An electrostatic positron beam for materials characterisation

Elena Abadjieva
Propositions accompanying the thesis
"An electrostatic positron beam for materials characterisation"

1. The time resolution of positron lifetime spectrometers in which the start-signal is triggered by secondary electron emission can be improved by optimising the optical design for the transport of the electrons.

   *this thesis Chapter 6*

2. A lens system characterised by two minima in its linear magnification can be formed by a two-tube lens ending in an aperture.

   *this thesis Chapter 7*

3. The micro-lensing effect, caused by grids in an optical system, can not be analyzed by computer codes based on the Finite Difference Method.


4. An efficient positron trap can be realized using stationary hybrid magnetic and electrostatic fields; this can not be accomplished by only electrostatic fields.

5. The residual stress in thin films and coatings can not be directly measured by the \(\sin^2\Psi\)-method if texture is present. In this case the orientation distribution function should be used to correct the strain measured by X-ray diffraction.


6. The internal decoration of cavities in silicon with hydrogen can be performed much more efficiently by infusion of gaseous hydrogen at elevated temperatures than by \(H^+\)-ion implantation and subsequent annealing.

7. The orientation relationship of crystalline precipitates in crystalline matrices is mainly determined by matching of the lattice parameters; in some cases, however, symmetry considerations are decisive.

8. A 'spiderweb' of a material with a high magnetic permeability was used at the Paul Scherrer Institute as a field terminator to extract a positron beam from a magnetic to a field-free area. However, switching from magnetic to electrostatic beam transport can be achieved even more successfully without using a 'spiderweb'.


9. The cell aging theory predicts the failure of cloning as a reproductive method.

   M. Ridley "Genome" Harper Collins Publ. 1999, Chapter 14

10. Antonie van Leeuwenhoek could very well have been posing for the artist Johannes Vermeer when he painted "The astronomer" and "The geographer" in 1668.

These propositions are considered defensible and as such have been approved by the supervisor Prof. Dr. A. van Veen
Stellingen behorende bij het proefschrift

"Een elektrostatische positronenbundel voor materialenonderzoek"

1. De tijdsresolutie van positronenlevensduur-spectrometers waarbij het startsignaal gegeven wordt door de emissie van secundaire elektronen kan worden verbeterd door het optimaliseren van het optisch ontwerp voor hun transport.

_Hoofdstuk 6 van dit proefschrift_

2. Een lenssysteem dat gekarakteriseerd wordt door twee minima in zijn lineaire vergroting kan worden geconstrueerd door een lenssysteem bestaande uit twee achter elkaar geplaatste cilinders eindigend in een apertuur.

_Hoofdstuk 7 van dit proefschrift_

3. Het micro-lens effect dat roosters kunnen veroorzaken in een deeltjesoptisch systeem kan niet geanalyseerd worden door simulatieprogramma's die op de 'Finite Difference Method' gebaseerd zijn.

4. Een efficiënte positronenval kan gerealiseerd worden door middel van stationaire hybride magnetische en elektrostatische velden. Met enkel elektrostatische velden is dit niet te bereiken.

5. De restspanning in dunne films en coatings kan niet direct worden gemeten door de sin²Ψ-methode als er een textuur aanwezig is. In dit geval moet de 'orientation distribution function' gebruikt worden voor de correctie van de met röntgendiffractie gemeten deformatie.

6. De inwendige decoratie van holtes in Si met waterstof kan veel efficiënter gedaan worden door middel van infusie met waterstofgas bij hoge temperaturen dan via de implantatie van waterstofionen en daarop volgende annealing.

7. De oriëntatie van kristallijne precipitaten in kristallijne roosters wordt in belangrijke mate bepaald door overeenkomst in de roosterparameters; in sommige gevallen is de symmetrie doorslaggevend.

8. Een "spinnenweb" bestaande uit materiaal met hoge magnetische permeabiliteit als veldbegrenzer is bij het Paul Scherrer Instituut toegepast om een positronenbundel van een magnetisch naar een veldvrij gebied te brengen. Het omschakelen van magnetisch naar elektrostatisch bundeltransport kan echter, met een zelfs beter resultaat, bereikt worden zonder het 'spinnenweb' toe te passen.

9. De celverouderingstheorie voorspelt de onmogelijkheid van het klonen als reproductiemethode.
_M. Ridley "Genome" Harper Collins Publ. 1999, Chapter 14_

10. Antonie van Leeuwenhoek zou zeer goed in 1668 bij Johannes Vermeer model hebben kunnen staan voor de schilderijen "De astronoom" en "De geograaf".

Deze stellingen worden verdedigbaar geacht en zijn als zodanig goedgekeurd door de promotor Prof. Dr. A. van Veen.
An electrostatic positron beam for materials characterisation
The research described in this thesis was performed in the Department of Defects in Materials of the Interfacultair Reactor Instituut, Delft University of Technology, Mekelweg 15, 2629 JB Delft, The Netherlands.
An electrostatic positron beam for materials characterisation

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Introduction

1.1 General

Positrons, a form of anti-matter, are a very sensitive probe for defects in materials because of their strong preference for open volumes. The product of the annihilation process, gamma radiation with an energy of 511 keV, is easily detected. The formation of beams of positrons with a variable energy allows depth profiling of the defects and defect analysis at interfaces and layered structures [1]. Another advantage of the positron probing techniques is that they do not influence the defect structures and therefore provide non-destructive methods of defect analysis.

Defects in solids are a consequence of atomic displacements. Usually they are associated with regions where the electron density is lower than in the perfect material, e.g. vacancies and vacancy clusters. As a result the energy level occupied by the positron will be lower than in the bulk and therefore the positron will tend to be trapped in the defect. The trapped positron will eventually annihilate with electrons in its vicinity. By monitoring the annihilation properties information on the defects can be obtained. In semiconductors and insulators the defects can be charged. Positively charged defects effectively repel positrons. Negatively charged defects enhance the initial positron density in the defect region and increase the trapping rate. This can be used to identify the charge state of the defect [2],[3]. The way in which positron trapping is identified depends on which property of the 511 keV annihilation gammas is measured.

The understanding of the effects of the electronic structure of defects on the positron behaviour, which become manifest in Doppler-broadening and positron lifetime measurements, has improved greatly during the last decade as a result of developments in the theory of electron-electron and positron-electron correlations [4],[5]. The advent of positron beams has enabled the performance of depth analysis of the defects. With the standard positron beams a relative depth resolution of 10% can be reached. The defect concentrations detected by positrons are in the order of $10^{-7}$ to
Defects can be identified from mono-vacancies to nanometre-size pores. In another positron technique positron lifetimes can be measured from a few hundred ps to more than a few ns.

The progress in the capabilities of positron spectroscopy, achieved in the last decades, is mainly due to the developments in the positron beam technology. The main efforts in this area can be summarized as follows:

- Beam production (in particular source-moderator geometry and moderation efficiency)

  A successful technology of producing thin crystal films has been established by Chevallier [7]. Jørgensen et al [8] studied a new rectifying sandwich W-Mo foil. Lynn and MacKee have proposed the field enhanced moderator [9]. While Zecca et al tested new materials and methods for moderator production [10].

- Electrostatic transport and focusing

  New optical systems have been proposed by Beling [11], Zecca [12, 13] and Nunogaki [14].

- New intense positron sources (based on nuclear reactors and LINACs)

  An intense positron beam based on a source installed in a nuclear reactor was built by van Veen et al [15] in the Positron Centre Delft. Lynn constructed an intense beam employing strong $^{64}$Cu sources produced in the HFBR (High Flux Beam Reactor) at Brookhaven National Laboratory. In Munich the newly designed intense positron source is ready for operation. Intense positron beams based on LINACs are available at the Lawrence Livermore National Laboratory (LLNL), the Oak Ridge National laboratory (ORNL), and at the Universities of Osaka and Tokyo [16].

- New applications of brightness enhanced micro-beams (positron micro-probe, positron re-emission microscopy, high-resolution low-energy positron diffraction (LEPD))

  Micro-beam facilities have been built or are under construction in Bonn [17], Munich [18], LLNL [19] and Delft [20]. However, the first results of micro-beam construction were achieved at Brandeis University [21].

- Improved beam-based positron lifetime spectrometers, requiring MeV and pulsed positron beams

  Pulsed positron beams are available in Japan [22] and Germany [23]. A MeV positron beam has been built in Stuttgart [24]. A recently constructed pulsed positron beam is in operation in Gent [25].
This thesis intends to contribute to the further development of positron beam techniques by presenting a design for an electrostatic positron beam with the following options:

1. **Doppler-broadening measurements in the low-mm scale**

   Historically, the instruments for the positron annihilation techniques for material defect analysis, Doppler-broadening and beam-based lifetime measurements have been based on magnetic systems. The main advantage of using magnetic fields is the high transport efficiency. They are therefore applied in intense beam transportation [15]. Standard laboratory-based positron beam systems use solenoids or permanent magnets, employed both to transport and to focus the beam to a small size at the target [26]. Magnetic-transport beam systems are relatively straightforward to design and construct. At the same time a number of disadvantages have emerged. Intensity, beam size, shape and beam position on the sample surface vary when the energy of the beam is changed. This makes it difficult to control the geometrical characteristics of the beam [27], and consequently the positron beam will explore different parts of the sample at different beam energies. These effects can be reduced when the earth magnetic field is compensated.

   The majority of the investigated samples can not be produced with uniform properties over areas of about one cm². Usually some of them are subjected to ion implantation, where the implanted area has a size of a few mm. Therefore, motion of the beam on the target can not be tolerated. In Chapter 7 a design of an electrostatic positron beam is presented that gives a fixed position, size and intensity at the target when varying the beam energy. It is useful for studying samples with sizes in the low millimetre range, as well as non-homogenous samples.

2. **Transmission re-moderation**

   In most measurements based on the detection of positrons that are reflected, transmitted, diffracted or re-emanated from solid surfaces, it is advantageous that the incident positrons are implanted in the sample in a small spot in a field-free environment [28]. When information on the energy and angular distribution of the positrons is needed, a magnetic field-free environment facilitates the measurements of these distributions. Also for transmission re-moderation this is essential. The description of the beam facility designed for transmission re-moderation is given in Chapter 4.

3. **Positron lifetime measurements with a continuous beam**

   The value of the a positron beam is increased further if the lifetimes of the annihilated positrons can be measured in addition to the Doppler-broadening parameters. However, pulsed positron beams require a considerably greater
design effort than continuous beams. Therefore it is investigated whether a
start-signal can be generated by interaction of the beam with a foil at an
intermediate position or at the target. In Chapter 6 two designs are presented.
The triggering of the start-signal is given by the secondary electron emission
from a thin carbon foil placed in front of the sample (transmission option:
positron beam passes through the foil and is focused on the target), or from
the sample itself (backscattering option: the positron beam is focused on the
target, which emits secondary electrons in the backward direction. Electrons
are detected by a Micro-Channel Plate (MCP) which has a central hole to
allow the positron beam to pass through it).

First an overview of the existing electrostatic positron beams and their applications
will be given.

1.2 Electrostatic positron beams and their applications

Positron beams are used for studies in atomic and molecular physics, condensed matter, surface science and materials science. Depending on the specific applications of the instrument the positron beams are designed to have different properties regarding the micro-beam dimensions, paraxiality, energy range, intensity and brightness. In order to achieve the required beam properties the positrons are subjected to electrostatic, magnetic or hybrid (electrostatic and magnetic) forces. The electrostatic and/or magnetic field distributions along the beam-line are created by lenses with specific shapes and dimensions. The basic knowledge of the properties of electrostatic and magnetic lenses and their construction can be found in the literature [29, 30]. A summary of the existing electrostatic positron beams and their applications is given in Table 1.1.

1.2.1 Materials Science

Worldwide there exist two variable energy positron beams for Doppler-broadening experiments based on an electrostatic system, designed by Zecca [12] and by Nunugaki [14], respectively. Electrostatic optics has also been employed in micro-beam technology for designing brightness enhancement stages. This has been done by Seijbel et al [20], Zecca and Brusa [13] and Gerola et al [37]. A positron source with electrostatic extraction and focusing is applied in the MeV Stuttgart beam used for beam-based positron lifetime measurements and the beam-based age-momentum correlation technique [24].
<table>
<thead>
<tr>
<th>University</th>
<th>Applications</th>
<th>Source/moderator</th>
<th>intensity ($e^+$/s·mCi)</th>
<th>reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>University of Trento, Italy</td>
<td>Doppler-broadening measurements</td>
<td>$^{22}$Na W (1µm)</td>
<td>$10^3$</td>
<td>[12]</td>
</tr>
<tr>
<td>University of Osaka, Japan</td>
<td>Doppler-broadening measurements</td>
<td>$^{22}$Na W (10µm)</td>
<td>$10^2$</td>
<td>[14]</td>
</tr>
<tr>
<td>University of Tokyo, Japan</td>
<td>Positron induced ion desorption spectroscopy</td>
<td>$^{22}$Na W (1µm)</td>
<td>$2 \times 10^3$</td>
<td>[31]</td>
</tr>
<tr>
<td>University of East Anglia, UK (presently at University of Bath)</td>
<td>Re-emitted positron spectroscopy (RPS), Re-emitted positron energy loss spectroscopy (REPELS)</td>
<td>$^{22}$Na W (6µm)</td>
<td>$10^3$</td>
<td>[32]</td>
</tr>
<tr>
<td>University of Texas, USA</td>
<td>Positron annihilation induced Auger electron spectroscopy (PAES)</td>
<td>$^{22}$Na W (1µm)</td>
<td>$3 \times 10^2$</td>
<td>[33]</td>
</tr>
<tr>
<td>University College London, UK</td>
<td>Atomic and molecular physics</td>
<td>$^{22}$Na W (meshes)</td>
<td>$10^2$</td>
<td>[34]</td>
</tr>
<tr>
<td>University of Western Ontario, Canada</td>
<td>Condensed matter</td>
<td>$^{58}$Co Ar (frozen rare gas)</td>
<td>$2 \times 10^2$</td>
<td>[35]</td>
</tr>
<tr>
<td>Brandeis University, USA (until 2000)</td>
<td>Low energy positron diffraction (LEPD)</td>
<td>$^{58}$Co W</td>
<td>20</td>
<td>[36]</td>
</tr>
</tbody>
</table>
1.2.2 Surface Science

One of the important subjects of surface science is the bonding mechanism and atomic structure of surface adsorbates. The atomic structure of the surface of the substrate is also significant for the successful application of molecular beam epitaxy. In order to study the dynamics of atoms on a surface, positron-induced ion-desorption spectroscopy has been proposed [38, 39]. To carry out investigations in this field an electrostatic slow positron beam has been designed at the University of Tokyo, Japan [31]. This instrument delivers a positron beam of 2 to 4 keV at the sample position within a spot with a diameter of 10 mm. Furthermore, positron re-emission studies have been extended to include re-emitted positron energy spectroscopy (RPS) and re-emitted positron energy-loss spectroscopy (REPELS). These techniques exploit the positron’s unique property of re-emission from surfaces. The RPS technique has been performed using both magnetic and electrostatic-transport positron beams. Magnetic systems are advantageous for confining all positrons scattered or re-emitted from the sample of interest. Electrostatic systems are advantageous in that angle-resolved measurements of positron re-emission can be performed more easily. A re-emitted positron energy spectrometer based on an electrostatic system was designed at the University of East Anglia, UK [32].

The well-known electron-induced Auger electron spectroscopy (EAES) uses electrons to induce vacancies in the electron core levels. In some cases it is advantageous to use positrons to create the vacancies. This becomes clear when the underlying processes are considered. The primary electron beam penetrates deep into the solid, causing a cascade of backscattered and secondary electrons to appear in the Auger spectrum [40]. The core holes in positron-annihilation induced Auger electron spectroscopy (PAES) on the other hand, are generated via matter-antimatter annihilation rather than by impact ionization [41]. Therefore no backscattered electrons contribute to the background and thus the background present in EAES is eliminated. The annihilation-induced Auger electrons originate almost exclusively from the topmost atomic layer, providing PAES with a high degree of surface specificity [42]. PAES spectrometers based on magnetically guided positron beams suffer from relatively poor energy resolution, because of the large acceptance angles needed for high transmission. That is why at the University of Texas at Arlington, USA, a high-resolution positron-annihilation-induced Auger electron spectrometer was designed based on an electrostatically guided and focused positron beam [33]. Its energy resolution is improved by a factor of five compared to the previous magnetic beam based instrument. Low-energy positron diffraction (LEPD), like LEED, relies on measurements of the diffraction of elastically scattered particles from ordered surfaces to obtain information on the arrangement of atoms in the first few atomic layers (surface structure). The Brandeis University LEPD system made use of an electrostatic brightness enhanced positron beam [36].
1.2.3 Atomic physics and condensed matter physics

Atomic physics and condensed matter studies involve the investigation of the positron-atom (molecule) collision and scattering process, positron-electron scattering and energy loss in solids. In order to study the energy dependence and angular distribution of the scattered positrons as well as possible coupling effects between the elastic and other scattering modes, a positron electrostatic beam was developed at University College London, UK [34]. The electrostatic positron beam at the University of Western Ontario, Canada, [35] has a variable energy from 1 to 60 keV. It can be used for the measurement of positron and electron backscattering, positron and electron energy loss processes in thin films and cross-section ratios for inner-shell excitations.

1.2.4 Design principles

Source-moderator assembly

The recipe for designing an electrostatic variable energy positron beam involves several basic points. First, a radioactive isotope is used as a generator of positrons. This is usually $^{22}$Na but sometimes $^{58}$Co is employed. The source activity is typically between 5 and 100 mCi. The energy spectrum of the $\beta$-production of both isotopes is wide, up to 0.5 MeV. In order to create a monochromatic beam the positrons have to be moderated. The classical approach is to use a W foil (with a thickness in the order of several $\mu$m) or W meshes. The application of a frozen inert gas (Ar, Kr, Xe) as positron moderator could be more efficient. It is used in the backscattering mode at the University of Western Ontario, Canada [35]. The energetic positrons, originating from the radioactive source, enter the solid and rapidly lose energy by undergoing inelastic collisions with core and conduction electrons. At low energies the energy loss mechanism is via plasmon excitations, which becomes important in the 10 eV region, and by phonon scattering below eV energies. The positrons reach thermal equilibrium with the solid lattice within picoseconds and diffuse until they annihilate or reach the surface of the solid. If the material contains only a few defects which may act as trapping and annihilating sites a large number of thermalised positrons will reach the surface. There they can: 1) get trapped into a surface potential well and annihilate, 2) pick up an electron and leave as positronium, or 3) be emitted as a free positron into the vacuum with an energy determined by the positron work function, as long as the work function has a negative value. The process that leads to slowing down and emission of slow positrons is called positron moderation. A small fraction of the thermalised positrons, which are close to the surface (e.g. within a distance equaling the diffusion length) and branch into free positrons, leave the W moderator with an energy of 3 eV. Their direction is almost perpendicular to the solid surface (maximum angle $\pm 6^\circ$) [6]. In order to ensure a good performance of the moderator material (a material with a long diffusion length and a clean surface),
the design of the facility should allow repeated annealing of the moderator in high vacuum.

**Positron gun**

The next element of the electrostatic positron beam is the so-called ”positron gun”. In most of the beams cited above a modified Soa immersion lens has been used as a positron gun. It is described in detail by Canter in [43]. Briefly, a modified Soa gun has five electrodes. The moderator surface constitutes the first electrode followed by a grid, Wehnelt cylinder, Soa tube and anode. Once the positrons are extracted from the source-moderator assembly they are transported and focused by a combination of Einzel lenses or two-tube lenses at the entrance of a deflector.

**Deflector**

The deflector bends the positron beam over 90° and serves to prevent gamma rays and un-moderated high-energy positrons from reaching the sample, as well as delivering the beam at ports for different experiments. Some facilities do not have a deflector and the beam is directly focused on the sample with a combination of electrostatic lenses. Examples of such facilities are given in [14], [32], [35]. A parallel-plate analyzer [29], [30] or a spherical electrostatic prism [44] can be used as a deflector for all beam energies.

**Lens types**

The optical system between the deflector and the sample is specific and generally consists of apertures, Einzel/zoom and two-tube lenses. It produces the required beam properties at the sample position. Therefore we summarize this last optical section taking into account the corresponding application of the positron beam:

- **Electrostatic positron beam for high-resolution positron-induced Auger electron spectroscopy**
  
  Two Einzel lenses transport the beam to a four-element zoom lens. The beam energy is in the 100 eV range. The last element is cone shaped to avoid obstructing the path of the Auger electrons into the cylindrical mirror analyzer and to reduce the electric field penetration from the lens into the region near the sample [33]. The beam diameter is 10 cm at 10 eV.

- **Electrostatic positron beam for positron-gas scattering experiments**
  
  The beam is focused by a five-element cylindrical lens at 30 eV to a spot smaller than 10 mm at the centre of the collision chamber [45]. The energy spread is less than 2 eV in the range 10 - 100 eV.
• Electrostatic positron beam for positron-induced ion-desorption spectroscopy

Three Einzel lenses are used to transport and focus the beam with an energy between 2 keV and 4 keV at the sample position onto a spot of the order of 10 mm [31].

• Electrostatic positron beam for low-energy positron diffraction

It is characterized by a three-element zoom lens, which produces a beam at the target with 1 mm diameter and up to 1° convergence angles in the 10 - 240 eV energy region [36].

• Electrostatic positron beam for Doppler-broadening experiments

The beam energy may vary up to 50 keV and at the same time the spot size and position should stay constant. The design presented by Zecca and co-authors in [12] consists of three lenses. The first one is a three-tube lens with a fixed voltage, the second one is also a three-tube lens at a flexible voltage as an asymmetric Einzel lens and the last one is a two-tube lens of a relatively large size, with a fixed voltage ratio, which works in both the deceleration and acceleration mode. This electrostatic system focuses the beam from a 4 mm primary size to a spot of 3 mm from 50 eV to 2 keV, and 2 mm from 1 to 50 keV. Its schematic view is given in Figure 1.1.

Every electrostatic beam can be steered. This can be done using deflection plates, by dividing one of the cylindrical electrodes into four segments in order to steer the beam with the aid of electrical field in two directions or by external magnetic coils. Special care has to be taken to eliminate the earth magnetic field and the residual magnetization of materials in and around the electrode system. The earth magnetic field should be shielded by μ-metal or mutually orthogonal Helmholtz coils.

**Beam quality**

A measure of the quality of the beam design and performance is the ratio of the number of positrons reaching the target $N_T$ to the number of the isotope disintegrations per second $N_d$. For beams with a conventional radioactive source and transmission moderator the efficiency is given by Zecca [12] as

$$
\epsilon = \epsilon_M \epsilon_T \epsilon_S B_P W \frac{\delta \Omega}{4\pi} = \frac{N_T}{N_d}
$$

(1.1)

where $\epsilon_M$ is the moderation efficiency of the chosen moderator foil, $\epsilon_T$ is the optical transport efficiency, $\epsilon_S$ is the source self-absorption, $B_P$ is the positron branching ratio of a radioactive isotope, $W$ is the source capsule window transmission for positrons and $\delta \Omega$ is the solid angle under which the moderator is viewed from the radioactive source. This angle depends on the distance of the moderator from the isotope.
Figure 1.1: A schematic view of the electrostatic positron beam at the University of Trento, Italy (with permission from Zecca [12]).

