XAFS-DET: a new high throughout X-ray spectroscopy detector system developed for synchrotron applications

F. Orsini^{a,*}, S. Aplin^b, A. Balerna^c, P. Bell^d, J. Casas^e, M. Cascella^d, S. Chatterji^f, C. Cohen^g, G. Dennis^f, P. Fajardo^g, H. Graafsma^h, H. Hirsemann^h, F.J. Iguaz^a, K. Klementiev^d, T. Kołodziejⁱ, L. Manzanillas^a, T. Martin^g, R. Menk^k, M. Porro^{b,l}, M. Quispe^e, B. Schmitt^j, N. Tartoni^f, M. Turcato^b, C. Ward^d, E. Welter^h

a Synchrotron SOLEIL, L'Orme des Merisiers, Départementale 128, Saint-Aubin, 91190, France b European XFEL, Holzkoppel 4, Schenefeld, 22869, Germany
c Laboratori Nazionali di Frascati, Via Enrico Fermi 54 (già 40), Frascati (Roma), 00044, Italy d MAX IV Laboratory, Lund University, Fotongatan 2, Lund, 224 84, Sweden
c ALBA-CELLS Synchrotron Radiation Facility, Carrer de la Llum 2-26, Cerdanyola del Valles, Barcelona, 08290, Spain f Diamond Light Source Ltd, Harwell Science and Innovation Campus, Didcot, OX1 10DE, United Kingdom The European Synchrotron Radiation Facility (ESRF), 71 avenue des Martyrs, Grenoble, 38000, France h Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, Hamburg, 22607, Germany i Jagiellonian University, ul. Golebia 24, Kraków, 31-007, Poland j Paul Scherrer Institute, Forschungsstr 111, Villigen PSI, 5232, Switzerland k Elettra-Sincrotrone Trieste, S.C.p.A., S.S. 14-km 163.5 in AREA Science Park, Basovizza, Trieste, 34149, Italy l Department of Molecular Sciences and Nanosystems, Ca' Foscari University of Venice, Dorsoduro 3246, Venezia, 30172, Italy

Abstract

The high brilliance and coherent beams resulting from recent upgraded synchrotron radiation facilities open the way for a large range of experiments, where detectors play a key role in the techniques and methods developed to fully exploit the upgraded synchrotron. For instance, one of the major limitations of XAFS experiment is the performance of the detectors. In order to be able to measure more challenging samples and to cope with the very high photon flux of the current and future (diffraction limited) sources, technological developments of detectors are necessary. In this framework, the germanium detector developed in the European project LEAPS-INNOV aims at improving several technological aspects. This type of detector represents a very important class of instruments for X-ray spectroscopy due to the fact that they enable to detect efficiently photons of considerable higher energy with respect to silicon detectors. The objective of this project consists in pushing the detector performance beyond the state-of-the-art. Preliminary layout and main choices for the design studies of this new detector are presented in this paper.

Keywords: Germanium detectors, X-rays spectroscopy, XAFS, Synchrotons Applications

1. Introduction

- With continuous improvements and upgrade of synchrotron radiation facilities, detection technologies beyond current capabilities are essential. In particular, in X-ray spectroscopy ap-
 - *Corresponding author

Email address: fabienne.orsini@synchrotron-soleil.fr (F. Orsini)

plications, germanium detectors are a class of detectors which offer energy resolution not far from the Fano limit. They are generally used in synchrotron experiments which require excellent energy resolution, for instance, when it is necessary to separate the fluorescence photons of an element from the elastically scattered radiation used to excite the sample. Spectroscopy grade Silicon detectors (either Si(Li) or SDD) are the only other class of detectors which offer similar energy resolution but they are not as effective when the photon energy becomes higher than 30 keV because of the lower stopping power of Silicon with respect to Germanium. In addition, Silicon detectors can lead to some artefacts in techniques such as XAFS (X-rays Absorption Fine Structure) because of the close distance of the escape peak from the main peak.

At synchrotron facilities, the major challenge is to exploit effectively all the photons produced by the machine and this means that the detector must have high throughput. Multi-element detectors enable to enhance the throughput by distributing the incoming photon flux on different detecting elements with independent readout channels. If the elements are built on the same sensor material, i.e. the detector is monolithic, the size of the system turns out to be particularly compact, which is an important advantage for many applications.

