$$-\frac{d}{dt}N = \frac{1}{\tau}N.$$

An operation time of 6000 h per year is assumed. A simplified assumption of equal operation time in each mode yields $1.5 \times 10^{16}$ lost electrons per year for PETRA III and $2.5 \times 10^{16}$ lost electrons per year for PETRA IV from the stored beam. If a very pessimistic transfer efficiency of only 50% is assumed, one has to double the lost electrons per year. In the worst-case scenario, all electrons are considered to be lost within a length of 115 m (or 5% of the circumference), as opposed to losses being equally distributed around the ring. This scenario corresponds to a typical local loss rate of $1.5 \times 10^{15}$ lost electrons per year for PETRA III and $2.5 \times 10^{15}$ lost electrons per year for PETRA IV. Measurements at PETRA III have shown that a loss rate that is about a factor of four or five higher than the typical loss rate is still tolerable from a radiation protection point of view. Therefore, the PETRA IV storage ring can be safely operated based on the parameters listed in Table 6.27. Even a lifetime of only 0.5 h in the timing mode of PETRA IV would just be tolerable.

The location of the beam dumps has not yet been finalised. The frequently used beam dump for the swapped-out beam will be inside the heavily shielded booster tunnel. Detailed calculations for the dump area will be part of the technical design.

Personnel Interlock Systems

A personnel interlock system has to be built to provide safety functions that secure radiation-restricted areas in order to protect personnel from ionising radiation created by accelerator components, such as RF cavities. In case of danger, the safety functions have to switch off all relevant radiation-producing devices. Additionally, the personnel interlock system will provide safety functions for the safe operation of magnets. The specification of each safety function and its requirements regarding the safety integrity level (SIL) will have to be determined during a risk assessment process. From previous experience, we know that these kinds of safety functions typically require SIL values of two to three. This already places requirements on the components that comprise parts of the safety functions, e.g. beam shutters and modulator conductors or switches. In order to reach high SIL values, it seems necessary to use SIL-certified components as much as possible. This also holds for the implementation of the safety function logic. To combine SIL-certified components with the long-standing experience with relay-based interlock systems we have at DESY, a hybrid so-
### Table 6.27: Typical parameters for radiation protection.

<table>
<thead>
<tr>
<th>Design parameter</th>
<th>PETRA III</th>
<th>PETRA IV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy / GeV</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>Operation time per year / h</td>
<td>6000</td>
<td>6000</td>
</tr>
<tr>
<td>Operation mode</td>
<td>Continuous Timing</td>
<td>Brightness Timing</td>
</tr>
<tr>
<td>Total current / mA</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>Total number of electrons / $1 \times 10^{12}$</td>
<td>4.8</td>
<td>4.8</td>
</tr>
<tr>
<td>Number of bunches</td>
<td>960</td>
<td>40</td>
</tr>
<tr>
<td>Beam lifetime / h</td>
<td>20</td>
<td>1.5</td>
</tr>
<tr>
<td>Loss rate / $1 \times 10^{16}$/year</td>
<td>0.2</td>
<td>2.8</td>
</tr>
</tbody>
</table>

A solution may be considered, e.g., a two-channel safety programmable logic controller (PLC) plus one channel implemented using relay modules. This architecture would be similar to the solution used at the LHC.
6.4. Technical Risks

From the present point of view, there is no unmanageable technical risk for the civil construction, including the new experimental stations and those to be reconstructed. DESY has many years of experience in performing such tasks and a similar project has already been successfully implemented at DESY in the context of PETRA III. A big technological step forward will be taken in terms of the storage ring construction. The very tight alignment tolerances in the range of 30 µm for the magnets on the girders and 100 µm for the girders relative to each other are a significant challenge for a large-scale facility with a circumference of 2.3 km. The current conceptual design of the new storage ring takes into account the experience at the first fourth-generation synchrotron radiation source MAX IV in Lund, Sweden, that is in operation since mid 2016, the EBS project at the European Synchrotron Radiation Facility in Grenoble, France, that is currently in the construction phase, and the upgrade of the Advanced Photon Source near Chicago, USA, that is currently in the technical design phase. Until the concrete implementation of the PETRA IV project, additional similar projects will be carried out, e.g., SIRIUS, Brazil, SPring8-II, Harima, Japan, or HEPS, Beijing, China. Through continuous exchange with colleagues from these facilities in the context of joint meetings and through exchange of personnel it shall be ensured that know-how developed at other locations will be included into the PETRA IV project, thus minimising the technical risks.

6.4.1. Risk Management

The ambitious performance goals of the PETRA IV machine are approaching the limits of the present state-of-the-art of accelerator physics and technology. Therefore, considerations of risks in this highly complex project are mandatory. The risk of serious conceptual flaws is counteracted very efficiently by thorough analyses and detailed studies performed by the accelerator design team. A continuous exchange with other colleagues in the worldwide accelerator community and with DESY’s Machine Advisory Committee (MAC) are extremely valuable to avoid overlooking design mistakes or missing opportunities for further design optimisation. Participation of team members in workshops and conferences related to low-emittance storage rings as well as in advisory committees of other projects are also particularly helpful in this respect.

Technical risks can already be mitigated early on in the project preparation phase by relying on existing, proven technology (at DESY or at other labs) or by building and testing prototypes of the most critical components of the machine. For larger volume procurements in the construction phase, pre-series component fabrication and tests are necessary to safely avoid technical flaws for the larger-scale series.

6.4.2. Design Risk Mitigation

The major challenge for the reconstruction consists of modification of the magnet arrangement and therefore the beam optics in the arcs of the PETRA ring. The aim is to obtain a horizontal emittance that is almost two orders of magnitude smaller than the emittance of the PETRA III storage ring operated today. The main risks here are in conceptual design flaws of the new facility, including the injector complex, the storage ring lattice, current limitations due to collective effects. The risk mitigation strategy to avoid design flaws has focused on the storage ring optics and beam instabilities.

Beam Optics

The risk of serious conceptual flaws is mitigated by thorough analyses and detailed studies performed by the accelerator design team. Specifically, the risk mitigation strategy for design flaws includes: usage of different simulation tools, collaborations within the accelerator community, benchmarking of the simulations against existing accelerators, and dedicated machine studies at PETRA III. Beam steering algorithm will be tested at PETRA III. New methods to detect optics errors have already been studied in 2019 in collaboration with CERN.
Instabilities
The risk mitigation strategy related to beam instabilities is based on a risk analysis of the PETRA IV impedance model as well as tests and measurements at PETRA III. The required single bunch current for the PETRA IV timing mode is at least 1 mA per bunch. The peak current of the bunch is significantly reduced with a harmonic cavity system. Together with high chromaticity we found the timing mode is possible. However, the conclusion depends on the impedance model represented in the CDR. To mitigate the uncertainty embedded in the impedance model we also analyse the conditions to deliver an intensity of 2 mA per bunch. By increasing or decreasing the transverse impedance by a factor we learned that an increase of the impedance of up to 40% from the current model (see Figure 6.84) can be tolerated. With this we allocate the impedance budget in three major categories as shown in Table 6.28. The small aperture of round chamber was the first risk we considered down to 17 mm from 20 mm. Then the undulator chambers of 6-mm gap chambers were allowed to increase by 30%. Finally, the geometric impedance of unknown components can be added to the model with up to a 40% increase in the magnitude.

Figure 6.84.: The single bunch current limit as a function of impedance factor with the lattice chromaticity at 5.

The reliability of the PETRA IV impedance analysis can even be improved further by updating/refining the impedance model for PETRA III and a comparison of the results with measurements. If resources permit, a very valuable preparation for the PETRA IV project would be to build a prototype 3rd harmonic RF system, install it in PETRA III and test bunch lengthening/low synchrotron frequency at 3 GeV beam energy where the 1st harmonic voltage can be strongly reduced. The possibility of this approach will be assessed and depends on funding availability.

6.4.3. Technical Risk Mitigation
The risk mitigation strategy is based on two pillars: (1) building and testing of prototypes and (2) the possibility of testing prototypical PETRA IV components or diagnostic, correction concepts, and controls with beam in the PETRA III ring and the present injector complex. The risk mitigation strategy is covering all subsystems of PETRA IV, including:

Magnets
Most of the magnets for PETRA IV do not have significantly higher strengths than the ESRF-EBS magnets. Therefore prototype magnets could be purchased from the ESRF-EBS production manufacturers for test purposes. Nevertheless, a few quadrupole and all sextupole and octupole magnets are significantly stronger than those used at the ESRF-EBS and therefore prototypes will be built and tested. Critical skills related to magnet design and measurements will be developed by the magnet group at DESY. This will include the establishment of collaborations with laboratories and institutes with strong magnet capabilities, and the hiring of additional personnel.

Alignment and Stability
The risk mitigation for this important topic is based on the experience at PETRA III [63] and the European XFEL, where a precise fiducialisation was achieved for the undulator section quadrupoles. Based on the experience, a precise (few µm) fiducialisation of magnets will be developed and tested. Girder prototypes will be developed and magnet alignment on them will be tested extensively, including transport into the tunnel and verification of the alignment after transport. Furthermore, studies will be performed to investigate the stability of the PETRA III tunnel. Tests of the temperature stabilisation of a section of the PETRA III tunnel for mitigation of tunnel floor motion have al-
Table 6.28.: Impedance Budget at Chromaticity 5.

<table>
<thead>
<tr>
<th>Impedance</th>
<th>Normalised</th>
<th>Risk Analysis</th>
<th>Increase</th>
<th>Budget</th>
</tr>
</thead>
<tbody>
<tr>
<td>RW (Ring)</td>
<td>0.286</td>
<td>20.6 smaller aperture (17 mm)</td>
<td>63</td>
<td>0.47</td>
</tr>
<tr>
<td>RW (ID)</td>
<td>0.701</td>
<td>50.3 smaller gap NEG surface</td>
<td>30</td>
<td>0.91</td>
</tr>
<tr>
<td>Geometric Impedance</td>
<td>0.404</td>
<td>29.1 unknown elements</td>
<td>40</td>
<td>0.56</td>
</tr>
<tr>
<td>Total</td>
<td>1.390</td>
<td>100</td>
<td>40</td>
<td>1.94</td>
</tr>
</tbody>
</table>

ready started and will be intensified during the TDR phase.

**Power Supplies and Utilities**
The requirements for a single power supply are quite similar to the ESRF-EBS and most of the components are available from industry. DESY has long experience in building high reliability power supplies for large machines as HERA, PETRA III, and the European XFEL. The challenges are the large number of power supplies and the demanding reliability requirements for this system. The mitigation strategy is based on the implementation of redundant power supplies in connection with a hot swap switching mechanism between power supplies. This system will be prototyped at an early stage of the project. Furthermore, a close collaboration with the ESRF will be implemented.

**Vacuum System**
The concept for the PETRA IV vacuum system is based on compact NEG coated chambers without antechambers. The successful commissioning of the MAX IV facility has demonstrated the applicability of this concept to a compact storage ring. Any risk can be mitigated in the framework of collaborations with other institutes and tests at PETRA III, which have already started in 2019. There exists considerable experience at DESY with NEG coated wigglers and undulator chambers. The vacuum group has been operating a NEG sputtering facility for several years with capability of coating multi-meter long tubes. In 2019 about 50 m of dipole chambers were installed in the PETRA III ring to study activation properties of NEG coating surfaces.

**Radio Frequency System**
DESY has since its inception 60 years ago developed world leading expertise and experience in the operation of large scale RF systems in storage rings and linacs. The PETRA IV RF system will use 500 MHz cavities for the basic RF system (as for PETRA III) and 1.5 GHz cavities for the third harmonic system. The risk mitigation strategy is based on a collaboration with BESSY II and ALBA in connection with tests at PETRA III. It is planned to use single-cell 500 MHz cavities based on the design and operating experience at BESSY II. The RF power generation will be based on solid state transmitters which are available from industry. A test at DESY will be done at an early stage to mitigate risks related to this new technology. A similar approach is also planned for the third harmonic system.