1.2.5 Positron beam detection

Positron beam detection is performed by two groups of detectors. The first group, consisting of scintillation detectors, is used to detect the annihilation radiation (e.g. to measure the Doppler-broadening of the 511 keV gamma line from annihilations in the target). Mostly used are Ge, NaI and BaF$_2$ detectors. Occasionally these detectors are employed to check the size and position of the beam. The second group of detectors consists of channeltrons, micro-channel plates with phosphor screens, hemispheric energy analyzers etc. These are used for direct counting of the number of positrons. Channeltrons coupled with a retarding element in front are easily transformed into simple energy analyzers. Micro-channel plates (MCP) with a phosphor screen are used for beam imaging. Usually two MCPs are mounted in series followed by a phosphor screen, connected to a CCD camera and computer controlled image processing software. Both channeltrons [29] and MCP can be used for the determination of positron beam size and for beam alignment.
1.3 Development of positron beams at the Positron Centre Delft

There are several facilities for positron annihilation studies at the Positron Centre Delft: two set-ups for conventional (i.a. based on a radioactive source) positron lifetime techniques, a slow variable energy positron beam with magnetic transport for 1D and 2D Doppler-broadening measurements, and the most advanced one a 2D-ACAR set-up coupled to an intense positron beam. The intensity of this positron beam is $4 \times 10^8$ positrons per second and it is based on the MeV $\gamma$-production of the Delft nuclear reactor [15]. Further development of the instrumentation of the positron centre requires a facility for beam-based positron lifetime measurements, used for polymer films and ceramic coatings. A variable energy beam for Doppler-broadening measurements on a sub-mm scale with improved beam performance, used for mm-scale samples, MOS systems and for materials, which have damaged zones with sizes in the low-mm range is another apparatus under consideration. A facility for studying the moderation properties of materials in transmission mode, used to support the research for the construction of a positron micro-probe facility is needed.

The latter project involves several major steps. The intense positron beam, produced by the nuclear reactor and guided magnetically to the experiment hall where the facilities are positioned, needs to be injected into the so-called re-moderation section. Prior to the injection of the beam the guiding magnetic field has to be terminated. The changeover from magnetic to electrostatic transport and focusing causes enlarged beam diameters. The positrons acquire a large transverse momentum when leaving the field, regardless of their velocity or whether the magnetic field is terminated abruptly. The first major step is to take the beam out of the magnetic field taking into account the acceptance of the following re-moderation section. Most likely additional electrostatic focusing in front of the re-moderation section will be needed. Another approach is to place a positron moderator at the exit of the magnetic field area in order to reduce the divergence. The role of the re-moderation section is to enhance the brightness of the beam by means of repeated moderation (re-moderation) and focusing performed in transmission mode. The focusing is done by electrostatic lenses in a special $\mu$-metal chamber. The optical design of this section is given in [20]. The second major step is to obtain thin foils, which possess a high moderation efficiency in transmission mode over a long period of time without additional treatment. This step is a complicated materials science task. Stability of the moderation properties of the foils is essential for the operational success of the project. The third and last major step is to insert the positron beam into the Scanning Electron Microscope (SEM) and getting the facility to work with both electron and positron beams, providing depth profiling analysis on a micrometre scale. The lateral resolution of this instrument is designed to be better than 1000 nm. Generally the improvement of the lateral resolution is limited by the diffusion
length of the positrons in the solids.

1.4 Outline

In this thesis a brief description of the positron annihilation techniques is given in Chapter 2. In Chapter 3 the basic definitions of positron beam optics, design methods of the optical systems and some construction principles are presented. The electrostatic positron beam designs presented in this thesis are summarized in Figure 1.2. In Chapter 4 the optical design and performance of the facility for positron remoderation experiments is discussed. In Chapter 5 we present the experiments with thin W and WMo foils carried out with this set-up.

![Diagram showing positron beam design with Na source and W target]

**Figure 1.2:** Overview of the electrostatic positron beam designs presented in this thesis.

The design of a positron lifetime spectrometer is described in Chapter 6. The optical design and the construction of the instrument for Doppler-broadening measurement in the low-mm scale are given in Chapter 7. Chapter 8 presents the depth profiling analysis done with the latter set-up on a mm-size p-n junction, Si samples implanted with Xe and Kr ions to different doses and SiC implanted with 50 MeV Cu ions.
Chapter 2

Principles of positron annihilation techniques

2.1 Positron implantation and transportation in solids

The interaction of a beam of monoenergetic positrons with a solid takes place via a number of different processes. Firstly, at the surface of the solid diffraction, positron backscattering and secondary electron emission may be observed. After implantation a positron may return to the surface, in which case so-called surface branching processes take place. This happens with non-thermalized as well as with thermalized positrons. For a detailed overview of the possible interaction channels we refer to the literature [6, 16]. The implanted keV positrons lose energy inside the material via electronic mechanisms. This includes core ionization and excitations, electron–hole excitations and collective plasmon like excitations of valence electrons. When their energy is in the order of a few eV, inelastic scattering follows the ionic mechanism via phonon scattering. Taking into account the cross-sections for the different scattering mechanisms the statistical profile of the depth at which the implanted positrons reach thermalization is best described by a Makhovian function. This implantation profile is given by

\[ P(x, E) = -\frac{d}{dx} [\exp(-\frac{x}{x_0})^m]. \]  \hspace{1cm} (2.1)

The mean implantation depth \( \langle x \rangle \) scales with the initial energy as

\[ \langle x \rangle = AE^n, \]  \hspace{1cm} (2.2)

where \( A, m, \) and \( n \) are material dependent parameters and \( x_0 \) is given by

\[ x_0 = \frac{\langle x \rangle}{\Gamma\left(\frac{1}{m} + 1\right)} \]  \hspace{1cm} (2.3)
in terms of the gamma function, \( \Gamma \). After being thermalized in a picosecond time scale positrons diffuse in the solid until they get trapped in a potential well and annihilate. The statistical behaviour of positrons after their thermalization in a solid can be modelled by the following equation given by van Veen et al. [46],

\[
D^+ \frac{d^2c(x)}{dx^2} - \frac{d}{dx} (v_d c(x)) + P(x) - \kappa_t n_t(x) c(x) - \lambda_0 c(x) = 0,
\]

(2.4)

where \( c(x) \) is the time averaged positron density and \( v_d(x) \) is the drift velocity,

\[
v_d(x) = \mu E(x).
\]

(2.5)

Here the positron mobility is indicated by \( \mu \) and \( E(x) \) is the electric field strength at a depth \( x \) in the solid. The energy dependent positron stopping rate at depth \( x \) is given by \( P(x) \). The defect density at depth \( x \) is \( n_t(x) \) and the rate constant for positron trapping at defects is \( \kappa_t \). The bulk annihilation rate is given by \( \lambda_0 \) and \( D^+ \) is the positron diffusion coefficient. The positron diffusion coefficient \( D^+ \) and the positron mobility \( \mu \) are connected by

\[
D^+ = \frac{k_B T \mu}{e},
\]

(2.6)

where \( k_B \) is the Boltzmann constant, \( e \) the elementary charge and \( T \) the absolute temperature. This diffusion model provides the framework for defect-profile analysis. It can be solved numerically. At large depths the concentration of positrons will become negligible and the solution of the diffusion model should satisfy

\[
\lim_{x \to -\infty} c(x) = 0.
\]

(2.7)

A second boundary condition is specified at the interfaces and surfaces

\[
-D^+ \frac{dc(x)}{dx} \bigg|_{x=0} + \mu E(x) = -\nu c(x)
\]

(2.8)

where \( \nu \) is the transition rate from the surface to the vacuum or to the surface state. The ejection current at the surface is assumed to be proportional to the positron density at the surface. The initial condition for the positron density in case we neglect epithermal positrons is represented by the implantation profile.

Part of the implanted positrons survive the defect trapping and annihilation and can diffuse to the back- (backward mode) or front-surface (transmission mode). They can be fully or partly thermalized. The energy and momentum distribution of the epithermal fraction depend on the implantation energy. The thermalized fraction has an isotropic Maxwellian velocity distribution which is determined by the temperature of the substrate. The surface interaction can be characterized by the surface dipole barrier, caused by the spill-over of electrons into the vacuum. The chemical
potential of a positron in the solid is a function of the correlation potential, which
is due to the positron's interaction with conduction electrons and its repulsive in-
teraction with ion cores. Positrons that reach the surface can be i) trapped into
an image-potential surface state, ii) reflected by the positron surface potential, or
iii) emitted into vacuum as positronium or free positrons. The positronium work
function or emission potential is given by

\[ \phi_{ps} = \phi_+ + \phi_- - 6.8 \]  

(2.9)

where the positronium binding energy is 6.8 eV. The electron work function and the
positron work function are respectively given by

\[ \phi_- = D - \mu_- \]  

(2.10)

\[ \phi_+ = -D - \mu_+ \]  

(2.11)

Here \( D \) is the surface dipole barrier and \( \mu_- \) and \( \mu_+ \) are the electron and positron
chemical potentials in the solid. Free positron emission from metal surfaces with
a negative work function is an adiabatic process. The positrons escape elastically
along the surface normal with an angular distribution proportional to \( k_B T/|\phi_+| \). A
more detailed discussion of the physics of positron surface processes can be found
in the literature [47, 48].

Positronium can be formed in insulators or materials with large open vol-
umes. The ground states of positronium consist of the singlet state \( ^1S_0 \) (para-
positronium) and the triplet \( ^3S_1 \) (ortho-positronium). Para-positronium decays via
emission of two gammas. In vacuum it has a lifetime of 125 ps. Ortho-positronium
has a lifetime of 142 ns and decays into three photons. In materials it decays faster
due to a "pick-off" process in which the positron annihilates with an electron of a
nearby atom.

2.2 Observables

The microscopic information of a material obtained with a positron beam is provided
by the gammas, which are the product of the annihilation of a positron with an
electron in its vicinity. The energy and angular distribution of the gammas are used
in positron annihilation spectroscopy. The positron lifetime is a third quantity from
which information can be extracted about the material. The electron density and
the electron momentum density in vacancy-type and open-volume defects differ from
those in the bulk. This can be observed using the techniques mentioned below. In the
centre-of-mass frame the two gamma rays are emitted in exactly opposite directions
and have equal energies. In the laboratory frame the momentum of the electron-
positron pair causes an energy shift and a deviation from the collinearity of the two
gammas. The energy shift ($\Delta E$) is dependent on the longitudinal component (with respect to the detector) of the positron-electron pair momentum, $p_t$

$$\Delta E = \frac{cp_t}{2}.$$  \hfill (2.12)

The deviation in the angle of emission can be calculated from the transverse component of the positron-electron momentum, $p_t$

$$\theta = \frac{p_t}{m_0c}$$  \hfill (2.13)

where $m_0$ is the rest mass of the positron and $c$ is the velocity of light.

**Doppler-broadening technique**

In the Doppler-broadening technique one measures the energy shift of one or both of the annihilation quanta. The measured energy distribution is characterised by the line shape parameter $S$ [49]. This parameter is calculated as the ratio between the central region of the annihilation peak and its total area (Figure 2.1). The annihilations with valence electrons contribute to the central region of the peak. The wing-parameter $W$ provides information on the core electrons. It is defined by the area of the two energy windows in the tails of the annihilation peak divided by the total area. The absolute values of the two parameters depend on the resolution of the instrument and the limits of the window intervals. The experimental data obtained

![Diagram](image)

**Figure 2.1:** Doppler-broadened 511 keV peak with the intervals used to define the $S$ and $W$ parameters.

by the Doppler-broadening technique can be analyzed with the aid of a computer program that simulates the implantation, diffusion, trapping and annihilation of the
positrons. A diffusion model with specific boundary conditions has been
to interpret the measured spectra. The program VEPFIT [46] solves numerically the
diffusion and trapping equation for the positrons. One of its options is to treat the
sample as a combination of different positron trapping layers, each defined to have
a certain thickness, line-shape and wing-shape parameters ($S$ and $W$) and positron
diffusion length, which are connected to the defect concentration. The measured
data are expressed as

$$S(E) = \sum_{i=1}^{n} f_i(E)S_i + f_{surface}(E)S_{surface} + f_{bulk}(E)S_{bulk}$$  
(2.14)

$$W(E) = \sum_{i=1}^{n} f_i(E)W_i + f_{surface}(E)W_{surface} + f_{bulk}(E)W_{bulk}$$  
(2.15)

where $f_i(E)$ is the fraction of the positrons implanted with energy $E$, which annihi-
late in layer $i$, and $S_i$ and $W_i$ are the values of the Doppler–broadening parameters
in layer $i$. The bulk and surface values are correspondingly defined. The so-called
$S - W$ map is obtained by plotting $W$ against $S$, using the implantation energy as
a running parameter. This allows a direct interpretation of the experimental data
and determination of the kind and number of annihilation sites in terms of layers
with distinct $S$ and $W$ values. In order to reduce the background and to improve the
resolution of the measured Doppler-broadening shift, two detectors are used in coin-
cidence. This is the so-called 2D Doppler-broadening technique. The two detectors
are positioned collinearly with the sample. For two identical detectors the resolution
is improved by a factor of $\sqrt{2}$.

**Positron lifetime technique**

The positron lifetime technique measures the lifetime of a positron in a solid as the
interval between its entry in the solid and its annihilation with an electron. The
positron lifetime, $\tau$, is the inverse of the annihilation rate, $\Gamma$, and thus is inversely
proportional to the electron density. The annihilation rate is determined by the
overlap of the electron and positron wavefunctions:

$$\Gamma = \pi r_0 \int \rho_-(r)\rho_+(r)dr$$  
(2.16)

where $\rho_-(r)$ and $\rho_+(r)$ are the electron and positron probability densities at position
$r$, respectively, and $r_0$ is the classical electron radius.

In conventional source-based ($\gamma\gamma$ coincidence) positron lifetime spectrometry
the start–signal is generated by the prompt $\gamma$-quantum emitted almost simultaneously
with the positron by the radioactive source $^{22}$Na. The stop–signal is triggered by
one of the two annihilation quanta. The reduced measuring time and the ability to
measure the low-intensity long-life components in the lifetime spectra (because of low background at high count rates) are advantages of the beam-based $\beta^+\gamma$ coincidence lifetime spectrometer. The start–signal is generated with 100% efficiency by passing the MeV positrons through a scintillator prior to implantation. When the positron lifetime measurement is combined with a depth resolution capability the start–signal can not be used as in the conventional circuitry. In order to perform beam-based positron lifetime studies pulsed beams or secondary electron emission from the surface of the sample are being used as the start–signal. Bunched positron beams with a pulse width of 150 ps and pulse repetition rates of $10^5$ Hz, available in Munich [23] and Japan [22], provide a time resolution of the positron lifetime measurement of around 200 ps. In an instrument where the secondary emission from the surface of the target is used as a start–signal an electrostatic beam is required. Such a setup has been built and achieves a time resolution of around 600 ps [50]. The resolution is limited by the positrons scattering off the sample surface and returning to it after some time and by the spread in the response time of the detector. In Chapter 6 in this thesis we present various designs for beam-based positron lifetime spectrometers, where the start–signal is triggered by secondary emitted electrons.

The measured lifetime spectrum can be modelled by

$$F(t) = \sum_{i=1}^{N} \frac{I_i}{\tau_i} \exp\left(-\frac{t}{\tau_i}\right)$$

(2.17)

where $N$ is the number of different annihilation states, $\tau_i$ is the lifetime of the positrons in state $i$ and $I_i$ is the intensity. The concentration of a particular defect type is related to the intensity for that defect state. For data analysis the POSITRONFIT and RESOLUTION programs are used. In POSITRONFIT the resolution function is given by a sum of gaussians and is assumed to be known. The spectrum is fitted by a sum of exponentials convoluted with the resolution function plus background in an iterative manner. The purpose of RESOLUTION is to extract the shape of the time resolution function. When the positron beam implantation energy is such that part of the positrons can reach the sample surface, the time spectrum cannot be described by a sum of exponential contributions. Methods to analyze the time spectrum in this case are reported in the literature [51, 52].
Chapter 3

Positron beam optics

3.1 Introduction

The first papers on slow-positron optics appeared in the eighties [43, 53] and serve as an alphabet in learning how to design electrostatic positron beams. Thanks to this pioneering work of Karl Canter and co-workers the number of electrostatic beams (E-beams) in the positron community has increased since then. Positron sources have a lower intensity and lower brightness compared to electron sources. Conventional bench-top positron beams are monochromatic, non-relativistic and have intensities in the order of $10^5$ positrons per second. Their intensity is restricted by the moderation efficiency of the moderator, the activity of the radioactive source and the source-moderator arrangement. Effects like mutual repulsion and space charge due to the interaction between the positrons are not present. The positrons also do not show collective behaviour. The properties of such beams are described by analyzing the motion of each anti-particle under the influence of the external forces. This question is dealt with by charged particle optics [29, 30]. However, differences between electron and positron optics arise from the optical differences between moderators and cathodes [10]. A general rule in positron optics is to maximize the number of positrons emerging from the moderator. In this chapter the basic definitions of beam theory will be given. The most frequently used electrostatic lenses and the design methods applied in this thesis will be described. Finally, some construction and lens performance principles will be reviewed, encountered in the building of electrostatic positron beams.

3.2 Definitions

Let us assume a system of non-interacting charged particles, influenced by conservative electrostatic forces. The motion of each individual particle is defined by the
three spatial coordinates \((x,y,z)\) and the three momentum coordinates \((P_x, P_y, P_z)\). An ensemble of particles forms a beam if their momentum component in one direction is much higher than the momentum component in the transverse directions. If we assume that in the cartesian coordinate system \(x\) is the direction of beam propagation then the necessary conditions for beam formation are: \(P_x >> P_y\) and \(P_z >> P_z\).

In order to define the basic beam properties the motion of the particles is considered in three spaces: three-dimensional geometric space or configuration space, four-dimensional trace space and six-dimensional phase space. At any given distance along the direction of the beam propagation every particle represents a point in \((y, y')\) (or \((z, z')\)) space, known as trace space. The parameter \(y'\) is defined by

\[
y' = \frac{dy}{dx} = \frac{\dot{y}}{\dot{x}} \approx \frac{P_y}{P_x}. \tag{3.1}
\]

In the \((x, y)\) plane, respectively in the \((x, z)\) plane,

\[
P_y << P_z \approx P \tag{3.2}
\]

The area occupied by the points representing all particles in the beam

\[
A_y = \int \int dy dy'
\tag{3.3}
\]

is called trace-space area. In the literature [29] this term is also defined as the emittance of the beam. The emittance provides a quantitative basis for describing the quality of the beam. It is the product of the width and the divergence of the beam and it is measured in [mm-mrad]. The emittance alone is not enough to define the quality of a beam. One can make the emittance as small as one desires for a particular application by the use of collimating slits. What counts, however, is the number of particles or the intensity of a beam with a given emittance. The figure of merit is the brightness of a beam, which is defined in equation 3.4. It equals the intensity divided by the total trace-space area. It is determined by the source-moderator arrangement.

\[
B = \frac{2I}{\pi^2 A_y A_z}. \tag{3.4}
\]

Optical elements like lenses can change the brightness. For example a change in potential changes the brightness linearly with the acceleration voltage \(V\) therefore the relevant parameter to use to characterize a source is the so-called reduced brightness \(B_r\), expressed in \([A/(cm^2.sr.V)]\)

\[
B_r = \frac{B}{V}. \tag{3.5}
\]

This quantity is a constant and does not change under the action of conservative forces. This is known as Liouville theorem. Every system for which a Hamiltonian can
be constructed can be treated via the concept of phase space. The six-dimensional space defined by the set of canonical coordinates \((q, p_i)\) is called phase space. The motion of the ensemble of particles representing the beam in actual configuration space is associated with an equivalent motion of the representative points in phase space. As the ensemble moves, the volume it occupies in phase space also moves and changes its shape. While the volume in phase space remains constant, the shape generally does not. In fact, non-linearities (aberrations) in the field configurations through which the particles move may cause considerable distortions in the shape of the phase space volume. The beam can be represented by projections of the six-dimensional (6D) phase space, called phase space diagrams. If the three components of motion are mutually independent in configuration space, then the motion in phase space is confined to three planes, which can be treated separately. If the system has axial symmetry one projection is enough to represent the beam. When there is a plane of symmetry, the beam can be presented by two two-dimensional projections of the 6D phase space.

For the development of low-energy positron diffraction (LEPD), the positron re-emission microscope (PRM) and the positron annihilation microprobe (PAM), brightness enhancement of the beams is necessary. The process, proposed by Mills [54], suggests repeated moderation (since positron moderation is a non-conservative process) and focusing to breach the Liouville theorem and thus to increase the brightness of a positron beam.

### 3.3 Electrostatic lenses and design methods

#### 3.3.1 Electrostatic lenses

The most frequently used electrostatic lenses in positron beam instruments are the TTL (two tube lens), the TAL (two aperture lens), and the Einzel lens (consisting of three electrodes). The latter may be a SEL (symmetric Einzel lens, when the outer electrodes are kept at the same potential and the middle one at a different potential) or an AEL (asymmetric Einzel lens, when the three electrodes are at different potentials). The focal properties of an electrostatic lens are determined by the diameter of the lens, the gap between the electrodes and the potential ratio (the ratio between the potentials on the electrodes). Using a SEL the beam size and divergence can be varied without affecting the beam energy. Another advantage of using a SEL rather than a TTL is that a small change of the voltage ratio alters the focal properties over a significant range which gives a higher flexibility for optimizing the beam characteristics. The most important aberration in positron optical systems is spherical aberration. In order to make this aberration negligible the diameter of the lenses should be at least twice the beam diameter and the trajectory angles with respect to the beam axis should not exceed 10°. Lenses should be separated by at least three times the lens diameter in order to keep them from interacting.
3.3.2 Design methods

Lens properties such as focal distances (focal lengths), positions of the principal planes (mid-focal lengths), and aberration coefficients have been calculated in the 70's. They are documented for the most frequently used electrostatic lenses in [55, 56, 57, 58]. These data are presented in so-called PQM diagrams (P and Q are the distances from the object and image to the reference plane respectively and M is the linear magnification) and corresponding aberration coefficient diagrams. They have been calculated by integrating the ray-equation under simplified approximations for the axial potential functions, which are solutions of the Laplace equation. These results are valid for paraxial beams only.

The matrix method is a simplified method for designing an optical system. In general, an optical system is formed by a sequence of drift (field-free) and lens (field) regions, which can be represented by sequential multiplication of the respective matrices. After analytical solution of the ray-equation for the simplest types of electrostatic lenses - the single aperture lens and the lens made by a homogeneous field - the matrix elements can be found. The basic types of electrostatic lenses (TTL, SEL) can be modelled as a combination of aperture lenses and lenses made by a homogeneous field [59]. The TTL can be modelled as a combination of two aperture lenses with zero field in front of the first aperture and behind the second aperture, and a homogeneous field in between. The SEL is a combination of four aperture lenses with zero field in front of the first and behind the last aperture and homogeneous fields of opposite signs between the first two and the last two apertures. There is no field between the two apertures in the centre. Knowing the matrix elements for these lenses ray-tracing is carried out using two characteristic rays [60, 61]. The remaining particle trajectories are expressed as a linear combination of these two characteristic ray trajectories. The transfer matrix subroutines for TTL, SEL and AEL are documented in [62].

Software packages

Versatile software is available nowadays providing accurate and simplified solutions for complex tasks. The main computational techniques for calculating electrostatic fields currently available are: FOFEM, SOFEM (first and second order finite element methods), FDM (the finite difference method) and CDM (charge density method). A detailed description of these methods can be found in [59]. They are mostly used when one has to design complicated optical systems consisting of three-dimensional components for lenses and deflectors. Programs based on computational techniques are capable of accurately simulating electrostatic fields near edges of electrodes and grids. The basic idea in the FDM is to cover the analysis region with grid points on a rectangular grid (some programs use a triangular mesh). The density of the mesh points can be varied according to the required accuracy. The electrode surfaces can be specified by a variety of line types (hyperboles, circles, ellipses etc.). The finite dif-
ference equations are obtained by a Taylor series expansion of the Laplace equation about the central mesh-point potential in which the first four (for a two-dimensional work-bench) or six (for a three-dimensional work-bench) peripheral mesh-point potentials are inserted. Terms higher than second order in the Taylor series expansion are neglected. This procedure is performed for each point of the mesh. The resulting set of finite difference equations is then solved by an algorithm called over-relaxation [63]. An important advantage of the FDM is that the potential values are obtained on a rectangular mesh. This permits a rapid and accurate evaluation of the electrostatic field components by numerical differentiation, and hence rapid and accurate ray-tracing is possible. The computed rays are accurate enough for direct extraction of the aberration coefficients. The computed image consists of the convolution of the geometrical and aberration spots and the effects of the possible aberrations can be found by convolution with a Gaussian or other relevant density distribution.

