Bachelor degree in Physics

Bachelorthesis

THz coupler design for electron accelerators

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On the side of the University of Oldenburg, I would like to thank Prof. Dr. Björn Poppe who supported my idea going to DESY after our first conversation.

Furthermore, traveling between Hamburg and Oldenburg during my work at CFEL could have been much more complicated without the help of my family and in particular Hermann Hiestermann and Lukas Köhneke for providing an accommodation.
2 ZUSAMMENFASSUNG


3 INTRODUCTION

Particle acceleration can be assumed to be one of the most popular and promising topics in physics with bright future. From tube television to the LHC at CERN, particle acceleration is demanded in various applications. The long storage rings at DESY and CERN produced loads of fundamental results. The synchrotron radiation as the main product is progressively used for chemical and biological science. To meet the requirements for screening applications linear accelerators received attention for their multiple possibilities. Due to the large dimensions of the available facilities, concepts have been developed for electron acceleration and free-electron-lasers (FEL) which pursue compact and table top sizes. This thesis is originated at CFEL in the "Ultrafast Optics and X-Rays Division" led by Prof. Dr. Franz X. Kärtner. The main goal is to design a waveguide coupler in the THz frequency range for use in an electron accelerator that is still under construction. The EM-fields in the coupler and all necessary physical behaviour is calculated with CST microwave studio. In the following the corresponding project called "CUBIX - Coherent Ultrabright Inverse Compton Scattering X-ray Source", a table top X-ray source, is presented. Furthermore the basics for Free-Electron Laser (FEL) and electron acceleration are explained with relations to the facilities used in CUBIX.

3.1 CUBIX

The "Coherent Ultrabright Inverse Compton Scattering X-ray Source" as described in the proposal [15] in the beginning of 2011 is a collaboration of the Massachusetts Institute of Technology (MIT), the Northern Illinois University and since 2013 the Center for Free-Electron Laser Science (CFEL). The project aims to construct an X-ray source which consists of a nano-tip field emitter delivering the electrons for direct laser acceleration with TW peak power pulses and finally an inverse compton scattering chamber for the generation of X-Rays.

Apart from the original proposal [15] other experiments are tested as well to investigate their applicability for the project. Concerning this thesis, the laser acceleration could be replaced or supported by THz acceleration to speed up the electrons from 0.95\(c\) to 0.99\(c\). A technical drawing of all the components is shown in figure [7]. The increased application of THz radiation in the CUBIX source is an outstanding feature and likewise a challenge due to several difficulties in the generation of THz radiation. The THz waveguide coupler designed in chapter [7] is positioned at the front or back of the THz linac depending on the position of the THz generation crystal. The ambition for the beam properties are a peak brilliance of \((10^{26} - 10^{27}) \text{ photons/mr}^2/\text{mm}^2/0.1\% \text{ bandwidth}\) by \(5 \times 10^{10}\) photons/s. The CUBIX Source can be considered as a new type of Free-Electron Laser. It will be possible to generate tunable coherent X-rays at high energies with a table top device.
Figure 1: An overview of the CUBIX project taken from [1]. The RF gun delivers pre-accelerated electrons with a speed of 0.5c. After that the THz- or Xband-linac are used for acceleration. To double the electron energy from 20MeV to 40MeV both accelerators can be used. The Emittance Exchange Line (EEX) supports microbunching for coherent radiation in the inverse compton scattering (ICS) generator. The red quadrupole magnets control the dispersion. In the end, an electron spectrometer measures the quality of the electron beam. The setup is about 8m long.

3.2 Free-Electron Laser

Common FELs work with an ultrarelativistic bunch of electrons that is sent through a magnetic undulator. The electromagnetic field in the wiggler drag the electron to a sinusoidal path and coherent synchrotron radiation is emitted because of the periodic change of direction. An outstanding advantage is the ability to tune the frequency of the laser beam by varying the electron energy or the electromagnetic (EM) field. The first FEL was invented and built up at Stanford University by the team of John Madey in the 1970s. Because of the low efficiency and the need for immense facilities there were just a couple of institutes making efforts to push the principle of the FEL forward. To name the famous ones there was the Stanford Linear Accelerator Center (SLAC) at Stanford built up in 1962 which was updated in 2009 and is known as LINAC Coherent Light Source (LCLS), holding the record for the brightest light source with about $8.5 \times 10^{32}$ photons/m$^2$/mm$^2$/0.1% bandwidth with light wavelength down to 0.15nm [16]. In Japan, they just released the SPring-8 Angstrom Compact Free-Electron Laser (SACLA) in March 2011 and raised the record for photon energy to $0.8 \times 10^{-9}$m [17]. In Hamburg, there will be two X-Ray sources with the first high energy FEL FLASH started in 2004 and in 2015 the European XFEL come in stream [16]. The European XFEL will be pioneering with wavelength down to 0.05nm and a peak brilliance of $8.5 \times 10^{32}$ photons/m$^2$/mm$^2$/0.1% bandwidth.

Free-electron lasers are generally categorized in Low-Gain and High-Gain facilities. A Low-Gain FEL is usually constructed with two mirrors on both sides to guide the laserbeam several times through the amplification area. Due to the small energy transfer, the laserfields can be assumed to be constant over the FEL length. Modern FEL with a high brilliance are constructed as High-Gain FEL [18]. The energy transfer happens in just one pass through the FEL therefore the laser field changes with it’s position in the undulator. The FEL sources functioning on strong electric fields are usually referred as the family of High-Gain FEL. High-Gain FEL rely on the principle of self-amplified spontaneous emission (SASE) to radiate coherent light. Due to the shot noise, random electrons in the beginning of the undulator radiate spontaneously. The radiation is used as the self-seeding and no other seeding laser is required. The electrons are distracted transversally on sinusoidal paths which cause synchrotron radiation. The resulting electromagnetic field
acts back on the electrons and accelerate or decelerate them depending on the phase. This leads to the so-called microbunching effect which is amplified along the undulator and creates coherent emission from the electrons. A schematic and the radiation behavior of a FEL is presented in figure 2.

![Figure 2: Sketch of the self-amplification of spontaneous emission (SASE) in an undulator. In the lower part of the figure the longitudinal density modulation (microbunching) of the electron bunch is shown together with the resulting exponential growth of the radiation power along the undulator][2].

The more the electrons are bunched the more coherent is the radiation. Additional the intensity of radiation field grows quadratically with the number of coherently interacting particles [3]. Space change effects restrict the maximum amount of electrons in a bunch and additionally introduce constraints on micro-bunching. To introduce to the analysis of Free-Electron Lasers the important forces and interactions are presented in the following equations. As the relativistic electrons travel through the undulator field they are affected by the Lorentz force. With $\gamma$ the relativistic factor, $m_e$ the mass of an electron and $e$ the electrons charge.

$$\gamma m_e \ddot{\vec{v}} = -e \vec{v} \times \vec{B}$$  \hspace{1cm} (1)

Solving the Lorentz equation results in two coupled differential equations for transversal and longitudinal motion and its solution yields the trajectory of the electron $x(t)$ in the undulator field (2) with a divergence $\Theta_{max}$ (3), the wavenumber of the undulator field $k_u$ and $\beta = v/c$.

$$x(t) \approx -\frac{eB_0}{\gamma m_e \beta c k_u} \cos(k_u \beta c t)$$  \hspace{1cm} (2)

$$\Theta_{max} \approx \left[ \frac{dx}{dz} \right]_{max} = \frac{eB_0}{\gamma m_e \beta c k_u} = \frac{K}{\beta \gamma} \ \text{with} \ K = \frac{eB_0 \lambda_u}{2\pi m_e c}$$  \hspace{1cm} (3)