In this context, the detector workpackage of the European project LEAPS-INNOV [1], also named XAFS-DET project, aims at pushing germanium detector performance beyond the state-of-the-art in the energy range from 5 to 100 keV that suits a large number of synchrotron facilities. In this project, the throughput per unit area for X-ray spectroscopy will be enhanced by developing a multi-element monolithic detector. In one version of the detector prototype, shrinking the germanium element size will also entail challenges such as the development of new miniaturized front-end electronics and the use of advanced Digital Pulse Processors (DPP) to avoid collimators in front of the sensing elements. The new technological developments proposed in this project would push the limit of current available detectors and open up new experimental possibilities.

2. Main specifications for the germanium detector and general layout

The main requirements for the High-grade Purity Germanium (HPGe) detector and its associated electronics are summarized in the following table 1 and presented in the CDR of the project [2].

One of the particularities of the HPGe detector is the need to be cryo-cooled to limit the leakage current of the germanium sensor. This condition leads to a complex detector layout as schematically illustrated with Figure 1. The detector consists of three main blocks:

- A very compact detector head under vacuum and cryogenic temperature. This part includes the detector window, the germanium sensor and its mechanical holder, the frontend electronics composed of boards equipped with specific readout preamplifiers, and the interconnections elements between the germanium sensor and the front-end electronics;
- A detector body with a part under vacuum and cryogenic temperature and another part that
 may include the back-end electronics in air and room temperature. This part includes the
 cryogenic cooling system needed to cool down the detector head, some shielded connections, the cryostat, and the flanges equipped with feedthroughs;
- Some external parts with the Digital Pulse Processing electronics, the power supplies and computers for the monitoring and control of the whole equipment and data recording.

Table 1: Main requirements for the XFAS-DET detector prototype.

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X-ray energy range	From 5 to 100 keV
Number of pixels	10
Pixel size and thickness	Small pixel version of 5 mm ² and large pixel version of
Energy resolution	20 mm ² , both versions are 4 mm thick < 200 eV FWHM at 5.9 keV and an Input Count Rate of
Detector efficiency	100 kcps/pixel and a shaping time (or equivalent) of 1 μs > 90% in the required energy range
Input Count Rate (ICR)	From 20 kcps/mm ² up to 250 kcps/mm ²
range per unit area	
Dead time (%) at 5.9 keV	30% at 1 Mcps and maintained at reasonable level at high
	energy (20-100 keV)
Peak to Background Ratio	> 1000 at 5.9 keV, defined as the ratio between the counts
	in the peak channel and the average background
Detector temperature	77 K (detector head and body)
Detector vacuum	1×10^{-7} mbar
Input Window	Beryllium window
Germanium sensor collimator	Multi-layer collimator

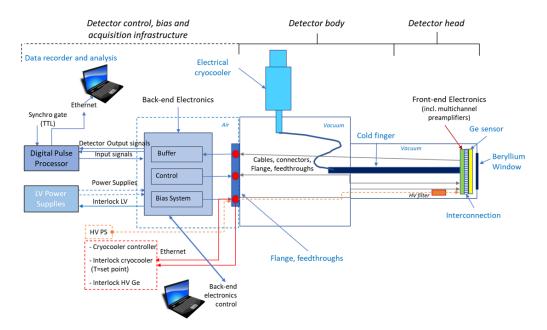


Figure 1: General layout of the XAFS-DET detector with main components.

The following sections give a general description of the main components with the on-going mechanical design of the whole detector.

3. Germanium sensors

The sensing part consists of a HPGe sensor. To avoid excessive complexity and costs of the prototype, it was decided to limit the number of segmentation elements of the germanium sensor to a reasonable and pragmatic maximum of ten pixels. Two-pixel versions will be designed in the project bearing in mind two different type of applications: the 5 mm² pixel area is dedicated to XAFS experiments and the future needs to scale up the number of channels [3], whereas the 20 mm² pixel area is considered for the needs of X-Ray Fluorescence (XRF) experiments, where the solid angle of collection needs to be maximized. The two versions, illustrated in Figure 2, differ only in a scale factor. The hexagonal and trapezoidal shape of pixels is appropriate to limit the charge sharing among fewer neighbouring pixels. The unusual ring-shape configuration of the three outermost pixels has been conceived to use them as ancillary pixels to electronically reject the charge sharing effect. All the pixels of one version have the same area so as the counting rate will not differ excessively between the pixels.

The frontside (facing the incident X-rays) is phosphorus implanted (N+ doped electrode) while the backside (segmented side with 2 pixels versions) is boron implanted (P+ doped). The inter-pixel spacing will be defined precisely later on by the manufacturer (depending on their process) to be compatible with an insulation of 10 TOhms. Aluminum contact will be evaporated on the implants (pixel surface) and on the frontside of the sensor. A bias voltage of +200 V is applied on the frontside, and the pixel electrode is grounded. The detector works in holes collection mode.