SIMION 7

SIMION 7 [64] is a software package for the simulation of charged particle optical systems. It has been used to design the electrostatic positron beam described in this thesis. This package allows a three-dimensional simulation of the optical elements, which in general may have different symmetries and positions in space. The entire optical system can be analyzed and viewed as well. Moreover, positron beams are not always paraxial. The electrostatic field distribution is analyzed with the 3D-FDM [65]. The design process follows a sequence of steps, which are described below:

- Creation of a virtual apparatus

  The different optical components (electrodes with different shapes, deflectors, quadrupoles, RF tuned devices, time-of-flight components etc.) are programmed. An editing program and debugger/compiler are used to develop, test and modify these programs (also called geometry files). Every geometry file represents one set of potential arrays - an 'instance' in the terminology of SIMION program. In a workspace it is allowed to have up to 200 different instances. In Figure 3.1 the simulation of an electrostatic mirror is presented, which is cut for inside view. The simulated optical system can be viewed in the real geometrical space frame and in a potential energy surface frame.

- Creation of virtual particles

  The particles can be generated via ASCII files (program segments) programmed with the HP RPN calculator language. Mass, charge, initial energy, angular and spatial distributions can be defined. The trajectories of the charged particles in three-dimensional space are obtained by numerical integration using the standard fourth order Runge-Kutta method. The coordinates
and the velocity (acceleration, energy, time-of-flight etc.) of the charged particles can be observed and recorded at each moment of their flight, as well as the gradients of the electrostatic field.

- Virtual detection and beam monitors

The position and size of the achieved beam can be viewed on a virtual target or a detector. It is shown in Figure 3.2. Changes in the trace space and the shape of the phase space can also be followed. Examples for calculated phase space diagrams are shown in Figures 3.3 and 3.4. They are derived using the optical element (electrostatic mirror) shown in Figure 3.1. In the given examples the

Figure 3.2: The coordinates of the particles on a virtual detector. The axis of beam propagation is x. The data can be exported for analysis by other software.
axis of beam propagation in front of the electrostatic mirror is $y$ and the beam can be represented with one diagram $(P_x, x)$ or $(P_z, z)$. At the exit of the mirror the axis of beam propagation is $x$ and the beam is then presented with the aid of two projections of the phase space $(P_y, y)$ and $(P_z, z)$.

**Figure 3.3:** The phase space diagrams $(P_x, x)$ and $(P_z, z)$ calculated at the entrance of the electrostatic mirror where the optical system has rotational symmetry.

**Figure 3.4:** The phase space diagrams $(P_y, y)$ and $(P_z, z)$ calculated at the exit of the electrostatic cylindrical mirror. The axis of beam propagation changes from $y$ to $x$. 
3.4 Lens performance and engineering design

The principal obstacle in the design of high-performance electrostatic lenses is caused by problems connected with electrical insulation and voltage breakdown. The field values that can be used in practice are between 10 and 20 kV/mm and depend on the choice of electrode material and on the surface preparation of the electrodes. As electrode materials, nonmagnetic (304 or 310) stainless steel, Ti, its alloys such as IMI TI-318, or Mo are preferred. Electrode edges must be rounded to avoid local enhancement of the fields. Good materials for insulators between the high-voltage supply line and the lens chamber are nonporous ceramics, glass and glass-ceramics, acryl-glass, and epoxy-glass. Insulators made of rexolite (cross-linked polystyrene) work well at 40 kV. One of the advantages of electrostatics is that the volume of the electrode does not contribute to the field distribution. Any metal can fulfill the requirements for producing an equipotential surface, although in practice the selection is much more restricted. Care must be taken in the choice of nuts, bolts and screws so that they can be annealed and are non-magnetic (materials like Cu-Be are preferred). All electrodes have to be matched with high accuracy and aligned on a common axis, and the electrostatic lens as a whole must be mechanically rigid so that individual electrodes do not move with respect to each other when the optical system is assembled, transferred or during bake-out. Misalignments and tilts of the electrodes nevertheless may occur. These introduce asymmetric fields and generate additional parasitic aberrations. Small misalignments and tilts produce additional weak deflection fields, whereas elliptical defects produce a quadrupole field. These can be calculated using the FDM. Elliptical defects are mostly caused by un-round bores. In addition we have to shield the system from external magnetic fields or compensate for them.
Chapter 4

A facility for positron re-moderation experiments

4.1 Introduction

The optical design, construction and performance of a facility for re-moderation experiments in the transmission mode will be presented in this chapter. The moderation efficiency as a function of the positron beam implantation energy (transmission measurements) and the energy spectrum of the emitted and thermalized positrons (retarding field measurements) will be studied for different materials. Of particular interest are thin foils with a thickness of about 100 nm made of materials with a negative work function for positrons. These are able to moderate in the transmission mode. The aim is to test the moderation capabilities of re-moderators, which possibly can be used in a brightness enhancement section, needed for the construction of a positron micro-probe. In some cases the candidates for re-moderators have a diameter size of only a few mm, therefore the positron beam used for such studies needs to be focused within the low-mm range. The investigation of the positron moderation properties of such materials requires a variable energy positron beam with well defined and controlled characteristics.

4.2 Three-dimensional modelling of the optical system

The electrostatic positron beam consists of a positron source, a positron gun, a cylindrical mirror to bend the beam over 90° which also removes non-moderated fast positrons from the beam, and transport and focusing lenses which guide and focus the beam onto the target [66]. The optical system has been simulated by trajectory calculations with program SIMION 7. An overview plot is shown in Figure 4.1.
Steering of the beam is provided by two sets of four cylindrical deflection plates installed at the entrance and the exit of the mirror. These are provided for the fine tuning of the beam position.

![Diagram](image)

**Figure 4.1:** Three-dimensional modelling of the optical system of the electrostatic positron beam for re-moderation experiments. The applied lens potentials are indicated. The positron trajectories are calculated with SIMION 7 [64]. For the scale of the picture see Figure 4.2.

**Positron gun**

The design of the positron gun (Figure 4.2) is similar to the modified Soa gun proposed by Karl Canter [67]. Our moderator has a radius of 3 mm. The Wehnelt

![Diagram](image)

**Figure 4.2:** Simulation of the positron gun.
cylinder is placed 2 mm from the moderator and has a diameter of 16 mm and a length of 10 mm. In our case a three-cylinder symmetric Einzel lens follows the Wernelt electrode. The Einzel lens begins 4 mm from the Wernelt cylinder and has a diameter of 26 mm. The gap between the electrodes is 4 mm and the length of the middle electrode is 24 mm. The anode tube is grounded and four deflection plates are introduced inside for fine tuning and steering of the positron beam. The positron trajectories, shown in Figure 4.2, have initial radial coordinates -3 mm, 0 mm and 3 mm and emission angles in the interval from -10 to 10 degrees. The positron gun produces a demagnified image at the entrance of the electrostatic mirror.

Mirror

The cylindrical mirror analyser consists of two concentric cylinders of each which half is cut away (Figure 4.3). The cylinders are electrically insulated and have a potential difference between them. Positrons enter the inner cylinder from the cutaway side from a point on the axis into the gap between the two cylinders. They are repelled by the field between the inner and outer cylinder. The axial distance $z$ travelled by a positron along the symmetry axis before it leaves the inner cylinder is given by

$$z = 2a \cos \theta \sqrt{\frac{\pi}{k}} \exp(k \sin^2 \theta) \text{erf}(\sqrt{k} \sin \theta),$$  \hspace{1cm} (4.1)

where $\theta$ is the injection angle (angle between the velocity of the positron and the

Figure 4.3: Schematic drawing of a cylindrical mirror electrostatic analyser.
symmetry axis). The parameter $k$ is defined as:

$$k = \frac{E_0}{V} \ln \frac{b}{a}$$

(4.2)

where $E_0$ is the kinetic energy of the positron in eV; $V$ is the potential difference between the two cylinders; and $a$ and $b$ are the cylinders radii. In order to ensure that the positrons do not hit the outer cylinder but exit the mirror, the following relation should be valid:

$$\sin^2 \theta < \frac{V}{E_0}.$$  

(4.3)

The energy of analysis and the energy resolution can be controlled by the voltages applied to the two cylinders, the angle of entry, and the size and position of the entrance and exit apertures. The energy resolution depends on the diameter $w$ of the exit aperture and on the quantity $D$ as:

$$\frac{\Delta E}{E} = \frac{w}{2D}$$

(4.4)

where $D$ is

$$D = E \frac{\partial z}{\partial E}.$$  

(4.5)

Focusing can be achieved for injection angles $\theta$ for which

$$\frac{\partial z}{\partial \theta} = 0.$$  

(4.6)

In our case positrons have injection angles of $45 \pm 1^\circ$ with respect to the symmetry axis of the two cylinders. The second aperture has a diameter of 10 mm, and is placed 50 mm away from the first entry aperture. The radius of the outer cylinder is 40 mm; that of the inner cylinder is 25 mm. For this geometry $\frac{\partial z}{\partial \theta}$ approaches zero for angles between 51 and 55 degrees. Therefore the mirror works slightly out of focus. This can be compensated partly by adjusting the beam at the entrance of the mirror. Other errors are introduced by the angular distribution of the positrons entering the mirror and by electric field penetration through the two apertures. These effects are taken into account in the 3D simulation of the mirror. The phase space diagrams calculated at the entrance and at the exit of the mirror are given in Figures 3.3 and 3.4 in Chapter 3. The potential difference between the cylinders for which all positrons with an energy of 3 keV exit the mirror was found to be 1.85 kV.

**Transport lens**

The moderated fraction of the positrons exiting the mirror can be directed into one of the three horizontal branches of the system. The left branch is designed for re-moderation experiments and continues with a second set of Einzel lens which is used.
4.2 Three-dimensional modelling of the optical system

To transport the beam. The potentials applied to the middle and outer electrodes are given in kV by

\[
V_{\text{middle}} = V_{\text{source}} - 1.55 \quad (4.7)
\]
\[
V_{\text{outer}} = V_{\text{source}} - 3 \quad (4.8)
\]

where \(V_{\text{source}}\) is the voltage applied to the source. The source and the moderator foil are kept at the same potential. This potential determines the beam energy. The beam is always transported with an energy of 3 keV. The entire system can be floated at high voltage. The target as well as the following re-moderation section are placed in a region kept at ground potential.

**Focusing lens**

The final lens will focus the beam from the floated to the grounded region. At a distance of 400 mm from the transport Einzel lens a focusing lens is placed. This is also a three-tube lens with the outer electrodes kept at the same voltage. The potentials applied to the middle and the outer electrodes are given in kV by:

\[
V_{\text{middle}} = V_{\text{source}} - 1.3 \quad (4.9)
\]
\[
V_{\text{outer}} = V_{\text{source}} - 3. \quad (4.10)
\]

In Figure 4.4 a simulation of the focusing lens is presented. It consists of three tubes with diameters 36 mm, 20 mm, and 10 mm, respectively, and lengths of 114 mm, 67 mm, and 50 mm, respectively. At this position the beam crosses from the

![Diagram](image)

**Figure 4.4:** The focusing lens with the simulated positron trajectories. The positron beam is focused at the target within a spot of 1 mm. This is the position of the first re-moderator of the transmission mode brightness enhancement section. Equipotential surfaces are shown as well.
high voltage to the grounded region. The three electrodes overlap each other with 22 and 20 mm respectively to ensure that the field between the lens electrodes is not influenced by the potential difference between the floated and the grounded vacuum chambers. An aperture of 4 mm diameter is placed 5 mm away from the last electrode and 2 mm in front of the target. It is kept at ground potential and is an element of the optical system of the following re-moderation section. The target is in an electric field free region.

Programming and simulation results

![Image](image-url)

**Figure 4.5:** Calculated beam size at the target when the lens potentials correspond to those given in Figure 4.1.

The three-dimensional simulation of the entire optical system was carried out using the SIMION 7 program. The electrodes were programmed as geometry files and inserted into the workbench as four independent instances. The calculated voltages are presented in Figure 4.1. The simulated positrons are emitted with an energy of 3 eV and a uniform angular distribution with an opening angle less than 20° and 0° beam angle. The positron emission is spatially simulated by a uniform distribution from a square area with sides of 6 mm. The initial positron parameters have been programmed as well. The result of the ray-tracing procedure run in SIMION 7 produces a final beam size at the target position of 1 mm diameter for the lens potentials given in Figure 4.1. The calculated beam image on the target is shown in Figure 4.5.
4.3 Apparatus

Vertical part

A technical drawing of the vertical part of the system is given in Figure 4.6. The

![Technical drawing of the vertical part of the electrostatic positron beam](image)

Figure 4.6: Technical drawing of the vertical part of the electrostatic positron beam (from Jørgensen [8]).

positron source $^{22}$Na (1.4 GBq on 21.01.1999) is encapsulated in a thick Ti foil. It was installed in the beam line in June 1999. It was calculated that the source
delivered $1.1 \times 10^9$ positrons per second at that time, taking into account the geometry, source self-absorption and the fraction of $\beta$-decay. The source is attached to an electrical insulated copper rod. Source and rod are placed on a linear motion drive, which is used to retract the source whenever the in situ annealing of the moderator foil is performed. As a moderator a 3.5 $\mu$m thick polycrystalline tungsten foil is used. The foil has a diameter of 6 mm. Annealing is done by resistive heating at 1200°C from 5 up to 10 minutes. In principle it is advisable to anneal the moderator after baking out the system in order to increase the moderation efficiency. The positron gun and the two sets of Einzel lenses with the four deflection plates on either side of the mirror are made of copper. They are gold plated in order to avoid charging effects of copper oxides present on the surfaces. The electrostatic cylindrical mirror is made of solid gold-plated copper. The mirror rests on a ball-bearing that allows it to rotate. In this way the beam can be switched between three available beam ports. In Figure 4.7 the beam line is shown under construction. The radioactive source and the moderator were not yet installed. At that time the front port was used for pressure monitoring.

The other two ports, at the left and the right, were planned for the construction of electrostatic positron beams for re-moderation and transmission experiments, Doppler-broadening and positron lifetime measurements. Manual vacuum valves are placed on both sides. This allows us to construct and modify the left and right hand branches of the beam system while keeping the source in vacuum. This prolongs the lifetime of the moderator foil. It also avoids the long evacuation time of this part of the facility due to the radiation shielding and the $\mu$-metal compensator for the earth magnetic field. The in-vacuum part of the radiation shielding consists of solid copper cylinders with grooves cut in them for better pumping. The vertical part of the system is covered entirely by $\mu$-metal to shield the system from magnetic fields. This part of the beam-line is electrically isolated and can be floated up to 30 keV. It rests on five ceramic insulators. The transport beam energy inside the UHV housing was chosen to be 3 keV. The source, Wehnelt, moderator foil, first Einzel lens and the mirror are connected to a resistance network fed by one power supply. The electric diagram is given in Figure 4.8. The power supply input is 3 kV. The source, denoted by S, and the moderator M are kept at that potential. The resistors were chosen after beam tuning for maximum intensity and were in agreement with the SIMION 7 simulation results shown earlier in this chapter. The four quarter-cylinder deflection plates are connected to separate power supplies.

The source region is pumped by two turbo molecular pumps that are electrically insulated from the rest of the set-up. After bake out the vertical part has a pressure of $10^{-8}$ mbar. The pressure can be measured by ion gauges at two positions: at the front port (in front of the mirror), and before the manual valve on the left back side. When the system is floated up to high voltage these pressure monitors are disconnected.
Figure 4.7: Photograph of the electrostatic positron beam, taken in June 1999, when the apparatus was being built at its present position in the new experiment hall. The source and moderator were not yet installed. The position of the source is denoted by S. The vertical part is separated from the two horizontal branches by vacuum valves (V). It is evacuated by two turbo pumps (P), which are electrically insulated from the system. The facility rests on five ceramic insulators (C), which permits floating up to 30 kV. The beam can be directed into one of the horizontal branches by rotating the mirror (M).

Horizontal left part

The drawing of the horizontal left part of the system is shown in Figure 4.9. The left branch is equipped inside with \( \mu \)-metal shielding. A ceramic insulator is inserted behind the bellows to separate floating from grounded regions. The bellows are needed to compensate for mechanical stresses and to protect the ceramic chamber from breaking or cracking. Inside the bellows a \( \mu \)-metal tube is fixed to the flange by three screws. This tube has a fixed position even if the bellows are exposed to distortion. The three screws have been included in the simulation with the SIMION 7 program, but no effect on the positron trajectories has been found. The presence of the bellows introduces difficulties with respect to the mechanical alignment of the optical system. The magnetic shielding continues in the ceramic insulator, where
Figure 4.8: Electrical diagram of the resistive network used to supply voltages to the optical elements of the vertical part of the facility. The resistances are given in MΩ. The power supply provides a voltage of 3 kV. The source S and the moderator M are kept at the same potential.

Figure 4.9: Technical drawing of the horizontal left branch of the facility. A and B indicate the positions where the beam intensity and size were measured, i.e. before and after the focusing lens, respectively.

the first electrode of the focusing lens is positioned. It is electrically connected to the floating region. The three tubes, which compose the focusing lens, are made of stainless steel. They have been annealed at 850°C for 1 hour to remove possible local magnetization. The electrodes are fixed mechanically to each other by alumina spacers. The outer electrodes of the focusing lens are connected to the floating region while the middle electrode is fed by a separate power supply. The aperture and the target are grounded. The left branch rests on two legs. These are positioned so as to align the various elements of the facility. The vacuum in this horizontal branch is maintained by a turbo-pump with a capacity of 150 liter per second. The pressure
is measured by an ion gauge mounted in the grounded region. The target can be inspected from outside through a glass window mounted on the six-tray vacuum piece. The rest of the beam line houses the detection system.

**Detection system**

For positron beam detection three options were available:

- A Ge-detector and a NaI-detector for beam intensity measurements
- A Micro-Channel Plate coupled to a phosphor screen, Charged Coupled Device (CCD) Camera and computer controlled imaging system for beam size estimation
- A Channeltron with retarding field analyser for beam intensity monitoring and re-moderation experiments

### 4.4 Performance

The beam performance was studied by means of a combination of detectors described above. The beam size and intensity profiles were monitored at two different positions of the beam line, indicated in Figure 4.9 as A and B. Position A is in front of the focusing lens while position B is at the position of the target (at the first re-moderation foil).

**Positron beam size and intensity at position A**

In Figure 4.10 a photograph of the facility before mounting of the focusing lens is shown. In this configuration the beam properties are observed at A. The intensity at a beam energy of 3 keV was first measured by a calibrated Ge-detector and was found to be $2.2 \times 10^4$ positrons per second. According to equation 1.1 (Chapter 1) the overall efficiency of the positron beam is estimated at $2 \times 10^{-5}$. In additional measurements set-ups with a channeltron and MCP were used. The channeltron was calibrated using the results obtained by the Ge-detector. Beam image taken with the MCP assembly at position A for a 3 keV beam is given in Figure 4.11. The image of the positron beam in front of the focusing lens has a non-circular shape. This is probably caused by the electric field penetration through the openings of the electrostatic mirror [66]. The spot shown in the Figure 4.11 is the smallest spot achieved by varying the voltage applied to the second Einzel lens (transport lens). Its size was determined to be 6 mm wide by 4 mm high.
Figure 4.10: Photograph of the set-up for measuring the beam properties at position A (see Figure 4.9). The lead shielding (Y) is mounted around the source-moderator area. The power supply line (P) feeds the elements from the optical system via resistance network (R). The channeltron, mounted on the outer flange of the target chamber (D), is used for beam intensity measurements. The left branch is supported by one aluminium leg (L).

Figure 4.11: Beam image at A for the 3 keV beam (in front of the focusing lens, see Figure 4.9).

Positron beam size and intensity at position B

The construction of the facility for observing the beam properties at position B is shown in Figure 4.12. The beam intensity was measured by the channeltron and is 96% of that measured at position A.

Beam image of a 3 keV beam is given in Figure 4.13. When the focusing lens is not used only 25% of the beam is transmitted through the lens and the aperture in front of the target. In this case the resulting beam image represents the last aperture
Figure 4.12: Photograph of the set-up for measuring the beam properties at position B (see Figure 4.9). The ceramic insulating tube (C) separates the electrically grounded part from the floating part of the facility. The bellows (B) are mounted to compensate for mechanical stress and distortion. The target chamber (T) contains the MCP with phosphor screen (for beam size measurement) on a linear drive motion (H), which allows the re-moderation foil under examination to be subsequently positioned on the beam-line. The left branch is pumped by one turbo pump (P). The mechanical support and alignment are achieved by two aluminium legs (L). The beam intensity can be controlled by a NaI $\gamma$-detector (D).

Figure 4.13: Beam image at B for the 3 keV beam (position of the target, see Figure 4.9).

in front of the MCP and its size equals the acceptance (see Figure 4.4). This image is shown in Figure 4.14 (a). The diameter of the aperture is known (4 mm) and we used it for beam size determination. The positron beam spot size at the target (at the
Figure 4.14: Images of the positron beam at the target position: (a) beam is not focused; the image represents the size of the aperture in front of the target, (b) image at 4 keV, (c) 5 keV, (d) 6 keV, (e) 7 keV, (f) 8 keV.

Figure 4.15: Count rate versus grid voltage.

first re-moderation foil) was found to have a diameter of 1 mm. The circular shape was achieved by fine tuning the potentials on the deflection plates. The focusing lens is necessary to reduce the beam size at the target [68]. The positron beam was imaged at the target position while the beam energy was varied. These images are given in figure 4.14 (b-f) and present the positron beam with an energy of 4 to 8 keV,
respectively. The beam size and position remain constant while the beam energy is changed. The beam image files (data files) were made by adding the recorded CCD camera frames. The frames collected at "background" conditions, when the vacuum valve of the left branch is closed and there are no positrons in the horizontal left side of the facility, form the "background" file. The final image file is produced by subtracting the "background" from the "beam + background" file. The data files thus obtained are processed by other software to visualize the image. The noise observed in some of the images originates from a defect in the CCD camera and could not be removed by the software used. The energy spread of the positron beam at the target position was measured using a channeltron with three grids in front of it. The outer two are kept at ground potential while a positive potential is applied on the middle one. When this potential reaches the value of the positron beam energy, positrons are retarded and the measured count rate decreases. The result of this experiment is shown in Figure 4.15. Its derivative represents the longitudinal energy distribution of the positrons at the target. The longitudinal energy is given by:

\[ E = E_0 \cos \theta \]  

(4.11)

where \( E_0 \) is the positron energy and \( \theta \) the angle with the beam axis. It is given in Figure 4.16. The energy spread at the target can be estimated from the FWHM of the peak, which is 0.12 keV at 3 keV.