At this point it is appropiate to name the difference between wiggler and undulator. Mathematically one refers to an undulator when the undulator parameter $K \leq 1$ that means the trajectory stays within the cone of synchrotron radiation. In an undulator, the undulator and emission fields interfere and microbunch the electrons supporting the advantageous monochromatic light emission. The magnetic structure is called a
wiggler when the divergence is higher $K > 1$. Figure 3 shows that the field vector of the EM-field must be synchronized with the electrons trajectory to enable efficient energy transfer. If the synchronization is not fulfilled, the energy transfer from EM-field to electron and other way around would reverse. Because the electron can not travel faster than light especially on the sinusoidal trajectory, the phase of the EM-field has to slip by integer numbers of $\pi$ expressed in equation 4 where $k$ is the wavenumber of the light wave.

$$ (k_u + k)z - \omega t = 0 $$

Generally it is one basic requirement to synchronize the electron speed and phase velocity of the EM-wave to generate a directed energy flow from electron to wave. The same task should also be done for electron acceleration. The adjustments on phase velocity in the waveguide is done with dielectric coating in section 7. The power of radiation emitted by a high gain FEL is given in equation 5.

$$ P = N^2 \cdot \frac{e^2 x_0^2}{6\pi \epsilon_0 c^3} \cdot \omega_0^4 $$

With $x_0$ the amplitude of electron motion, $\omega_0$ the frequency and $e, \epsilon_0, c$ constants. The number of electrons $N$ increases the power quadratically. One thing that all of these high power X-Ray sources have in common are their huge dimensions up to 3.4 km [16]. The longer the undulator magnets are, the better the bunching effect and the higher the achievable energies. The undulator facility at XFEL for example is about 200m long [19]. The size and the costs limit the availability of these X-Ray sources for investigations in medicine, biology or chemistry. As described before, CUBIX pursues a tabletop facility and does not require long undulator magnets. To generate high energy photons the principle of Inverse Compton Scattering (ICS) is used. In contrast to the usual Compton Scattering, the electrons are moving at high velocities when photons and electrons collide and energy is transferred from the electrons to the photons. ICS is capable to produce radiation from the X-ray to optical frequencies [20]. For the CUBIX project one plans to use bunched electron beams and generate coherent ICS. The advantages over other compact X-ray sources like the bremsstrahlung sources are (1) small opening angle (2) coherent radiation accompanied by squared flux gain with the number of electrons and (3) tunable frequency. A laser in the optical range or a THz field can be used for ICS. The THz radiation is located between the microwave und infrared spectrum at the frequency from 0.1 to 10 THz [21]. Despite a lot of advantages over other wavelengths the usage of THz radiation in commercial products remains negligible to this day due to its difficult generation. To close
the gap in the frequency spectrum physicists put in great efforts in the last 10 years \cite{22} to develop new THz sources. Taking such THz sources to perform inverse Compton Scattering it is possible to build up an efficient tabletop X-Ray laser. The CUBIX radiation source as shown in figure 1 delivers a high quality beam which is comparable to the large FELs as illustrated in figure 4 at a fraction of size.

Figure 4: An overview of free-electron laser in terms of peak brilliance and photon energy \cite{4}. The CUBIX marked by the green dot in comparison with FELs around the world.

Currently the set up for the X-Ray source is about 5m long including the RF gun, LINAC, beam focusing and the ICS chamber. It is delivering a peak brilliance of $10^{26} - 10^{27}$ photons/mm$^2$/mm$^2$/0.1\% bandwidth \cite{23}. These qualities make it possible to install such facilities even in hospitals to use the high quality beam for medical applications such as ablation in the high absorption peak around $\lambda = 6.4\mu$m for water and proteins \cite{24}. The tunable frequency range makes it more flexible as common small X-ray sources.

### 3.3 Electron Acceleration

The demand for relativistic electrons in a FEL relates the science of electron acceleration to FEL science. The way of affecting an electron bunch by radiation is well known in the RF and optical regime. Some technique will be presented in comparison with THz acceleration. It was always challenging to generate THz generation. That is why THz acceleration is so far an untouched topic but retains some good advantages towards RF and optical acceleration.

A lot of RF-cavities were designed and tested in the past decades, some details on RF-cavities used at several acceleration facilities are collected in table 1. RF-cavities require a big amount of low loss and good quality metals that are usually costly metal i.e. the superconductive niobium. Due to their limited acceleration field the string to get an electron energy of 17.5 GeV has to be about 1km long \cite{25}. In contrast to radio frequencies, laser wakefields deliver significantly higher acceleration fields as described in paper \cite{29}. With a pulse power of 1.9 TW generated by a Nd:YAG Laser they reach up to 8 GV/m and even higher acceleration gradients are possible with powerful laser facilities. Therefore particle accelerators
shrink from large machines to tabletop devices. This promising principle is limited due to space charge effects in the compressed electron bunch [5]. Compared with an RF-cavity generating an electron beam of energy \((50 - 100) \text{ MeV}\) the transverse dimension of the beam should be \((200 - 500) \mu\text{m}\) and even smaller than the longitudinal. For a laser particle accelerator working in the infrared the longitudinal length of the electron bunch must not exceed \(\approx 1 \mu\text{m}\) to ensure efficient acceleration in the wave of the laser field [30].

The debunching effect of the electrons due to the Coulomb force prevents achieving large enough electron bunches in such short scales.

The invention of THz sources delivering an efficient short pulse makes it possible to close the gap between RF-acceleration and optical laser acceleration. THz wavelengths do not demand extreme short bunches like the optical wavelengths and can increase the acceleration field compared to radio frequencies. To describe THz acceleration in detail the reader is referred to [5]. The designed waveguide coupler will be adapted to a very similar waveguide discussed in that paper, so it represents the requirements for the following design process in section [7]. The main issues of the waveguide accelerator are scheduled in table [2]. An illustration of the waveguide is given in figure [5].

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Frequency</th>
<th>Accelerating Field</th>
</tr>
</thead>
<tbody>
<tr>
<td>LHC / CERN [26]</td>
<td>400 MHz</td>
<td>5 MV/m</td>
</tr>
<tr>
<td>European XFEL [27]</td>
<td>1.3 GHz</td>
<td>23.6 MV/m</td>
</tr>
<tr>
<td>TESLA [28]</td>
<td>1.3 GHz</td>
<td>(\geq 25\text{ MV/m})</td>
</tr>
</tbody>
</table>

Table 1: Operation frequencies and accelerating fields for current linear accelerators using radio frequency EM-fields for electron acceleration.

<table>
<thead>
<tr>
<th>Operating frequency</th>
<th>Pulse Energy</th>
<th>Pulse duration</th>
<th>Electron charge</th>
<th>Interaction distance</th>
<th>Acceleration gradient</th>
<th>phase velocity</th>
<th>Waveguide radius</th>
<th>Dielectric thickness</th>
<th>mode</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.6 THz</td>
<td>20 mJ</td>
<td>10 cycle</td>
<td>1.6 to 16 pC</td>
<td>20 mm</td>
<td>450 MeV/m</td>
<td>(v_{ph} \approx c)</td>
<td>(r = 380 \mu\text{m})</td>
<td>(d = 32 \mu\text{m})</td>
<td>(TM_{01})</td>
</tr>
</tbody>
</table>

Table 2: The main issues of a 0.6 THz electron acceleration system in a diamond loaded waveguide which are numerically evaluated in [5].