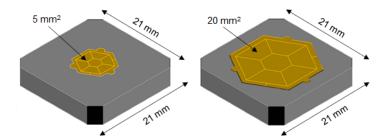


Figure 2: Germanium sensor segmentation on the back side: $10 \text{ pixels of } 5 \text{ mm}^2 \text{ each (left)}$ and $10 \text{ pixels of } 20 \text{ mm}^2 \text{ each (right)}$. The germanium dice is $21 \times 21 \times 4 \text{ mm}^3$.

4. Electronic chain

To cope with high segmented and compact germanium detector, operating in a large energy range from 5 to 100 keV, it is necessary to foresee a new electronic chain able to perform signal processing of several channels simultaneously.

The electronics of the project can be considered as a three-blocks system designed specifically for this development. The first block is the multi-channel integrated preamplifier (microelectronic circuit in CMOS technology). The second block is the front-end electronics equipped

with the ASICs (shown in Figure 3-left), followed by the third block, i.e. back-end electronics (shown in Figure 3-right). The two first blocks share the same environment under vacuum and cold temperature and are very close to the germanium sensor (as shown in Figure 1). The three blocks are strongly interfaced together.

The design studies of the new multi-channel integrated preamplifier will start in the coming months and the specifications are quite ambitious. The new ASIC must be compatible with the detector capacitance estimated to be from 1 pF to 3 pF for small and large pixels respectively. One discriminator per channel is required, as well as the possibility to disable individual channels. The implementation of three gains, compatible with the 3 energy ranges of interest of the detector (5-15 keV / 15-37.5 keV / 37.5-100 keV) is a constraint for the design. The power consumption is also an issue and it should be limited to 60 mW maximum per ASIC. The reset time duration should be as small as possible: < 2 μ s (including possible artefacts before and after the reset slope) and the number of events between two resets should be at least 20 events in the high energy end of the gain range of the preamplifier, in order to avoid energy resolution degradation and large increase of the total dead time due to reset time at high counting rate and high photon energy.

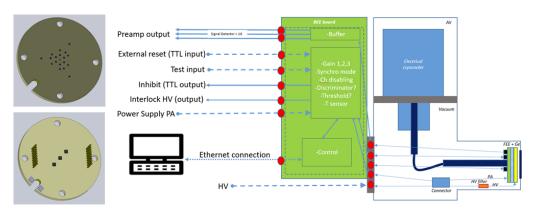


Figure 3: Overview of the front-end board electronic (left): top side of the board matching both the small and large pixels arrangement (top-left) and its back side (bottom-left); Schematic overview of the functionalities of the back-end electronics (right).

The front-end board consists of a multi-layer printed ceramic board, equipped with the integrated low-noise multi-channel preamplifiers. This board, also under design, will also enclose a set of resistances and decoupling capacitances and connectors for I/O signals and power supplies. The front-end board must be compatible with high vacuum (10^{-7} mbar) and liquid-nitrogen temperature (77 K).

The back-end electronic board is the third electronic block at the interface between the detector head and the 'external world' with I/O communication lines. This electronic board will include different functionalities, such as providing and filtering the different power supplies to the front-end board, managing the reset mode, the multi-channel preamplifiers internal gain, and buffering/amplifying the outputs signals. The overall design of the back-end boards will be low noise (few tens of μV max for each power supply). The Figure 3-right illustrates the schematic of this board with its various functionalities.

The readout system, also called the Digital Pulse Processor (DPP), will reconstruct the energy

of X-ray events impinging on each germanium pixel and will present the resultant energy spectra to the user. To do this, it digitises the analogue output associated with each pixel and transferred by the back-end electronics, then uses digital algorithms to identify any events in the digital stream and measure their amplitude (energy). Each measured X-ray energy is then binned in a histogram of all those previously measured to form an energy spectrum. The DPP for this project should comprise a minimum of 10 channels with the analogue inputs matching the electrical characteristics of the back-end electronics.

The main specifications for the DPP have been defined by the consortium early in the project, and after a review of existing commercialized systems, it was decided to purchase a 10-channel modified Xspress4 DPP developed by DIAMOND. One of the unique features of the Xspress4 is its ability to characterise and potentially correct for inter-pixel effects in segmented monolithic detectors [4].

5. Mechanical design and preliminary thermal simulations

The current mechanical model under design is illustrated in Figure 4-left. This design is preliminary and progress iteratively with the thermal simulation studies. There is a wide-but-close interaction between the mechanical design, the thermal simulations, the components under development and the overall system integration.