### 4.5 Conclusion

The results of the three-dimensional modelling of the optical system of the variable energy positron beam using the SIMION 7 program have been shown. An additional focusing lens was added to reduce the beam size. The beam can be focused within
1 mm diameter on the target in a field-free region. The beam size and position are constant under variation of the beam energy. The potentials applied to the lenses are in agreement with those calculated with SIMION 7. The facility can be used for re-moderation experiments in the transmission mode. The beam system can easily be coupled to a brightness enhancement section.
Chapter 5

Re-moderation experiments

5.1 Introduction

The development of brightness enhancement positron beams with applications in positron micro-probe, positron re-emission microscopy and high-resolution low-energy positron diffraction requires the use of re-moderation [54]. Extensive studies of the moderation properties of different materials have been performed during the last decade. Some of the summarized results can be found in the literature [6]. Thin metallic foils are considered to be re-moderators in case re-moderation takes place in transmission mode. Preferred materials are those with a negative positron work-function. Tungsten foils were studied by Chen and co-workers [69]. The moderation efficiency of Ni foils with a thickness of 150 nm was measured by Schultz [70]. Brusa and co-workers [71] studied the moderation properties of thin Cu foils of different thicknesses. They also provide an overview of the maximum measured re-moderation efficiency of thin metallic foils and the positron implantation energy at which this efficiency was achieved as a function of the foil thickness. The thickness of the re-moderator should be in the order of the sum of the positron mean implantation depth and the diffusion length in the re-moderator [69]. In order to enhance the re-moderation yield van Veen proposed a system of a bi-metallic foil, where the internal potential step at the interface is used. It consists of a thin tungsten layer deposited on a layer of molybdenum. The measured re-moderation efficiency in transmission mode with such a bi-metallic foil is reported by Jørgensen [8]. The positron moderation efficiency depends on the positron diffusion length (defect structure) and the surface branching into free positrons (surface condition). Several attempts have been made to calculate the positron implantation profile for thin metal foils and thus to derive a theoretical model for the measured moderation efficiency as a function of the implantation energy [69, 8]. The standard Makhov function as well as its modifications fail, however, to give a quantitative model of positron moderation from surfaces of thin metal foils.
The brightness enhancement section in development in the Positron Centre Delft, uses triple re-moderation in transmission mode. The intensity of the positron beam for testing the re-moderation efficiency of the candidates for this section is $10^4$ $e^+/s$ (see Chapter 4). The intensity of the positron beam to be inserted in the re-moderation section is $4 \times 10^8$ $e^+/s$ and the final intensity at the target of the positron micro-probe to be constructed should be in the order of $10^5$ $e^+/s$, taking into account possible transport losses.

This chapter contains the results of the measurements of the re-moderation yield in transmission mode of two series of identically produced thin foils (W foils and W-Mo foils) by means of an electrostatic variable energy beam. The foil is kept in a field-free region. On this basis the best foils can be selected. This can contribute to the discussion whether the transmission or the reflection geometry of re-moderation is preferable in the brightness enhancement sections.

### 5.2 Experimental techniques

**Transmission and Retarding field measurements**

![Diagram](image)

*Figure 5.1: Schematic drawing of the experimental set-up. A channeltron with retarding field analyser is used for beam intensity measurements and re-moderation experiments.*

A schematic drawing of the experimental set-up for the transmission and retarding field measurements is shown in Figure 5.1. The detailed view on the detection configuration is presented in Figure 5.2. The positron beam is guided and focused at the position of the sample by a set of electrostatic lenses (see Chapter 4). When one intends to measure the energy spectra of the transmitted positrons it is necessary
to keep the sample in a field-free region. A channeltron is mounted 24 mm behind the sample. The cone of the channeltron has a diameter of 20 mm. The pulses from the output of the channeltron are fed into an amplifier, followed by a single-channel analyzer (SCA) and a counter. There are three copper grids between the sample and the channeltron. The middle grid serves as a retarding element. The outer two grids are placed to avoid the presence of stray electric fields that can influence the experiment at low energies. The three-grid retarding device may lead to a lower transmission efficiency. The foil holder consists of a ceramic plate with a hole of 10 mm and a thick 30 μm tungsten foil with a hole of 6 mm mounted on it. These are annealed prior to the measurements up to 800°C in a separate oven. The foils are mounted on a tungsten grid and placed between the ceramic holder and the thick tungsten foil. The latter is used to assure that only positrons transmitted through the foil will be counted. The foil and each of the grids have a separate electrical connection. The total beam intensity is measured through the holder, when no foils are mounted. The number of transmitted (moderated and fast) positrons can be measured directly with the channeltron. In order to separate the fast from the slow transmitted positrons a positive voltage is applied to the middle grid. When the applied voltage is higher than the energy of the moderated positrons, they will be retarded. Only the fast (non-moderated) positrons will then reach the channeltron. The fraction of slow positrons can be found as the difference between the two measured values, with and without applied retarding voltage. The energy spectrum of the moderated positrons can be calculated from the result of the retarding field measurement. By increasing the applied voltage on the middle grid, the measured count rate will decrease and finally saturate. The derivative of the number of transmitted positrons as a function of the grid bias is the energy spectrum of the emitted slow positrons. It is an important characteristic of the material studied. It reveals the
positron work function and possible epithermal fraction, which gives information about the surface conditions.

5.3 Experiments with Tungsten foils

Five single crystal W (100) foils with a thickness of 100 nm were studied as possible candidates for positron re-moderators. These were produced by J. Chevallier at the University of Aarhus, Denmark. The results for each foil are given below in the order of the measurements. The energy scale in the retarding field measurements is given by:

\[ E_+ = eV_{\text{grid}} + \phi^\text{Cu}_- - \phi^W_- \]  

(5.1)

where \( \phi^\text{Cu}_- \) is the electron work function of the grid material (Cu) and \( \phi^W_- \) is the electron work function of the surface of the studied foil. The retarding field measurements are performed with an energy of the incident positron beam of 5 keV.

Results for tungsten foil A

![Graph](image)

**Figure 5.3:** Retarding field measurement of positrons transmitted through foil A.

The retarding field measurement was performed with foil A as received. The result, shown with black dots in Figure 5.3, presents the ratio between the number of transmitted positrons and the total number of implanted positrons. Moderated positrons were not detected. The fraction of fast positrons transmitted through this foil is 0.75%. The foil was subjected to a Doppler-broadening measurement using the variable energy positron beam (VEP) [72]. The result is given in Figures 5.4 and 5.5, respectively, for the S and the W parameter. The diffusion length was found to
be $17 \pm 1.68 \text{ nm}$ by using the one-layer model in the fitting program VEPFIT [46]. The next step was to anneal the foil in a separate oven ($10^{-5}$ mbar) for 10 minutes up to $1100^\circ$C in order to remove oxygen from the surface and possible intrinsic defects. The Doppler-broadening measurement was repeated. The measured $S$ and $W$ parameters are compared with those before the annealing (Figures 5.4 and 5.5). The diffusion length after the annealing procedure was found to be $19 \pm 1.58 \text{ nm}$, in agreement with the modelling of the data before the annealing. Annealing causes a change in the defect state of the surface, which is reflected in the decrease of the $S$ parameter measured at the surface. The diffusion length is only little changed by the applied annealing procedure. The foil was transported in air to the experimental set-up and the retarding field measurement was repeated. The result is shown in Figure 5.3 with open symbols. The fraction of the transmitted fast positrons has increased three times after the annealing. This is due to the fact that the heating process has caused holes in the foil. Moderated positrons were not found. This result may be explained by the low diffusion length and/or the surface conditions of the foil. In order to find evidence of possible surface contaminants surface branching ratio measurements have been performed. The branching ratios derived depend on the incident positron beam energy. The large statistical uncertainty of the branching ratios even at low beam energies (1 - 2 keV) is due to the fact that the fraction of positrons reaching the surface is statistically small. Because of the fragility of the foil a second cycle of treatment could not be applied.

**Results for tungsten foil B**

Foil B has been subjected to retarding field measurements before and after a treatment procedure. Before the annealing procedure no moderated positrons were detected. The foil was annealed in a separate vacuum oven ($10^{-7}$ mbar) up to $1600^\circ$C for 10 minutes. After this it was transported in air for 5 minutes and installed in
Figure 5.6: Retarding field measurement of positrons transmitted through foil B. The derivative of the fit presents the energy distribution of the moderated positrons.

the experimental set-up. The result from the retarding field measurement is shown in Figure 5.6 by open circles. It is fitted with the following function

\[
y = a \left( 1 - \frac{1}{1 + \exp \left( -\frac{x - x_0}{b} \right)} \right) + c
\]

(5.2)

where \( c \) is the fraction of the transmitted fast positrons, \( a \) is the fraction of the emitted moderated positrons, \( x_0 \) and \( b \) are fitting parameters, \( x \) and \( y \) are respectively the grid bias and the transmitted fraction of positrons. A fit is found for \( x_0 = 3 \) and \( b = 0.25 \). The fraction of moderated positrons is measured to be 0.8% while the fraction of transmitted fast positrons is 1.1% (Figure 5.6). The derivative of this function is also drawn (broken line). It gives the energy distribution of the emitted moderated positrons. The negative positron work function for the surface studied is \(-2.88 \text{ eV}\). It is derived taking into account the difference in electron work-function of 0.12 eV between the tungsten surface and the copper grid.

Results for tungsten foil C

In an attempt to achieve a higher positron re-emission yield foil C has been treated in a different way. It is known that carbon is the dominant surface impurity for tungsten. This means that heating in oxygen and subsequent annealing may reduce the carbon and other surface contaminants. The applied procedure was as follows: when the vacuum pressure reached \(10^{-7} \text{ mbar}\) the foil was treated first by heating in oxygen \((10^{-5} \text{ mbar})\) at 1600°C for 10 minutes and then in vacuum \((10^{-8} \text{ mbar})\) at 2000°C for 3 minutes. The foil is then transported in air to the experimental set-up. The result of the retarding field measurement after the treatment is shown in Figure 5.7. The result is fitted with the function given in equation 5.2 with the following
5.3 Experiments with Tungsten foils

Figure 5.7: Retarding field measurement of positrons transmitted through foil C. The derivative of the fit presents the energy distribution of the moderated positrons.

fitting parameters: \( x_0 = 3.09 \) and \( b = 0.258 \). The measured slow positron fraction is 3.6\% while the fast positron fraction is 4.2\%. A work-function for positrons of \(-2.97\) eV is derived from this.

Results for tungsten foil D

A retarding field measurement was performed with foil D as received. The result is shown with open circles in Figure 5.8. The fit was done with the following parame-

Figure 5.8: Retarding field measurement of positrons transmitted through foil D before and after heating with a halogene lamp.
ters: \( x_0 = 3 \) and \( b = 0.25 \). The measured fraction of emitted slow positrons was 1%; the fraction of transmitted non-thermalized positrons was 0.6%. In order to heat the foil in situ without exposing it to air after the treatment the foil holder was modified. Its schematic drawing is shown in Figure 5.9. A halogène lamp was installed

![Schematic drawing of the experimental set-up](image)

**Figure 5.9:** Schematic drawing of the experimental set-up for in situ annealing of the re-moderator foil. The heating is performed with a halogène lamp.

![Photograph of the modified foil holder](image)

**Figure 5.10:** Photograph of the modified foil holder with the mounted halogène lamp. The channeltron is denoted by C, the three grids by G, the lamp for in situ annealing by L and the foil by F.

in front of the foil. Figure 5.10 shows a picture of the modified foil holder. The lamp
has a power of 250 W. The heating procedure was performed as follows: the vacuum pressure was $7 \times 10^{-8}$ mbar before the current and the voltage applied to the lamp were gradually increased. When a power of 86 W was reached the vacuum pressure was $10^{-5}$ mbar. This condition was maintained for one hour. The next retarding field measurement was performed at a vacuum pressure of $4 \times 10^{-8}$ mbar. The result is given by closed circles in Figure 5.8. It was fitted similar to the results for foils B and C. The fitting parameters $x_0$ and $b$ were 2.9 and 0.18, respectively. The fraction of slow positrons was 2.4%, i.e. increased almost by a factor of two as a result of the in situ annealing. The fraction of fast positrons was also increased slightly to 1.3%. The resulting positron work-functions before and after the treatment were $-2.78$ eV and $-2.88$ eV, respectively.

Results for tungsten foil E

Foil E was not subjected to any annealing procedure. The transmitted slow and fast positrons versus the incident beam energy were measured as the foil was received. These are given in Figure 5.11. The maximum fraction of emitted slow positrons was

![Graph](image)

**Figure 5.11:** Transmitted slow and fast positron fractions versus the positron beam energy.

measured with a 5 keV incident beam energy and was found to be 8%. The fraction of transmitted fast positrons increased gradually with the implantation energy.

Discussion

A summary of the treatment procedures applied, the measured moderation efficiency $\varepsilon$ and the positron work-function $\phi_+$ derived is given in Table 5.1. The results for the positron work-function are compared with experimentally found values for
monocrystalline tungsten published by Lynn and co-workers [6]. The five identically produced thin tungsten foils have different positron moderation properties.

**Table 5.1**: Summary of the applied treatments and experimental results for the moderation efficiency $\varepsilon$ and positron work-function $\phi_+$.  

<table>
<thead>
<tr>
<th>Foil</th>
<th>treatment</th>
<th>$\varepsilon$ (%)</th>
<th>$\phi_+$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>time (min.)</td>
<td>temperature (°C)</td>
<td>pressure (mbar)</td>
</tr>
<tr>
<td>A</td>
<td>10</td>
<td>1100</td>
<td>$10^{-6}$</td>
</tr>
<tr>
<td>B</td>
<td>10</td>
<td>1600</td>
<td>$10^{-7}$</td>
</tr>
<tr>
<td>C</td>
<td>10(3)</td>
<td>1600(2000)</td>
<td>$10^{-6}(10^{-8})$</td>
</tr>
<tr>
<td>D</td>
<td>60</td>
<td>300</td>
<td>$10^{-5}$</td>
</tr>
<tr>
<td>E</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$W(100)$ [6]</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$W(100) + C$ [6]</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

This could be due to the different non-ideal surface conditions as well as to the different defect structure manifesting itself in a low positron diffusion length. Although there are surface changes caused by the treatment applied to foil A, the positron diffusion length of around 19 nm is too small to allow the implanted and moderated positrons to diffuse to the surface. The carbon removal procedure applied to foil C is effective and the derived positron work-function has a value, which is in agreement with that found by Lynn et al [6] for a no-contaminated tungsten surface. The other foils B and D have a value of the positron work-function that is lower than for the other foils. A lowering of the work-function might be due to carbon contamination. Exposing the foil to air after such a treatment may have an influence on the surface condition. Although some of the applied annealing procedures helped to improve the moderation efficiency, the highest measured moderation efficiency of 8% was achieved with a non-treated foil. The cycling of the sample-cleaning procedures appeared not to be advisable. After a second round of treatment the foils were damaged. Their integrity was broken and their moderation properties degraded.
5.4 Experiments with Tungsten-Molybdenum foils

The moderation efficiency of five W-Mo foils was measured. These foils consist of a two-layer system. A tungsten (100) layer with a thickness of 10 nm is epitaxially grown on 100 nm Mo (100). Both materials have the bcc crystal structure with a lattice misfit lower than 1%. The Fermi levels of the two materials become equal due to the charge transfer across the junction. Therefore a dipole potential step is introduced at the interface. The size of the dipole step equals the difference between the electron chemical potentials of the two metals $\mu^W_-$ and $\mu^{Mo}_+$. There is a difference between the ground state positron energy in both metals. Thus the internal potential step also depends on the positron chemical potentials of the two metals $\mu^W_+$ and $\mu^{Mo}_+$, respectively. It is given by

$$\delta E^{W,Mo}_{W} = \mu^W_- + \mu^W_+ - \mu^{Mo}_- - \mu^{Mo}_+. \quad (5.3)$$

This equation can be re-written using the electron and positron work-functions for both surfaces.

$$\delta E^{W,Mo}_{W} = \phi^{Mo}_- + \phi^{Mo}_+ - \phi^W_- - \phi^W_+. \quad (5.4)$$

The positrons gain an energy equal to this internal potential step when they enter Mo from the W side. During thermalization, positrons are reflected from the interface between the two metals when they enter from the Mo side. The potential step has a theoretical value of 0.61 eV [5] and an experimental value of 0.64 eV [73].

The retarding field measurements were performed on the foils as received. Even one round of surface treatment destroys the moderation properties of these foils. The energy of the incident positron beam was 3.5 keV. The positrons were implanted from the W side.

Results for bi-metallic foil F

The result of the retarding field measurement on foil F is given in Figure 5.12. The result is fitted with the function described by equation 5.2. The fitting parameters are $b = 0.3$ and $x_0 = 2$. The fraction of slow re-emitted positrons is 0.18%; that of fast transmitted positrons is 0.7%. A negative work-function was derived, taking into account the difference between the electron work-functions of the grid material (Cu) and the Mo surface (see equation 5.1). The latter is 0.06 eV. The positron work-function for the Mo surface is found to be $-1.94$ eV. This value is lower than the one experimentally found for Mo (100)(-1.7 eV) [6], probably due to oxygen impurities. The theoretically calculated value by Boev and co-workers is $-2.65$ eV [74]. The energy spectrum of the slow positrons emitted from the Mo surface is shown by a broken line in Figure 5.12.
Figure 5.12: Retarding field measurement of positrons transmitted through foil F. The derivative of the fit presents the energy distribution of the moderated positrons.

Results for bi-metallic foil G

Figure 5.13: Retarding field measurement of positrons transmitted through foil G. The derivative of the fit presents the energy distribution of the moderated positrons.

The result of the retarding field measurement on foil G is shown in Figure 5.13. The fitting parameters are $b = 0.3$ and $x_0 = 1.7$. The fraction of transmitted fast positrons is 0.17% while the fraction of slow positrons emitted from the Mo surface is 0.08%. The positron work-function derived for this Mo surface is $-1.64$ eV.
Results for bi-metallic foils H, I and J

The fraction of slow positrons emitted from the Mo surface for foils H, I and J was measured versus the incident positron beam energy. The positron beam energy was varied from 1 to 12 keV. The results are shown in Figure 5.14. These foils have considerably higher moderation efficiencies than the previous two foils. Foil H has the maximum moderation efficiency of 9% at 3.5 keV. This foil has been subjected to an argon plasma treatment. The treatment consists of a foil exposure to a 0.5-watt argon plasma at 0.4 mbar argon pressure for 5 minutes, followed by annealing at 600°C for 10 minutes in a separate vessel with 10⁻⁷ mbar vacuum pressure. This

![Graph](image)

**Figure 5.14:** Transmitted slow positron fractions through foils H (before and after treatment), I and J versus the positron beam energy. The result for the I and J foils is also given for the reverse direction, when the positron beam is implanted from the Mo side.

procedure is used to reduce the surface contaminants. As a result the moderation efficiency decreases 3 times in comparison with the result before the treatment. This might be due to the increased oxygen on the surface, observed for the argon cleaning procedures. Foils I and J have not been subjected to any treatment. Their moderation efficiencies were measured to be 20% and 22% at 3.5 keV, respectively. The results achieved for the reverse direction when positrons are implanted from the Mo side and emitted from the W surface are presented as well. They demonstrate the effect of the potential step between the two metals. The trend which the moderation efficiency follows (see Figure 5.14) is similar to that measured by Jørgensen et al [75].
Discussion

A summary of the measured moderation efficiency for WMo foils and the derived positron work-function for the Mo surface is given in Table 5.2. The derived positron work-function for the Mo surface of two foils is compared with the theoretically calculated value and with the experimentally obtained value for a non-contaminated surface. Most likely the surfaces of foils F and G are contaminated. Although the foils were produced and stored in an identical manner they show different re-moderation properties. These differences may be due to the different defect concentrations at the interface between the W and Mo parts. The defect concentrations in the bulk of both foils may differ as well. No treatment (such as surface cleaning or defect annealing) could be applied to increase the re-moderation yield because of the fragility of this type of foil. A comparison of the highest reported moderation efficiency with thin metallic foils in transmission mode is presented in Table 5.3. The moderation efficiency achieved depends on the production method, the treatment applied for surface cleaning and the thickness of the foil. The highest values are found using bi-metallic foils.

Table 5.2: Summary of the measured moderation efficiency ε and the positron work-function φ+ for WMo foils.

<table>
<thead>
<tr>
<th>Foil</th>
<th>F</th>
<th>G</th>
<th>H</th>
<th>I</th>
<th>J</th>
<th>Mo (100) exp. [6]</th>
<th>Mo (100) th. [74]</th>
</tr>
</thead>
<tbody>
<tr>
<td>ε(%)</td>
<td>0.18</td>
<td>0.08</td>
<td>9</td>
<td>20</td>
<td>22</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>φ+ (eV)</td>
<td>-1.94</td>
<td>-1.64</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-1.7</td>
<td>-2.65</td>
</tr>
</tbody>
</table>

Table 5.3: Overview of the highest reported moderation efficiencies for thin metallic foils used in transmission mode.

<table>
<thead>
<tr>
<th>material</th>
<th>efficiency ε (%)</th>
<th>thickness (nm)</th>
<th>Implantation energy (keV)</th>
<th>reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>W</td>
<td>18</td>
<td>100</td>
<td>5</td>
<td>[69]</td>
</tr>
<tr>
<td>Ni</td>
<td>19</td>
<td>150</td>
<td>5</td>
<td>[70]</td>
</tr>
<tr>
<td>Cu</td>
<td>11.5</td>
<td>100</td>
<td>6.5</td>
<td>[71]</td>
</tr>
<tr>
<td>WMo</td>
<td>18</td>
<td>110</td>
<td>3.5</td>
<td>[8]</td>
</tr>
<tr>
<td>WMo</td>
<td>20</td>
<td>110</td>
<td>3.5</td>
<td>this work</td>
</tr>
<tr>
<td>WMo</td>
<td>22</td>
<td>110</td>
<td>3.5</td>
<td>this work</td>
</tr>
</tbody>
</table>
5.5 Conclusion

Measurements of the moderation efficiencies of ten thin foils were performed for the purpose of use in a brightness enhancement stage in a positron beam. The foils are divided in two groups: five W foils with a thickness of 100 nm and five WMo foils with a thickness of 110 nm. The foils of each group were identically produced, but they have different moderation properties. Various treatments which may have influence on the recovery of the moderation properties and the lifetime of the foil were applied to increase the re-moderation yield. For the first group of foils the carbon removal procedure was found to be successful, although the highest moderation efficiency was measured for the non-treated foil. After a second cycle of treatments the foils were damaged and lost their moderation properties. The two-layered WMo foils were also fragile. After exposure to annealing or to other surface cleaning treatments their integrity was ruined and the measured fraction of slow positrons considerably decreased. This means that these foils can not be subjected to a recovery procedure and once their moderation efficiency decreases they have to be renewed. Before being considered as successful re-moderators the stability of their moderation properties has to be evaluated. Although brightness enhancement in transmission is considered advantageous because of its comparatively simple optics, the re-moderation yields achieved are still orders less than those in the reflection mode. Typical backward yields are in the order of 40% [69].
Design options for a positron beam lifetime spectrometer

6.1 Introduction

Positron annihilation spectroscopy is a fruitful method to study microscopic properties in condensed matter. Positron lifetime measurements are particularly valuable because they allow, in principle, the quantitative identification of various structural defects that are simultaneously present [76]. The positron lifetime in a solid is measured as the time interval between the entry of the positron into the solid and its annihilation with an electron. The product of the annihilation is $\gamma$ radiation, which is detected as a function of time. The moment of the positron entry into a solid is more difficult to observe. Various techniques have been developed to trigger a time counter. The instruments for measuring the positron lifetime can be divided according to the method used to start the clock:

- $\gamma\gamma$ coincidence method, applied in conventional set-up's
  
  In conventional set-up’s ($\gamma\gamma$ coincidence method) the start-signal for the measurement of the positron lifetime is given by the prompt $\gamma$ quantum, which is emitted almost simultaneously with the positron by the radioactive source $^{22}$Na. Instruments based on this type of triggering have a time resolution of about 250 ps.

- $\beta^+\gamma$ coincidence method, using MeV beams
  
  In the $\beta^+\gamma$ coincidence method the start-signal is generated by passing a MeV positron beam through a scintillator prior to the implantation in the sample. Positron lifetime spectrometers that make use of this method have a reduced measuring time and the ability to measure the low intensity long-life components in the lifetime spectra.
• pulsed beams, where the pulse sets the clock

When lifetime spectra need to be measured in a depth-profiling manner, a variable energy positron beam is needed. For that purpose the positron beam is pulsed using a radio-frequency electrical field. Available pulsed beams [23, 22] have a pulse width of 150 ps and a pulse repetition rate of $10^5$ Hz, providing a time resolution of 200 ps.

• $\beta^-\gamma$ coincidence method, using secondary emitted electrons

Another approach to construct a beam-based positron lifetime spectrometer avoiding the laborious beam chopper and bunch-systems is to use the secondary emission from the surface of the target as a start-signal. The time resolution of a set-up employing this technique is around 600 ps [50]. The relatively large time resolution is due to the energy and angular distribution of the backscattered electrons.