**Beam Diagnostics**
The precise measurement of the beam size (emittance) at PETRA IV will be based on further developments of the beam size monitor at PETRA III. Tests at PETRA III will clearly mitigate the risk for PETRA IV. In 2019 it was demonstrated in a study period that PETRA III can provide beams with an emittance as low as 300 pm rad at a beam energy of 3 GeV, which was significantly lower than the emittance of 1300 pm rad at 6 GeV.

BPM prototypes will be built to investigate them on a test bench (including fiducialisation with stretched wire) and perform beam tests using PETRA III. For that purpose they should ideally be installed into a short section with a PETRA IV type vacuum chamber, installed at a suitable (sufficiently low-beta) position of the PETRA III ring.
6.5. Cost and Schedule Risk

Cost risks with regards to uncertainties of the cost estimates in the CDR and TDR phase are minimised by relying on DESY’s extensive experience with previous successful large-scale accelerator projects (in particular PETRA III and the European XFEL) and by using actual cost information obtained from other ongoing projects, especially the ESRF upgrade project. Early interaction with possible manufacturers and well-prepared tender procedures are essential for successful and economic procurements in the project phase. Tight supervision of the budgets and costs during the course of the project will be provided by the project office to ensure that deviations between planned and real costs, as well as accurate predictions of remaining costs, can be assessed at any point in time. Special attention will be given to issues with respect to cost estimates for the tender for civil construction as well as availability of construction companies, and for the procurement of rare earth materials for the manufacturing of magnets. Due to the boom in construction in the Hamburg area, many of the major civil construction companies are currently extremely busy. Thus, at the present time the market development for civil construction is hard to predict. The same holds true for the market of some raw materials. Here, the price fluctuations have been very significant in the past. A careful survey of the market, early engagement of the construction companies and early material procurement combined with ensuring ample contingency in funds and schedule will be pursued to minimise the risk here.

One important aspect of the mitigation of schedule risks is a tight follow-up on all critical milestones in all phases of the project. This includes the supervision of the manufacturers of accelerator components. Time critical decisions have to be scheduled early, e.g. civil construction approval for the new experimental hall by the local authorities. The organisation of the project and the applied tools and procedures for project follow-up, enable the project management to obtain a complete overview of schedule-critical issues at any point in time.

To mitigate the different risks discussed above, the PETRA IV Management Board will be supported by the PETRA IV project office. It will be the task of the project office to keep track of the different organisational, technical, and financial jobs in processing by the different work packages, to identify and report occurring issues of the project as soon as possible to the PETRA IV Management Board. In this way, the issues can be discussed and addressed finding solutions before they can delay the project. Another key aspect of the project office will be the dissemination of information between the different work packages keeping everyone working for the PETRA IV project up-to-date of all developments.
References


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[92] Instrumentation Technologies.


[104] Bergoz, Online.


7. Photon Beamlines

The methods enabling the novel science and technology case of PETRA IV described in Chapter 4 require a highly advanced beamline portfolio. Taking full advantage of the ultra-low emittance of the storage ring, the photon beamlines need to be optimised in all aspects, from the source over the optics and the sample environment to the photon detection and the data handling. The transition from the current beamline portfolio to that of PETRA IV will be managed taking into account both highest performance standards, in view of the science and technology case (cf. Chapter 5), and sustainability, in order to make optimal reuse of the existing infrastructure and instrumentation. This chapter presents the design concepts for the photon beamlines at PETRA IV.

In Section 7.1, we describe our strategy for developing the optimal beamline portfolio for PETRA IV. A detailed list of beamlines and experiments will be compiled in the TDR phase of the project, involving the user community and the advisory bodies of DESY.

7.1. Beamlines

PETRA IV will provide exceptional beam properties that will offer transformative experimental opportunities (cf. Chapter 3, Chapter 4 and Chapter 5). Compared to PETRA III, the ultra-low-emittance storage ring of PETRA IV imposes new boundary conditions on the photon beamlines. Most prominently, the number of sectors in the arcs changes from nine to eight, and substantial canting of the straight sections in order to increase the number of independent undulator stations is no longer compatible with the ultra-low emittance. This implies that most of the beamlines at PETRA III will have to be relocated. While this is a substantial task, it is also an opportunity to upgrade the beamline portfolio in view of both its scientific focus and the instrumentation. We plan to define the PETRA IV beamline portfolio during the TDR phase.

7.1.1. PETRA III Beamline Portfolio

Currently, at PETRA III, there are 15 straight sections for undulators distributed over three experimental halls (cf. Figure 7.1). To accommodate a large number of beamlines, most straight sections are canted, allowing for the independent operation of two independent beamlines from one straight section. Only four straight sections in the Max von Laue Hall and one in the Paul Peter Ewald Hall (Figure 7.1) are equipped with a single insertion device. In
Figure 7.1.: DESY with the existing PETRA III experimental halls: Paul Peter Ewald in the north, Max von Laue in the north-east and Ada Yonath in the east. The inset shows details of the beamline distribution. Red beamlines are located at straight sections of PETRA III that are long enough to accommodate IDs up to 10 m in length. The canting angle between closely neighbouring beamlines in the Max von Laue Hall is 5 mrad and scaled up a factor of 4 for better visibility. The canting in the other other halls is 20 mrad and correctly scaled.

All this allows for 25 independently operated undulator beamlines. Table 7.1 summarises the current beamlines at PETRA III.

For most beamlines, the available sector length is more than 100 m from the undulator source, allowing the installation of one to two optics and three to four experimental hutchs. One straight section can accommodate two canted beamlines by introducing a small bending magnet between two shorter insertion devices, separating their optical axes in angle. The optical axes of the canted beamlines are separated by 5 mrad and 20 mrad in the Max von Laue hall and the two extension halls (Paul Peter Ewald and Ada Yonath), respectively. Each canted insertion device (ID) can have a maximal length of 2 m. The two canted IDs in a straight section generate two independent X-ray beams that are guided to two individual experiment beamlines sharing the 100 m long sector. Therefore, each beamline has space for one optics and one to three experimental hutchs.

The beamlines (P01, P21 and P61) at the first straight section in each of the experimental halls are special. Their insertion device is located in the longer straight section preceding the respective arc, which provides special freedom. As a result, P01 is fed by a 10 m insertion device, P21 has two slightly canted devices, one of them being a 4 m in-vacuum undulator, and P61 is fed by a 40 m long damping wiggler. The opportunity to accommodate such exceptional insertion devices is unique to PETRA and can be exploited further for PETRA IV.

At beamline P02, two experiments share one undulator in parallel operation by branching off one beamline using a semitransparent Laue monochromator. As the deflected beam has to be operated at a fixed energy, the experiments cannot be operated completely independently. This solution may be adequate for some PETRA IV beamlines to increase the number of stations that can run simultaneously.
### Max von Laue Hall

<table>
<thead>
<tr>
<th>#</th>
<th>Name</th>
<th>Energy / keV</th>
<th>Undulator</th>
<th>$\beta$</th>
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<tbody>
<tr>
<td>P01</td>
<td>High Resolution Dynamics</td>
<td>5 - 70</td>
<td>U32-10 m</td>
<td>high</td>
</tr>
<tr>
<td>P02.1</td>
<td>Powder Diff. &amp; Total Scat.</td>
<td>60</td>
<td>U23-2 m</td>
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<td>Extreme Conditions</td>
<td>9 - 77</td>
<td>U23-2 m</td>
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<tr>
<td>P03</td>
<td>Micro &amp; Nano Focus X-ray Scat.</td>
<td>8 - 23</td>
<td>U29-2 m</td>
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</tr>
<tr>
<td>P04</td>
<td>Variable Polarization XUV</td>
<td>0.25 - 3</td>
<td>U65-5 m</td>
<td>high</td>
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<tr>
<td>P05</td>
<td>Imaging (HZG)</td>
<td>5 - 50</td>
<td>U29-2 m</td>
<td>low</td>
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<tr>
<td>P06</td>
<td>Hard X-ray Micro/Nano-Probe</td>
<td>2.4 - 100</td>
<td>U32-2 m</td>
<td>low</td>
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<tr>
<td>P07</td>
<td>High-Energy Mat. Sci. (HZG)</td>
<td>50 - 200</td>
<td>IVU21-4 m</td>
<td>high/low</td>
</tr>
<tr>
<td>P08</td>
<td>High-Resolution Diffraction</td>
<td>5 - 30</td>
<td>U29-2 m</td>
<td>high</td>
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<tr>
<td>P09</td>
<td>Resonant Scattering &amp; Diffraction</td>
<td>2.7 - 50</td>
<td>U32-2 m</td>
<td>high</td>
</tr>
<tr>
<td>P10</td>
<td>Coherence Applications</td>
<td>4 - 25</td>
<td>U29-5 m</td>
<td>low</td>
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<tr>
<td>P11</td>
<td>Bio Imaging &amp; Diffraction</td>
<td>2.4 - 30</td>
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<td>BioSAXS (EMBL)</td>
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<td>high</td>
</tr>
<tr>
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<td>Macromolec. Cryst. (EMBL)</td>
<td>5 - 20</td>
<td>U29-2 m</td>
<td>high</td>
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<tr>
<td>P14</td>
<td>Macromolec. Cryst. (EMBL)</td>
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### Ada Yonath Hall

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<tr>
<td>P21</td>
<td>Swedish Mat. Sci. BL</td>
<td>40 - 150</td>
<td>U29-2 m/IVU21-4 m</td>
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<td>P22</td>
<td>Hard X-ray Photoel. Spect.</td>
<td>2.4 - 15</td>
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<td>P23</td>
<td>In-situ &amp; Nano Diffraction</td>
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<td>P24</td>
<td>Chemical Crystallography</td>
<td>8, 17 - 44</td>
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<td>P25</td>
<td>HIMAX</td>
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<td>planning stage</td>
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### Paul Peter Ewald Hall

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<tr>
<td>P61</td>
<td>High-Energy Wiggler BL</td>
<td>50 - 200</td>
<td>wiggler-40 m</td>
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<td>P62</td>
<td>Small-Angle X-ray Scat.</td>
<td>10 - 35</td>
<td>U32-2 m</td>
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<tr>
<td>P63</td>
<td>Catalysis Beamline</td>
<td>planning stage</td>
<td>planning stage</td>
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<td>P64</td>
<td>Advanced XAS</td>
<td>4 - 44</td>
<td>U32-2 m</td>
<td>high</td>
</tr>
<tr>
<td>P65</td>
<td>Applied XAS</td>
<td>4 - 44</td>
<td>U32-0.35 m</td>
<td>high</td>
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<td>Time-Resolved Luminescence</td>
<td>UV</td>
<td>BM</td>
<td>N. A.</td>
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</table>

**Table 7.1.**: *PETRA III beamlines as of mid 2019*. Uxx denotes a normal undulator with xx mm period length. IVU: in-vacuum undulator.

X-rays from bending magnets are not used at PETRA III, mainly due to space constraints. One separate beamline (P66, cf. Figure 7.1) for UV spectroscopy is currently being set up at a bending magnet.

### 7.1.2. PETRA IV Beamline Portfolio

Due to the ultra-low emittance of PETRA IV, the current scheme of accommodating a large number of insertion device beamlines in only relatively few straight sections will no longer be possible. According to the conceptual design of the storage ring, eight straight sections will be available per arc (cf. Section 6.1.1). Moreover, only a very small number of beamlines can be canted by only a few mrad without significantly affecting the emittance (cf. Section 6.1.1). Therefore, most of the PETRA IV beamlines will be allocated to an individual straight section. In the three present experimental halls, $8 + 2 \times 3 = 14$, i.e. fourteen straight sections will be available. In order to preserve the number of beamlines and experiments and to be able to extend the beamline portfolio in the future, a fourth experimental hall in the west of PETRA is planned that can accommodate another $2 \times 8 = 16$ beamlines. With this, a total of 30 straight sections will be available for undulator beamlines.

Figure 7.2 shows the beamline locations at PETRA IV. The first beamline in each arc has
its insertion device in a long straight section (marked in red in Figure 7.2). These beamlines can be equipped with particularly long (e.g., 10 m) and optimised undulators with optimised beta functions (cf. Section 6.1.1) to match the electronic and photonic phase space. For these “flagship” beamlines, the spectral brightness can be pushed to extremes, exceeding that of any other planned fourth-generation source by at least one order of magnitude (cf. Figure 4.3). The flagship beamlines will be selected and designed to make optimal use of this extreme brightness (cf. Section 7.1.3).