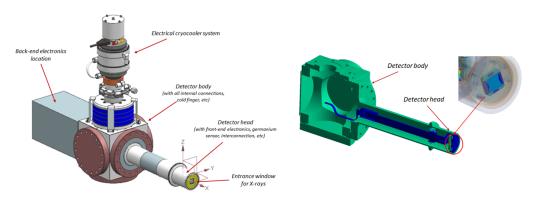


Figure 4: Simplified mechanical model of the XAFS-DET detector (left); Preliminary results of the thermal studies (in case of optimized contacts and copper braid, and a ceramic front-end electronic board)(right).

The preliminary thermal studies have been performed based on the current mechanical design. The very first results feature an efficient cooling of the germanium sensor close to 77 K, in case of optimized contacts and copper braid, and with a ceramic front-end electronic board, as illustrated on Figure 4-right. As the thermal contacts are essential in this project and are based on 'ideal' assumptions for the moment, a dedicated set-up is foreseen to get soon more realistic experimental values which could be included in the thermal simulations.

6. Cooling system

The baseline option for the cooling at 77 K consists of replacing the usual LN2 cryostat by an electrical cryocooler. The goal is to simplify detector operation, make it more compact, and

suppress the tedious LN2 refilling. In practice, it requires a meticulous selection of components under vacuum to avoid high level of outgassing and reduce the needs of power cooling. After a survey of different commercialized systems, and due to budget constraints, a SunPower system has been chosen.

This system is operated by the Stirling cycle, that compress and expands a fixed quantity of Helium gas. The available 11 W cooling power is large enough for our needs. Nevertheless, this system can induce high vibration to the cold finger, and this aspect can be an issue on beamlines requiring low induced vibration for high beam stability. In order to assess this potential negative effect, a dedicated test bench is under preparation to study the efficiency of a vibration cancellation system, inspired from the existing Maroon-X detector system [5] (as shown in Figure 5) and first results are expected in the coming months.

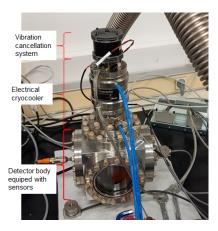


Figure 5: Vibration induced by the electrical cryocooler under assessment with a dedicated testbench.

7. Simulation of detector performances

A strong effort has been made by the project consortium on simulation tools to provide guidelines for the detector design studies. A dedicated simulation chain has been implemented and it includes all the steps from the interaction of X-rays with matter to a reconstructed energy spectrum using simulated raw-data-like waveforms. This simulation chain, based on Geant4, COMSOL MultiphysicsTM (Semiconductor module) linked to Allpix-squared framework [6] and also on SSD software packages, is schematically represented in Figure 6-left and is described in details in [7].

As an example of output, the energy spectrum obtained for one configuration of our detector has been simulated with an incident 30 keV direct beam (with 2 millions of photons). The results are presented in Figure 6-right. In this figure, the Signal-to-Background ratio is of the order of 800 for the large pixels, which is close to our requirements. This work will continue with more realistic parameter definitions inserted in the simulations (detector secondary component material, front-end electronic features, etc) as the design will be refined.

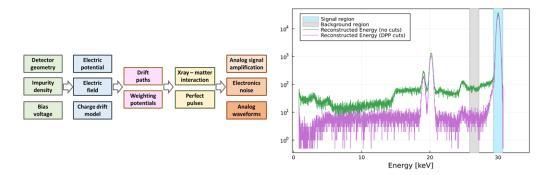


Figure 6: Flowchart of the multiphysics simulation chain (left), reconstructed energy spectrum for a direct X-ray beam of 30 keV. The two peaks around 20 keV come from the germanium fluorescence peaks (right).

8. Summary and next steps

The XAFS-DET project is an ambitious R&D European project launched in April 2021 for the development of a new generation of monolithic pixelized germanium detectors for synchrotron applications. Several design studies have started in parallel (germanium sensor, mechanics, thermics, cooling, etc). Multi-physics simulations are used to guide the detector design and will assess the future detector performances.

The next steps in the coming months will consist in finalizing the mechanical and thermal design studies of the detector head (taking into account the integration of all the critical components which compose the head and which are already under development in different tasks), finalizing the design studies of the multi-channel preamplifier and front-end and back-end electronics, manufacturing the 2 germanium sensors (one of each version), assessing the vibration cancellation system of the cooling system with a dedicated set-up, and progressing in the thermomechanical design of the complete detector (including the body part and the electrical cryocooler).

9. Acknowledgments

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