A set-up for measuring the positron lifetime is described in this chapter. The use of an electrostatic beam offers better possibilities for detection of the secondary electrons than a magnetically guided beam. It is designed in two versions. The first version (transmission design) is characterized by the use of a thin carbon foil installed in front of the target, which serves as a secondary electron emitter. This emission is used to provide the start-signal for the positron lifetime measurement. The annihilation radiation gives the stop-signal. In the second version (backscattering design) the target itself is used to generate the backward emitted electrons due to the incident positron beam. The position of the target in both designs is fixed. The modelling of the electrostatic optical system as well as the engineering design for both versions are given below in detail.

6.2 Transmission design

A schematic drawing presenting the operating principle of the facility in the first version is given in Figure 6.1. The positron beam is transported and focused on a thin foil. This foil is able to emit secondary electrons due to the impact of the positrons transmitted through it. The foil is mounted on a movable holder and tilted under 45° with respect to the beam axis. The secondary electrons emitted backwards are detected by a micro-channel plate (MCP) with its anode assembly positioned normal to the foil surface on the side where the positrons enter the foil. The output pulses of the MCP are fed into a time-to-amplitude converter (TAC) giving the start signal for the positron lifetime measurement. Then the transmitted positrons are focused on the target, where they annihilate. The gammas are detected by a BaF$_2$ detector providing the stop-signal of the TAC.
6.2 Transmission design

![Figure 6.1: Schematic view of a positron beam lifetime spectrometer - Transmission design. The positron beam is transmitted through a carbon foil. The secondary electron emission in the backward direction is used to generate the start-signal. The annihilation gammas give the stop-signal.](image)

6.2.1 Positron optics I

The electrostatic optical system is designed in two parts: before (positron optics I) and after the foil (positron optics II), as far as the positron beam transmitted through the foil has changed properties. The 3D simulation of the lens system from the first part including the carbon foil is presented in Figure 6.2. By rotating the electrostatic mirror, the positron beam is directed into the right branch of the facility.

![Figure 6.2: Three-dimensional modelling of the optical system up to the carbon foil.](image)
(see Chapter 4), where it is transported and focused on the foil by two identical Einzel lenses. The source and the moderator are kept at 5 keV, the Wehnelt electrode at 4.8 kV. The outer electrodes of the vertical Einzel lens are at 3.77 kV, while the middle electrode is at 4.41 kV. The electrostatic mirror is kept at 3.85 kV. The horizontal Einzel lens (lens 1) has its outer electrodes at 2 kV and the middle electrode at 3.3 kV. It is mounted at a distance 112 mm away from the mirror. The lens has a diameter of 26 mm, a length of the middle electrode of 24 mm and a gap of 4 mm. The part of the set-up that can be floated up to 30 kV ends behind this lens. The following focusing lens (lens 2) placed 60 mm in front of the foil and 370 mm behind lens 1, belongs to the grounded part of the set-up. Its outer electrodes are at ground potential and the middle electrode is at 2.5 kV. The foil is kept at −2 kV, while the front of the MCP is kept at −1.7 kV in order to ensure optimal detection of the secondary emitted electrons. The results from the simulation of the positron trajectories are given in Figure 6.3, where the trace space diagrams of the positron beam at the carbon foil are shown. In a cartesian coordinate system the axis of beam propagation is \( X \), the two orthogonal directions are \( Y \) and \( Z \), the angles \( \gamma' \) and \( \varphi' \) are given with respect to the beam axis (see Chapter 3). Using the potentials given in Figure 6.2 the positron beam with an energy of 7 keV can be focused within a 1 mm spot at the foil. The angles under which the positrons enter the foil have a spread of ±2 degrees. In case the energy of the positron beam needs to be re-tuned, keeping the beam diameter at the foil the same, the operating regime of the lenses from the vertical part of the facility should follow the relations given in Chapter 4. The voltages on the Einzel lenses from the horizontal part obey the following relations (in kilovolts).
For lens 1:

\[ V_{\text{middle}} = V_{\text{source}} - 1.7, \quad (6.1) \]
\[ V_{\text{outer}} = V_{\text{source}} - 3. \quad (6.2) \]

For lens 2:

\[ \frac{V_{\text{middle}}}{V_{\text{source}}} = 0.5, \quad (6.3) \]
\[ V_{\text{outer}} = 0, \quad (6.4) \]

where \( V_{\text{source}} \) is the potential applied to the source of the positron beam.

### 6.2.2 Electron optics

![Simulation of the trajectories of the secondary emitted electrons from the carbon foil up to the MCP presented in the frame of the potential energy surface. The distance between the foil and the MCP is 40 mm. For scale see Figure 6.5.](image)

The simulation of the trajectories of the secondary emitted electrons is performed using the SIMION 7 program. It is shown in Figure 6.4 in the frame of the potential energy surface. The time-of-flight (TOF) of the electrons and its distribution are calculated, supposing that the foil is kept at \(-2\) kV, while the front plate of the MCP is kept at \(-1.7\) kV. The secondary emitted electrons are assumed to have an average energy of 20 eV. The TOF is calculated to have an average value of 2.165 ns, while its total spread is 52 ps. The total spread of the TOF is defined as the interval between the arrival of the slowest and the fastest electron at the MCP. The distance between the foil and the detector is chosen to be 40 mm. The technical drawing of the configuration in which the elements of the electron optics are mounted in the beam-line is shown in Figure 6.5. A picture of the linear motion drive with the MCP and foil holder is shown in Figure 6.6. The engineering design allows the foil and MCP assembly to be fully retracted from the beam-line.
Figure 6.5: Technical drawing of the section of the beam-line in which the MCP (B) and the carbon foil holder (A) are mounted under 45 degrees with respect to the beam axis. Secondary emitted electrons are detected in the reflection geometry. The linear motion drive allows fine positioning of the carbon foil on the beam axis.

Figure 6.6: Photograph of the Micro-channel plate device for detecting the emission of secondary electrons, which give the start signal for the positron lifetime spectrometer. The carbon foil, denoted by A, is mounted on a holder. The MCP is denoted by B. Both are mounted on a linear motion drive.

6.2.3 Positron optics II

The energy of the positron beam passing through the foil can be chosen in a compromise between:

- number of generated electrons
- quality of the transmitted positron beam (in terms of intensity, monochromaticity, beam divergence)
The number of generated secondary electrons from the carbon foil is proportional to the inverse of the kinetic energy of the incoming beam [77], [78], [79]. Positrons undergo inelastic and elastic scattering processes while being transmitted through the foil. Monte Carlo simulations have been performed for a set of selected energies of the incoming beam to calculate the fraction, energy and angular distributions of the transmitted positrons. The methodology used is described in [80].

Monte Carlo simulations

The results for the calculated fraction of positrons transmitted within a given angular interval, as well as the average energy loss, due to the inelastic scattering of the positrons with the medium of the foil are shown in Table 6.1 as a function of the incident positron beam energy. The interactions of the positrons with the atoms of the carbon foil reduce the quality of the positron beam. Beam divergence, monochromaticity and beam intensity are changed. The transmitted fraction of positrons increases with the energy of the incoming beam. However, the averaged energy loss decreases with increasing positron beam energy. The secondary electron emission yield therefore decreases. For the case of a 7 keV positron beam the calculated angular distribution is presented in Figure 6.7. The peak in the intensity at 45° is due to the non-scattered positrons passing directly through the foil. The angles are given with respect to the normal to the foil surface. At that energy 90% of the beam is transmitted within an angular interval of 15°.

Table 6.1: Results from the Monte Carlo simulations. Calculated fraction of transmitted positrons through a 25 nm thin carbon foil and average energy loss for incident positron beam energies varying from 1 to 7 keV.

<table>
<thead>
<tr>
<th>positron energy (keV)</th>
<th>fraction within ΔΩ (%)</th>
<th>average energy loss (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ΔΩ = 10°</td>
<td>ΔΩ = 15°</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>11</td>
</tr>
<tr>
<td>1.5</td>
<td>7</td>
<td>15</td>
</tr>
<tr>
<td>2</td>
<td>11</td>
<td>22</td>
</tr>
<tr>
<td>3</td>
<td>23</td>
<td>41</td>
</tr>
<tr>
<td>5.5</td>
<td>49</td>
<td>71</td>
</tr>
<tr>
<td>7</td>
<td>81</td>
<td>90</td>
</tr>
</tbody>
</table>
Figure 6.7: Angular distribution of positrons with an energy of 7 keV transmitted through a 25 nm thin carbon foil. It is supposed that the positrons enter the foil under 45° with respect to the surface normal.

The average energy loss is calculated to be 1.5% of the initial value. These data determine the optical design of the lens system between the carbon foil and the target, because an angular spread of 15° can be accepted in the optical system that follows the foil.

SIMION 7 simulations

An earlier design of the optical system between the carbon foil and the target can be found in [81]. An improved solution is given in Figure 6.8. It consists of nine electrodes. The first electrode behind the foil has a conical shape with a grid mounted on it. It is kept at the same potential as the carbon foil, namely −2 kV. The second electrode is partly conically shaped and its potential is fixed at 4.6 kV. The potential difference between the first two electrodes is used to minimize the divergence of the positron beam. The beam is subsequently transported by two Einzel lenses, the electrodes of which overlap each other. This is done to prevent positrons "seeing" the potential difference with the grounded beam-line. Finally the beam is focused a by two-tube lens ending with an aperture at the target. The potentials of all electrodes are fixed and are shown in Figure 6.8. The potential applied to the target is variable and determines the implantation energy of the positron beam. Positrons are simulated with the following initial parameters: an energy of 7 keV, an angular distribution, as shown in Figure 6.7, and a random spatial distribution from an
Figure 6.8: Optical design of the system between the carbon foil and the target. The distance between the foil and the target is 423 mm. The lens potentials are indicated.

area of 2 mm. The calculated potentials at the target, the corresponding spot size and the spread in the time-of-flight of the positrons from the foil to the target are listed in Table 6.2. The spot size of the positron beam changes from 8 mm to 3.6 mm when the implantation energy is varied from 1 keV to 25 keV. Between the last electrode and the target the positron beam is decelerated for beam energies from 1 keV to 5 keV and accelerated for the other beam energies. This means that only homogeneous samples with a minimum size of 8 mm can be studied with this

<table>
<thead>
<tr>
<th>$E_{\text{impl}}$ (keV)</th>
<th>Voltage on the target (kV)</th>
<th>$\Delta$TOF (ps)</th>
<th>beam size (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4</td>
<td>207</td>
<td>8</td>
</tr>
<tr>
<td>2</td>
<td>3</td>
<td>209</td>
<td>7.2</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>186</td>
<td>6.6</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>203</td>
<td>6.2</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
<td>196</td>
<td>6</td>
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<td>6</td>
<td>$-1$</td>
<td>194</td>
<td>5.8</td>
</tr>
<tr>
<td>7</td>
<td>$-2$</td>
<td>188</td>
<td>5.6</td>
</tr>
<tr>
<td>8</td>
<td>$-3$</td>
<td>190</td>
<td>5.2</td>
</tr>
<tr>
<td>9</td>
<td>$-4$</td>
<td>183</td>
<td>5</td>
</tr>
<tr>
<td>10</td>
<td>$-5$</td>
<td>170</td>
<td>5</td>
</tr>
<tr>
<td>15</td>
<td>$-10$</td>
<td>180</td>
<td>4.4</td>
</tr>
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<td>20</td>
<td>$-15$</td>
<td>175</td>
<td>4</td>
</tr>
<tr>
<td>25</td>
<td>$-20$</td>
<td>170</td>
<td>3.6</td>
</tr>
</tbody>
</table>
instrument. The time resolution of the apparatus is determined by the spread in the
time-of-flight of the electrons from the emitter to the MCP and the spread in the
time-of-flight of the positrons from the carbon foil to the target. The time-of-flight
distributions have been calculated for the electrons (giving the start-signal) and the
positrons. Positrons have a broader time-of-flight distribution in comparison with
the electrons. The time spread of the positrons is approximately $200 \pm 10$ ps. The
contribution of the electronics is in the order of $250$ ps. The total time resolution of
the facility is estimated to be around $320$ ps.

6.2.4 Apparatus

![Figure 6.9: Technical drawing of the lifetime beam apparatus in transmission design.](image)

The technical drawing of the apparatus (horizontal branch) in the transmission
design is presented in Figure 6.9. The two Einzel lenses, which transport and fo-
cus the beam at the carbon foil, are indicated. The separation of the floated and
grounded parts of the set-up is done by a ceramic tube. The bellows are included to
compensate for mechanical stress and distortion. The vacuum valve separates the
vertical from the horizontal branches of the instrument. The position of the carbon
foil and the mounting of the nine-electrode lens system for focusing the positron
beam on the target are shown as well.

6.3 Backscattering design

In the second version of the design of the positron beam lifetime spectrometer the
target itself is used as an emitter of secondary electrons as shown in Figure 6.10. The
Figure 6.10: Schematic view of the operating principle of a positron beam lifetime spectrometer - Backscattering design. The positron beam is transported through a MCP with a central hole. The secondary electron emission in backward geometry is used for start-signal. The annihilation gammas give the stop-signal.

The positron beam is focused on the target, passing through the central hole of the MCP, which is mounted in front of the target. The secondary electrons are detected by the MCP, which triggers the TAC (time-to-amplitude convertor) with the start-signal for measuring the positron lifetime. In this case the materials to be investigated by this set-up must be good electron emitters. In order to build this apparatus the same beam-line can be used after the carbon foil assembly is retracted from its position on the axis of the beam.

6.3.1 Positron optics

The three-dimensional simulation of the optical system, which transports and focuses the positron beam on the target, is shown in Figure 6.11.
Three identical Einzel lenses are used. The first two lenses are placed as in the transmission design; the third one is mounted at a distance of 185 mm away from the second Einzel lens, while the distance from the last lens to the target is 83 mm. The implantation energy is varied by changing the potential on the source, keeping the potential on the target fixed. The lens potentials are derived as follows. The potentials of the lenses in the vertical part of the set-up are given in Chapter 4. Lens 1 from the horizontal branch works as in the transmission design. The potential on lens 2 is kept fixed at $-1.1$ kV. The applied voltage on lens 3 is given in kilovolts by

$$ V_{\text{middle}} = \frac{V_{\text{source}}}{1.92} + 0.2, $$

(6.5)

where $V_{\text{source}}$ is the voltage applied to the source of the positron beam. The outer electrodes of lens 3 are at ground potential. The beam spot at the target is calculated using the operational regimes for the lenses given above. It is found that the overall spot has a diameter of 3 mm. The total demagnification is a factor of two for a diameter of the source-moderator assembly of 6 mm. The intensity of the positron beam is measured at the position of the target after it has been transmitted through a 5 mm hole. The experimentally found lens potentials for lens 3 that give a $95 \pm 5\%$ transmission of the beam are compared with the calculated ones. The result from the comparison between simulation and experiment is shown in Figure 6.12. It is clear that theory and experiment agree rather well.

![Figure 6.12: Comparison of the calculated potential for lens 3 using the optical design given in Figure 6.11 with the experimentally found values. In this case the earth magnetic field is compensated by six orthogonal coils (see Figures 6.15 and 6.16).](image)
6.3.2 Electron optics

The optical design of the system between the target and the MCP aims at optimizing the collected number of secondary electrons, which are emitted by the target after the impact of the positron beam. The optical design is shown in Figure 6.13. The secondary electrons are simulated to be emitted from a spot of 6 mm with a uniform angular distribution within ±90° and an energy between 1 and 150 eV. Using the potential difference between the front of the MCP, the target (T) and the cylindrical electrode (E) all electrons are collected by the effective area of the MCP except those emitted within 0 – 15° with respect to the surface normal, which escape through the central hole of the MCP. The calculated potential difference between the front

![Figure 6.13: Simulation of the electron optical system between the target and the MCP. The trajectories of the secondary electrons are plotted together with the equipotential surfaces. The target is denoted by T and the cylindrical electrode by E. The applied potentials are given in Figure 6.14.]

of the MCP and the target is 300 V and between the front of the MCP and the electrode is 200 V. These relations are expressed in volts as follows:

\[ V_{MCP} = V_{\text{target}} + 300, \]  
(6.6)
\[ V_{MCP} = V_{electrode} + 200. \]  \hfill (6.7)

The electron trajectories are presented in the frame of the potential energy surface in Figure 6.14. They are accelerated on their way to the MCP. The spread in the time-of-flight of the electrons from the target to the MCP determines the time resolution of the positron lifetime spectrometer. This is due to the energy and angular distributions of the electrons. The calculated total spread is 191 ps. The backscattered positrons have also been simulated. Backscattered positrons with an energy of 30 keV will arrive at the MCP after 200 ps, while positrons with 2 keV energy will arrive after 1 ns. For comparison the fastest electrons (150 eV) arrive at the MCP after 2.9 ns. The presence of the backscattered positrons influences the accuracy of the generation of the start-signal.

Figure 6.14: The electron trajectories are shown in the frame of the potential energy surface. The target is kept at $-2.5$ kV, the electrode $E$ at $-2.4$ kV and the front plate of the MCP at $-2.2$ kV. For scale see Figure 6.13.

6.3.3 Apparatus

A technical drawing of the instrument in the backscattering design is shown in Figure 6.15. A new focusing lens is mounted in the target chamber. The elements of the electron optics are installed as shown. The horizontal branch of the facility is evacuated by a turbo- and a rotary pump, keeping a vacuum pressure of around $10^{-8}$ mbar. The $\mu$-metal shielding is placed inside the beam-line up to the vacuum valve. The earth magnetic field is compensated by six orthogonal magnetic coils. Compensation is achieved with a current of 2.08 A through the horizontal pair of coils. In Figure 6.16 a picture of the apparatus is shown. The target chamber is denoted by A. The 3D frame with the magnetic coils is denoted by B. The ceramic tube (C) separates floating from grounded parts of the system. The bellows are mounted immediately behind the ceramics in order to protect it from distortion. The vertical part of the apparatus (D) is surrounded by a metal cage to protect from electrical shocks.
Figure 6.15: Technical drawing of the apparatus in the backscattering design.

Figure 6.16: Photograph of the positron lifetime spectrometer based on an electrostatic variable energy beam. A is the target chamber, B shows the magnetic coils for earth magnetic field compensation and C denotes the ceramic tube, which separates the floated from the grounded regions. D is the vertical part of the facility, that is surrounded by a metal cage.
6.4 Detection system and timing electronics

The diagram of the detection system is shown in Figure 6.17. The 511 keV annihilation gammas are detected by a BaF$_2$ crystal coupled to a Photo Multiplier Tube (PMT) with built-in Constant Fraction Discriminator (CFD). This detection system produces negative output pulses with a pulse width of approximately 5 ns. The lower

![Diagram of the detection system and timing electronics.](image)

**Figure 6.17:** Diagram of the detection system and timing electronics. Both detectors are indicated. A constant-fraction-discriminator (CFD) triggers for any pulse height at the optimum fraction of the pulse height. A time-to-amplitude-converter (TAC) converts small time intervals to pulse amplitudes. Its output is fed into an analog-to-digital converter (ADC). A micro-channel-analyzer (MCA) and personal computer (PC) are used to sort and display the measured spectrum.

level (LL) and walk adjust (WA) potentiometers of the CFD are adjusted to obtain an optimal count to background ratio and best timing definition, respectively.

The secondary electrons generated at the target surface when it is hit by a positron are detected by a Micro Channel Plate assembly. The front of the first plate (1, see Figure 6.17) is put at $-2.2$ kV. By means of a simple resistor network the back of the second plate is kept at $-100$ V. The inner surfaces of the two plates are internally connected. The anode is kept at ground potential and the pulses are fed into an amplifier through a fast, ring-shaped transformer. The output pulses of the amplifier are typically 10 ns wide with an amplitude of 100 mV. For a good
6.5 Conclusion

A set-up for positron lifetime measurements based on a variable energy positron beam has been designed in two versions. In the first version the positron beam spot at the target varies between 8 and 3.6 mm when the implantation energy is changed from 1 to 30 keV. The spread in time-of-flight of the electrons and positrons to the detectors that feed the Time-To-Amplitude Convertor (TAC), caused by the angular and energy spread, determines the time resolution. The total time resolution was calculated to be around 320 ps, taking into account the contribution of the electronics as well. In the second version the positron beam is focused on the target within a spot of 3 mm for the whole range of implantation energies. The time resolution is determined by the spread in the time-of-flight of the electrons from the target to the MCP. The total time resolution in this case is approximately 315 ps. The advantage of the transmission design is that the lens potentials are fixed which allows full automation of the electrical system. The measuring time, however, will be longer in comparison with the backscattering design for which there are no intensity losses in connection with the triggering of the start-signal. A disadvantage of the second design can be the presence of backscattered positrons. The set-up in both its versions can be used for studies of porosity in ceramics, polymer coatings and other materials with long lifetime components.
Chapter 7

A facility for Doppler-broadening measurements in the low-mm range

7.1 Introduction

The Doppler-broadening technique with applications in material science has been developed and improved in the last decade [16, 6]. At the Positron Center Delft the variable energy positron beam for Doppler-broadening studies (VEP) has been in operation since 1988. It has been used for the investigation of a wide range of materials: semiconductors, polymers and layered structures. This facility has a magnetic positron beam transport. The beam diameter of the VEP is between 8 and 10 mm [72]. The beam spot at the target is subjected to movement and broadening when the positron energy is changed, which causes oscillations in the count rate but also introduces fluctuations in the Doppler-broadening parameters, especially in the case of small samples. Most of the defect structures studied with the Doppler-broadening technique are produced by keV ion implantation or other types of low energy irradiation, e.g. sputtering and deposition, often followed by a thermal treatment. The implanted spot usually has the size of a few mm, while the size of the sample is in the cm range. When one aims studying such samples one needs a positron beam of a size comparable to the size of the interesting area. The position and size of such a beam should not change while the beam energy is varied. These requirements led us to design a new variable energy positron beam based on an electrostatic optical system. The left branch of the facility described in Chapter 4 has been modified for Doppler-broadening experiments. The details of the optical design, the apparatus and the beam performance are presented in this chapter.
7.2 Three-dimensional modelling of the optical system

The three-dimensional model of the optical system of the apparatus is given in Figure 7.1. The vertical part is described in chapter 4. The optics of the left horizontal branch consists of two lenses: an Einzel lens for beam transport and a two-tube lens for beam focusing. The two-tube lens is positioned 404 mm from the transport lens. The target is kept at ground potential. The instrument can be floated up to 30 kV except for the target chamber which is grounded. The implantation energy is determined by the potential difference between the source and the target. The voltages of the lenses of the vertical part and the transport lens of the horizontal part are given in Figure 4.1 in Chapter 4. The first tube of the focusing lens is attached to the floating region. This means that it is kept at the potential applied to the floating region. The behaviour of the focusing two-tube lens is simulated using a three-dimensional model taking into account the walls of the grounded target chamber. The two dimensional projection of the focusing lens and the positron trajectories are shown in Figure 7.2.

![Diagram showing three-dimensional modelling of the optical system](image)

**Figure 7.1:** Three-dimensional modelling of the optical system of an electrostatic positron beam for Doppler-broadening measurements.

Focusing lens

The combination of two tubes separated by a small gap acts as a converging lens. The length of the first tube is 188 mm, its diameter 36 mm. The gap between the two tubes is 10 mm. The second tube is 61 mm long and has a diameter of 46 mm.
It ends in an aperture with a diameter of 24 mm. The grounded target is placed at a distance of 10 mm from the aperture. Positron trajectories were simulated for a number of beam energies. The input data for the initial coordinates of the positrons for 3D simulation are generated by a program using SIMION 7. The simulated positrons are emitted and an energy of 3 eV with a uniform angular distribution within a 20° cone, the axis of which is perpendicular to the moderator surface. The positrons are emitted with a uniform distribution from an area with a diameter of 6 mm.