With the current design, many beamlines will gain both in brightness and in flux, as the electron beam emittance is significantly reduced and the length of most insertion devices can be increased to 5 m or more in the case of the flagship beamlines. Generally, there is more space at each beamline compared to PETRA III today to add the lab space and infrastructure needed for in-situ/operando and high-throughput experiments. The number of beamlines could be increased beyond 30 by canting, although the canting budget is very limited (cf. Section 6.1.1). A maximum of three sectors with two undulators canted by an angle of 2 mrad would be possible without significantly compromising the emittance. Canting would be an option to increase the number of beamlines that are highly productive but with methods not requiring the full brightness and flux of a 5 m undulator, such as macromolecular crystallography, automated powder diffraction or XAFS. The parallel operation of two experiments by splitting the beam in a scheme similar to that at P02 today (cf. Section 7.1.1) is also conceivable.

No X-ray bending magnet beamlines are considered in the PETRA IV design for similar reasons as for PETRA III (cf. Section 7.1.1). The evolution of the PETRA III beamline portfolio into that of PETRA IV will be carried out in the upcoming TDR phase. The next section details the strategy for selecting the beamline portfolio.

7.1.3. Scientific Case and Selection of PETRA IV Experiments

During the TDR phase, a detailed design of the beamlines at PETRA IV will be worked out. The new boundary conditions at PETRA IV open up exceptional experimental opportunities, but they also require a substantial logistic and construction effort. On the other hand, the relocation of most beamlines opens up the possibility to make changes to the beamline portfolio and rearrange and extend experiments in a way not possible otherwise. In the TDR phase, the beamline portfolio will be analysed in view of this. User workshops in all fields of science will be carried out, surveying the needs of the user community and identifying the experiments to be implemented at PETRA IV. We expect that many experimental techniques at PETRA III will evolve rather continuously into those needed at PETRA IV,

Figure 7.2.: Distribution of PETRA IV beamlines assuming eight beamlines per PETRA octant. Red lines mark the PETRA IV flagship beamlines located in long straight sections.
but that some disruptive new techniques will appear in addition. The new beamline portfolio will be developed with advice from the DESY Photon Science Committee and submitted for approval to the DESY Scientific Council (cf. Section 1.2). This selection process will be carried out in the first half of TDR phase within work package WP 3.08 “Beamline and Experiments Design” (cf. Figure 1.3 in Section 1.2). This work package will define the full beamline portfolio, including the new flagship beamlines (cf. Section 7.1.2).

To be able to manage the transition from PETRA III to PETRA IV with reasonable effort and in a sustainable manner, the existing infrastructure and instrumentation will be reused as much as possible (cf. Section 7.1.4). In the coming years, the PETRA III beamlines will be constantly kept up to date, already taking the requirements for PETRA IV into account. This effort will be complemented by a dedicated development of beamline components, as covered by the work packages WP 3.01 to WP 3.07 and described in the following Sections 7.2 to 7.7.

At the PETRA IV flagship beamlines, there will be particular freedom to optimise the insertion devices for optimal beam parameters in terms of flux, brightness, energy and polarisation. The experimental conditions at these beamlines will exceed those at any other source, making PETRA IV worldwide unique. The se-

Figure 7.3.: DESY Hamburg site with existing and planned PETRA IV experimental halls: Paul Peter Ewald in the north, Max von Laue in the north-east, Ada Yonath in the east and the new experimental PETRA IV Hall West (in blue). The beamlines are indicated by lines, with the red ones being the PETRA IV flagship beamlines.
lection of the experiments at these beamlines is driven by both the exceptional capabilities and the resulting strong science and technology case for a large user community (cf. Chapter 5). Without preempting the future beamlines and their scientific case, here are some of the options for the flagship beamlines:

- 10 m in-vacuum undulator with intermediate period for ultimate X-ray microscopy: Exploiting the brightest coherent hard X-ray nanobeam, multimodal 3D X-ray imaging down to 1 nm resolution could be realised using scanning coherent diffraction microscopy (cf. Section 4.2). The beamline could accommodate different stations optimised for different sample environments. Depending on the sample environment, this experiment could provide unique insights into many different fields of science.

- 10 m undulator (cf. for example Figure 7.4) with intermediate period for hard X-ray scanning microscopy with inelastic scattering (nanoIXS) or nuclear resonant scattering (nanoNRS) as contrast (cf. Section 4.2 and 5.1).

- 10 m in-vacuum undulator with intermediate period for dynamic coherence applications: This beamline would be optimised for a high coherent photon flux in the hard X-ray range to perform correlation spectroscopy experiments (XPCS) with high temporal resolution. It will reach time resolutions that are about 100 times faster than at any other synchrotron radiation source worldwide (cf. Section 4.3), enabling for example studies of the dynamics of complex liquids and solutions, e. g. in chemistry and biology, and with a special emphasis on water science (Section 5.4.3).

- 10 m cryo-cooled or superconducting in-vacuum undulator with short period for high-energy X-ray applications. As the worldwide brightest synchrotron radiation source (Figure 4.3), this device would be ideally suited for Compton tomography (cf. Section 4.5) of biological specimens (cf. Section 5.2).

- Two-colour beamline with two independent, optimised undulators for combined spectroscopy and structure determination (e. g. 5 m APPLE in sequence with 5 m standard undulator). In this way, electronic band structure information could be combined with the atomic structure of the sample, both with high spatial and temporal resolution. This combination would find applications in materials science in the fields of energy research (cf. Section 5.1 and information technology (cf. Section 5.5).

As part of the work package WP 3.08 “Beamline and Experiments Design” (Figure 1.3), these and further options will be evaluated.

7.1.4. Reusability of PETRA III Components at PETRA IV and Logistics Considerations

Relocating beamlines is a huge effort and requires a detailed logistic planning. In order to be able to have a substantial number of beamlines operational when starting the operation of PETRA IV, long-lead planning and preparation are needed. According to the schedule (cf. Figure 1.4), parts of the TDR and the project phase can be used for this, giving about a five years lead time before the actual dismantling and rebuilding of the beamlines. The beamline portfolio will be determined during the first part of the TDR phase. In the remaining part of the TDR phase, the new locations and the layout of the beamlines will be fixed together with the technical design. This will include the identification of experimental stations at PETRA III that will be relocated and those that are to be newly built. Based on the design of the new beamlines, a detailed planning of the reuse of components and new purchases will be made. During the first part of the PETRA IV construction phase (cf. Figure 1.4), i.e. when PETRA III is still in operation, detailed preparations for the dismantling and rebuilding phase are foreseen. A large fraction of the experimental stations and optical components at PETRA III will be transferred to PETRA IV. The necessary upgrades of these instruments and components will be made already during their operation at PETRA III, keeping the instruments at the state of the art. In addition, an inventory of
the reusable beamline components at the existing beamlines will be made. In parallel, all new components needed for the beamlines at PETRA IV will be procured. When PETRA III is shut down, the beamlines in the old experimental halls will be dismantled, carefully recovering all reusable components. In parallel, the new experimental hall will be built. As soon as the experimental floor is ready, the PETRA IV beamlines will be set up in parallel to building the storage ring. During this dark period, the scientific and technical personnel for the experiments at PETRA will have to focus their work implementing the new beamlines. The beam transport group at DESY will have to be expanded in terms of personnel, and additional external manpower will have to be allocated.

7.2. Radiation Sources

**Boundary Conditions**
In the PETRA IV lattice, it is planned to have 25 straight sections for insertion devices (IDs) of 5 m length. The horizontal and vertical beta functions in these undulator cells are $\beta_x = 6.86$ m and $\beta_y = 2.36$ m, respectively. A major improvement for the ID performance at PETRA IV will be the considerably smaller magnetic gap that can be realised. This is a result of the largely reduced size of the injected beam after refurbishment of the booster, which will allow for a smaller “beam stay clear” aperture of 6 mm. The smaller magnetic gap can be used to increase the magnetic peak field and/or to shorten the period length of the undulators. In addition, with the new on-axis injection scheme, the particles will be injected essentially without horizontal oscillations, which also reduces the required width of the transverse “good field” region in the undulators down to about $\pm 5$ mm. This allows for an improved design of the magnet structure, which is narrower and thereby reduces the magnetic load on the support structure and at the same time increases the magnetic peak field on the beam axis.

**Undulator Types**
The choice for a specific type of undulator depends on the needs of the associated beamline. In general, the use of an ID customised for a specific spectral range will result in a better performance and/or a reduced heat load on the frontend components compared to a generic all-purpose device. For example, an effectively 4 m long in-vacuum undulator with a period length of 25 mm would
provide a photon spectrum that is continuously tuneable from 3.7 keV onwards. It would also put a heat load of more than 9 kW on frontend and optics. The same would hold for a cryogenic permanent-magnet undulator with a period length of 18 mm optimised for higher-energy photons. This device would provide a three times higher brightness for most photon energies above 8 keV; however, the range from 17 keV to 24 keV would not be accessible. Thus, in order to fully exploit the potential gain in brightness available from a source like PETRA IV, it is highly favourable to design a multitude of diverse beamlines, each of them specialised in a limited photon energy range. On the other hand, equipping each beamline with an identical multipurpose ID that can be tuned continuously would allow for maximum flexibility and interchangeability of devices. All this adaptability would come with the trade-off of a brightness reduced by a factor of about 3 phasing of adjacent modules and does not require the installation of a separate phase shifter between the individual undulators within the 10 m straight section.

Radiation Properties
The brightness, which serves as a figure of merit in the design of an undulator source, is defined as the photon flux normalised to the phase space. At a diffraction-limited light source like PETRA IV, the electron beam emittance \( \epsilon_{x,y} = \sigma_x \cdot \sigma_y \) is of the same order of magnitude as the natural emittance \( \epsilon_r = \sigma_r \cdot \sigma_r' \) of the emitted radiation. While the emission characteristics are largely diffraction-limited in the soft X-ray energy range (approx. a few keV and below), the spectral and spatial properties are still significantly emittance-limited in the classical X-ray regime \((\approx 10 \text{ keV and above})\). For such conditions, the convoluted phase space distributions are not fully dominated by the electron beam properties, so that the commonly used Gaussian approximation of the undulator radiation phase space is not any more an appropriate description in all cases. A widely used description of the photon density in phase space is based on the Wigner distribution function, which has been implemented in various codes for simulation of synchrotron radiation. Parameter studies in the course of the PETRA IV conceptual design phase have mainly been made by means of Spectra [115] and SRW [116, 117].

Insertion Device Technology
Currently, conventional pure permanent magnet (PPM) or hybrid magnet structures (such as the majority of the present PETRA III IDs) are the most commonly used techniques for insertion devices. In-vacuum undulators (IVUs) are another already well established technology that is used to increase the brightness further. They use the available “beam stay clear” aperture more efficiently and thus allow for shorter period lengths and/or higher magnetic fields in comparison to out-of-vacuum devices. Therefore, IVUs are used at many medium-energy storage rings to extend the spectral range of the experiments towards high-energy photons. For high-energy storage rings such as PETRA, this may not be the main motivation for using IVUs, since high-energy photons

Nick Leithold
Spectronet Cluster Manager

“We need leading interdisciplinary research in photonics in Germany in order to be able to support all high-tech companies and applications coming out of this field. PETRA IV is exactly that, and a project on this scale has the potential to spur innovations and new products. DESY and the GSI Helmholtz Institute Jena have already shown, with the very successful start-up Class 5 Photonics, that research in this area can lead to very interesting new companies. As an innovation cluster strengthening photonic measurement engineering and quality assurance, we strongly support PETRA IV, as we are sure that we will see a lot of advancements in this area with the development of this synchrotron.”