Figure 5: Schematic of proposed waveguide and simulation setup. In this study, the dielectric is diamond \((\epsilon_r = 5.5)\). The initial relativistic electron bunch is shot along the THz pulse, which propagates at a non-relativistic group velocity [5].
As described in section 5 the $TM_{01}$ mode is the considered mode as an electron located close to the axes is solely accelerated in the longitudinal direction. Equation 6 sums up all the appearing forces which affect the electron. Of course $\vec{p}_i(t)$ is the relativistic momentum of the electron that is composed of the force $\vec{F}_d^i(t)$ derived by the electromagnetic field, the interaction forces of the electrons $\vec{F}^{pp}_{i,j}(t)$, the force produced by image charges from reflected electrons at the inner wall $\vec{F}^{wf}_i(t)$ and at least $\vec{F}^{rr}_i(t)$ a force resulting from the electrons own radiation.

$$\frac{d\vec{p}_i(t)}{dt} = \vec{F}_d^i(t) + \sum_{j=1, i \neq 1}^N (\vec{F}^{pp}_{i,j}(t) + \vec{F}^{wf}_i(t) + \vec{F}^{rr}_i(t))$$ (6)

The analysis of the electromagnetic field in the waveguide is based on the Helmholtz equations and is explained in [5]. To check the damage threshold of the structure the temperature increase is simulated to investigate thermal damage and beam breakdown in the dielectric. All simulations use $20 \, mJ$, $10$ cycle beam centered at $0, 6 \, THz$ and a $1, 6 \, pC$ electron bunch with kinetic energies from $(1 - 10) \, MeV$. The temperature rise can be calculated by equation 7

$$\Theta(t = \infty, z) - \Theta_0 \approx \frac{P_0 \alpha T_0}{\rho Cu \sqrt{\pi r_2 \delta_s C}} e^{-2\alpha z}$$ (7)

With $\rho_{Cu} = 8940 \, kg/m^3$, $C = 385 \, J/kg/°C$ and $\delta_s = 0.084 \, \mu m$ the simulation calculates a temperature rise of $\approx 320\,°C$ which is far below the melting point of $1084\,°C$. Another important point when dealing with strong electric fields is the possibility of electric breakdown in the wall materials. The electric field in the dielectric region is reported to $8 \, MeV/cm$ which is suitable for diamond (breakdown at $10 - 20 \, MeV/cm$). Diamond is a hard material and is difficult to be shaped for specific applications. Moreover, it is an expensive material which makes the waveguide fabrication process very costly. Therefore, we later change to Quartz for the waveguide material. Quartz has an electric breakdown of $10 \, MeV/cm$ [31] with slightly decreasing stability at higher temperatures. Looking at the thermal conductivity, we see that Diamond ($k \geq 1000 \, W/mK$) dissipates a lot better than Quartz ($k = 1.5 \, W/mK$). That might cause a problem when using the same energies like in the diamond waveguide. The coupler will always have less problems than the waveguide concerning heat and breakdown because of the bigger diameter and thinner dielectric coating.

The presented waveguide coupler plays a key role in combining the THz waves generated in a cryogenically cooled congruent Lithium-Niobate [1] crystal to the dielectric waveguide where the electron acceleration shall occur.

## 4 Guided Electromagnetic Waves

The following chapter introduces the theory of electromagnetic waves especially in hollow (dielectric) waveguides. The focus is set on radio- to optical frequencies with a specialisation in THz frequencies. The electromagnetic spectrum has a massive range of about 20 orders of magnitude in frequency measured against the long-wave transmitter for submarine communications $(15 - 60) \, Hz$ and gamma rays $(10^{20}) \, Hz$ from nuclei. A lot of processes in nature and engineering are described with the help of EM-field theory.
4.1 Maxwell Formulation

In 1873 James Clerk Maxwell published the groundbreaking Maxwell Equations in the Royal Society and proofs that electric and magnetic fields are not independent and can be combined in the EM-field theory. Maxwell united the research from Faraday, Coulomb, Ampere and others to get a set of four differential equations. Since then the description of electromagnetic fields rely on Maxwell’s equations, given in equation\[8\]

\[
\begin{align*}
(1) \quad & \text{div} \vec{D} = \rho \\
(2) \quad & \text{div} \vec{B} = 0 \\
(3) \quad & \text{rot} \vec{E} = -\partial_t \vec{B} \\
(4) \quad & \text{rot} \vec{H} = -\partial_t \vec{D} + \vec{J}
\end{align*}
\]

Where \( \vec{D} \) and \( \vec{B} \) is the electric and magnetic flux density, \( \vec{H} \) and \( \vec{E} \) the magnetic and electric field strength and \( \rho \) is the electric charge density. As Maxwell did not derive the formulas from scratch some former physical laws can be recognized. Coulomb’s law is presented by the first Maxwell equation and Faraday’s law can be found in the third maxwell equation. The second equation expresses that there are no magnetic monopoles and equation, and four is also known as Amperes’s circuit law. The basic differential formulation can be translated to integral equations\[10\] by the Gauss’ and Stokes’ theorem. The electric field strength \( \vec{E} \) and the magnetic field strength \( \vec{B} \) are coupled to \( \vec{D} \) and \( \vec{H} \) by equation\[9\]

\[
\begin{align*}
\vec{D} &= \epsilon_0 \vec{E} \\
\vec{B} &= \mu_0 \vec{H}
\end{align*}
\]

The integral equations provide the basis for the numerical simulation presented later in chapter\[6\].

4.2 Helmholtz Wave Equation

When the EM-fields impinge on a surface the characteristics of the wave changes. Mathematically one can set specific boundaries to solve the Maxwell equations in different electromagnetic environment. All EM-waves have to fulfill the Helmholtz wave-equations, given in equation\[12\] and \[13\] derived from the third maxwell equation with the use of the fourth. Exerting the curl operator to the equation\[8\] by using the identity \( \nabla \times \nabla \times \vec{E} = \nabla (\nabla \cdot \vec{E}) - \nabla^2 \vec{E} \) delivers the three dimensional wave equation, similar for \( \vec{E} \) and \( \vec{B} \) field. The speed of light is \( c^2 = \frac{1}{\mu_0 \epsilon_0} \) in SI units.

\[
\nabla \cdot (\nabla \cdot \vec{E}) - \nabla^2 \vec{E} = -\frac{\partial}{\partial t} (\nabla \times \vec{B}) = \frac{\partial}{\partial t} (\mu_0 \epsilon_0 \frac{\partial}{\partial t} \vec{E})
\]

\[
(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}) \cdot \vec{E}(\vec{r}, t) = 0
\]

\[
(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}) \cdot \vec{B}(\vec{r}, t) = 0
\]
4.3 Free Space Wave Equation

For the propagation in free space the following equations describe the electric (E) and magnetic (H) field. The equations are basics and the best known solution for the wave equation when assuming neither boundaries.

\[ E = E_0 \cdot e^{i(\vec{k} \cdot \vec{r} - \omega t)} \]  
\[ H = H_0 \cdot e^{i(\vec{k} \cdot \vec{r} - \omega t)} \]  

For example the plane waves \[14\] and \[15\] solve the wave equations and it can be shown that \( c = \frac{1}{\sqrt{\mu_0 \epsilon_0}} \) as it should be in vacuum for free space propagation \[33\].

4.4 Circular Waveguides

The first theoretical description of guided EM waves were made by A. Sommerfeld \[34\]. The guided frequency in wire or coaxial lines is limited due to the total reflection from the waveguide walls. To guide EM waves in the THz spectrum hollow waveguides support a low loss propagation. Lord Rayleigh was the first one in 1897 with the idea of using hollow waveguides for the optical spectrum \[35,36\]. In 1961 Snitzer and in 1964 Marcatili and Schmeltzer published their papers concerning the transmission and mode selection in dielectric waveguides.