![Figure 7.2: The two-dimensional projection of the focusing lens. It consists of two tubes. The second tube ends in an aperture. The two-tube lens acts as a converging lens. The positron trajectories and equipotential surfaces are shown. (HV = 10 kV, potential at the first tube \( V_{\text{tube}_1} = 10 \) kV, potential at the second tube \( V_{\text{tube}_2} = 12.5 \) kV.)](image)

The spot size at the target and the maximum angle of convergence were calculated as a function of the potential on the second tube. The results are given in Figure 7.3 for a number of beam energies between 1 and 30 keV. The beam size, indicated by black dots and solid curves (Figure 7.3), has two minima for all calculated cases. The one at the lower voltage is caused by the effect of the two-tube lens and gives a spot size of 0.5 mm. In this case the beam is focused on the target using "two-tube lens (TTL)" focusing. The voltages (in kV) applied to the two electrodes are as follows:

\[
V_{\text{tube}_1} = V_{\text{source}} - 3, \tag{7.1}
\]

\[
V_{\text{tube}_2} = V_{\text{source}} - 19, \tag{7.2}
\]

where \( V_{\text{source}} \) is the potential applied to the source of the positron beam. The other minimum (which appears at a higher voltage) is due to the effect of the potential difference distribution between the aperture, the target and the grounded chamber and gives a spot size of 0.2 mm. This focusing we call "aperture" focusing. The
Figure 7.3: The spot size and the maximum converging angle for number of beam energies. (a) at 3 keV, (b) at 5 keV, (c) at 10 keV, (d) at 16 keV, (e) at 20 keV and (f) at 30 keV.

"aperture" focusing is applied when:

\[ V_{\text{tube}_1} = V_{\text{source}} - 3, \]  
\[ V_{\text{tube}_2} = V_{\text{source}} - 0.5. \]  

(7.3)  
(7.4)

Using the two parameters (beam size and converging angles at the target) we can find the potentials at which the beam emittance (the product of the beam size and the angles which the positron trajectories form with the beam axis) has a minimum.
The beam emittance has its minimum when "two-tube lens" focusing is used, while the smallest spot size (0.2 mm) is achieved with the "aperture" focusing.

The operational regime of the focusing lens should be chosen taking into account two criteria: minimum beam emittance to ensure high-quality beam performance and working in the low-voltage range to avoid electrical breakdowns and discharges. The latter is a practical limitation of the "aperture" focusing method at higher beam energies. Voltages higher than 20 kV cause breakdowns for the design shown here.

Two operational regimes were considered and tested:

- hybrid regime: The working regime of the focusing lens is chosen to change from "aperture focusing" at lower energies (between 0.5 and 10 keV) to "two-tube lens" focusing at higher beam energies (between 11 and 30 keV), thus varying the potential at the second tube between −11 kV and +11 kV. When the type of focusing changes the polarity of the power supply for the second tube of the focusing lens changes from positive to negative. For the lens potentials thus chosen the maximum beam size at the target will be around 0.5 mm.

- two-tube lens (TTL) focusing: The voltage applied to the second tube of the focusing lens changes from −15.5 kV to 15 kV when varying the beam energy from 0.5 keV to 30 keV. The polarity of the power supply feeding this electrode changes from negative to positive for beam energies higher than 16 keV. The potential of the first tube is varied with the positron beam energy according to equation 7.1.

The calculated spot size at the target using the three-dimensional simulation of the electrostatic system when both operational regimes are assumed is not larger than 0.5 mm. This result will be compared with the experimentally measured beam diameter presented in Section 7.4 of this chapter.

### 7.3 Apparatus

A technical drawing of the left branch of the facility is shown in Figure 7.4. Two modifications were made in this branch, which was previously described in Chapter 4. The first is the construction and mounting of the new focusing lens. Both electrodes of the focusing lens are made of stainless steel, subsequently annealed at 800 °C to prevent the presence of local magnetic domains. The second modification is the new sample holder, attached to a linear motion drive. It is mounted on a flange with a seven pin feedthrough, which allows electrical measurements and in situ annealing of the sample. The target chamber is made of stainless steel and is supported by two aluminium legs. A top view of the target chamber is shown in Figure 7.5.
Figure 7.4: Technical drawing of the left branch of the facility. A ceramic insulator separates floating parts of the instrument from the grounded ones. The bellows are introduced for mechanical stress compensation.

7.3.1 Mechanical alignment

The optical system was aligned using the following procedure. The bellows, indicated in Figure 7.4, are disconnected from the beam line on the right-hand side and compressed. Together with the target chamber they are moved 10 cm to the left. A laser beam of 1 mm diameter is mounted on the flange where the bellows were disconnected. Four round plates, each with a hole of 2 mm at the centre, are placed: two at both ends of the first tube of the focusing lens, one at the aperture in the second tube and one in the middle of the end flange of the target chamber (see Figure 7.5). The alignment was considered successful when these four points appeared to be on one line and the laser beam passed through the holes of all plates. Afterwards the target chamber and the ceramic insulator were moved back and the bellows were attached to the rest of the left branch. The height and the horizontal position of the target chamber (including the lenses inside) can be adjusted by means of the two supporting aluminium legs.

7.3.2 Detection system

The detection system for Doppler-broadening measurements consists of a Ge-detector, placed at the end of the target chamber as indicated in Figure 7.5. It is used for detection of the annihilation photons with an energy of 511 keV. The resolution is 1.76 keV (FWHM) at 1.33 MeV. The schematic drawing of the de-
Figure 7.5: Top view of the target chamber. Position of the sample holder and the Ge-detector are shown. The two electrodes of the focusing lens are included. The points, where the apertures were mounted used for mechanical alignment with a laser, are indicated with crosses.

detection set-up is shown in Figure 7.6. The Doppler-broadening measurements are controlled by an Excel-based program which sets the beam energy, starts and ends the measurement, calculates the values of the Doppler-broadening parameters, the count rate and the positronium fraction. Since the polarity of the power supply for the second tube of the focusing lens can only be changed manually the automation of the facility is only partial.

Figure 7.6: Schematic drawing of the detection set-up. It consists of a Ge-detector with a power supply indicated by HV. The detector is connected via an amplifier (A), and an Analog-to-Digital Convertor (ADC) to a Multi-Channel Analyzer (MCA) and personal computer (PC).
7.4 Performance

The beam performance has been studied taking into account the locally present sources of magnetic field which may influence the beam size and position at the target. There are three sources of magnetic field which are considered to be important for the positron beam behaviour:

- the earth magnetic field (with components of 0.3 - 0.4 Gauss)
  \[1 \text{ Gauss} = 10^{-4} \text{ T}\]
- the magnetic parts of the target chamber which locally induce magnetic fields up to 1 Gauss
- the field, created by the magnetic coils for transportation of the intense positron beam (POSH) which are situated at a distance of less than one metre from the electrostatic set-up. When the intense positron beam is in operation the non-homogeneous magnetic field in the vicinity of the electrostatic beam reaches values of 0.3 up to 0.7 Gauss.

A \(\mu\)-metal shielding is provided for the entire beam-line except for the target chamber. Two different types of additional magnetic field shielding are considered. They are tested by performing two sets of measurements. The results are given in the next section.

7.4.1 First set of measurements

The first set of measurements is performed using the hybrid operational regime for the focusing lens. In order to minimize the influence of the magnetic fields on the positron trajectories two \(\mu\)-metal plates (60 mm \(\times\) 70 mm \(\times\) 3 mm) were installed, which form a "roof" over the target chamber. In this way the measured field strength under the "roof" is reduced to 0.2 Gauss. The positron beam intensity profiles are measured with a 45° tilted slit, placed at the target position (see Figure 7.7). The slit is mounted on a linear motion drive. The width of the slit is 2.28 mm. It can cross the beam line and as a result a pattern of peaks will be found in the measured annihilation count rate, corresponding to the passing of the positron beam through the slit or to the situation in which the slit is fully retracted from the beam. From the experimental results the beam size and the horizontal and vertical positions at different beam energies can be obtained. The model used to fit the experimental data is based on the assumption that a one-dimensional gaussian describes the positron beam at the target:

\[
G(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp \left( -\frac{(x-x_0)^2}{2\sigma^2} \right). 
\] (7.5)
Subsequently this Gaussian is convoluted with the function $H(x)$ that describes the slit:

$$H(x) = \begin{cases} 
1 & x > 0 \text{ and } d_1 < x < d_2 \\
0 & \text{otherwise.}
\end{cases}$$

When the positron beam passes through the opening the function $H(x)$ is equal to 1; when the positrons annihilate on the holder the function is 0. The result of the convolution is a function $F(x)$ which is represented by a series of error functions.

$$F(x) = \int H(x)G(x - x_0)dx$$

$$F(x) = \frac{1}{2} \left[ \frac{\text{erf}(x - x_0)}{\sqrt{2}\sigma} + \frac{\text{erf}(x - x_0 + d_2)}{\sqrt{2}\sigma} - \frac{\text{erf}(x - x_0 + d_1)}{\sqrt{2}\sigma} + 1 \right].$$

In equation 7.7, $\sigma$, $x_0$ and $d_1$ are the fitting parameters where $\sigma$ is related to the FWHM of the positron beam as follows:

$$\text{FWHM} = 2\sigma \sqrt{2\ln(2)}.$$

The parameter $x_0$ indicates the position where the holder is half-retracted from the beam-line and thus, where half the full beam intensity is measured. The parameters $d_1$ and $d_2 = d_1 + 2.28$ indicate the distances, measured from $x_0$ to the left and right end of the slit, respectively. The holder is horizontally and vertically aligned with

![Schematic diagram of the slit](image)

**Figure 7.7:** Schematic drawing of the slit used to monitor the beam profile. The width of the slit $(d_1 - d_2)$ is 2.28 mm.
Figure 7.8: Normalized intensity versus slit position: (a) at 3 keV, (b) at 5 keV, (c) at 10 keV and (d) at 15, 20 and 25 keV.

The full beam intensity will be measured. The fraction of the beam intensity, \( Z \), is related to the width of the slit, \( d \), and the FWHM of the positron beam as follows:

\[
Z = \text{erf} \left( \frac{d}{\sqrt{2}\text{FWHM}} \right).
\]  \hspace{1cm} (7.9)

The experimental results and the model functions are given in Figure 7.8 for beam energies of 3, 5, 10, 15, 20 and 25 keV.

The measured beam intensities are normalized to the maximum count rate. The results for the fitting parameters are summarized in Table 7.1. For beam energies of 3, 5 and 10 keV the beam is focused using "aperture" focusing and the agreement between experiment and model is fairly good. The error is less than 5% of the values obtained for the parameters given in Table 7.1. This means that in these cases the beam can be approximated by a one-dimensional Gaussian. The model fails to describe the experimental results achieved for the high-energy beams (15 to 25 keV), which are focused using "TTL" focusing. Probably the "TTL" focused beam has a
non-symmetric shape for the present magnetic field shielding. The beam diameter was determined using the results from the fitting functions and formula 7.9. For the "aperture" focused beam it varies with the beam energy from 2.8 mm to 3.1 mm FWHM. While the size of the "TTL" focused beam can not be determined accurately from the fitting parameters of the model function, it is clear that it is smaller than the width of the slit since the beam intensity reaches a value of 100%. Moreover, in that case the beam size does not change when the beam energy is changed. The horizontal and vertical positions of the beam at the target can be found with respect to the axis of the mechanical system. The horizontal shift equals the deviation from the zero value of the fitting parameter $d_0$. For a vertically unshifted beam the value of the fitting parameter $d_1$ should be 9 mm (see Figure 7.7). The deviation from this value equals the vertical shift. The absolute values of the horizontal and vertical shifts versus the beam energy are summarized in Table 7.2. The position of the "aperture" focused beam moves when the beam energy is varied and the beam spot at the target wanders within a distance of 2.3 mm horizontally and 1.9 mm vertically. The "TTL" focused beam has a fixed, stable position at the target, which deviates from the centre of the mechanical axis by 1.2 mm horizontally and 0.2 mm vertically. The experimentally found results for the beam size and position at the target for both types of focusing do not agree with calculated values using SIMION 7, when the simulation is performed supposing pure electrostatic conditions. The reason for the disagreement is the influence of the magnetic fields present in spite of the applied magnetic screening. When the modelling of the magnetic fields was included in the three-dimensional simulation of the optical system it was found that the observed deviation of the beam position is mainly due to a vertical magnetic field component. Figure 7.9 shows a comparison of the beam profile at 5 keV with and without the magnetic screening (by the two $\mu$-metal plates), and with the magnetic coils of POSH switched off or on. From these measurements it is clear that the effect of the POSH coils on the positron trajectories can be largely compensated by the $\mu$-metal "roof" construction, but that this does not hold for the influence of the magnetic parts of the target chamber. This means that the effect of spread and shift of the beam spot at the target should be attributed to the non-homogeneous magnetic fields originating from the welds of the target chamber, which play a major role in the deviation of the positron trajectories.

### Table 7.1: Summary of the fitting parameters.

<table>
<thead>
<tr>
<th>Beam energy (keV)</th>
<th>FWHM (mm)</th>
<th>$d_1$ (mm)</th>
<th>$x_0$ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>2.8</td>
<td>10.3</td>
<td>-1.8</td>
</tr>
<tr>
<td>5</td>
<td>2.9</td>
<td>10.7</td>
<td>0.3</td>
</tr>
<tr>
<td>10</td>
<td>3.1</td>
<td>10</td>
<td>0.5</td>
</tr>
<tr>
<td>15, 20, 25</td>
<td>0.7</td>
<td>10</td>
<td>-1.2</td>
</tr>
</tbody>
</table>
Table 7.2: Results for the horizontal and vertical shifts of the positron beam versus the beam energy. The shifts are given with respect to the axis of the mechanical system.

<table>
<thead>
<tr>
<th>Beam energy (keV)</th>
<th>horizontal shift (mm)</th>
<th>vertical shift (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>-1.8</td>
<td>-0.5</td>
</tr>
<tr>
<td>5</td>
<td>0.3</td>
<td>1.42</td>
</tr>
<tr>
<td>10</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>15, 20, 25</td>
<td>-1.2</td>
<td>0.2</td>
</tr>
</tbody>
</table>

An example of a Doppler-broadening measurement with this set-up is shown in Figure 7.10. It is performed on a Si sample with 4 mm diameter, mounted on the holder shown in Figure 7.7 (on top of the slit). The $S$ parameter and the count rate were measured, when the type of focusing from "aperture" focusing to "two-tube lens" focusing is switched at 8 keV (indicated by open symbols) and 10 keV (denoted by closed symbols).

![Graph showing beam profiles with and without shielding](image)

Figure 7.9: Beam profiles at 5 keV beam compared with and without μ-metal shielding.

The Doppler-broadening parameter $S$ and the count rate are measured between 8 keV and 10 keV beam energy using both types of focusing. It is clear that the $S$ parameter takes on different values at these energies when we switch from one type of focusing to the other. This change also causes a decrease of the count rate. The different values of the Doppler-broadening parameter can be explained by the changes in the size of the beam spot and the shift of the beam position at the sample. In the case of "aperture" focusing the size of the beam spot is larger and the annihilation takes place only partly in the sample (part of the beam goes through
the slit). Part of the annihilation gammas are absorbed by the sample (Si) and the holder (Ni-Cr alloy), while in the case of "TTL" focusing the whole beam is focused on the sample. The difference in the count rate when the type of focusing is changed is thus attributed to the fraction of the beam which goes through the slit and reaches the detector without interaction with the sample and/or holder.

The $\mu$-metal shielding does not provide the required non-magnetic conditions. Although it shields from the earth magnetic field and the magnetic coils of POSH to a large extend, it is not good enough to ensure acceptable beam performance for measurements in the low-mm range, because the influence of the magnetic parts of the target chamber remains. We must therefore look for other ways of magnetic field compensation which includes the magnetized parts of the target chamber, and also make a detailed study of the beam properties under the new conditions of magnetic field compensation.

Figure 7.10: The $S$ parameter and the count rate versus beam energy. Switching from one type of focusing to the other took place at 10 and 8 keV, respectively.
Figure 7.11: Photograph of the set-up for Doppler-broadening measurements with the six orthogonal magnetic coils, denoted by (C), installed around the target chamber (T). The detector (D) is placed behind the target chamber, which is supported by two construction legs (L).

7.4.2 Second set of measurements

A system of magnetic coils was designed in order to compensate for the above-mentioned sources of magnetic fields. It consists of six-square orthogonal coils with sides of 40 cm length. A photograph of the coils mounted around the target chamber is shown in Figure 7.11. We measured the three components of the local magnetic field at a number of positions along the beam-line. It was found that, using the vertical pair of the coils, the magnetic field could be compensated either in the region of the gap between the two electrodes of the focusing lens or in the region of the sample. When the current was set at 3.5A the measured transverse components of the magnetic field reached minimum values in the region of the gap of the focusing lens. The results are given in Table 7.3.

The three components of the magnetic field are defined as follows: the $x$ component is oriented along the beam-line, the $y$ component lies along in the vertical direction and the $z$ component is perpendicular to the $(x, y)$ plane. The study of the influence of the two types of focusing on the spot size and position in the presence of the magnetic fields, given in Table 7.3, was performed using a new target holder.
Table 7.3: Magnetic field components, measured at the sample position and at the position of the lens gap, when the current in the vertical coils is 3.5 A.

<table>
<thead>
<tr>
<th>Magnetic field component (Gauss)</th>
<th>at the sample</th>
<th>at the lens gap</th>
</tr>
</thead>
<tbody>
<tr>
<td>$B_x$</td>
<td>0.13</td>
<td>0.71</td>
</tr>
<tr>
<td>$B_y$</td>
<td>0.15</td>
<td>0.02</td>
</tr>
<tr>
<td>$B_z$</td>
<td>0.02</td>
<td>0.02</td>
</tr>
</tbody>
</table>

(Figure 7.12). The new holder with slits and holes was installed on a linear motion drive at the target position. It can be moved 53 mm across the beam. In this way the positron beam is scanned by two slits and two holes. The result is a pattern of four peaks in the measured intensity profiles corresponding to the overlap between the beam and the slit or hole in the holder. The first hole has a diameter of 3 mm, the second hole of 5 mm. One slit is tilted at 45 degrees and has a width of 2.28 mm while the other slit is vertical and has a width of 2 mm.

![Diagram of the new holder](image)

Figure 7.12: The new holder with a combination of slits and holes for the determination of beam size and position.

In Table 7.4 the types and size of the openings in the new holder are given. The distances indicated in the same table are measured from the right end of the holder.

Table 7.4: Summary of the sizes and distances of the openings in the holder, used for beam intensity profile measurements.

<table>
<thead>
<tr>
<th>Openings</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>type</td>
<td>hole</td>
<td>hole</td>
<td>tilted slit</td>
<td>vertical slit</td>
</tr>
<tr>
<td>diameter/width (mm)</td>
<td>3</td>
<td>5</td>
<td>2.28</td>
<td>2</td>
</tr>
<tr>
<td>distance (mm)</td>
<td>10</td>
<td>20</td>
<td>35</td>
<td>51</td>
</tr>
</tbody>
</table>
to the centre of each opening. The holder is aligned with the mechanical system of the set-up in a way similar to the alignment in the first set of measurements. The function that models the experimental results is a convolution of a two-dimensional Gaussian, representing the positron beam, and a two-dimensional function representing the holder, similar to the function used in the previous experiment. The analytical convolution of the two functions is complicated. For this reason the model function is approximated using a program that calculates the beam intensity profile on a 2D grid with a spacing of 0.1 mm for those grid points that lie within the opening. The positron beam intensity for different beam energies was measured

![Graph](image)

**Figure 7.13:** A scan through a 9 keV beam, using "aperture" focusing (a) and using "TTL" focusing (b). The model function is based on the assumption that the positron beam can be described by a two-dimensional Gaussian.

while scanning it through the holder. The result for a 9 keV beam focused using "aperture" focusing is presented in Figure 7.13 (a). The result for a 9 keV "TTL" focused beam is given in Figure 7.13 (b). A comparison of the experimental results
and the applied model shows that in both cases the beam intensity profile at the target can be described by a two-dimensional Gaussian. The experimental results are modelled supposing that the beam has a FWHM of 2 mm. From the peak positions (listed in Table 7.5) we can conclude that the horizontal beam position at the target is the same for both types of focusing and that it is not shifted from the centre of the mechanical system. The vertical beam position of the "aperture" focused beam is 1 mm higher than that of the "TTL" focused beam. The "TTL" focused beam at 9 keV shows no shift with respect to the mechanical axis, so for this case the optical and mechanical systems are aligned. The same measurement was performed for a 3 keV positron beam. In Figure 7.14 the results for the two types of focusing are compared. The result for the "aperture" focused beam is shifted upwards in order to make the details visible. There is a significant difference in the beam profile for

![Graph showing beam intensity profile comparison](image)

**Figure 7.14:** Scan through a 3 keV beam for "aperture" and "TTL" focusing. The result for the "aperture" focused beam is shifted upwards in order to make the details visible.

the two types of focusing. The "aperture" focused beam does not have a Gaussian profile. The beam is larger than the "TTL" focused beam and is most likely shifted both horizontally and vertically. The experimental data for the 3 keV "TTL" focused beam and the model function are compared in Figure 7.15. The beam has a FWHM of 2 mm and its position at the target coincides with the position of the 9 keV "TTL" focused beam (see Table 7.5). The measurements performed for 1 keV, 5 keV and 20 keV "TTL" focused beams show the same beam size and position as found for the 3 keV and 9 keV beams. All experimentally achieved beam sizes are four times larger than the calculated ones, resulting from SIMION 7 simulation without magnetic fields. The difference between the calculated and measured beam spot is caused by the residual magnetic field, which is difficult to compensate fully. The aim of the positron beam described is to perform Doppler-broadening measure-
Figure 7.15: Scan through a 3 keV beam, focused using "TTL" focusing. The model function is based on the assumption that the positron beam can be described by a two-dimensional Gaussian.

ments in the low-mm range. A beam size of 2 mm and a constant beam position at the target are sufficient to achieve this goal. If we use "TTL" focusing the beam size and the position at the target do not change when the implantation energy is varied between 0.5 and 25 keV. "Aperture" focusing is not applicable since the magnetic field compensation at the position of the aperture is only partial and the beam spot at the target therefore experiences broadening and wandering. The hybrid regime for the focusing lens can not fulfill the requirements of constant beam size and position at the target with the present residual magnetic fields. The chosen operational regime for the focusing lens in the presence of the magnetic fields is therefore the "TTL" focusing regime. The maximum measured count rate at the target position is about 1420 counts per second, which allows the Doppler-broadening measurements

Table 7.5: Comparison of the positions, where the peaks of the beam intensity profile appear for different types of focusing (see also Figure 7.12).

<table>
<thead>
<tr>
<th>Peak positions</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aperture focusing at 9 keV</td>
<td>9.5</td>
<td>20</td>
<td>34</td>
<td>52</td>
</tr>
<tr>
<td>TTL focusing at 9 keV</td>
<td>10</td>
<td>20</td>
<td>35</td>
<td>51</td>
</tr>
<tr>
<td>TTL focusing at 3 keV</td>
<td>10</td>
<td>20</td>
<td>35</td>
<td>51</td>
</tr>
<tr>
<td>Aperture focusing at 3 keV</td>
<td>9</td>
<td>20</td>
<td>33</td>
<td>50</td>
</tr>
</tbody>
</table>
to be performed in the relatively short time of about 5 minutes per energy. The beam intensity normalized to the averaged count rate measured above 6 keV beam energy versus the implantation energy is shown in Figure 7.16. The stability of the count rate is mainly due to the electrostatic optical system used for beam transport and focusing and is better than the one achieved with a magnetic system [72]. The decrease of the beam intensity at the target for energies lower than 4 keV is due to the fact that the backscattered and epithermal positrons, reflected from the surface of the target, can not be re-implanted because there is no retarding electric field as in the case of higher energies (see equation 7.1). In order to calibrate the set-up, Doppler-broadening measurements were performed on a silicon single crystal. The results are shown in Figure 7.17. The $S$ and $W$ parameters were modelled with the VEPFIT program [46]. The bulk parameters obtained were $S = 0.575$ and $W = 0.03$. The diffusion length was found to be 200±10 nm, which is comparable with the literature value of 250 nm for single crystal silicon.