For some beamlines that require very special photon characteristics, such as variable polarisation, or beamlines that need to cover a unique spectral range, it is inevitable to use specialised IDs instead of universal ones. There will be five straight sections available that are long enough for the installation of undulators of up to 10 m length. For these straights, dedicated short-period undulators are planned, which will consist of several units of 3 m to 5 m length each. These devices will be built in in-vacuum technology, which allows for a continuous magnet structure with proper
are already easily available using conventional IDs. Nevertheless, IVUs offer an increased brightness and enable the use of even harder X-rays. Advanced cutting-edge technologies even outperform IVUs, namely superconducting undulators (SCU) and cryogenically cooled permanent-magnet undulators (CPMU). They allow for even smaller period lengths without a trade-off in magnetic field strength [118, 119]. At cryogenic temperatures, the magnetic properties of rare-earth magnet materials such as NdFeB or PrFeB improve considerably. The remanence $B_r$ increases by 15% to 20%, the coercivity $H_{C,J}$ even by a factor of 3 or more. CPMUs can be considered as just an extension of the conventional IVUs. Therefore, the technology can be regarded as well developed. An increasing number of these devices are already successfully operated at other synchrotron radiation facilities (e.g. ESRF, SOLEIL, DIAMOND, PSI). Another advanced concept for IDs is the use of superconducting coils. Several prototype IDs were built based on NbTi coils. Especially at the APS, some superconducting undulators are routinely operated, and there are strong development efforts for additional ones within the scope of the APS upgrade. Considering the maximum magnetic fields that can be achieved using this technology, these devices clearly outperform all other devices based on permanent magnets for a large range of period lengths. Although the technology of winding NbTi coils has matured during the last years, it still lacks the perfection that is required for routinely achieving phase errors below maximally 2° for full-length devices. In addition, there are only limited methods for phase and trajectory shimming after fabrication of the superconducting coils. A significant advantage of SCUs over room temperature permanent-magnet undulators is their much higher radiation resistivity. Advanced SCUs based on Nb$_3$Sn coils could provide magnetic fields that are even a factor of 1.4 higher than those of SCUs based on NbTi coils. However, for Nb$_3$Sn or even high-temperature superconductors, the coil-winding and activation procedure is way more complex than for NbTi. Despite the existence of a few prototypes, these technologies should not be considered as the desired baseline standard for PETRA IV IDs, due to the involved risks. DESY currently has neither built SCUs nor CPMUs. However, experience in all of the technologies required for building and operating CPMUs is available on site. The required liquid N$_2$ cooling infrastructure will be available at PETRA IV anyway, since it is also needed for the cryogenic monochromators. SCUs on the other hand would require an additional elaborate liquid He cooling infrastructure. The risk of quenching must be considered as a potential peril for stable machine operation, but APS has reported good experience in this regard. The heat load induced by the beam on the superconducting coils cannot be calculated with high accuracy as it also sensitively depends on actual operation conditions and orbit distortions. Since there isn’t even reliable data on this issue for PETRA III, the design of SCUs for PETRA IV would require a substantial safety margin.

Recycling of Current IDs
The support structures of most IDs currently operated at PETRA III are still in a state that would meet the specifications for new devices. Besides the update of some electronics, no distinct improvements need to be implemented. Experience from previous devices has shown that it is even possible to refurbish and retune magnet structures that suffered from radiation damage. Therefore, reusing some of the current out-of-vacuum devices could be considered as an intermediate cost-effective or backup scenario for some beamlines. However, a smaller vacuum chamber with $\leq 8.0$ mm thickness should be considered. Since most of the current IDs are 2 m long, their most efficient reuse would be an installation in a potentially canted straight section. Whether or how many canted beamlines will be implemented will be considered in the TDR phase. Undulators for beamlines working at low X-ray energies could be considered for reuse because IVUs develop their full advantages only towards higher photon energies. This holds in particular for the present UE65 APPLE undulator. In addition, the two more recently installed IVUs will be used further in PETRA IV. They will be compatible with the new machine, but need to be magnetically retuned as they will then be used with smaller gaps. The downside of recycling some of the present IDs is the lacking optimisation in terms of period length and
transverse geometry of the magnet structure, which both result in a spectral performance somewhat below the maximum possible.

New Magnetic Measurement Technologies

Conventional out-of-vacuum undulators with a C-shaped support frame provide convenient access to the magnet structure for measuring and tuning. For advanced insertion devices such as (cryogenic) IVUs or even SCUs in their fully assembled operational state, measuring the magnetic field distribution on the beam axis can be quite challenging from a technical point of view. Either magnetic measurements have to be done under ambient conditions and the operando state has to be extrapolated from these data, or new measurement tools and techniques have to be developed that allow for measurements in the operational state. One of the key requirements for such a system is compactness. Vacuum and cryo compatibility may be necessary in addition. Several compact Hall probe systems \[120\] have already been built at other facilities, and as of late, HZB \[121\] operated such a system under vacuum and cryogenic conditions. Even if purchasing of turn-key-ready devices is considered an option, these kinds of tools need to be developed also at DESY to allow for independent site acceptance tests. This may happen on the basis of a collaboration with other institutes or industry, e.g. within LEAPS. The required system will include a miniaturised vacuum-compatible Hall probe setup and a stretched wire system.

Radiation Damage

In the current operation scheme of PETRA III, there are considerable particle losses in particular during timing operation, which lead to a degradation of the magnetic field quality in the undulator and thus of its performance ahead of time. By choosing magnet grades with increased coercivity and operating them at cryogenic temperatures, this problem can be mitigated, but might go along with a decrease in ID performance due to lower remanence. From the currently available data on magnet degradation and beam lifetime at PETRA III, a correlation can be estimated between beam lifetime intended for PETRA IV and expected undulator life span. Besides passive measures (i.e. increasing the radiation hardness of the magnet material), it is absolutely essential to also implement active measures such as a loss monitor system to ensure the longevity of the IDs. Further, the amount of timing mode operation (low Touschek lifetime) must be restricted to the absolute minimum by scheduling as many experiments as possible with this requirement in parallel.

7.3. X-Ray Optics

To make best use of the extraordinary properties of PETRA IV, the X-rays from the undulator sources need to be filtered and transported to the experiments, shaping the photonic phase space to optimally fit the experiments while minimising losses in intensity and coherence. In addition, aberration-free nanofocusing will be needed at many experiments. This section describes the concepts for the X-ray optics for beam transport (Section 7.3.1) and nanofocusing (Section 7.3.2). Considerations about ultra-high-precision mechanics and stability are given in Section 7.4 and 7.5.

7.3.1. Beam Transport

Frontends

The generic frontend concept as installed in PETRA III will be the basis of all the PETRA IV beamlines \[122, 123\]. The main task is to provide a hydrocarbon- and dust-free vacuum system and to transport and tailor the photon beam from the undulator to the experiment, conserving the unique photon beam properties. Concepts for relocating all the beamlines to the new eight-sector scheme and dealing with the source point shift of \( \approx 20 \) cm outboard for the flagship beamline positions in the long straight sections of the PETRA tunnel, which are currently occupied by the PETRA III beamlines.
Figure 7.5.: Sketch of the PETRA III frontend setup.

P01, P21 and P61, will be developed on this generic basis. Most of the beamlines at PETRA IV will occupy an entire straight section with one undulator (up to 5 m in length). For these beamlines, the frontend design can be based on that of the current PETRA III beamlines P07 or P10. Canting will be possible at PETRA IV at the expense of increased horizontal emittance. Therefore, only a few beamlines may be canted with small canting angle ($\leq 5$ mrad).

At present, solutions for potential electron beam canting schemes are available based on the designs for:

- 1 mrad canting at P21a/b,
- 5 mrad canting at beamlines in the Max von Laue hall. Smaller angles, i.e. 4 mrad, will require a redesign of the girder structure, but the design will still use original standard components.
- 20 mrad canting at the PETRA III extension beamlines. This canting angle is too large for PETRA IV and this design can not be carried over to PETRA IV.

Solutions for further optical separation of canted undulator photon beams are available based on:

- the horizontal side station optics at P21b,
- vertical separation schemes, e.g. large offset monochromator (LOM) at P02/P03 and P08/P09.

The flagship beamlines (cf. Section 7.1.2 and 7.1.3) will be optimised for highest brightness and flux. They are located in the longer straight sections at the beginning of each arc, allowing for up to 10 m long insertion devices with adapted beta function. DESY has extensive experience in coping with high heat load from long insertion devices, such as the 10 m IDs at P01 and the 40 m damping wiggler at P61. The heat-load management of the white ID beam at the flagship beamlines will be based on that of the high-heat-load beamlines at PETRA III. The increased electron beam current (200 mA) will require a careful heat-load management and an adaptation of the design. As the beamline portfolio and the resulting design requirements will be considered in the upcoming TDR phase, a detailed planning of the design, construction and implementation can only be developed at a later time (cf. Section 7.1.4).

Monochromators

The generic vertically deflecting direct-drive monochromator with LN$_2$ cooling offers the most versatile option for providing the largest Bragg angle / energy range. The critical parameter for these systems is the relative angu-
lar movement of the crystals in a crystal set. Current systems in operation at PETRA III and worldwide are achieving values in the 50 nrad (rms) angular range, with frequencies up to the few kHz range [124]. Developments are ongoing, i.e. at SIRIUS and ESRF, to lower this value down to 20 nrad. To preserve the source parameters of PETRA IV in an optimal way, this target value will even have to be lowered down to 5 – 10 nrad. From a mechanical and stability point of view, a horizontal setup of the monochromator mechanics and crystal sets is favourable compared to the commonly used vertically deflecting systems [125]. Due to the polarisation-dependent reflectivity of the monochromator crystals, horizontally deflecting monochromators will provide limited energy ranges. These systems will be either a tailored solution for special scientific needs or a more general scheme with several horizontally deflecting monochromators with different crystal sets arranged in a line to cover larger energy ranges. A fundamentally different, very stable solution is the use of channel-cut systems. At PETRA III, these systems are installed as add-ons in the high-heat-load double-crystal monochromators (DCMs) at Beamlines P06 and P10. Conceptionally, these setups provide limited energy ranges and a vertically shifted beam depending on the energy setting [126]. At the expense of mechanical complexity and potentially new stability and synchronisation issues, a second channel-cut would be able to provide a fixed exit beam again (e.g. cryogenically cooled two-channel-cut monochromator successfully demonstrated at the Diamond Light Source) [127]. All design options would benefit from decreasing the mandatory bremsstrahlung offset at PETRA and reevaluating the photon beam height above ground, currently 20 mm and 1.4 m, respectively. The exact boundary conditions concerning these aspects will be finalised in the TDR phase. The total white beam power generated at PETRA IV by the IDs will only slightly change (in the 10% range) due to customised undulator structures with smaller gaps. The current PETRA III monochromator design is already based on 6 GeV operation with up to 200 mA. Therefore, the current design is considered to already fulfil the heat-load requirements of PETRA IV. A detailed evaluation will be done in the TDR phase. All high-heat-load silicon crystal optics at PETRA III have been manufactured in-house in a specialised crystal optics laboratory. Only this capability ensures the availability of very-high-quality crystal optics, including custom made systems for special applications. The current crystal optics quality used at PETRA III is appropriate for future use at PETRA IV. It is DESY’s strategy to maintain the knowledge and infrastructure to make high-quality crystal optics in house.

Mirrors

The requirements on mechanical stability of mirrors are similar to those of monochromators. Horizontally deflecting systems are already successfully in operation at many beamlines at PETRA III and FLASH. Their performance will be evaluated in view of the new requirements of PETRA IV. The mechanical design will be updated according to the design concepts presented in Section 7.4 and 7.5. All PETRA III mirror optical elements are custom made for PETRA III photon beamlines by commercial vendors. The same scheme will be followed for all reflective optics at PETRA IV. Currently, the vendor base for highest-quality synchrotron radiation mirror optics is very small with JTEC (Japan) dominating the market for high-end mirrors. The mirror quality requirements of PETRA IV are the same as for hard X-ray free-electron lasers, such as the European XFEL. High-end mirrors developed for the European XFEL fulfil the surface quality requirements for PETRA IV already today, however, they are expensive and have long delivery times. In order to extend the vendor base, DESY collaborates with partners within LEAPS to qualify other companies to secure the supply for high-quality reflective optics for all sources in Europe.

Beam Position Monitors

Regarding photon beam diagnostics, white beam and monochromatic beam X-ray beam position monitors (XBPMs) will be needed in order to characterise and control the photon beam. Monochromatic beam XBPMs are available with sufficient spatial resolution. Effects on the beam quality, especially when used in
a transparent mode, have to be further investigated. Further development of transparent white beam monitors is still needed [128, 129].