According to the theoretical description of the fields in hollow waveguides, the guided modes can be categorized as Transverse Electric (TE) and Transverse Magnetic (TM) Modes. The properties are shown in table 3. Since the interaction between THz wave and electrons will take place in a circular cross-section waveguide an introduction to the analysis of this waveguide is given in the following. The mathematical description is based on the formalism used in \[6\]:

\[ \nabla \cdot \vec{B} = 0 \Rightarrow \nabla \cdot (\nabla \times \vec{A}) = 0 \]  
\[ \nabla \cdot \vec{D} = 0 \Rightarrow -\nabla \times \vec{F} = 0 \]  
\[ \vec{B} = \nabla \times \vec{A} \Rightarrow \vec{H} = \frac{1}{\mu} \nabla \times \vec{A} \]  
\[ \vec{D} = -\nabla \times \vec{F} \Rightarrow \vec{E} = -\frac{1}{\epsilon} \nabla \times \vec{F} \]

Where \( \vec{A} \) is the vector potential belonging to the B-field and \( \vec{F} \) is the vector potential belonging to the E-field. Equations \[18\] and \[19\] follow from the fact that the maxwell equation 1 and 3 are equal to zero on the right hand side in a source free region (see equations \[16\] and \[17\]). For the TE modes the vector potentials \( \vec{A} \) and \( \vec{F} \) can be set to

\[ \vec{A} = 0 \]  
\[ \vec{F} = \hat{a}_z F_z(\rho, \phi, z) \]
For time-harmonic fields of the form $e^{i\omega t}$ the wave equations simplify to equation (22) and (23)

\[ \nabla^2 \vec{E} = -\omega^2 \mu \epsilon \vec{E} = -\beta^2 \vec{E} \]  
\[ \nabla^2 \vec{H} = -\omega^2 \mu \epsilon \vec{H} = -\beta^2 \vec{H} \]  

The assumed vector potentials 20 and 21 must satisfy the wave equation.

\[ \nabla^2 F_z(\rho, \phi, z) = \beta^2 F_z(\rho, \phi, z) \]  

The derivation for the vector-wave equation is done in chapter 3.4.2 of [6] and the result is presented in equation 25.

\[ F_z(\rho, \phi, z) = [A_1 J_m(\beta \rho) + B_1 Y_m(\beta \rho)] \times [C_2 \cos(m \phi) + D_2 \sin(m \phi)] [A_3 e^{-i\beta z} + B_3 e^{+i\beta z}] \]  

The unknown coefficients are given by the boundary conditions which are (1) $E_\phi(\rho = a, \phi, z) = 0$, (2) the fields must be finite everywhere and (3) the fields must repeat every $2\pi$. Solving the wave equation for a circular cross section provides the condition for cutoff frequency besides the electric and magnetic field components and wave impedance. Since the coupler has a continuously varying radius, the fields in the waveguide are delivered by CST MWS as described in section 6. It can be helpful to make an estimate for the cutoff frequency given by equation 26 to suppress higher order modes. The cutoff frequency is the lower limit in terms of frequency for the propagating modes. Owing to the first boundary condition, $f_{cutoff}$ depends on the zeros of the derivative of the Bessel function, the waveguide radius $a$ and some constants. The zeroes of the derivative of the Bessel functions can be looked up in [6].

\[ (f_c)_{mn} = \frac{X'_{mn}}{2\pi a \sqrt{\mu \epsilon}} \quad (TE) \]  

For the EM waves with an electrical field in the longitudinal direction, called TM waves the procedures is similar with slightly varying factor $X'$ because of the initial conditions change for TM-fields in equations 27 and 28. In the end the zeros of Bessels function are needed in equation 29.

\[ \vec{A} = \vec{a}_z A_z(\rho, \phi, z) \]  
\[ \vec{F} = 0 \]  
\[ (f_c)_{mn} = \frac{X'_{mn}}{2\pi a \sqrt{\mu \epsilon}} \quad (TM) \]  

In figure 7 the first appearing modes are shown. All modes have a fixed bandwidth and the order they occur does not change with the radius of the waveguide. The cutoff frequency of the modes as derived from equation 29 is visualized in figure 6.
and the second term under the root can not be lower than zero.

The wave number is then given by equation 30:

\[ k^2 = \mu \varepsilon (\omega^2 - \omega_c^2) \]  

Assuming that the \( E_z \) component of the field vanishes at the outer radius \( r = a \) the wave number shall be \( \beta_c = \lambda_{mn} / b \). As defined in (33), \( \beta_c = \mu \varepsilon \omega^2 - \beta^2 \) for the longitudinal fields with \( \beta = \omega / c \) in general. The wave number is then given by equation (30)

\[ k^2 = \mu \varepsilon (\omega^2 - \omega_c^2) \]  

The phase velocity can be calculated with equation (31)

\[ v_{ph} = \frac{\omega}{\beta_{mn}} = \sqrt{\frac{1}{\mu \varepsilon} + \frac{\omega_c^2}{\beta_{mn}}} \]  

The phase velocity according to equation (31) should always be higher than the speed of light since \( \frac{1}{\sqrt{\mu \varepsilon}} = c \) and the second term under the root can not be lower than zero.

Figure 6: The mode distribution according to the normalized angular frequency. Where \( a \) is the waveguide radius.

Figure 7: E-field and H-field (dashed) of the first modes in a circular waveguide [6]
4.4.1 DIELECTRIC WAVEGUIDES

The opportunities using circular hollow metal waveguides are limited by varying the radius to change cutoff frequencies. Moreover, the phase velocity in a hollow waveguide is always higher than the speed of light which makes the phase-matching with electrons impossible. A lot of more possibilities can be realized with a dielectric coating on the inner side. The big range of dielectric materials from quartz to polystyrene with arbitrary permitivities make it possible to adapt the waveguide to its application. There are two outstanding enhancements: The hollow dielectric waveguide support the complete set of modes, the transverse electric and transverse magnetic fields can superimpose and form hybrid modes. Furthermore the phase velocity can be controlled by varying the thickness or permitivity of the dielectric coating. In the optical frequency range metal boundaries show increased dissipation and intensify the losses. A thin layer of dielectric coating can damp the wave and minimize reflections to reduce losses. Like B. Bowden showed, the loss for HE and TE modes is much lower using a thin layer of polystyrene compared to a pure metal waveguide.

In dielectric waveguides, the $HE_{11}$ mode will be the dominant one and just minimal penetrating in the dielectric in contrast to the dominant $TE_{11}$ mode in metallic waveguides. The $TE_{0x}$ and $TM_{0x}$ modes appear nearly unmodified and can be treated in a similar way as the ones in metallic waveguide.

5 COUPLING IN THE THZ REGIME

Coupler in general cover a large area of facilities used to couple EM-waves between various interfaces. The word "coupler" is mostly used from radio to optical frequencies and is equate with the "connector " in tethered systems. Generally you can distinguish coupler for mode conversion or signal distribution from coupler to guide free space waves in a waveguide or the other way around as horn antenna. According to the thesis’ task of free space coupling these design options are discussed in detail. Some basic approaches are discussed and the frequency response is valued.

A lot of couplers are designed for spectroscopy applications, that’s why the TE mode is highlighted in most papers because of of their usefulness for spectroscopy due to very low ohmic losses in the waveguide and the convinient field distribution with an transverse electric field. But keep in mind that the TM mode is indiependensible for electron acceleration because of the need for longitudinal electric field.

5.1 GRATING COUPLER

Over the past decades the grating coupler attracted large attention with its properties being experimentally and theoretically investigated. The paper presents a good review of the behavior of grating structures. Since the transmission coefficient can reach nearly 100 %, the grating coupler is superior for monochromatic signals. Due to the periodicity in the grating the transmission is highly dependent on the frequency as observed in figure.
The modulus of the transmission coefficient (in amplitude) of the grating coupler device vs the frequency is shown in Figure 8. The circles are the experimental data, and the solid line is data calculated with differential theory. The dashed line corresponds to the calculated transmission of a flat parallel 190-mm-thick silicon slab. The peaks labeled (m,p) originate from excitation of the guided mode is negative for contrapropagative guided modes through grating diffraction order p [7].

The angle, the periodicity, the depth and the filling with dielectrics of the grating has to be changed when the frequency varies [7]. Besides the parameters of transmission, the coupling structure must be able to guide relativistic electrons to match our desired application of electron acceleration. Therefore, the range limits to structures with a vacuum core. To keep the idea of a periodic grating the paper of R.B. Yoder and J.B. Rosenzweig describes a "side-coupled slab-symmetric structure for high-gradient acceleration using terahertz power" [8] illustrated in Figure 9.

Figure 8: Modulus of the transmission coefficient (in amplitude) of the grating coupler device vs the frequency. The circles are the experimental data, and the solid line is data calculated with differential theory. The dashed line corresponds to the calculated transmission of a flat parallel 190-mm-thick silicon slab. The peaks labeled (m,p) originate from excitation of the guided mode is negative for contrapropagative guided modes through grating diffraction order p [7].