### 7.5 Conclusion

A positron beam for Doppler-broadening experiments in the low-mm range has been designed on the basis of an electrostatic optical system. The optical lens system is aligned mechanically with the aid of a laser beam. Local magnetic fields originating from parts of the target chamber and fields from the magnetic transport coils of the intense positron beam (POSH) in the vicinity of the set-up cause deviations from the calculated positron trajectories. As a result the size and position of the beam spot at the target vary with the implantation energy. The influence of the magnetic transport coils of POSH can be compensated by two $\mu$-metal plates, placed outside
the target chamber forming a "roof" over it. Yet, the perturbations by the local fields, produced by the welds of the target chamber, do not allow an acceptable beam performance. These fields have been partially compensated by means of six orthogonal magnetic coils. Using so-called "TTL" focusing a beam size at the target of 2 mm FWHM is achieved, while its position is stable under variations of the beam energy. In this case the positron beam profile can be modelled with a two-dimensional Gaussian distribution. The count rate of 1420 counts per second is also remarkably stable in comparison with beams based on a magnetic system. Doppler-broadening measurements with this beam are shown in the next chapter.
Chapter 8

Doppler-broadening measurements

8.1 Introduction

The aim of this chapter is to demonstrate the feasibility of performing Doppler-broadening measurements with the millimeter-sized positron beam. In the previous chapter the beam characteristics were studied with the aid of specially designed apertures. The positron beam has a diameter of 2 mm FWHM and an intensity of $2.2 \times 10^4$ positrons per second. The energy range of the positron beam can be varied between 0.5 and 25 keV. Such a beam allows low-mm sized structures to be measured with lateral beam stability at different energies within this range. Three different systems have been subjected to analysis with this positron beam: i) SiC, partly implanted with Cu ions, ii) a p-n junction and iii) p- and n-type Si, implanted with Kr or Xe ions. As a material with various applications in the manufacturing of semiconductor devices [82], optical and electrical devices [83] and neutron detectors [84], SiC has been studied extensively. The p-n junctions are used in integrated circuits. Si has a wide range of applications in microelectronic and optoelectronic manufacturing.

8.2 SiC implanted with Cu

As a test of the applicability of the low-mm size positron beam a Cu implanted SiC sample with dimensions of 10 mm by 10 mm was used. The implanted area was 5 mm by 2 mm, the implantation dose was $10^{15}$ ions/cm$^2$, while the angle of implantation was 20 degrees with respect to the surface. The Cu ions had an energy of 50 MeV. The sample was mounted on the holder, made of Ni-Cr alloy and positioned in the positron beam-line for Doppler-broadening measurements. The sample was scanned horizontally by moving the sample holder in steps of 1 mm. At each position the Doppler-broadening parameters $S$ and $W$ were measured using a 3 keV positron
Figure 8.1: A positron beam scan over a SiC sample implanted with 50 MeV Cu ions. The values of the $S$ and $W$ parameters change when crossing through different regions on the sample holder. The model is a convolution of a Gaussian with a FWHM of 2 mm (describing the positron beam) and a block function (describing the holder and the sample). A schematic drawing of the sample on the holder is shown as well.

beam. The measuring time at each position was 5 minutes. The result is shown in Figure 8.1, where the $S$ and $W$ parameters are given versus the position of the sample. The $S$ parameter gradually increases while moving from the holder to the
8.2 SiC implanted with Cu

sample \((x_0 < x < x_1)\) (see the schematic drawing of the sample holder). Then it shows a shoulder, which corresponds to the non-implanted part of the sample \((x_1 < x < x_2)\). A further increase in the \(S\) parameter is observed when the positron beam probes the implanted area of the sample \((x_2 < x < x_3)\) after which it gradually decreases while the sample holder is moved further \((x_3 < x < x_4)\). The experimental data are modelled with the function, given in equation 8.1, which is a convolution of a Gaussian with a standard deviation \(\sigma = 0.9\) mm (describing the positron beam with a FWHM of 2 mm) and a block function \(H(x)\) which describes the sample on the holder.

\[
S(W(u_0)) = \int H(x)G(x - u_0)dx, \quad (8.1)
\]

\[
H(x) = \begin{cases} 
S_i & x_i < x < x_{i+1} \\
W_i & x_i < x < x_{i+1}.
\end{cases}
\]

In this way the experimentally observed dependence of the parameters \(S\) and \(W\) on the sample holder position can be described as a summation of different contributions:

\[
S(u_0) = \sum_{i=0}^{4} \int_{x_i}^{x_{i+1}} S_i G(x - u_0)dx. \quad (8.2)
\]

Finally, the parameters \(S\) and \(W\) are modelled with the functions

\[
S(u_0) = \sum_{i=0}^{4} S_i(\text{erf}(x_{i+1} - u_0) - \text{erf}(x_i - u_0)), \quad (8.3)
\]

\[
W(u_0) = \sum_{i=0}^{4} W_i(\text{erf}(x_{i+1} - u_0) - \text{erf}(x_i - u_0)). \quad (8.4)
\]

The result of the model shown by the solid line in Figure 8.1 is obtained for the parameters presented in Tables 8.1 and 8.2. The non-implanted SiC has a \(S\) value of 0.508 and a \(W\) value of 0.08, in agreement with an independent measurement done on virgin SiC with a magnetic beam system with a similar resolution of the detectors.

<table>
<thead>
<tr>
<th>(x_0)</th>
<th>(x_1)</th>
<th>(x_2)</th>
<th>(x_3)</th>
<th>(x_4)</th>
<th>(x_5)</th>
<th>(\sigma) (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>13.5</td>
<td>19</td>
<td>21</td>
<td>23.5</td>
<td>28</td>
<td>0.9</td>
</tr>
</tbody>
</table>

Table 8.1: Summary of the positions in the model function.

From the position parameters in the model function it follows that the sample has a size of 10 mm and the implanted spot a size of 2 mm, in agreement with the actual
sample characteristics. The experiment shows that a sample feature of 2 mm size can be resolved at 3 keV beam energy. In order to prove this result for the entire energy range depth profiling measurements were done. The non-implanted and implanted areas of the sample, where the depth analysis was performed, are identified by arrows in Figure 8.1. The results of the Doppler-broadening measurements at the indicated spots are given in Figure 8.2. The result of the measurement performed at the non-

![Image of Table 8.2: Summary of the S and W parameters in the model function.](image)

**Table 8.2:** Summary of the S and W parameters in the model function.

<table>
<thead>
<tr>
<th>$S_{Ni-Cr}$</th>
<th>$W_{Ni-Cr}$</th>
<th>$S_{SiC}$</th>
<th>$W_{SiC}$</th>
<th>$S_{Cu}$</th>
<th>$W_{Cu}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.485</td>
<td>0.08</td>
<td>0.508</td>
<td>0.05</td>
<td>0.54</td>
<td>0.038</td>
</tr>
</tbody>
</table>

![Image of Figure 8.2: Doppler-broadening parameter S measured versus the positron beam energy at the implanted and at the non-implanted region of the probe sample.](image)

**Figure 8.2:** Doppler-broadening parameter $S$ measured versus the positron beam energy at the implanted and at the non-implanted region of the probe sample.

implanted area shows a behaviour that is typical for virgin SiC. The data are fitted with the VEPFIT program with a one-layer model. The result is shown by the solid line. The result for the implanted spot reveals that the $S$ parameter gradually increases and even at higher energies does not reach the bulk value. At 25 keV the mean positron implantation depth in SiC is about 2 μm. Thus, the observation shows that the damage created extends beyond this depth. In order to understand the observed effect, the collision events of the Cu ions within the host material have been simulated using program SRIM 2000. The damage profile expressed in dpa (displacements per atom) and the concentration of Cu ions in the sample, given in
8.2 SiC implanted with Cu

appm, are presented in Figure 8.3. The sample is implanted and stored at room temperature thus some of the Frenkel pairs have a chance to re-combine, which may introduce changes in the final defect structure. The concentration of Cu ions in the host material is calculated using the following relation,

\[
\text{concentration[appm]} = \frac{N_{\text{ion}} \phi}{\Delta x N_{\text{total}} n_{\text{host}}} \times 10^6,
\]  

(8.5)

where \( \frac{N_{\text{ion}}}{\Delta x} \) is the fraction of the ions in the host material per depth interval which is the output of the SRIM 2000 calculation, \( N_{\text{total}} \) is the total number of Cu ions used in the simulation, and \( \phi \) is the implantation dose. The concentration of lattice atoms, \( n_{\text{host}} \), can be found from

\[
n_{\text{host}} \text{[lattice atoms/cm}^3\text{]} = \frac{\rho N_a}{(M_{\text{at}}^{\text{Si}} + M_{\text{at}}^{\text{C}})/2} = 9.6 \times 10^{22},
\]  

(8.6)

where \( \rho \) is the density of the host material, \( N_a \) is the Avogadro number, and \( M_{\text{at}}^{\text{Si}} \) and \( M_{\text{at}}^{\text{C}} \) are the atomic masses of Si and C, respectively. The damage caused by

\[\text{ Figure 8.3: Damage profile of SiC implanted with 50 MeV Cu ions (left) and concentration profile of Cu ions in SiC (right). The maximum implantation depth probed by the positron beam is shown by an arrow.}\]

the 50 MeV ion implantation is distributed up to 3 \( \mu \)m depth inside the sample. The majority of Cu atoms are found in the depth region between 2 and 3 \( \mu \)m. The maximum depth probed by the positron beam is indicated by an arrow in Figure 8.3. These results explain why the value of the \( S \) parameter, measured in the implanted area of the sample, does not decrease to the bulk value at higher positron beam energies. Probably a threshold of the defect concentration is reached beyond which the \( S \) parameter can not change any further. By increasing the positron beam energy the width of the implantation profile increases. Thus, the value of the \( S \) parameter gradually increases. The maximum depth probed by the positron beam lies within the damaged layer.
This study shows that the positron beam is able to resolve the implanted from non-implanted areas of the sample at all energies (from 0.5 to 25 keV). On this basis we can draw the following conclusions: i) the position of the positron beam at the target is stable over the entire energy range and ii) the size of the sample features that can be resolved laterally with this positron beam set-up is better than 2 mm.

8.3 P-N junction

A schematic drawing of the studied p-n junction is shown in Figure 8.4. Its dimensions are 7 mm by 7 mm; the p-Si layer has a diameter of 4.6 mm. The p-Si layer was produced by implantation of 15 keV boron ions to a dose of $6 \times 10^{14}$ cm$^{-2}$, while the n-type layer Si by ion implantation with 30 keV phosphor ions to a dose of $5 \times 10^{14}$ cm$^{-2}$. A thin Al ring was deposited on the top-surface of the sample. It has a thickness of 300 nm and a width of 300 μm. An Al layer with a thickness of 300 nm was deposited on the bottom surface. Both are used for electrical connections. Outside the Al ring, a layer of SiO$_2$ with a thickness 200 nm was deposited, which serves as an insulator. The positron beam is scanned over the p-n junction surface at 3 keV beam energy. From earlier measurements it is known that the $S$ parameters of Si and SiO$_2$ are almost equal, which is why we follow the changes in the $W$ parameter in order to resolve the different areas of the sample. The wing-parameters for Si and SiO$_2$ are different because the implanted positrons overlap with high-momentum electrons from oxygen atoms, which results in higher $W$ values for SiO$_2$. The result for the $W$ wing-parameter versus the beam position on the sample is shown in Figure 8.5. There is clear evidence that the beam subsequently crosses regions of SiO$_2$ via Si to SiO$_2$. The experimental data are modelled in the same way as explained in the previous section. The resulting model function is shown by the solid line in Figure 8.5 and the parameters used to obtain this result correspond to the actual size of the scanned regions. In order to perform a depth analysis the beam was positioned at the centre of the sample, where the p-Si was located.
Figure 8.5: Positron beam scan over p-n junction surface.

Figure 8.6: Doppler-broadening measurement of the p-n junction and the model resulting from VEPFIT program

Prior to the Doppler-broadening measurement an estimate of the thickness of the p-Si layer was made. The collision events of the boron ions with the host material
were simulated with the SRIM 2000 program. The result shows that the p-type Si layer has a thickness of about 100 nm. The results for the $S$ and $W$ parameters as well as the VEPFIT modelling are given in Figure 8.6. The VEPFIT modelling was performed using two models: a one-layer and a two-layer model (including the p-Si as a separate layer). The best fit, shown in Figure 8.6, is found with a one-layer model. A diffusion length of $140 \pm 20$ nm for positrons in the sample was derived. The values for the Doppler-broadening parameters for surface and bulk were found as follows: $S_{\text{surf}} = 0.554$, $W_{\text{surf}} = 0.0395$, $S_{\text{bulk}} = 0.575$ and $W_{\text{bulk}} = 0.0295$. There is no response from the interface between the p- and n-type layers.

### 8.4 Si implanted with Kr and Xe

Samples of differently doped Si, implanted with 500 keV Xe and Kr ions to different doses, have been studied by means of positron beam analysis. The implantations were performed in Argonne National Lab, USA. The samples were divided in three groups. Each group contains 7 samples. The first group consists of samples of p-type Si with a resistivity of $10 - 20 \ \Omega \ \text{cm}$. Three of the samples were implanted with Kr to doses of $2 \times 10^{12}$ ions/cm$^2$, $4 \times 10^{12}$ ions/cm$^2$ and $10^{15}$ ions/cm$^2$, respectively. Another three samples were implanted to the same doses with Xe ions and one sample was non-implanted and was used for reference. The second group consists of samples of n-type Si with a resistivity of $10 - 20 \ \Omega \ \text{cm}$. The last group consists of samples of n-type Si with a resistivity of $50 - 100 \ \Omega \ \text{cm}$, also implanted with Xe and Kr ions to the doses mentioned above. The damage profiles for all implantation doses were estimated using the SRIM 2000 program. The results are shown in Figure 8.7.

![Figure 8.7: Calculated damage profile of Si implanted with 500 keV Kr and Xe ions to different doses. The figure on the left shows the results for Kr and Xe ion implantation to doses of $2 \times 10^{12}$ (ions/cm$^2$) and $4 \times 10^{12}$ (ions/cm$^2$). The right-hand figure shows the results for Kr and Xe ion implantation to a dose of $10^{15}$ ions/cm$^2$.](image-url)
The damage level in the samples varies with the implantation dose. The depth of the damage profile depends on the ion type. The Xe implantation produces a damage profile with a depth of 300 nm for all implantation doses, while the Kr implantation is characterized by a depth of the damage profile of 400 nm.

In order to study the defect structure of the samples described above Doppler-broadening measurements were performed. The $S$ and $W$ parameters were measured over 0.5 - 24 keV energy range of the positron beam.

### 8.4.1 p-type Si

The results for the p-Si samples implanted with Kr ions to different doses are shown in Figure 8.8 below.

**Figure 8.8:** Measurements of the $S$ and $W$ parameters for p-type Si implanted with Kr ions to different doses and for a non-implanted sample. The results are modelled with VEPFIT.

The measurement for the non-implanted sample is given as a reference. The
VEPFIT modelling was performed for each of the measurements. The results for the non-implanted sample are as follows: $S_{\text{surf}} = 0.54$, $W_{\text{surf}} = 0.045$, $S_{\text{bulk}} = 0.578$ and $W_{\text{bulk}} = 0.029$. The diffusion length for positrons was found to be $194 \pm 1.2$ nm, which is less than the value for a perfect Si single crystal (250 nm). The implanted samples were modelled using a two-layer model. The bulk values and the value of the diffusion length in the bulk were kept fixed. The fitted parameters were the values of $S$ and $W$ at the surface, inside the damaged layer ($S_l$ and $W_l$), the diffusion length in the damaged layer ($L_+$) and its width. The results for p-Si samples, obtained from VEPFIT modelling, are given in Table 8.3. The values of the Doppler-broadening parameters in the damaged layer for the samples implanted to the two lower doses are the same, while the $S$ parameter is slightly higher for the higher dose. The diffusion length decreases with the implantation dose (there are more trapping sites), while the width of the damaged layer increases. The measurements and the modelling of the Xe implanted p-Si samples are shown in Figure 8.9. The fitted parameters are given in Table 8.3. Comparing the results in Table 8.3 for both ion implantations we see that the same trend is observed for the Xe implanted as for the Kr implanted samples. Implantation with Xe ions results in a shorter diffusion length in the damaged layer and a 20% smaller width of that layer. This is in accordance with the trend obtained by the SRIM calculations. On the other hand, the width of the damaged layer is always larger than the predicted value. The reason for such a "tail" in the damage profile may be a channelling effect during the implantation process.

Table 8.3: Summary of the fitted parameters for the p-type Si samples implanted with Kr and Xe ions. The resistivity of this type Si is 10-20 $\Omega$ cm.

<table>
<thead>
<tr>
<th>p-type Si</th>
<th>$S_l$</th>
<th>$W_l$</th>
<th>$L_+$ (nm)</th>
<th>width (nm)</th>
<th>$S_{\text{surf}}$</th>
<th>$W_{\text{surf}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kr $2 \times 10^{12}$</td>
<td>0.597</td>
<td>0.025</td>
<td>40 $\pm$ 1</td>
<td>906</td>
<td>0.57</td>
<td>0.035</td>
</tr>
<tr>
<td>Kr $4 \times 10^{12}$</td>
<td>0.597</td>
<td>0.025</td>
<td>40 $\pm$ 1</td>
<td>906</td>
<td>0.57</td>
<td>0.035</td>
</tr>
<tr>
<td>Kr $1 \times 10^{15}$</td>
<td>0.598</td>
<td>0.025</td>
<td>13 $\pm$ 1</td>
<td>1100</td>
<td>0.574</td>
<td>0.032</td>
</tr>
<tr>
<td>Xe $2 \times 10^{12}$</td>
<td>0.597</td>
<td>0.025</td>
<td>30 $\pm$ 1</td>
<td>740</td>
<td>0.57</td>
<td>0.035</td>
</tr>
<tr>
<td>Xe $4 \times 10^{12}$</td>
<td>0.597</td>
<td>0.025</td>
<td>30 $\pm$ 1</td>
<td>740</td>
<td>0.57</td>
<td>0.035</td>
</tr>
<tr>
<td>Xe $1 \times 10^{15}$</td>
<td>0.6</td>
<td>0.0245</td>
<td>14 $\pm$ 1</td>
<td>787</td>
<td>0.577</td>
<td>0.032</td>
</tr>
</tbody>
</table>
Figure 8.9: Measurements of the $S$ and $W$ parameters for p-type Si implanted with Xe ions to different doses and for the non-implanted sample. The results are modelled with VEPFIT.
8.4.2 n-type Si (I)

The second group of samples of implanted n-Si with a resistivity of 10 - 20 Ω cm was studied analogously to the first group. The results of the Doppler-broadening measurements are shown in Figure 8.10 for the Kr implanted samples.

![Graph showing measurements of S and W parameters for n-type Si (I) implanted with Kr ions to different doses and for the non-implanted sample. The results are modelled using VEPFIT.](image-url)
Figure 8.11 shows the results for the Xe implanted samples. The parameters derived from the VEPFIT analysis for the non-implanted n-Si sample are the same as for the virgin p-Si sample. The two virgin p-type and n-type (I) Si samples are indistinguishable for positrons. The VEPFIT modelling was done in the same way as the modelling for the previous group of samples. The results of the fit are presented in Table 8.4.
Table 8.4: Summary of the fitted parameters for the n-type Si (I) implanted with Kr and Xe. The resistivity of this type Si is 10-20 Ω cm.

<table>
<thead>
<tr>
<th>n-type Si (I)</th>
<th>$S_i$</th>
<th>$W_i$</th>
<th>$L_+$ (nm)</th>
<th>width (nm)</th>
<th>$S_{surf}$</th>
<th>$W_{surf}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kr $2 \times 10^{12}$</td>
<td>0.595</td>
<td>0.026</td>
<td>54 ± 2</td>
<td>806</td>
<td>0.57</td>
<td>0.035</td>
</tr>
<tr>
<td>Kr $4 \times 10^{12}$</td>
<td>0.595</td>
<td>0.026</td>
<td>54 ± 2</td>
<td>806</td>
<td>0.57</td>
<td>0.035</td>
</tr>
<tr>
<td>Kr $1 \times 10^{15}$</td>
<td>0.599</td>
<td>0.025</td>
<td>23 ± 1</td>
<td>993</td>
<td>0.57</td>
<td>0.035</td>
</tr>
<tr>
<td>Xe $2 \times 10^{12}$</td>
<td>0.595</td>
<td>0.026</td>
<td>58 ± 2</td>
<td>805</td>
<td>0.57</td>
<td>0.035</td>
</tr>
<tr>
<td>Xe $4 \times 10^{12}$</td>
<td>0.6</td>
<td>0.025</td>
<td>26 ± 1</td>
<td>790</td>
<td>0.57</td>
<td>0.035</td>
</tr>
<tr>
<td>Xe $1 \times 10^{15}$</td>
<td>0.6</td>
<td>0.025</td>
<td>26 ± 1</td>
<td>790</td>
<td>0.57</td>
<td>0.035</td>
</tr>
</tbody>
</table>

The Doppler-broadening parameters, the diffusion length and the width of the damaged layer are the same for the samples implanted with Kr ions at the two lower doses, while the $S$ parameter for the highest dose Kr implanted sample is higher and the $W$ parameter is lower. The diffusion length in the damaged layer decreases for the highest implantation dose while the width of the damaged layer increases. For the samples implanted with Xe ions the highest two doses give indistinguishable Doppler-broadening parameters, diffusion length and width of the damaged layer, while the $S$ parameter for the lowest dose Xe implanted sample is lower and the $W$ parameter is higher. The diffusion length and the width of the damage layer have higher values for the lowest implantation dose.
8.4.3 n-type Si (II)

The measurements performed on the Kr implanted samples of the third group are presented in Figure 8.12, while Figure 8.13 shows the results for the Xe implanted n-Si samples.

![Graph showing S parameter for n-Si (II) Kr implanted samples](image1)

![Graph showing W parameter for n-Si (II) Kr implanted samples](image2)

**Figure 8.12:** Measurements of the S and W parameters for n-type Si (II) implanted with Kr ions to different doses and for the non-implanted sample. The results are modelled using VEPFIT.
Figure 8.13: Measurements of the $S$ and $W$ parameters for n-type Si (II) implanted with Xe ions to different doses and for the non-implanted sample. The results are modelled using VEPFIT.

The result for the virgin n-Si (II) sample with a resistivity of 50 - 100 Ω cm is identical to that for the non-implanted n-Si (I) from the previous group. The values of the fitted parameters (Doppler-broadening parameters at the surface and inside the damaged layer, the diffusion length for positrons in the damaged layer and the width of the damaged layer) are given in Table 8.5.

The Kr implanted samples have higher Doppler-broadening parameters at the surface in compared to all other samples. The Doppler-broadening parameters in the damaged layer, the diffusion length and the width of the damaged layer are the same for the samples implanted with Kr ions to the two lower doses, while the $S$ parameter for the highest dose Kr implanted sample is higher and the $W$ parameter is lower. The diffusion length decreases while the width of the damage layer increases for the highest implantation dose. The Doppler-broadening parameters of the Xe implanted samples depend on the implantation dose. The values of $S$ and $W$ in the damaged layer, as well as at the surface, increase with the implantation dose while
Table 8.5: Summary of the fitted parameters for the n-type Si (II) implanted with Kr and Xe ions. The resistivity of this type Si is 50-100 Ω cm.