Resources and Staffing
The in-house design and manufacturing of critical beamline components, especially high-heat-load systems in the frontends and high-precision UHV-systems, i.e. mirror chambers, proved to be very valuable for the timely implementation and operation of the PETRA III beamlines. This concept will be carried over to PETRA IV and the scope will be re-evaluated in respect of the volume of systems to be manufactured.

There will be a considerable increase in staff needed in the design, preparation and implementation phase. This increase includes all levels of expertise. Especially during the implementation phase staff trained at beamline components from PETRA III or equivalent sources is needed in order to keep the shutdown time as short as possible.

When the beamline portfolio for PETRA IV will be defined in the TDR phase, a detailed planning of the resources will be made, including staffing and logistics.

7.3.2. Nanofocusing

The advent of synchrotron radiation sources of the third generation and their significant boost in brightness compared to previous sources has boosted X-ray microscopy and spawned the development of high-quality X-ray optics. Today, high-quality focusing optics are available based on diffraction, reflection and refraction of X-rays. Diffraction-limited performance has been reached for all three types of optics. For PETRA IV, nano-focusing optics of the highest quality will be crucial to achieve an optimal performance of the facility. The following section presents the DESY nano-optics strategy.

The “ultimate X-ray microscope” PETRA IV aims at highest spatial resolution for the study of processes in special sample environments. This requires highest possible numerical apertures and long working distances. In addition, spectroscopic studies call for achromatic optics, and investigating small objects in tight sample environments, e.g. double diamond anvil cells (cf. Section 5.4.2), need to be probed with a beam with low background to avoid excessive signal from the sample environment. All these requirements cannot be fulfilled by one single optics, excluding a “one-fits-all” solution.

At PETRA IV, various nano-focusing X-ray optics will be needed depending on the particular application:

Diffractive Optics

Fresnel zone plates (FZPs, cf. Figure 7.7a), multilayer mirrors and multilayer Laue lenses (MLLs, cf. Figure 7.7b) are all diffractive optics. Among today’s X-ray optics, they have the highest numerical apertures and reach focus sizes in the single-digit nanometre range [131, 132]. Theoretically, these optics can reach (sub-)one-nanometre focusing [133–135], but they are currently still limited by fabrication technologies. All these optics are chromatic, i.e. their optical properties depend on the wavelength.
Indeed, for highest numerical apertures, these optics need to be specifically designed for a certain wavelength, and the working distances of FZPs and MLLs become very short (in the millimetre range). Due to their large numerical aperture, diffractive optics – in particular MLLs – will play a crucial role at PETRA IV. DESY has a world-leading development programme for these optics, pursued by the X-ray Optics for Extreme Conditions group, that is decisive for the optics strategy of DESY.

Reflective Optics
Today, mirrors based on external total reflection can reach focal spot sizes of a few ten nanometres [136]. Their numerical aperture is limited by the length of the mirror and can reach at best half the critical angle of total reflection. For this reason, the current record focal sizes of 25 nm [136] of these optics cannot be improved much further. The main advantage of reflective optics is their achromaticity, which makes them particularly useful for spectroscopic techniques, in which the incident energy is scanned, e.g. X-ray absorption spectroscopy.

Reflective optics will play an important role for PETRA IV for spectromicroscopy (cf. Section 4.2). There are not many vendors for high-quality X-ray mirrors, in particular for focusing ones. Currently, DESY relies on the availability of commercial mirrors. Activities within the LEAPS consortium (cf. Section 2.4.2) will ensure a reliable availability of mirror optics in the long term.

Refractive Optics
Refractive X-ray lenses can currently reach focal spot sizes of a few ten nanometres [138, 139]. While there is no fundamental limit in numerical aperture for refractive optics [140], the numerical aperture is practically limited around the 10 nm range. As for diffractive optics, highest numerical apertures come with very short working distances (sub-millimetre range), limiting the focal spot size for in-situ/operando experiments to several tens of nanometres. Due to the approximately Gaussian aperture of these optics, the background outside of the focus can be made very low, resulting in a very high signal-to-background ratio in scanning microscopy experiments. Refractive lenses are strongly chromatic, and for high numerical apertures their design depends on the wavelength [140]. Refractive optics often suffer from spherical aberrations. Perfect, diffraction-limited focusing can be achieved by correcting these optics with special phase plates [137] (cf. Figure 7.8).

Refractive optics will play an important role for scanning microscopy, in particular in small sample environments where low background is crucial. Currently, there is only one commercial vendor for refractive lenses, but some research institutions provide refractive optics. DESY has a world-leading development programme for refractive optics, in particular for nanofocusing, that is pursued by the X-ray Nanoscience and X-ray Optics group.

The X-ray optics need to be integrated into the X-ray microscopes at PETRA IV. Highest mechanical stability and precision alignment...
are required to make full use of these optics. These issues are addressed in Section 7.5. In addition, a systematic metrology is required for these optics, in particular at X-ray wavelengths. There are several expert groups at DESY dealing with the at-wavelength metrology of X-ray nano-optics, using wavefront sensors, the Ronchi method and ptychography. The latter is particularly suited to directly measure the wave field in the focus with high sensitivity [141].

With increasing numerical aperture, it becomes more and more challenging to fabricate optics without aberrations (i.e., distortions of the wavefront). This holds for all types of X-ray optics. To achieve optimal focusing in spite of aberrations in the optics, the aberrations can be corrected for in the experimental setup using appropriate phase plates (cf. Figure 7.8). This technique was pioneered by DESY’s X-ray Nanoscience and X-ray Optics group [137]. As this method can be applied very generally to all kinds of X-ray optics, a phase plate fabrication lab is currently being implemented at DESY. These corrective schemes are decisive for the optics strategy of DESY.

X-ray optics development is expected to continue along with the improved experimental possibilities at the upcoming fourth-generation synchrotron radiation sources (cf. Section 2.3). In addition, specially tailored wave fields will become more and more relevant, such as orbital angular momentum beams (cf. Section 5.5.3).

### 7.4. Building Infrastructure

The ultra-low-emittance synchrotron radiation source PETRA IV offers experimental possibilities that go significantly beyond what is currently state of the art. The achievable beam properties enable scientific experiments with unprecedented requirements on spatio-temporal stability. With new focusing optics, focus sizes in the single-digit nanometre range can be achieved with very good beam quality. This means that equipment operating in the nanometre range must fulfill very special requirements, which can only be achieved if all influencing factors are taken into account.

For this reason, our strategy for the experiments and for the beamlines is based on five fundamental elements (cf. Figure 7.9). These are, on the one hand, reduction of noise and preserving constant environmental conditions in the infrastructure and, on the other hand, rigid supports, optimised designs and modern mechatronic concepts in the experimental instrumentation. With the operation of PETRA III, DESY engineers have gained a lot of experience along these lines.
7.4.1. Design Features of the Experimental Environment

Every change of the environmental parameters has a direct influence on the experiments. Temperature changes, for example, cause position drifts. Changes in air pressure and humidity have an influence on the measurement accuracy of high-precision sensors and instruments, etc. These fluctuations are often very difficult to compensate and must be avoided by a suitable infrastructure. A concept for an optimised infrastructure, which ensures that all environmental conditions are kept constant over a longer period of time, is shown in this section.

**Air Conditioning**

Constant temperature conditions require in particular very good air conditioning systems, which must enable precise temperature regulation and humidity control. Furthermore, external conditions such as day–night fluctuations, weather changes, etc. should be compensated or shielded as well as possible. Experiences from the PETRA III experiments in the Max von Laue Hall show that a temperature stability of $\pm 0.05 \text{ K}$ over 24 hours is feasible during user operation (cf. Figure 7.10). The room-in-room concept used here, with a well-tempered experimental hall and internally separated, much more precisely temperature-controlled experimental hutches, is also the favoured strategy for achieving the conditions required by the future experiments at PETRA IV. Last but not least, the system must not generate any additional disturbances, such as vibrations or sound emissions into the experiments. This point will be discussed in more detail in the following section.

**Environmental Conditions**

In order to avoid disturbances caused by heat sources, uncontrolled inflow of external air and air turbulence, access airlocks are provided for the climatic zones. The hutches are exposed to slight overpressure. Fine-meshed filters in the ventilation systems ensure low-dust operating conditions. The air-changing rate is set for a continuous laminar air flow around the experiment. This air flow with tempered air avoids heat turbulence and local temperature differences. For particularly sensitive experiments, this laminar flow can be temporarily switched off.
Radiation Protection Hutches
The main function of the experimental and optical hutches is radiation protection. Thanks to their special construction and the use of air locks, they also ensure stable temperature and air conditions, as described in the previous section. The structure of a radiation protection hutch used at PETRA III can be seen in Figure 7.11, where a modular concept consisting of different steel-lead elements is used. Recent studies at PETRA III experimental hutches have shown that the current steel-lead hutches are sensitive to induced vibrations (cf. Figure 7.13). They have many resonances, which lie in the range of typical excitation frequency spectra of the experimental halls.

Figure 7.11.: 3D drawing of a representative experimental hutch, located at PETRA III beamline P06. By courtesy of Roland Platzer (ZM1).

Figure 7.12.: FEA modelling results. Concrete wall segment of radiation protection hutch. The lowest resonance frequency modes lie between 350 Hz and 480 Hz as modelled with ANSYS.

Calculations have indicated that the construction of the hutch walls is the main factor causing the sensitivity, illustrated in the detail view in Figure 7.13. As a consequence, the hutch acts as a kind of vibration amplifier. These vibrations are propagated to the sensitive experiment in two ways: the direct path via in-coupling by airborne sound and the indirect path through the floor into the support structures of the experimental setup. Figure 7.14 depicts how a defined impact to one of the hutch walls is transferred to the experiment. Finite element analysis (FEA) calculations have shown that by using concrete and optimising the structural design, disturbing influences from outside can be significantly reduced by a factor of 40 to 50 compared to the steel-lead wall structures used at PETRA III. In this design, concrete fulfills two tasks at once: It provides both the shielding material and the supporting structure of the hutch. Furthermore the damping factor of the concrete walls, which is a factor of 2 higher than that of the steel-lead walls, has a positive effect especially in the case of strong excitations.

Figure 7.13.: Diagram of measured frequency spectra of an experimental hutch, induced by a defined impact. (a) Wall segments of a radiation protection hutch as implemented at PETRA III and two characteristic resonance frequency modes (48 Hz and 86 Hz) from FEM modal analysis with ANSYS, which indicate a good agreement with the vibrations measured in the hutch. (b) Measuring point for the vibration measurements [142]. By courtesy of Torben Reuß, HAW.
New Hutch Concepts

A group of specialists is now developing an optimised design for a prototype of this innovative hutch concept. Different strategies for a design of the module joints compatible with radiation protection and for an easy fabrication of the modules are currently being investigated. (cf. Figure 7.15 and Figure 7.16). For this purpose, the use of established components such as media chicanes and radiation protection doors is considered. In addition, new ideas from the construction industry are to be implemented here, providing a factory pre-installation of the infrastructure for power supply, internet, media, lighting, etc. in the individual modules. The modular set of a few custom-designed components allows for the construction of the experiments hutches with very flexible design.

Figure 7.12 shows results from an FEA calculation of a concrete wall segment with the same dimensions as a typical steel-lead segment used at PETRA III. Nevertheless, the advanced design also enables the provision of a modular system, consisting of standard wall and ceiling elements, which can be used to build any kind of hutch required for PETRA IV. This previously underestimated issue, particularly for experiments with very high demands on the position stability of the samples and the optics, such as 3D microscopy, coherence measurements or bioimaging experiments, will be significantly reduced with a new design of the hutches. In the new concept for radiation protection hutches, special attention will be paid to vibration optimisation of the structural design.