Figure 9: (a) Schematic drawing of the side-coupled slab-symmetric structure geometry. Two layers of dielectric-lined conductor surround a vacuum gap; a very wide electron beam is injected into the gap and travels in the z direction, while radiation (polarized in z) is coupled in from above through transverse slots in the conductor. (b) A cross-section in x, showing the parameters used in the analysis [8].
The slab-symmetric accelerator couples terahertz frequencies at \( \lambda = 340 \text{nm} \) or \( f = 882 \text{GHz} \) with the advantage of nearly single mode excitation. One thing that is not presented is the transmission coefficient of the coupled power. In addition to that there is no plot showing the frequency response around the frequency point \( f = 882 \text{GHz} \).

The frequency response is not promising at all even at a broader spectrum symmetrically located around the target frequency because the THz beam will be pulsed with a length of 10 cycle, hence the bandwidth is not negligible. The equations [32] and [33] are used to calculate the important frequency range: With \( \tau = \text{puls duration} \).

\[
T = \frac{1}{\nu} \rightarrow \tau = n \cdot T \quad (32)
\]

\[
\Delta \tau \cdot \Delta \nu = \frac{2\ln 2}{\pi} = 0.4413 \quad (33)
\]

With \( \tau = \text{puls duration} \), the time-bandwidth product appears when one performs a Fourier transformation of the intensity of a Gauss pulse as is done in [41]. The time-bandwidth product changes with the signal type due to the Fourier transformation. For our goals, the parameters are \( \nu = 450 \text{Ghz} \) and \( n = 10 \text{cycle} \) and the results are listed in table 4. Because of a bandwidth of \( \approx 20 \text{GHz} \) the waveguide coupler should show an almost uniform behaviour for this range around 450 GHz.

\[
\begin{align*}
\tau & = 22, 2 \text{ps} \\
\Delta \nu & \approx 20 \text{GHz}
\end{align*}
\]

Table 4: Results of the time-bandwidth product

### 5.2 Lens and Flare Coupler

A coupling structure without any periodic gratings are parallel plate waveguides (PPWG) with lenses [40]. Working with lenses is a basic principle developed in the optics. In terahertz frequencies, the amplitude suffers from the inherent Fresnel losses [9]. For that reason M. Theuer and colleagues used metal flares as shown in figure 10(a) and could increase the coupling ratio from 22% for Si lens to 35% for metal flares measured at 1 THz. Especially for frequencies \( \approx 2 \text{THz} \) the coupling efficiency for the Si lens and flare type divergates as spectrum divide in optical and microwave ranges. The advantages of flares against lenses are elaborated in [10] at a frequency of 1 THz. They simulate a gain of 56% using flares instead of lenses on the input side. It is worthwhile to point out that a continuous tapering reduces massive hotspots of radiation power compared to a coupler with a kink at the junction to the waveguide. The fields in the waveguide coupler are shown in figure 10(b). The coupler with an arch at the junction it is possible to observe a minimization of reflection. The reflection is more distributed in the horn as well, so the reflected energy is not concentrated in the center on the electrons trajectory. The structure is quite similar to the one assumed in this thesis even in regard to the dimensions. In section 7, the performance of an arch coupler and its dependence on the structure dimensions are investigated. The papers [9, 10] conclude that a flared waveguide coupler (the so-called an inverse horn antenna) is the best choice.
Figure 10: (a) Cross-sectional illustration of the two types of coupling schemes used for PPWGs. ((a)a) PPWG with coupling using silicon lenses. ((a)b) Same WG with flared coupling using copper shim [9]. (b) Tappered parallel-plate waveguide simulated at 1THz. Calculated input-side magnitude of THz field distribution. ((b)a)10Ð non-round TPPWG.((b)b) 10Ð round TPPWG with an 80mm-diameter circular arc [10].

To use the waveguide and its input coupler for electron acceleration in a FEL it is definitely needed to analyse propagation of different modes. To get a logitudinal electric field, the structure must provide the $T_{M01}$ mode. Since the waveguide structure is not designed for any mode conversion a radially polarized input beam is necessary [5]. The first beginnings to get a radial polarized THz beam were just done previously based on optical rectification [42] and laser excited GaAs antennas [43]. Another way is to use the experience of generating liniarly polarized beams and convert them into radial polarized ones presented in [44]. This thesis will no longer approach the THz generation, it is enough to check if there are useful radially polarized THz sources to run the electron accelerator.

6 Numerical Simulation with CST MWS

For the design and optimization of the THz waveguide coupler, it is necessary to make use of numerical simulation techniques. The structure of the coupler and thickness of materials changes continously hence a description based on an analytical solution would be hard to realize. Besides loads of codes developed in MATLAB or C for special projects there are a few commercially available software. To name the famous ones HFSS based on the Finite Element Method (FEM) was developed over several years by hewlett packard. Presently the American company ANSYS is one of the biggest vendor for numerical simulation software including HFSS and Maxwell2D/3D. A software based on the Finite Integration Method (FIM) is originated at DESY primal called MAFIA and was commercialized by Computer Simulation Technology (CST) in Darmstadt. A great summary is available on [45]. CST implemented different solvers for various problems leading to a structurized software in eight individual Studios. Due to the availability of licences and the efficient calculation in the time domain the choice falls on CST microwave studio for the design process in section 7. The Studio of interest in this thesis is the MicroWave Studio (MWS) for high frequency applications. Furthermore a graphical user interface with a comfortable 3D modelling interface is developed and matured over the years.

In 1976/77 Weiland proposed the Finite Integration Technique/Method (FIT / FIM) to solve Maxwells equations [10] even in the time or frequency domain. It is necessary to generate small grid cells to define a finite calculation domain. Since the E- and B-field assumend to be constant within one cell for the calculation, it is obvious that the results becomes more accurate with increasing the mesh resolution. The Maxwell equations are set up separately for each cell and solved with the boundary conditions defined on the primary and dual mesh. The schematic in figure [11] illustrates the voltages located on the grid and the fluxes located on
Figure 11: Meshing in CST MWS. The electric- \((e_i)\) and magnetic \((h_i)\) voltages are located on the grid and the electric- \((d_j)\) and magnetic \((b_n)\) fluxes are located on the facet [11].

\[
\oint_{\partial A} \vec{E} \cdot d\vec{s} = -\frac{\partial}{\partial t} \int_A \vec{B} \cdot d\vec{A} \tag{34}
\]

\[
\oint_{\partial A} \vec{B} \cdot d\vec{s} = \int_A \vec{j} \cdot d\vec{A} \tag{35}
\]

Now, CST can set up a matrix system and the continuous Maxwell equations are translated to Maxwell’s Grid Equations (MGEs). Three types of solvers, the transient solver, frequency domain solver and eigenmode solver can be chosen to calculate the EM-fields. The transient solver calculates the fields for the grid cells in time-domain as shown in figure [12]. As mentioned before, the accuracy of the results compared to real measurements or analytical results (if available) is mostly governed by the settings of mesh generation. A mesh with very small elements would cause infinitely long processing duration and is therefore not reasonable. Especially, on edges and material discontinuities the mesh design is important.

CST MWS
offers the "Perfect Boundary Approximation" (PBA) where the properties of a cell is weighted by the ratio of the materials in that cell. That offers a higher accuracy without affecting the mesh. Furthermore, CST MWS delivers a build-in "expert system" that detects significant changes in the structure and does an automatic mesh refinement in that region. The mesh can be also refined by setting a desired accuracy, for example a maximum of S-Parameters between each iteration steps. That takes for usual a long time and the mesh should be saved when it is produced once.

When the structure is modeled and the basic adjustments are set, CST offers various tools for optimisation and customized data generation. Parameters can be defined for every physical size and calculations can be done automatically with a parameter sweep. The results are organized in a 3D and 1D/2D result tree as you can see in figure [15]. These basic quantities can be used for calculations in the "template Based Post Processing" which contains a large amount of additional functions.