A prototype of this hutch is planned to be built at PETRA III. Figure 7.16 presents a model designed for verifying this concept. A wide range of different hutches are possible based on using only the basic wall elements. The information obtained from this work is used to calculate the design and construction time, which is extremely important considering the very tight time schedule for the construction phase of the PETRA IV project. We assume that there will be a significant reduction in costs and in the time of fabrication and installation of the hutches with the new concept.
Reuse of the Existing Hutches

However, not all experiments have the same high demands on the sample environment and vibration stability as the ones mentioned above. In these cases, it is planned to utilise the steel-lead design used in PETRA III (cf. Figure 7.11). This design is both space saving and proven. Currently, concepts for the re-use of the mostly module-based PETRA III hutches are under consideration. Here, on the one hand, the static requirements are considered in order to enable the engineers to combine the existing modules into new radiation protection hutches. Furthermore, concepts for the logistic organisation of the dismantling and the reconstruction have to be evaluated. It is also necessary to organise the availability and temporary storage of the components. In this context, the cooperation of structural engineers, experimental engineers and DESY Radiation Safety experts is essential to carry out the structural calculations and to meet the high radiation protection requirements. By combining the existing elements with adapted new modules, any hutch design can also be implemented in a very time-saving way. The time and effort required to dismantle the components in a clean and tidy operation is significantly higher than a normal breakdown. However, this work can be carried out very well by external staff, who are supervised and managed by logisticians and engineers from DESY.

Media Supply of Experiments

The experimental infrastructure of course also includes the central supply with all necessary media, such as electricity, cooling water, compressed air, process gases, liquid nitrogen, etc., as well as the corresponding supply lines and pipes in the experimental halls. Cable and pipeline routes must be planned during the construction of the radiation protection hutches. In particular, the central supply of liquid nitrogen from a ring line must be planned with special care. The routing must guarantee a reliable supply all the way to the experiments and should not introduce any additional disturbances into the experiments. This has to be ensured by a flow-optimised design of the lines. Additional acoustic dampers at critical points prevent the transmission of impact noise by the pipes. The infrastructure groups will be specially trained in advance so that appropriate precautions can be implemented during the planning of the routes and the installation of the media lines.

7.4.2. Prevention and Suppression of Disturbances

Any kind of interference source can have a negative effect on the experiments at PETRA IV. On the one hand, this should be prevented by a suitable infrastructure, but on the other hand, it is even more important to avoid the occurrence of disturbing vibrations. In general, it is easier to eliminate or shield a source of interference than to protect the relatively sensitive experiments from the influence of noise. A dedicated network of suitable measuring instruments will be installed in the experimental halls in order to identify changing sources of vibration and to eliminate them in order to keep the noise background as low as possible.

Decoupling and Damping

In order to prevent the occurrence of vibrations as effectively as possible, it is necessary to decouple the vibration sources, such as pumps, air conditioning systems, electronic racks etc., as well as possible from the critical areas of the accelerators, optics and experiments, or to damp them as much as possible. For this purpose, the disturbing components should
be stored on their own foundations if possible. These must not be connected to the concrete foundations of the experimental halls and accelerators. If this is not possible, suitable damping must be provided by using vibration dampers or vibration absorbers.

**Acoustic Protection**

The small sample structures that are used in the most experiments are influenced by airborne sound. This leads to an induced vibration in the nanometre range, which is clearly visible with the interferometer we use for sample position monitoring, but also in the measured data of the performed experiments. Sound sources such as shutters, valves, pumps, fans, etc. must be shielded and damped to avoid this effect. The air conditioning units will be equipped with *bionic loop fans* in order to minimise noise emission, which also ensure a more uniform air flow and additionally improve the efficiency of these units.

### 7.4.3. Laboratories and Preparation

A modern infrastructure naturally also includes areas for the preparation and storage of samples and the experimental equipment. For this purpose laboratory space is provided near the beamlines where experiments and measurement equipment can be set up and tested.

### 7.5. Ultra-High-Precision Mechanics

For the groundbreaking experiments planned at PETRA IV, it is important to prevent relative movements between the various components of the experiment. Any disturbance in the stability of the beamline optics or the experimental apparatus has a direct effect on the measurement performance. Such disturbances cause a blur or distortion in the measured data and limit the resolution of the results. Therefore, the entire design of the beamline instruments must be optimised for vibration behaviour and stiffness. On the other hand, the experimental stations should offer flexibility for a wide range of different experiments. These two requirements contradict each other and need to be weighted carefully for each particular case to find the optimal solution for the given application.

#### 7.5.1. Strategy and Implementation

In ultra-precision mechanics, the trend is going towards ever more compact and specially adapted individual systems. The high demands on stability and precision require a different way of thinking. On the one hand, the systems are designed to be as stiff and stable as possible. On the other hand, an active position correction is wanted, which requires light and highly dynamic systems. A good solution is to combine the two properties. To this
end, adaptable system concepts have to be developed and new control strategies have to be implemented. Due to the high complexity of the systems, this can only be achieved as part of a cooperation with developers from industry, using modern methods of engineering and the implementation of new manufacturing techniques.

7.5.2. Modern Mechatronic Concepts

Mechatronic engineering is a combination of mechanical, electrical and software engineering that integrates these three disciplines to design optimised hybrid systems (cf. Figure 7.17). With the help of microelectronics and ultra-precise sensors, modern mechatronic systems are providing high levels of precision and reliability. New functionality can be integrated more easily. Due to extremely fast signal processing, position corrections are possible almost in real time. This simplifies the synchronisation between data acquisition and sample movement and allows much faster measurement cycles at the different experiments at PETRA IV.

For this purpose, highly dynamic components have to be integrated into the instruments, and very high-performance and accurate sensor systems are required. The combination of mechanical and electrical engineering facilitates an optimised construction, which can be on the one hand very stiff and light and on the other hand very powerful and functional due to the integrated sensors and actuators.

Module-based Constructions

Modularity in construction offers the possibility to create and develop systems and subsystems independently from each other. This enables a functional separation into individual, scalable and multi-usable modules. Here, an exact definition of the module interfaces must be ensured and applied consistently, by structuring the system into individual components. Systematic improvement is facilitated by the fact that critical components can be identified and replaced by better-optimised units. In addition, modularity offers further benefits, such as cost reduction through standardisation of components and more flexibility of the system by replacing components and increasing the functionality.

Figure 7.17.: Framework for integration of modern mechatronic systems.

The implementation of this concept requires strategies to coordinate the different technical disciplines, such as mechanics, electrics, electronics, software, etc., in order to create a functional system, and the integration of industry standards for interfaces to ensure that the systems are open for adaptability and modernisation. Various international activities with DESY participation are going in this direction. The Nanoscience Foundries and Fine Analysis (NFFA) European Research Infrastructure project JRA5, for example, focuses on advanced nano-object transfer and alignment to enable reproducible sample positioning, with nanoscale precision, under different experimental probes.

Technically Optimised Devices

Along with the actual geometry design, comes the analysis of the components and assemblies. Simulation, validation and optimisation work will be carried out with computer-aided engineering (CAE) software. Calculations and simulations can be done either in computer-aided design (CAD) with integrated tools or with dedicated analysis software. These are used to perform tasks such as stress and
modal analysis for dynamic properties, with finite element methods (FEM), computational fluid dynamics (CFD) and so on.

Figure 7.18.: View of FEA modelling results as an example of a design of a supporting structure optimised for frequency behaviour and stiffness. The lowest eigenfrequency is about 340 Hz.

The experience gained shows that with a consequent implementation of these methods in the construction phase, the high demands on the PETRA IV beamlines can be realised. A further improvement in the stability and vibration behaviour of the instruments can be expected through the use of new manufacturing methods, such as selective laser melting (SLM). These will be used to manufacture functional components and supports, such as bionic structures, which can be produced at a reasonable budget, and enable designs that meet the highest requirements in terms of dynamic behaviour and stiffness of modules and instruments. An example of an optimised structure and its vibration behaviour is shown in Figure 7.18. A further optimisation of the instruments in terms of position stability, but also with respect to the signal-to-background contrast, is achieved by performing these experiments under vacuum conditions. For these applications, special developments have been initiated to simplify the equipment and sample handling. A practical reference is the automatic sample-changing device [143], which is already being used in ultra-high-vacuum experiments at the MiNaXS beamline at PETRA III (cf. Figure 7.19).

In order to optimise data acquisition in the experiments, adaptive detector setups are needed to flexibly adapt to changing experimental or scattering geometries. Various development projects have been successfully carried out in recent years and integrated into the beamlines at PETRA III. However, further developments are required in order to optimise the measurement technology inside the vacuum. This will help to generate significantly stronger and better-separated signals and even more accurate position measurements without atmospheric interference.

Figure 7.19.: In-vacuum sample changing robot at the highly automated sputter experiment at Beamline P03 [143]. Example for sample handling in vacuum with (a) sample changing robot, (b) measurement position and (c) sample cartridge. Reproduced with permission from [143]. © (2013) by the American Institute of Physics.

New Control Concepts

The realisation of modern mechatronics also requires highly specialised controllers. Figure 7.21 shows an example, which can process the high data rates of the sensors and also allows very fast control processes in order to provide position corrections in real time, for example. Engineers at DESY are currently working on the development of innovative control concepts to optimise the measurement technology and adapt it to the extreme requirements of position stability and precision mechanics. The enormous data quantities to be processed in real time for this task require very fast, bus-capable control systems. The MicroTCA.4 standard developed by DESY in cooperation with industry offers a very good opportunity for developing a modern, state of the art standard controller, usable at PETRA IV, which is fast, reliable and can be built in a very
modular way. The fast bus system allows synchronisation with the accelerator, the detectors and all other components of the beamline. A very close networking of the mechanical design process with the measurement and control technology as well as the software is a basic requirement for reliable operation and positioning in the nanometre range.

to be implemented that is able to provide the data for position, location, shape, speed, velocity, physical status, etc. with the adequate accuracy and the required rate. Supersensitive sensors and well-defined environmental conditions, for example, enable high-precision position measurements at the sample point in real time. With laser interferometers, 3D position data down to the sub-nanometre range can be simultaneously recorded and processed. Figure 7.22 shows the measuring principle and the setup for 2D data acquisition, developed for the PtyNAMi instrument at Beamline P06 of PETRA III, where a special glass lens is used as a retro-reflector (cf. Figure 7.20) [144, 145]. The position data can be used for a fast position feedback, to monitor the current conditions and for data correction during evaluation.

7.5.3. Operando Metrology

Based on the research and development requirements, scientists and engineers need access to all significant parameters related to the experiment. This is particularly important if the measurement has to be performed at high speed and with extreme precision, for example in scanning probe microscopes for nanoanalytic applications. In order to fulfill these requirements, an in-situ metrology has

Figure 7.20.: Principle of a ball lens working as a retro-reflector. Perfect retro-reflection is achieved for glass with a refractive index of 2. The back side of the lens is covered with chrome to obtain a higher reflectivity and thus a stronger interferometric signal.

Figure 7.21.: Schematic of a control loop for a voice coil drive. Fast feedback of multiple values such as position, current, field etc. are required for high-end position tracking.

Figure 7.22.: Setup for 2D position measurement with laser interferometers. The geometry allows for rotation around the ball axis, which is needed for example for tomographic scanning.
7.5.4. Sample Environments

Many of the types of sample environments currently used at PETRA III will also be used at PETRA IV beamlines. Nevertheless, we have to consider that samples can be smaller and measuring times shorter, which in some cases requires a modification of the sample holders or a new design of heating and reaction cells, for example. Furthermore, the highly bright beam conditions enable much faster measurements and significantly smaller beam sizes, which require a high degree of dynamics and precision also for sample movements and a very precise control and monitoring of all necessary parameters as well as an optimised synchronisation with the beamline and the detectors. For this purpose, new concepts are currently being developed and tested at various beamlines.

Automatic Sample Change
An automated sample change is already being performed in some experiments at PETRA III. This is very useful for crystallography or X-ray experiments with high sample throughput. It is also worth considering such systems for experiments with high demands on the stability of the environmental conditions, for example, to avoid disturbing influences from a manual sample changing procedures. Due to the better availability of industrial robots nowadays, several beamlines at PETRA III already offer successful concepts for the implementation of an automated sample exchange, which are also an option for experiments at PETRA IV.

Optical Sample Monitoring
Specimens are often studied with different analytical methods. Therefore, it is important to identify and analyse the same nanostructure or the same nano-sized area of a sample at the different instruments. These areas have to be provided with markers that need to be clearly identified in the various experiments. This requires optical microscopy, which has to be integrated into the experiments and must enable reproducible positioning. In combination with specific software and a high degree of automation, the sample positioning is dramatically simplified. Furthermore it allows for an integrated documentation of the different measurement methods. This enables a significantly more efficient use of the experimental time.

7.5.5. Manufacturing Techniques

As shown above, modern system engineering enables interdisciplinary design and development, with teams of engineers from various disciplines developing optimised and specialised components. However, in order to ensure a proper functionality, the production methods have to fulfill the highest demands as well.

Mechanical Manufacturing
The tolerances of parts are becoming more and more restrictive and the structures of the components will be also finer and more complex. Industrial manufacturing often does not have suitable solution for the special requirements of materials, tolerances and the limited number of individual components. With the organisation of the internal workshops in a collaborative workshop network, DESY has already established opportunities for very close cooperation between developers and producers. In this way, the manufacturing processes for the special requirements of materials and geometry of accelerator components and experimental instruments are improved. However, for the high level of precision required at PETRA IV, DESY needs to strengthen the department for manufacturing highly specialised components used in precision mechanics.

Electronics Manufacturing
The basic requirements for mechanical manufacturing also apply to the fabrication of electronic modules. DESY has several specialised electronics departments, where experts work together with scientists and engineers to develop and build highly specialised components for accelerators or experiments. One example is the Service Centre Electronics, with its own PCB production facility, which can develop and manufacture complete devices from the idea to CE certification. Another department is the MicroTCA Technology Lab. This offers a wide range of services for the development of MicroTCA-based electronic devices and the associated firmware, thus enabling the development and construction of high-tech components for the machine and the experiments.
7.5.6. Minimising Disruptive Factors

As already mentioned in the previous sections, the temperature stability in the experimental environment is also a critical parameter for positional stability. For example, temperature fluctuations lead to uncontrolled drifts and cause inaccurate positioning of the sample. FEA methods are applied to these aspects in order to identify weak points in advance and to compensate them with a dedicated mechanical design and the use of specially selected materials. By using these simulation methods, in combination with extremely stable environment conditions, thermal drifts can be avoided almost completely. Nevertheless, the disturbing influences from the sample environment need to be considered, as well. Here, especially during in-situ experiments, e.g. with heating cells, the region of interest must not drift out of the measurement range due to thermal effects. In addition, in dynamic experiments it must be ensured that the sample keeps a defined position during the measurement cycle. The equipment required for this kind of measurements is very complex, since large interfering factors have to be compensated by the design or an adaptive position correction. Figure 7.23 shows how the influence of a heating cell affects the sample environment. With thermal simulation, temperature gradients can be determined very precisely in advance, enabling a dynamic position correction. Measurements on PETRA III show that this method works very well and that the sample can be placed in a stable position over a longer period of time.

7.5.7. Commissioning, Tests and Documentation

Hardware tests have to be carried out in advance to ensure that the equipment performs properly during operation of the experiments. For this purpose, specific test procedures have to be defined and established. In order to realise this initial commissioning, special laboratories must be equipped in which conditions are similar to the experimental conditions. This enables the measurement, simulation and testing of function, stability and the integration of new devices into the software environment of the beamlines.

7.5.8. Risk Assessment and Additional Requirements

The requirements on many instruments and experimental stations are very high, reaching and even sometimes exceeding current technological limits. With the above-mentioned engineering schemes (cf. Section 7.4 and 7.5) together with continuous instrumental development that started several years ago, DESY engineers work on minimising the risk of not being able to take full advantage of the experimental capabilities due to instrumental shortcomings of the photon beamlines. DESY is part of international collaborations on solving engineering challenges for the next generation synchrotron radiation sources, such has NFFA and LEAPS. The detailed beamline portfolio will be defined in the TDR phase (cf. Section 7.1). A more detailed list of requirements will be compiled for the beamline instrumentation during that phase. Then, the instrumental development programme will we focused on solving the more specific engineering challenges. The engineering solutions can be tested at PETRA III. The very ambitious time schedule is also a significant challenge for the scientists and engineers, which requires a very good organisation of the work flows and a high level of teamwork during the upcoming phases of the project. A detailed planning of the necessary resources and logistics are part of the TDR. The infrastructure for the development, testing and specification of new equipment is currently in preparation.
7.6. Detectors

The dramatically increased brightness and coherence of PETRA IV will enable an exciting range of experimental methods, but also place greatly increased demands on X-ray detectors. Many of the detectors for PETRA IV will be acquired commercially or developed in collaboration with other institutes. In particular, European light sources within the LEAPS consortium are planning a programme of complementary detector developments in order to cover the diverse range of detectors needed by next-generation sources. At DESY, we will focus on a few key detector developments that are especially important to science at PETRA IV and the European XFEL. Developing a new detector typically takes at least five years, so these developments will need to begin early in the PETRA IV project. The detector group has developed systems for PETRA III and the European XFEL, so experienced personnel and lab infrastructure are already available. However, funding will be needed for new hardware and additional staff to build these systems for PETRA IV.

Two key aims of PETRA IV are to achieve X-ray microscopy covering length scales from macroscopic objects down to atoms and to study dynamics in materials on time scales down to microseconds and below. Both of these methods require faster detectors. New X-ray microscopy techniques generally involve raster-scanning a sample across a nano- or microfocused X-ray beam and taking X-ray data, such as a coherent X-ray diffraction pattern, at each scan point. The increased brightness and coherence of PETRA IV will reduce the acquisition time per scan point to as little as 10 µs, allowing scans of large areas and 3D volumes. However, this naturally requires detectors capable of acquiring data at 100 kHz rates. Likewise, studying fast dynamics in materials will require correspondingly fast detectors. These demands on detector speed will need to be met while maintaining and improving other performance parameters, such as pixel size, detection efficiency and dynamic range. A particular distinctive feature of PETRA IV is its capability to produce hard X-rays with high brightness and coherence. So, efficient detection of hard X-rays is an additional requirement.

In the following sections, we outline specific detector developments needed to make effective use of PETRA IV and briefly discuss opportunities to access detectors through collaboration with other institutes and from industry.

7.6.1. High-Speed Integrating X-Ray Imager

At third-generation synchrotron radiation sources such as PETRA III, photon-counting hybrid pixel detectors are the technology of choice for X-ray diffraction experiments, with their key strengths being effectively noise-free operation and high frame rate. However, photon-counting detectors have a maximum counting rate per pixel, which can prevent them from accurately measuring very intense X-ray diffraction signals, such as Bragg peaks or X-ray scattered signals close to the beam. The dramatic increase in brightness at PETRA IV and increased use of techniques such as coherent imaging mean that many measurements will require pixel detectors with a wider dynamic range. In addition, detector frame rates up to 100 kHz will be needed, compared to ~1 kHz frame rates today.

Detectors for X-ray free-electron lasers (XFELs), such as AGIPD [146] and Jungfrau [147], have been developed by DESY and PSI using an “adaptive gain” integrating amplifier design, which can achieve sensitivity to single photons while also measuring up to $10^4$ photons simultaneously hitting a pixel. In this design, each pixel has an amplifier, which measures the total integrated signal in the pixel during the image. In-pixel circuitry dynamically varies the amplifier’s gain in response to the magnitude of the incoming signal, on a pixel-by-pixel and image-by-image basis. If few photons hit the pixel, the high gain makes it possible to measure the total signal accurately enough to determine the exact number of photons. For higher signals, the gain is lowered, but the noise is significantly below Poisson statistics. As shown in Figure 7.24, in tests with AGIPD at Beamline P10, it was possible to see both the direct X-ray beam and single photons scattered from a sample within a single image.
Using this concept, we plan to build a high-frame-rate integrating hybrid pixel detector, suitable for use at both PETRA IV and future continuous-wave (CW) XFEL sources. Table 7.2 lists the planned specifications of this detector. In operation at PETRA IV, the maximum flux an integrating detector can detect is the product of the signal range per image and the frame rate. So, a 100 kHz frame rate imager with $10^4$ photon signal range could detect up to $10^9$ photons/second/pixel, which is a factor of about 100 higher than can be achieved with photon-counting detectors. The detector will have a modular design, similar to the detector systems mentioned above, so by tiling together many modules it will be possible to build large systems with pixel counts of 10 megapixels and above.

The main technical challenges of developing this detector are due to its extremely high data rate: The signal measured in each pixel must be rapidly digitised, passed from the sensor assembly to a specialised readout board over highly parallelised high-speed electrical links, serialised and transmitted out of the detector head over optical fibres. When building large-area X-ray detectors, the data bandwidth per unit area is a key limiting factor, and this creates a trade-off between frame rate and pixel size. A conceptual design study has been made for this detector, and it should be possible to exceed the minimum specifications listed in Table 7.2. This requires us to develop a new readout chip in a smaller technology scale (65 nm CMOS) and to take advantage of rapid improvements in commercial components such as optical links and field-programmable gate arrays (FPGAs). These developments will, in particular, require experienced electronic engineers. However, the benefits of working with these new commercial components can also be applied to other areas, such as high-speed data processing.

### 7.6.2. X-Ray Imager with Event-by-Event Readout

If we ignore the issue of data volume, the ideal detector for a photon science experiment would provide full information on each individual photon: exactly when and where it arrived at the detector, and its energy. New developments in detector technology make it possible to build pixel detectors with “event-by-event” readout capability, where the detector provides time of arrival and energy information on each photon. This type of detector could improve performance in experiments where the X-ray flux is more moderate. To take a specific example, X-ray photon correlation spectroscopy (XPCS) techniques would benefit greatly from the increased coherence of PETRA IV and could potentially measure dynamics in soft matter down to time scales of tens of nanoseconds (cf. Section 4.3). While it is currently unfeasible to continuously take full X-ray images at 100 MHz rate, a pixel detector with event-by-event readout could measure the time of arrival of each photon with single-bunch accuracy.

DESY is a member of the Medipix3/Timepix3 and Medipix4/Timepix4 collaborations, led by CERN. The Timepix3 [148] readout chip has event-by-event readout. It is currently used at DESY for experiments such as molecular imaging, but is limited to experiments with low flux. Within the Timepix4 collaboration, CERN is developing a readout chip capable of operating both in a photon-counting mode (with superior performance to existing photon-counting detectors) and in an event-by-event mode with improved data rate and time resolution. Based on data from PETRA III, the data rate capability
7.6.3. High-Z Sensor Materials for High-Energy X-Ray Detection

A unique feature of PETRA IV will be its high coherence at high X-ray energies, and to take advantage of this, hard X-ray detectors are needed. However, above 20 keV, typical silicon sensors have low efficiency. A common approach to hard X-ray detection is to convert hard X-rays to visible light with a scintillator and then to detect this light with a visible-light sensor, but this indirect detection process is inefficient and reduces performance. In particular, while visible-light imagers exist that are sensitive enough to detect the scintillation light from a single X-ray photon, these imagers tend to be limited in speed or signal range.

![Figure 7.25: A 2-megapixel GaAs photon-counting detector (LAMBDA), currently used by Beamline P02.2 at PETRA III. By courtesy of X-Spectrum GmbH.](image)
The two detectors described previously (Section 7.6.1 and 7.6.2) use a “hybrid pixel” structure, where a pixelated sensor layer is bonded face-to-face with a readout chip. While hybrid detectors typically use silicon as a sensor material, it is possible to use sensors with higher atomic number ("high-Z") for efficient detection of hard X-rays, provided the readout chip is appropriately designed. DESY has worked with suppliers of gallium arsenide, cadmium telluride and germanium to improve the quality of these materials. In recent years, we have built large (2-megapixel) detectors with high-Z sensors that are capable of measuring hard X-ray diffraction with frame rates of 2 kHz and single-photon sensitivity [149]. A system with GaAs is shown in Figure 7.25. While these sensor materials do not yet have the same level of uniformity as silicon, their quality has become sufficiently good for practical use in many experiments.