7 CIRCULAR DIELECTRIC COUPLER

The theory part of the thesis conveys the fundamentals to handle and design the dielectric circular acceleration structures. More details on the coupler performance are acquired during the design process with the help of the numerical simulation presented in this section. The task is to design a free space to waveguide coupler operating in the frequency interval \((425 - 475) THz\). The phase velocity is set constant and equal to the speed of relativistic electrons and the efficiency of the device is judged based on the power reflection coefficient which should be as low as possible. Other conditions are evaluated in the following sections to match the waveguide coupler in the best possible way. Some suggestions for the shape derive from the ones in the chapter [5], some from discussions with Dr. A. Fallahi and some from the weekly CUBIX meeting.

7.1 FULL PARAMETERIZED CAD MODEL

Before any calculations the physical model is transferred to CST MWS. The quantities listed in table 5 are collected from previous work done in the CUBIX research group. The quantities changed during the design process as the whole accelerator project is quite unique and still in progress. For example the radius in front of the coupler was first assumed to be around \(2.5 mm\) but then corrected to \(1.5 mm\) as the \(LiNbO_3\) crystal for THz generation does not produce a beam with such a large spot size. Figure [13] displays one of the first drafts to get an idea of the structure. At the beginning some preparatory simulations were done with the model made of PEC to save computation time. The coupler is refined bit by bit to record the effect of every modification.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>radius front</td>
<td>1.5mm</td>
</tr>
<tr>
<td>radius end</td>
<td>0.47mm</td>
</tr>
<tr>
<td>dielectric thickness end</td>
<td>0.06mm</td>
</tr>
<tr>
<td>length</td>
<td>(\approx 10mm)</td>
</tr>
<tr>
<td>frequency range</td>
<td>((425 - 475) THz)</td>
</tr>
<tr>
<td>basic material</td>
<td>copper</td>
</tr>
<tr>
<td>dielectric coating</td>
<td>quartz</td>
</tr>
<tr>
<td>input signal</td>
<td>gauss pulse (10 cycle)</td>
</tr>
</tbody>
</table>

Table 5: The intertial boundary conditions given for the waveguide coupler derived from earlier calculations done in the CUBIX group.
As mentioned in section 6, the parameter sweep is a powerful tool for saving time and generating a structured table of results. The parameters are defined during the modeling process. In table 6 all defined parameters are listed and explained. In each simulation, the port modes are checked first to ensure the

<table>
<thead>
<tr>
<th>parameter</th>
<th>unit</th>
<th>meaning</th>
<th>range</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>mm</td>
<td>coupler length (without straight parts, just flared)</td>
<td>6 - 16</td>
</tr>
<tr>
<td>b</td>
<td>mm</td>
<td>radius of blend</td>
<td>0 - 40</td>
</tr>
<tr>
<td>c</td>
<td>mm</td>
<td>dielectric thickness front</td>
<td>0 - 0.1</td>
</tr>
<tr>
<td>d</td>
<td>mm</td>
<td>dielectric thickness back</td>
<td>0.05 - 0.07</td>
</tr>
<tr>
<td>e</td>
<td>mm</td>
<td>waveguide radius back</td>
<td>0.4 - 0.6</td>
</tr>
</tbody>
</table>

Table 6: The parameters used for easy changes in the structure, including units and range. The range is just an assessment.

excitation of the accelerating mode. Analytically the third appearing mode should be the radial $TM_{01}$ mode. That agrees with the simulations for the circular waveguide. To accelerate the calculation, magnetic or electric symmetry planes can be defined in CST MWS. With each symmetry plane the calculation effort reduces by the factor of two. The shape permits to set two symmetry planes along the trajectory of the electrons. With the symmetry plane, the first two non radial modes are skipped and the desired $TM_{01}$ mode is the first occurring mode for all further simulations. There are three imagined initial designs with various dielectric inputs shown in figure 14. Below the design in figure 14 (a) is denoted as coupler design A. The coupler in figure 14 (b) as B and the coupler in figure 14 (c) as C. Design C is taken from E.Nanni and is mainly considered to compare the simulations from CST to the ones from HFSS E. Nanni did. Before the designs are approached in detail in section "Optimization" a further introduction to the results in CST MWS is given.
Figure 14: The initial designs for the waveguide coupler. The copper (yellow) is 0.5mm thin and the dielectric (blue) is 0.06mm thin. (a) The dielectric coating is simply put on the straight waveguide whereas design (b) is fully coated with dielectric. The straight dielectric rod in (c) should minimize impedance mismatch between the ports.
7.2 Result View and Post Processing

The challenge is to elicit the required results from CST MWS out of the abundance of calculations and interpret them in the right way. CST offers a wide range of standard results which are organized in the result tree (see figure 15). In addition to that the "Template Based Post Processing" enables customized results listed in the last orders containing all specially defined post processing calculations. Several faces, lines and points are defined to record signals by linked monitors. The names for these shapes appear in figure 15(a) and are related to the input- and output faces. The curve one is located along the electron trajectory, curve two is defined diagonally thru the input port and curve three diagonally thru the output port. Starting with the 1D scattering parameters especially $S_{21}$ to evaluate the designs and to optimize the appreciated quantities seems to be quite comfortable. The definition of scattering parameters is done in a standard way in microwave network theory. The concept is explained in figure 16.
Figure 17: The radial electric fields showing the $TM_{01}$ port modes at input (a) and output (b). The radial electric field confirm the formation of the $TM_{01}$ mode. The shown coupler is one of the latest designs made of copper with coating of quartz.

Figure 16: Schematic for a two port network with the definition of scattering parameters [12].

During the optimization of the design towards finding the maximum $S_{21}$, the parameter grew higher than one, which means amplification and is not allowed. The $S_{21}$ in CST MWS is just the ratio of amplitudes from in- and output signal without considering the port impedances. The following formulas show the problem when just the amplitudes are divided. The ports are quite different in diameter and dielectric coating therefore the port impedances are different as well, which can not be neglected. Due to the different impedances at the ports the results given by CST should be rectified as done in equation 37.

$$S_{21} = \frac{b_2}{a_1}$$

$$S_{21}^{opt} = \frac{b_2}{a_1} \sqrt{\frac{Z_1}{Z_2}}$$

To avoid problems and misleading results when using the $S_{21}$ parameter the $S_{11}$ can be used as well without any disadvantage. Since there are just two ports, minimization of $S_{11}$ is equivalent to the maximization of $S_{21}$. Disregarding the power dissipation in the copper and quartz, the energy conservation confirms this fact, see equation 39. Furthermore, we can be sure that CST is considering the same port modes as $S_{11}$ is solely calculated from port one, see equation 38.

$$S_{11} = \frac{b_1}{a_1}$$

$$S_{11}^2 + \frac{Z_1}{Z_2} S_{21}^2 = 1$$

To be sure if the results belong to the $TM_{01}$ mode the port modes for input and output are displayed in figure 17. The radial electric field confirm the formation of the $TM_{01}$ mode. The port signals and 2D/3D field monitors are always helpful to check how the signal behavior is in terms of time and spatial distribution of the fields. The accelerating electric field in the waveguide is observed by setting a field monitor for (1)
individual frequencies optimally around the center frequency \( f = 450 \text{GHz} \) or better for (2) a predefined time. As the incoming pulse travels from input to output port in about 80 ps the time dependend visualization of the E-field is calculated from 0 to 800 ps. Field monitors in CST are useful to see what’s going on in the structure, basically between the ports. The results of the field monitors are animated in relation to phase or time. Additional result templates can be defined as Postprocessing calculations. The defined results can be observed in figure 15(c). Some results like the number of meshcells and solvetime serve for observation of the simulation and some are there to gain information about the coupler itself. The delivered power is a post processed value calculated from the \( S_{11} \) (equation 40) and a mean value for evaluating the design.

\[
P_{\text{del}} = 1 - S_{11}^2 \quad (40)
\]

Most of the used results share the property to be just ratios of different signals. There are no absolute numbers giving the amplitudes or energy of the beam. To figure out the specific energy coupled into the waveguide, the following derivation based on [6] and [46] yields the energy going through the input port and the energy going through the output port. Thereby the input port and output port are considered as a metallic ones. So the calculation are applicable to the symmetric designs. At the end of the derivation the E-field at the input port \( E_{\text{in}} \) and at the output port \( E_{\text{out}} \) are needed to solve the equations. The E-fields are measured by Probe Monitors, set at the center of input and output port.