For PETRA IV, the X-ray imagers described above can be designed to be compatible with both silicon and high-Z materials, allowing them to be used at high-energy X-ray beamlines. The quality and availability of high-Z materials should continue to improve over time, thus leading to better image quality. An important requirement for some experiments is the stability of the sensor material under high X-ray flux; in particular, the response of CdTe is known to change temporarily under intense irradiation. To meet these requirements, we will investigate the performance of different materials under high flux, including a wider range of materials such as cadmium zinc telluride.

### 7.6.4. Detectors for Spectroscopy

By micro- and nanofocusing the full PETRA IV beam, it will be possible to combine microscopy with a wide range of spectroscopic techniques; for example, X-ray fluorescence measurements provide additional information on elemental composition, and photoelectron measurements provide information on band structure (cf. Section 4.2). These spectroscopic techniques can be grouped into different categories. In some cases, the experiment is designed to encode energy information with position. For example, as described in Section 4.2, it will be possible to perform resonant inelastic X-ray scattering (RIXS) experiments where a combination of incoming and scattered photon energies are encoded by position on a pixel detector. For these experiments, the pixel detectors described above could be used. Likewise, the Timepix4 development could be used for techniques such as photoelectron detection. Other spectroscopic techniques would require other specialised detectors.

Energy-resolving detectors for X-ray fluorescence measurements are readily available, but rapid scanning measurements require both a large number of detector elements, to make it possible to detect hundreds of millions of photons per second, and a large solid angle, to increase efficiency. Detector developments such as the MAIA detector [150] from Brookhaven National Laboratory (with 384 silicon elements) have made significant progress, making it possible to perform X-ray fluorescence scans with 50 µs dwell time per scan point. Likewise, Rutherford Appleton Laboratory has developed a spectroscopic hybrid pixel detector called Hexitec [151] and built systems with 160 000 pixels. Both of these systems are already being used at DESY, and over the coming years we expect further improvements in these detectors. For experiments requiring high energy resolution, cryogenic detectors such as superconducting tunnel junctions have a lot of potential, and the Helmholtz Association plans to develop lab infrastructure for these detectors within its Matter and Technologies programme.

### 7.6.5. Imagers with Small Pixel Sizes

Certain X-ray techniques such as full-field X-ray microscopy require imaging detectors with as small an effective pixel size as possible. This is typically achieved by coupling a thin scintillator to a visible-light detector with small pixels, using optics to magnify the image. In coming years, this approach can benefit from rapid improvements in commercially available visible-light imagers using CMOS technology (where a single silicon wafer performs both light detection and signal processing). Additionally, DESY is currently developing a CMOS imager called Percival [152] in collaboration with other light sources. Percival offers a unique combination of high dynamic range, sensitivity to low signals and relatively high
7.6.6. High-Speed Processing of Detector Data

To make full use of the capabilities of PETRA IV, large quantities of experimental data must be processed. This is a complex topic, which is discussed fully in the next section. As a first step, however, the raw data stream from the detector must be converted into meaningful images; in integrating detectors, for example, the raw data consists of digitised voltages from each pixel, which must be converted into numbers of X-ray photons. This should be performed in real time, so that beamline scientists and users have immediate access to useful experimental data. For a given detector, converting raw data into images is a relatively fixed process, which can also be highly parallelised. So, this task can be efficiently performed by a specialised layer of hardware, before the data is passed to a high-performance computing cluster. This could consist, for example, of multiple FPGAs within a MicroTCA crate. This layer could also perform data compression and other processing tasks in order to reduce the workload on later stages of data handling. The development of this specialised processing layer can take advantage of existing expertise within DESY (e.g. the MicroTCA Technology Lab) and other Helmholtz institutes in the Matter and Technologies programme.

Improving detector performance to make effective use of PETRA IV is a significant challenge. We will focus on a few key detector developments that are needed to meet the specific requirements of PETRA IV, and which complement developments by other photon sources and industry.

7.7. Data Handling and Experiment Control System

The PETRA IV computing model covers all IT services that are necessary to control the experiments and to collect, store, process and visualise the data. Figure 7.26 shows the main components of the system, which will be discussed in the following sections. The primary objectives leading to the specifications of the model are:

- Fast data reduction, high-speed data transfer and efficient storage to cope with the data rates of modern 2D detectors,
- Near real-time analysis for a rapid experiment feedback to ensure the data quality,
- Offline analysis executed in parallel with the data taking and finished by the end of the beamtime,
- Standard visualisation tools to display raw and derived data,
- Web portal to browse and download data.

These ambitious goals can only be achieved by an integration of services provided by the DESY Photon Science division (FS) and the DESY computer centre.

7.7.1. Experiment Control System

When setting up an experiment control system (CS), several issues have to be considered. The CS has to be very flexible to cope with the frequent changes of the experimental setups at the beamlines. The standard operating systems (Linux, Windows) have to be supported. The CS needs bindings to scripting (Python) and programming languages (C++). The performance has to be adequate to handle motors, counters, timers, etc. Additional methods are needed to transfer data from 2D detectors, which create by far the highest data rates. Furthermore, experiments requiring logical decisions or synchronisations on a time scale below a ms need customised electronics to
cope with the speed. These applications need a deterministic behaviour and therefore cannot be implemented on PCs. Instead, field-programmable gate arrays (FPGAs) have to be employed. They run sufficiently fast and can be adapted to a variety of tasks by preparing a suitable firmware. FPGAs are operated by the control system, but they run independently. In addition to these technical aspects, there is another important issue that needs to be considered. An experiment control system should be supported by an international community for several reasons:

- The reuse of code that has been written elsewhere saves resources, and the quality of the code usually improves if it is developed by a group of programmers.

- The communication among the members of the collaboration about new ideas, procedures and experiences is advantageous.

- Collaborations help to develop common user interfaces. At PETRA III, the user interfaces are prepared within the Sardana\(^1\) framework, which was created at ALBA and is now being further maintained by a collaboration of ALBA, DESY, MAX IV and Solaris, leading to a standardisation in the area of control clients. PETRA IV intends to follow the same path.

- Sustainability: The software in the experimental area is programmed against the application programming interface (API) of a particular CS. This code is a major investment that is best protected by selecting a CS that is supported by a strong community.

The PETRA IV control system will support all relevant field bus systems, including MicroTCA. This modular bus system is specialised for high-throughput applications and adaptable to very specific needs. MicroTCA will play an important role in the readout of fast 2D detectors (see below), and it will be applied to synchronise data acquisition with the arrival times of bunches in the accelerator.

At PETRA III, Tango\(^2\) serves as the device access layer. This CS is supported by a community of ten core members and about 50 partners from academia and industry organised as a consortium. It is remarkable that the Square Kilometre Array (SKA), a large project from outside the photon science area, became a core member recently.

For the reasons mentioned above, it was decided not to start a new development, but to use Tango for PETRA IV. In case requirements will arise that are not covered by the current

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1. sardana-controls.org
2. www.tango-controls.org

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**Figure 7.26.:** PETRA IV computing model.
functionality of the program, Tango will be extended. The work should be carried out in collaboration with other institutes. A project within LEAPS\(^3\) seems to be an ideal platform for organising such a common effort (cf. Section 2.4.2).

7.7.2. Data Acquisition, Storage and Processing

The primary goal of a data acquisition system is to transfer all detector data to a storage system. The transfer process can be divided into three sections. Each of these contributes to the overall performance, and each of the steps has to be reconsidered when new, faster detectors are installed:

1. **Readout:** Usually, detectors are read out by dedicated PCs executing some raw data processing and compression. The detector PCs should be able to forward the data to the transfer step without any delay. If time lags occur, the detector PCs can be equipped with more RAM or more cores to make them faster. This procedure applies for detectors that have been purchased from commercial manufacturers.

   For detectors built by DESY or by a collaboration including DESY, data processing can be integrated more deeply. As pointed out in the detector section (cf. Section 7.6), raw data processing can be done by FPGAs hosted in MicroTCA crates, resulting in a higher performance.

2. **Transfer:** For an optimal data transfer, it has to be assured that the protocol is able to saturate the network line speed. If this is assured, the transfer speed can only be increased by upgrading the network infrastructure or by parallelising I/O.

3. **Storage:** Data will be stored in the DESY computer centre. For PETRA III, the storage system is divided into two subsystems: the beamline file system (BL-FS) and the core file system (C-FS). The BL-FS receives the data coming from the detectors. It has multiple entry points to cope with the parallel I/O requirement. The BL-FS is optimised for write operations. To make data available for near real-time and offline analysis, they are copied to the C-FS within seconds. The C-FS has a high-throughput connection to the compute servers and a full authorisation management.

   The core file server can be considered as a first-level storage. It is highly performant but rather expensive. Therefore, a second-level storage needs to be installed, where the data are migrated after they have been analysed. Currently dCache, a collaborative initiative between DESY and Fermilab, serves as the second-level storage.

   Data processing is executed on a cluster of multicore compute nodes optionally equipped with GPUs.

   The standard data format will be based on HDF5, because this format allows for annotation of the data with information describing the data sources, the experiment setup and the measurement technique. During the ingest procedure, metadata are extracted and stored in a metadata catalogue.

   Data taken at PETRA IV will be managed under a policy largely following the recommendations of the PaN-data Europe project (D2.1) on data ownership, data curation, data archiving and open access to data. The main points of the policy are: DESY acts as a custodian of the experimental primary data and metadata; data and metadata become open access after an embargo period; a searchable catalogue gives access to the data and metadata.

7.7.3. Scientific Computing Support

The goals mentioned in the introduction can only be achieved by a scientific software group (SSG). The members of this group need an in-depth knowledge of advanced computing techniques including parallelisation, data science, mathematical methods and hardware-accelerated computing. They have to understand the scientific background and the experiment procedures.

The members of the SSG will be assigned to improve the data processing for specific experimental techniques. They will optimise the
Data Handling and Experiment Control System

algorithms for near real-time and offline analysis.
The members of the SSG will find the best technical solutions in terms of cluster computing, possibly with GPU utilisation or other hardware-accelerated computing techniques. They will know how to utilise the storage system to reach the best performance. Eventually, they will create interfaces that allow the users to utilise the whole framework efficiently. The members of the SSG will instruct the users how best to use the experiment control and data processing framework.

After work on a specific project is completed, the scientific programmers will take on a new task. The completed project will continue to be supported, however. Since the scientific programmers are organised in a group, it will easily be possible to exploit synergies.

Currently, there are plans to establish the Centre for Data and Computing in Natural Science (CDCS), a joint initiative of DESY and the universities in Hamburg (cf. Section 2.1.1). According to the current state of planning, CDCS will focus on topics that are relevant for the user support of the DESY facilities, such as machine learning, methods in imaging, automation and control as well as computational methods. A close collaboration with the scientific groups within CDCS will be needed to tackle the big-data challenge created by PETRA IV.

Data handling and experiment control at PETRA IV requires an integration of several IT-related services. The big challenge of coping with the huge data rates of modern 2D detectors will be addressed by preparing an adapted data acquisition, data transfer and data storage chain. Since the success of a beamtime may depend on fast feedback information, a near real-time analysis framework has to be prepared. It is almost equally important that the off-line analysis is completed during the beamtimes. These two activities have to be supported by a powerful scientific computing group with links to the Interdisciplinary Data Analysis Facility (IDAF) and CDCS (Section 2.1.1).

**Staffing**

Since the PETRA IV experiment control system will be an evolution of the PETRA III software, no fundamental changes requiring a significant increase of the personnel are expected. The staff development in this field will be proportional to the number of experimental stations and beamlines. However, high throughput applications and the synchronisation of experiments and accelerator (arrival times of bunches) will create new demands that can only be fulfilled by hiring additional staff.

Furthermore, the experiment control support of the PETRA III experiments is limited to the regular working hours. If this service will be extended for PETRA IV, the personnel has to be extended accordingly.

Regarding the scientific computing support (SC), PETRA IV will benefit from the experiences made at PETRA III. Data reduction, near real-time data processing for rapid experiment feedback and offline analysis have recently been identified as critical tasks to accomplish the facilities mission. Therefore, a group will be established to work on this matter. Since the data rates at PETRA IV will lead to an increase of data volumes by several orders of magnitude a strong SC group will be of vital importance for the success of the facility.
References


Deutsches Elektronen-Synchrotron DESY
A Research Centre of the Helmholtz Association

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