CST is giving the values for the E-field in x-direction over time \( E_{z,\text{CST}}(t, r = 0) \). The electric fields in the circular waveguide are of the type

\[
\begin{align*}
E_z &= A(t) \cdot f(r, \phi) \\
E_r &= A(t) \cdot g(r, \phi) \\
H_\phi &= A(t) \cdot h(r, \phi)
\end{align*} \quad (41)
\]

with varying function \( f, g, h \) for all three components \( E_z, E_r, H_\phi \). The energy is generally given by the time-integral of the power

\[
E = \int P \, dt \quad (42)
\]

The power for the ports is obtained from the transverse fields using:

\[
P = \int \frac{E_r^2}{Z} \, ds \quad (43)
\]

Then, the energy going through the port is

\[
E = \int \frac{1}{Z} \int A^2(t)g^2(r, \phi) \, ds \, dt. \quad (44)
\]

On the other hand, one can write for \( A(t) \):

\[
A(t) = \frac{E_{z,\text{CST}}(t, r = 0)}{f(0, 0)} \quad (45)
\]

and with respect to equation 41 the energy can be derived by an integration over the electric field given by CST.

\[
E = \frac{C}{f^2(0, 0)} \cdot \int E_{z,\text{CST}}^2(t, r = 0) \, dt \quad \text{with} \quad C = \frac{1}{Z} \int g^2(r, \phi) \, ds \quad (46)
\]
The functions $f$ and $g$ are given in [46] and solved analytically.

$$f(r, \phi) = J_0(k_1 r) \quad \text{with} \quad k_1 = \omega \sqrt{\frac{1}{\varepsilon^2} - \frac{1}{v_p^2}}$$

(47)

With phase velocity equal to the speed of light:

$$k_1 = 0 \rightarrow f(0, 0) = J_0(0) = 1$$

(48)

Before the integral of $g(r, \phi)$ is solved in cylindrical coordinates for a radius $0 < r < a$ with $a = 1.5 \text{mm}$ and the hole circle one can benefit from the limes $v_p \rightarrow c$

$$\lim_{v_p \rightarrow c} E_r = \frac{\beta J_1(k_1 r)}{k_1} = \frac{\beta r}{2}$$

(49)

$$\int g^2(r, \phi) \, ds = \int_{\phi=0}^{2\pi} \int_{r=0}^{a} \frac{\beta^2 r^2}{4} \, r \, dr \, d\phi = \frac{\pi \beta^2 a^4}{8}$$

(50)

The Energy is then given by

$$E = \frac{1}{Z} \int E^2_{z,CST}(t, r = 0) \, dt$$

(51)

The integral over the electric field $\int E^2_{z,CST}(t, r = 0) \, dt$ is done numerically in matlhb.

### 7.3 Optimization

After the CAD model was parameterized and the result templates were set, the first performed parameter sweeps gave an impression on the impact of the dimensions on the transmission efficiency. In the beginning the simulations were done for the PEC coupler to save computation time. This thesis concentrates on the later drafts made out of copper and dielectric to keep it simple.

The delivered power plots for the initial designs $A$, $B$ and $C$ (figure [14]) are shown in figure [18]. In some frequency ranges the delivered power to port two with about $0.8 - 0.9$ of the input power is quite acceptable. A disadvantage are the massive dips down to 0.1 for design $B$ and $C$. The coupler $A$ shows attenuation down to 0.6 at specific frequencies. It is assumed that the notches occur from reflections arisen from standing wave interference due to inconvenient length of the coupler or from reflections at the edges. Therefore the couplers are optimized subsequently to minimize reflections.

The second design step approaches the edges from quartz coating. The quartz is tapered off in the beginning for design $A$ and $B$ shown in figure [19] with the corresponding delivered power plots. While there is just little improvement for coupler design $A$ the delivered power plot indicates a big leap in quality for design $B$. The notches at 448 $GHz$ and 462 $GHz$ show the reduction of the signal to maximum 0.93 the input power. That means an enhancement of about 90% compared to the results without tappering. For a transmission of a broad bandwidth pulse it’s more important to gain a flat frequency response than having a maximum signal value at single frequencies. That is an important evaluation criterion for all coupler designs. Except the small ripples the notches at 448$GHz$ and 462$GHz$ are still outliers and need to be improved.

In the third design step the edges in copper and for design $B$ in dielectric are blend. For comparison with previous designs, the power plot is shown in figure [20].

30
Figure 18: The delivered power as described by equation 40 for the coupler A, B, C. The simple design A shows the best results compared to B and C. The length of the flared part is $a = 8\, \text{mm}$ for all designs.

Figure 19: Design of the second design step with tapered dielectric for design A and B in comparison to the initial design without tapered dielectric. The delivered power is increased but still contains notches at defined frequencies. The length is kept unchanged ($a = 8\, \text{mm}$) and there is no blending ($b = 0\, \text{mm}$).
Figure 20: Design step number three for coupler design A, B and C. In addition to the tapered dielectric, all designs have blended edges in copper and dielectric. See figure (a),(b) and (c) for a blending radius of $b = 20$. The length for the coupler is still $8\,\text{mm}$. The plots (d),(e) and (f) show the delivered power for a blend radius of $(b = 0/6/12/18/24/30)$. The blending does not effect the performance considerably. A blending of $b = 20$ show minimal improvements compared to design step No.2.

The optimized coupler A and C are not affected by the third design step in terms of transmission efficiency. The notches are just shifted but the magnitude is nearly unchanged. For coupler design B the maximum attenuation for a blend of $b = 20$ is reduced to 0.94 at 459GHz instead of 0.91. This improvement may not be overrated since it is very little and not broad enough. For example small variation in the
blend radius \((b = 24 \text{ at } 435\,GHz)\) can cause hard dips.

The fourth and last optimization step concerns the length of the coupler. The main interest is to observe if the dips in the power plot shift when the length varies. For all designs a parameter sweep with \(a = (4, 6, 8, 10, 12)\,mm\) is performed. The power plots are shown in figure 21.

Figure 21: The delivered power in terms of frequency for the coupler drafts A, B and C. A parameter sweep delivers automatically the plots for a hornlength of \(a = (4, 6, 8, 10, 12)\,mm\). The blending is fixed at \(b = 20\). The plots for design C do not show any improvement. The power plot for coupler A and B show a flattening behaviour for \(a > 12\,mm\).
At this point it is important to mention that all calculations were done with two ports and just allowing the $TM_{01}$ mode propagating through a port. The sharp resonances hint at a problem in the calculation process. The problem can be caused if the structure has a resonating behavior or a problem of the numerical simulation. Due to mode conversion during the reflection process in the horn, it is necessary to define the waveguide ports for at least 10 modes to allow the reflected energy passing out. Several simulations were done with different port adjustments to get the best compromise of accuracy and computation time. Finally, a number of 10 modes at the input port and an exclude of an output port to avoid any blockades for the wave are chosen for all further simulations.

The Energy plot from MWS shown in figure 22 indicates that the amount of energy resting in the structure is nearly going down to $-40 \text{dB}$ for most designs. Previous calculations with just one mode at the input port indicated an energy of $\approx -10 \text{dB}$ resting in the coupler.

![Figure 22: The Energy all three designs in the latest design step (symmetric and unsymmetric). The calculations were done involving 10 modes to let the reflected energy passing out.](image)

There is another possibility for optimization when using the previously optimized structures and construct them symmetrically. It is not sure that a structure with an output port can be used in the CUBIX project but it is worth while to have a look at the performance. The symmetric waveguide has the advantage of exactly the same port geometry which facilitates the analytical calculation for the transmitted energy. It is assumed that a shaped output coupling minimizes irritations on the wave and accelerated electrons. The symmetric waveguide couplers based on the three previous designs are shown in figure 23 for a horn length ($a = 12 \text{mm}$) and a blending radius of ($b = 20 \text{mm}$) with the corresponding delivered power plot.
Figure 23: Symmetric waveguide coupler with tapered dielectric in the horn part (a), tapered dielectric in the waveguide (b) and a straight dielectric rod (c). The designs are originated from the ones in figure 14 with a hornlength of 12\,mm and a blending radius of 20\,mm. The delivered power plot (d) indicates a very good power transmission for all three designs with a small disadvantage for design (A). The delivered power does not fall below 99.5\% in the frequency range from (425 − 475)\,GHz. The calculations for the nonsymmetric structures are displayed in (e) to compare the results. Figure (e) contains an additional zoom-in for a detailed view.

All symmetric structures show superb power transmissions based on the $S_{11}$ coefficient. In addition to that, the energy remaining in the symmetric design (C) is very low, down to $−80\,dB$ in figure 22. A quick decrease of the stored energy in the structure is worthwhile to prepare the coupler for the next pulse. It is conspicuous that the performance of the nonsymmetric structure (C) differ from the one of design (A) and (B) though all simulations were done with the same adjustments. In symmetric style all designs show nearly the same performance. One can point out that coupler (C) benefits most from a smooth output coupling.

The optimization for all three designs is finished at this point. Especially for the nonsymmetric design A and B and the symmetric design (B) and (C) the performance could be increased and the frequency response is nearly flat.
As design $B$ seems to be the most promising one, no matter if symmetric or not, it is discussed in more detail in the following part.

### 7.4 Final Draft

The best performance is observed for the symmetric waveguide coupler made of copper with a quartz coating tapered at the input horn with a hornlength of $a = 12\text{mm}$ and a blending radius of $b = 20\text{mm}$. To study the details for acceleration application of the symmetric coupler design $B$, some additional capabilities of CST MWS are used. Specific lines and planes are defined in the structure to obtain the electric field in detail. The amplitude of the electric field gradient right on the longitudinal axis can be seen in figure 24. The plot is compatible with the fields indicated by the colour scale in figure 27. In the beginning the signal is quite low. Because of the decreasing radius of the coupler the energy is concentrated to the center. From $4\text{mm}$ to $12\text{mm}$ some inhomogeneties occur with a small hotspot at $a \approx 11$. In the straight waveguide ($a = 12\text{mm}$) the electric field is periodical and the amplitude is constant. The field amplitude for the accelerating field component gains about 15 times from the input port to the waveguide. When the acceleration ends, the wave decouples smoothly to free space without any phase irritations.

![Figure 24: A plot of the x-component of the electric field (f=450GHz) along the trajectory of the electrons. Some field inhomogenities occur along the hornpart ($4\text{mm} < a < 12\text{mm}$) but enter the waveguide at $a=12$ periodically.](image)

Apart from the signals in frequency range it is useful to keep an eye on the results in a timing diagramm. To check the accelerating E-field in particular, field probe monitors are set at the center of port 1, some along the axis and one at the output coupler to record the E-field in x-direction for the propagating pulse in time. It was not expected that the probe monitor signal, displayed in figure 25 at the input indicates a longtime electric field. The remaining field might occur from the reflections during the coupling process. In addition to that the number of modes defined in the port settings might be still too low and the port is reflecting instead of absorbing. At the center of the acceleration path, the gaussian pulse is undistorted as indicated by the probe monitor at $x = 15\text{mm}$. At the end at $x = 30\text{mm}$ the electric field is attenuated to a maximum field strength of about $1500 \text{V/m}$.
Figure 25: Signals detected by probe monitors for the symmetric design $B$ with $a=12\text{mm}$ and $b=20\text{mm}$. The monitors are set at the center of the input port ($x=0\text{mm}$), in the horn part ($x=15\text{mm}$), in the waveguide and at the output port ($x=30\text{mm}$).

To prove that the reflections do not affect subsequent incoming signals the same simulation run is performed for a pulse train of five times the gaussian signal used in the simulations before. The result is presented in figure 26. The signal in the waveguide part is again very clean and undistorted. It is satisfying that the reflections do not affect the output signals in such a big way as the probe monitor at the input may constitute.

Figure 26: The time evolution of the E-fields along the x-axis measured by probe monitors at $x=0\text{mm}$ and $x=15\text{mm}$. The E-field at the input port is lasting due to reflections but the gaussian pulses at the output are undistorted.

The two dimensional plots of the electric field can be visualized in a color plot. Figure 27 is a sectional drawing in the xy-plane and visualizes the E-field in x-direction for time steps $t = (80, 120, 160, 200, 240)\text{ps}$. The incoming beam reaches the waveguide at $80\text{ps}$. At $120\text{ps}$ the peak of the THz pulse enters the waveguide and little distortions occur from $x=6\text{mm}$ to $x=12\text{mm}$. The powerful part of the beam enters the waveguide after $140\text{ps}$. While the signal in the waveguide is clean, the reflections in the horn part increase. At $160\text{ps}$ the beam passes out to free space. The simulations at $200\text{ps}$ and $240\text{ps}$ indicate that the beam remains in the horn part as assumed by figure 25. At least it is good that the waveguide part is not affected by any distortions.
Figure 27: The electric field in x-direction for a time from 0ps to 500ps, longitudinal to the electron trajectory. The figures plot the field amplitude dependent on the time. Starting with a snapshot at 100ps in (a) the signal propagates thru the coupler, leaves the output in (d) at 170ps and finally figure (f) indicates the remaining resonances. The colour scale indicate the strength of the electric field. Beware of different scaling for the figures. While the colour scale ranges from $-15000 \text{ V/m}$ to $15000 \text{ V/m}$ for the pulse in the waveguide the resonances are visualized using a scale from $-500 \text{ V/m}$ to $500 \text{ V/m}$. 
The energy efficiency is calculated by dividing the Energy going through the input port by the energy leaving through the output port as done in equation 51. The port impedance is $Z = 370 \Omega$ and the integration is done over the first gaussian pulse. For the input signal from $(0 - 107) \text{ps}$ and for the output signal from $(140 - 400) \text{ps}$. The efficiency over the whole bandwidth is than $E_{in} / E_{out} = 0.50$.

8 CONCLUSION AND PROSPECT

The research in this thesis was done to design a waveguide coupler for electron accelerators. The coupler should support the aimed frequency range from $425 - 475 \text{GHz}$ and fit to a circular acceleration structure. Starting with some basics concerning electromagnetic field theory, the theory section ended up with the analysis of circular waveguides. To find a suitable coupler design, a revision of recent papers concerning THz acceleration was given. The grating coupler, lens coupler and flared coupler all have their advantages and all of them are presented in recently published papers. The purpose to couple in a circular waveguide and a bandwidth of $\approx 10\%$ lead to the decision for a circular flared waveguide coupler.

The design process was mainly done with the help of CST MWS to compute the electromagnetic fields numerically. The rudimentary structures were refined as well as the software was adjusted step by step to fit the needs for a precise simulation. Several sweeps for blendings, angles and length of the coupler were performed. In the end, three different designs and their symmetric structures promised an efficient power transfer and an high acceleration gradient in the waveguide. One coupler design was chosen as the "final draft" and observed in detail. The structure has an input radius of $1.5 \text{mm}$, tapered to $0.47 \text{mm}$ to match the waveguide radius. A dielectric coating out of quartz with a thickness of $0.06 \text{mm}$ is needed to match the phase velocity. The quartz is tapered towards the input port to couple the THz pulse smoothly to the waveguide and minimize reflections. The thesis presents a waveguide coupler with high power transmission and just small phase distortions.

Because of this thesis does not include any electrons in the simulations, it has to be considered how the electrons react while passing through the waveguide coupler. A working waveguide coupler will be able to concentrate the hardly generated THz radiation and enables electron acceleration with high acceleration gradients.
REFERENCES


9 DECLARATION


I declare that I wrote the thesis on myself and no other than the specified sources were used. I also assure that I followed the general principles of scientific work and release, as declared in the guidelines of good scientific practice at the Carl von Ossietzky University of Oldenburg.

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Fabian Scheiba