<table>
<thead>
<tr>
<th>n-type Si (II)</th>
<th>$S_i$</th>
<th>$W_i$</th>
<th>$L_+$ (nm)</th>
<th>width (nm)</th>
<th>$S_{surf}$</th>
<th>$W_{surf}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kr $2 \times 10^{12}$</td>
<td>0.594</td>
<td>0.0255</td>
<td>140 ± 20</td>
<td>970</td>
<td>0.582</td>
<td>0.03</td>
</tr>
<tr>
<td>Kr $4 \times 10^{12}$</td>
<td>0.594</td>
<td>0.0255</td>
<td>140 ± 20</td>
<td>970</td>
<td>0.582</td>
<td>0.03</td>
</tr>
<tr>
<td>Kr $1 \times 10^{15}$</td>
<td>0.595</td>
<td>0.025</td>
<td>90 ± 10</td>
<td>1100</td>
<td>0.585</td>
<td>0.029</td>
</tr>
<tr>
<td>Xe $2 \times 10^{12}$</td>
<td>0.585</td>
<td>0.027</td>
<td>70 ± 5</td>
<td>900</td>
<td>0.562</td>
<td>0.038</td>
</tr>
<tr>
<td>Xe $4 \times 10^{12}$</td>
<td>0.595</td>
<td>0.026</td>
<td>48 ± 2</td>
<td>650</td>
<td>0.57</td>
<td>0.035</td>
</tr>
<tr>
<td>Xe $1 \times 10^{15}$</td>
<td>0.602</td>
<td>0.024</td>
<td>25 ± 1</td>
<td>540</td>
<td>0.576</td>
<td>0.033</td>
</tr>
</tbody>
</table>

the diffusion length and the width of the damage layer decrease.

On the basis of the results presented above several conclusions can be made. The virgin samples of the three types of Si are identical to positrons: the diffusion length and the Doppler-broadening parameters ($S$ and $W$) at the surface and in the bulk have the same values. The width of the damaged layer in the implanted samples is greater for Kr implanted samples than for Xe implanted samples, which is in agreement with SRIM calculations. The width of the damaged layer of all implanted samples has been found to be larger than the value calculated by SRIM. The error in the estimate using VEPFIT is 10%. The effect of ion type and dose of implantation on the changes in the defect structure is less pronounced than the influence of the type and resistivity of the material. The changes in the width of the damaged layer in n-type Si (I) are smaller than those observed in the other types of Si; the largest being found in n-type Si (II). The same is true also for the changes in the positron diffusion length in the damaged layer. The highest diffusion length is found in n-type Si (II), the smallest, however, in the p-type Si. Most likely the charge state of the created defects is of significance for the positron trapping.
8.4.4 Annealing experiments

A sample of p-Si implanted with Xe to a dose of $2 \times 10^{12}$ ions/cm$^2$ was annealed in steps of 50°C for 10 minutes. The measurements of the Doppler-broadening parameters after annealing at 150°C, 250°C, 300°C and 350°C are shown in Figure 8.14. At these temperatures changes were observed in the values and the behaviour of the

![Graph showing Doppler-broadening measurements](image)

Figure 8.14: Measurements of the S and W parameters for p-type Si implanted with Xe ions to a dose of $2 \times 10^{12}$, for the non-implanted sample and after annealing of the implanted sample. The results are modelled using VEPFIT.

$S$ and $W$ parameters. The measurements at 150°C and 250°C were modelled using the two-layer model and those at 300°C and 350°C using the one-layer model. The results are given in Table 8.6. At 300°C $S_{surf} = 0.578$, $W_{surf} = 0.035$, $S_{bulk} = 0.578$ and $W_{bulk} = 0.028$. The diffusion length could not be determined in this case. At 350°C $S_{surf} = 0.57$, $W_{surf} = 0.034$, $S_{bulk} = 0.578$ and $W_{bulk} = 0.028$. The high value at 150°C of $S$ at the surface is probably due to changes in the top-surface
Table 8.6: Summary of the fitted parameters for p-type Si implanted with Xe $2 \times 10^{12}$ ions/cm$^2$ after the annealing procedure.

<table>
<thead>
<tr>
<th>p-type Si (Xe $2 \times 10^{12}$)</th>
<th>$S_t$</th>
<th>$W_t$</th>
<th>$L_+$ (nm)</th>
<th>width (nm)</th>
<th>$S_{surf}$</th>
<th>$W_{surf}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>implanted</td>
<td>0.597</td>
<td>0.025</td>
<td>30 ± 1</td>
<td>740</td>
<td>0.57</td>
<td>0.035</td>
</tr>
<tr>
<td>150°C</td>
<td>0.605</td>
<td>0.025</td>
<td>40 ± 5</td>
<td>500</td>
<td>0.59</td>
<td>0.0285</td>
</tr>
<tr>
<td>250°C</td>
<td>0.593</td>
<td>0.034</td>
<td>15 ± 2</td>
<td>150</td>
<td>0.59</td>
<td>0.035</td>
</tr>
</tbody>
</table>

oxygen layer. There is a partial recovery of the "tail" of the damage profile and a slight increase of $S_t$ in the damaged layer. This suggests possible rearrangements of the damage structure. The "tail" is fully recovered at 250°C and there is a partial recovery of the damaged layer. The $S_t$ parameter reaches the bulk value at 300°C. The re-crystallization in Si occurs at that temperature and the amorphous zones disappear. It is possible, however, that the damage is still present. Probably Xe atoms diffuse to the vacancies and cause re-arrangements in the defect structure. At 350°C there are changes in the surface conditions, most likely due to oxygen related trapping sites at the surface.

8.5 Conclusion

Doppler-broadening measurements were performed on i) SiC implanted with 50 MeV Cu ions, ii) a p-n junction with a diameter of 4.6 mm and iii) differently doped samples of Si implanted with 500 keV Kr and Xe ions. The implanted area of the SiC sample was 5 to 2 mm$^2$. The positron beam was able to resolve the implanted from non-implanted regions of the sample at all energies (from 0.5 to 25 keV). A positron beam scan over a p-n junction was performed as well as a depth profiling analysis. Furthermore, the defect structure of three types of Si samples after Kr and Xe implantation and thermal annealing was studied. The damage profile of Kr implanted Si is extended to a larger depth than for Xe implanted Si. However, the damage level produced by Xe ions is higher than that caused by Kr ions. The width of the damaged layer, created by both Kr and Xe implantation is larger than the calculated. The ion type and the implantation dose play a lesser role in the defect structure changes than the type and resistivity of the material. Recovery of the defect structure of p-Si implanted with Xe to a dose of $2 \times 10^{12}$ ions/cm$^2$ has been found to occur at 300°C. This study of various materials demonstrates the defect profiling capabilities of this electrostatic positron beam in the low-mm range.
List of symbols

\( \epsilon \) overall efficiency
\( \epsilon_M \) moderation efficiency
\( \epsilon_S \) source self-absorption
\( \epsilon_T \) transport efficiency
\( \mu \) positron mobility
\( \mu_+ \) positron chemical potential
\( \mu_- \) electron chemical potential
\( \kappa_t \) rate constant for positron trapping at defects
\( \lambda_b \) bulk annihilation rate
\( \nu \) positron transition rate between surface and vacuum
\( \rho \) mass density
\( \rho_+(r) \) positron probability density at \( r \)
\( \rho_-(r) \) electron probability density at \( r \)
\( \sigma \) standard deviation of a Gaussian distribution
\( \tau \) positron lifetime
\( \tau_i \) lifetime of positrons in state \( i \)
\( \phi_- \) electron work function
\( \phi_+ \) positron work function
\( \phi_{ps} \) positronium work function
\( \Gamma \) annihilation rate
\( \Gamma(m) \) Euler's gamma function
\( \delta E \) dipole potential step
\( \delta \Omega \) solid angle
\( \varphi \) implantation dose
\( \vartheta \) angular deviation from collinearity
\( k_b \) Boltzmann constant
\( r_0 \) classical electron radius
\( a \) fitting parameter in the model for the retarding field measurement data
List of symbols

\( a \)
radius of the outer cylinder of the mirror

\( b \)
radius of the inner cylinder of the mirror

\( b \)
fitting parameter in the model

for the retarding field measurement data

\( c \)
velocity of light

\( c \)
fitting parameter in the model

for the retarding field measurement data

\( c(x) \)
time averaged positron density

\( e \)
elementary charge

\( m \)
shape parameter for the Makhovian implantation profile

\( m_0 \)
mass of positron or electron

\( n \)
exponential constant in the formula

for the mean implantation depth

\( n_{host} \)
density of lattice atoms

\( n_d(x) \)
defect density

\( p_{lt} \)
longitudinal (transversal) component

of the momentum of the electron–positron pair

\( q, p_i \)
canonical coordinate, canonical momentum

\( t \)
time

\( v_d(x) \)
drift velocity

\( w \)
aperture width

\( x_0 \)
penetration parameter

\( x_0 \)
fitting parameter in the model

for retarding field measurement data

\( \langle x \rangle \)
mean implantation depth

\( z \)
distance travelled by the positrons

along the axis of the mirror

\( A \)
materil dependent parameter

\( A_y, A_z \)
trace space projections

\( B_x, B_y, B_z \)
cartesian components of magnetic field

\( B \)
brightness

\( B_r \)
reduced brightness

\( B_P \)
positron branching ratio of an isotope

\( D \)
surface dipole barrier

\( D^+ \)
positron diffusion coefficient

\( E \)
positron beam energy

\( E_0 \)
kineitc positron energy

\( E_p \)
potential energy

\( \Delta E \)
energy shift

\( E(x) \)
electric field strength

\( L_+ \)
positron diffusion length

\( M_{at} \)
atomic mass
\[ N_d \] rate of isotope disintegrations

\[ N_T \] rate of positrons reaching the target

\[ N_A \] Avogadro constant

\[ P(x, E) \] positron implantation profile

\[ P_{x,y,z} \] cartesian components of the classical momentum

\[ S \] line-shape annihilation parameter

\[ T \] absolute temperature

\[ W \] wing-shape annihilation parameter

\[ W \] source capsule window transmission for positrons

\[ V \] potential applied to an electrode
List of abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D-ACAR</td>
<td>Two-dimensional angular correlation of annihilation radiation</td>
</tr>
<tr>
<td>A</td>
<td>Amplifier</td>
</tr>
<tr>
<td>ADC</td>
<td>Analog to Digital Converter</td>
</tr>
<tr>
<td>AEL</td>
<td>Asymmetric Einzel Lens</td>
</tr>
<tr>
<td>bcc</td>
<td>body centered cubic</td>
</tr>
<tr>
<td>BNL</td>
<td>Brookhaven National Laboratory</td>
</tr>
<tr>
<td>CCD</td>
<td>Charged Coupled Device</td>
</tr>
<tr>
<td>CFD</td>
<td>Constant Fraction Discriminator</td>
</tr>
<tr>
<td>EAES</td>
<td>Electron-induced Auger Electron Spectroscopy</td>
</tr>
<tr>
<td>E-beam</td>
<td>Electrostatic Positron Beam</td>
</tr>
<tr>
<td>FDM</td>
<td>Finite Difference Method</td>
</tr>
<tr>
<td>FOFEM</td>
<td>First Order Finite Element Method</td>
</tr>
<tr>
<td>FWHM</td>
<td>Full Width at Half Maximum</td>
</tr>
<tr>
<td>HFBR</td>
<td>High Flux Beam Reactor</td>
</tr>
<tr>
<td>HP RPN</td>
<td>Hewlett Packard Reverse Polish Notation</td>
</tr>
<tr>
<td>IRI</td>
<td>Interfaculty Reactor Institute</td>
</tr>
<tr>
<td>LEED</td>
<td>Low Energy Electron Diffraction</td>
</tr>
<tr>
<td>LEPD</td>
<td>Low Energy Positron Diffraction</td>
</tr>
<tr>
<td>MCA</td>
<td>Multi-Channel Analyser</td>
</tr>
<tr>
<td>MCP</td>
<td>Micro-Channel Plate</td>
</tr>
<tr>
<td>LINAC</td>
<td>Linear Accelerator</td>
</tr>
<tr>
<td>LL</td>
<td>Lower level</td>
</tr>
<tr>
<td>LLNL</td>
<td>Lawrence Livermore National Laboratory</td>
</tr>
<tr>
<td>MOS</td>
<td>Metal Oxide Silicon</td>
</tr>
<tr>
<td>ORNL</td>
<td>Oak Ridge National Laboratory</td>
</tr>
<tr>
<td>PAES</td>
<td>Positron Annihilation Induced Auger Electron Spectroscopy</td>
</tr>
<tr>
<td>PAM</td>
<td>Positron Annihilation Micro-probe</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>-------------</td>
</tr>
<tr>
<td>PC</td>
<td>Personal Computer</td>
</tr>
<tr>
<td>PMT</td>
<td>Photo Multiplier Tube</td>
</tr>
<tr>
<td>POSITRONFIT</td>
<td>Program for analyzing positron lifetime data</td>
</tr>
<tr>
<td>POSH</td>
<td>Intense positron source at the Positron Centre Delft</td>
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<tr>
<td>PQM</td>
<td>Diagram of optical lens properties</td>
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<td>REPELS</td>
<td>Re-emitted Positron Energy-loss Spectroscopy</td>
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<tr>
<td>RESOLUTION</td>
<td>Program for positron lifetime data analysis</td>
</tr>
<tr>
<td>RPS</td>
<td>Re-emitted Positron Energy Spectroscopy</td>
</tr>
<tr>
<td>SCA</td>
<td>Single Channel Analyzer</td>
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<tr>
<td>SEL</td>
<td>Symmetric Einzel Lens</td>
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<td>SEM</td>
<td>Scanning Electron Microscopy</td>
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<tr>
<td>SIMION 7</td>
<td>Computer code for charged particle system analysis</td>
</tr>
<tr>
<td>SRIM 2000</td>
<td>Program for ion scattering simulation in solids</td>
</tr>
<tr>
<td>SOFEM</td>
<td>Second Order Finite Element Method</td>
</tr>
<tr>
<td>VEP</td>
<td>Variable Energy beam at Positron Center Delft</td>
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<tr>
<td>VEPFIT</td>
<td>Program for Doppler-broadening data analysis</td>
</tr>
<tr>
<td>TAC</td>
<td>Time to Amplitude Converter</td>
</tr>
<tr>
<td>TAL</td>
<td>Two-Aperture Lens</td>
</tr>
<tr>
<td>TC</td>
<td>Time Calibrator</td>
</tr>
<tr>
<td>TOF</td>
<td>Time Of Flight</td>
</tr>
<tr>
<td>TTL</td>
<td>Two-Tube Lens</td>
</tr>
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<td>WA</td>
<td>Walk adjust</td>
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Bibliography


An electrostatic positron beam for materials characterisation

by Elena Abadjieva

Summary

Positron annihilation spectroscopy is a relatively new method for studying the microscopic properties of condensed matter. The progress in the capabilities of the positron annihilation techniques is due to the development of positron beam technology. During the last decade the instrumentation for positron studies has been extended with: i) new brightness enhanced positron beams for positron re-emission microscopy, high resolution low energy positron diffraction and the positron micro-probe, ii) new intense positron sources and iii) improved beam transport and focusing. This thesis describes the design and performance of an electrostatic variable energy positron beam with several separate beam-lines. It is developed for Doppler-broadening and positron lifetime measurements with an improved lateral resolution and for re-moderation studies in the transmission mode. The latter is a step forward in the development of a high-brightness positron micro-beam.

Chapter 1 gives an overview of the existing electrostatic positron beams and their applications, as well as the basic design principles for such beams. A brief description of the positron facilities of the Positron Centre Delft is also included.

Chapter 2 presents the theory of positron behaviour in condensed matter and describes some of the positron annihilation techniques.
The basic definitions of positron optics and the design methods used in this thesis are given in Chapter 3.

Chapter 4 presents the design of an apparatus for re-moderation experiments. It contains the three-dimensional modelling of the optical system, a description of the apparatus and test results. The beam is transported and focused to a 6 times smaller diameter. A symmetric einzel-lens is used to focus the beam at the target, which is kept in an electric field-free region. The beam spot at the target has a diameter of 1 mm over the entire beam energy range. The re-emitted positrons are detected by a channeltron coupled to a retarding field element. It is used to perform transmission and retarding field measurements, which yield information on the positronic properties of moderation materials.

The re-moderation measurements with five identically produced single crystal W (100) foils with a thickness of 100 nm and five bi-metallic W-Mo foils with a thickness of 110 nm, consisting of a W (100) layer epitaxially grown on a 100 nm Mo (100) layer are shown in Chapter 5. Various treatments have been applied to improve the moderation efficiency. The highest measured moderation efficiency is 8 % for a W foil and 22 % for a WMo foil.

The design and construction of a positron lifetime spectrometer based on an electrostatic variable energy positron beam is given in Chapter 6. The design is made in two versions. In the first version the start-signal for the positron lifetime measurement is given by the secondary electron emission from a thin carbon foil, placed in front of the target in the path of the positron beam. In the second version the start-signal is given by the backward emitted secondary electrons due to the positron beam impact on the target. The three-dimensional simulation of the optical system and the positron trajectories for both versions are presented. For facilities with this type of triggering of the start-signal the time resolution is around 300 ps. This allows investigation of ceramic coatings, polymers and materials with long lifetime components.

Chapter 7 presents the design, construction and performance of the facility for Doppler-broadening measurements on the low-mm range. The beam is transported and focused on the target within a spot of 2 mm by a two-tube lens. The size, position and intensity of the positron beam at the target do not change when the beam energy is varied. The beam profile has been studied experimentally. The results show good agreement with the model function, which describes the intensity distribution of the entire positron beam as a two-dimensional gaussian with a FWHM of 2 mm over the entire energy range (from 0.5 keV to 24 keV). Doppler-broadening measurements have been performed with this set-up.

The results on different defect structures are presented in Chapter 8. It concerns i) defect structures in SiC implanted with Cu ions, ii) three types of Si, implanted with Kr and Xe ions and iii) a p-n junction. Depth-profiling analysis has been carried out for the different layered structures in order to yield the thickness and positronic properties of the individual layers.
Een elektrostatische positronenbundel voor materiaalonderzoek

door Elena Abadjieva

Samenvatting

Positronen-annihilatiespectroscopie is een relatief nieuwe, niet-destructieve methode voor het onderzoek van de microscopische eigenschappen van de vaste stof. Met name door de ontwikkeling van positronenbundeltechnologie heeft deze techniek een grote vlucht genomen. Zo zijn er in het afgelopen decennium nieuwe bundels met sterk verbeterde helderheid (i) in gebruik genomen voor positronen-reëmissie-microscopie, hoge-resolutie lage-energie positronendiffractie en positron micro-probes. Verder hebben nieuwe intense positronenbronnen (ii) en verbeterd bundeltransport en focussering van positronenbundels (iii) de mogelijkheden van deze techniek aanzienlijk uitgebreid.

In dit proefschrift worden het ontwerp en de prestaties van een nieuwe elektrostatische variabele-energie positronenbundel beschreven. Het ontwerp omvat een sectie voor Dopplerverbredingsmetingen en een sectie voor positronenlevensduur experimenten, beide met verbeterde laterale resolutie. Verder kan de opstelling ingericht worden voor positron transmissie-remoderatie studies. Deze laatste optie is relevant voor de ontwikkeling van een positronen-microbundel met hoge helderheid.

In hoofdstuk 1 van dit proefschrift wordt een overzicht gegeven van de bestaande elektrostatische positronenbundelsystemen. De ontwerpprincipes en toepassingen van deze bundels worden kort besproken. Verder wordt een beknopt
overzicht gegeven van de positronenfaciliteiten aanwezig binnen het Positron Centre Delft.

Vervolgens wordt in hoofdstuk 2 ingegaan op de theorie van het gedrag van positronen in de vaste stof en wordt een beschrijving gegeven van de experimentele positronen-annihilatie technieken. In hoofdstuk 3 worden de benodigde definities uit de positronenoptica gegeven, en worden de gebruikte methoden voor het ontwerpen van de elektrostatische positronenbundel besproken.

In hoofdstuk 4 wordt het ontwerp van de faciliteit voor remoderatie-experimenten gepresenteerd. Achtereenvolgens komen de driedimensionale modellering van het optisch systeem, de technische beschrijving van het instrument en de eerste experimentele resultaten aan bod.

In dit instrument is het preparaat geplaatst in een veldvrije omgeving. De positronenbundel wordt door middel van elektrostatische velden van de moderatiesectie naar de preparatkamer geleid en aldaar met behulp van een symmetrische Einzel-lens op het preparaat gefocuusseerd. Het resultaat is een reductie in bundeldiameter met een factor 6. Vastgesteld is dat de bundeldiameter op het te onderzoeken monster binnen 1 mm blijft voor alle mogelijke bundelenergieën. In geval van reëmissie experimenten worden de positronen welke het preparaat verlaten eerst op energie geselecteerd en vervolgens gedetecteerd door een channeltron. Deze opstelling kan eveneens gebruikt worden voor transmissiemonderatie- en "retarding field" experimenten, waarmee informatie over de positronische eigenschappen van moderatormaterialen kan worden verkregen.

In hoofdstuk 5 worden remoderatie-experimenten aan verschillende dunne moderator folies beschreven. Voor deze experimenten zijn vijf op identieke wijze geproduceerde wolfram (100) folies en vijf bimetaallische wolfram/molybdeen moderator folies onderzocht. De 110 nm dikke WMo folies bestaan uit een laagje W (100) dat epitaxiaal gegroeid is op een 100 nm dik 100 Mo folie. Deze folies zijn vervolgens onder diverse condities behandeld (zoals temperatuur, vacuumcondities) om hun moderatie-efficiëntie te vergroten. Voor de in dit werk onderzochte folies is een maximale moderatie-efficiëntie van 8 % voor de W folies en 22 % voor de WMo folies gemeten.

Het ontwerp en de constructie van de positronenlevensduur opstelling, welke is gebaseerd op de hier behandelde elektrostatische variabele-energie positronenbundel wordt beschreven in hoofdstuk 6. Van dit instrument zijn twee ontwerpen beschouwd. In het eerste ontwerp wordt het startsignaal voor de positron levensduurmeting gegeven door de secundaire elektronen die geëmitteerd worden door een in de bundellijn, voor het meetmonster geplaatst dun koolstoffolie. Het startsignaal in het tweede ontwerp wordt verkregen door detectie van de secundaire elektronen die worden gecreeëerd wanneer de positronenbundel het preparaat treft. Voor beide ontwerpen worden in dit hoofdstuk de driedimensionale simulatie van het optische systeem en de berekende banen van de positronen en secundaire elektronen gepresenteerd.
Het blijkt dat met de hierboven beschreven methodes voor het verkrijgen van een startsignaal een tijdresolutie van 300 ps haalbaar is. Hierdoor wordt het mogelijk levensduurmetingen te verrichten aan polymeren, keramische coatings en andere materialen met ‘lange levensduur’ componenten.

In hoofdstuk 7 wordt aangetoond dat het mogelijk is Dopplerverbredingsexperimenten te doen met een positronenbundel met een diameter in de orde van millimeters. Het ontwerp, de constructie en de eigenschappen van dit instrument worden achtereenvolgens besproken.

In deze opstelling wordt de positronenbundel getransporteerd en op het preparaat gefocuseerd door middel van een lenssysteem bestaande uit twee achter elkaar geplaatste cilinders. Hiermee wordt ter plaatse van het preparaat een bundeldiameter verkregen van 2 mm. Het bundelpatroon is voor diverse bundelenergieën experimenteel bepaald. De positie, diameter en intensiteit van de positronenbundel blijken niet te veranderen met de energie van de inkomende positronen. De laterale intensiteitsverdeling van de bundel is voor alle energieën zeer goed te beschrijven door een tweedimensionale gaussische verdeling met een breedte (FWHM) van 2 mm.

Met het hiervoor beschreven instrument is een reeks experimenten uitgevoerd. Deze worden in hoofdstuk 8 gepresenteerd. De defectenstructuur van met koper geïmplanteerd siliciumcarbide(i), silicium geïmplanteerd met xenon en krypton (ii) en een p-n junctie (iii) zijn gemeten. Deze resultaten zijn gebruikt voor een diepteprofielingsanalyse van de diverse gelaagde structuren aan de hand waarvan o.a. de dikte en positronische eigenschappen van de individuele lagen zijn bepaald. Uit deze experimenten blijkt dat het instrument aan de verwachtingen voldoet.
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Curriculum Vitae

The author of this thesis was born on the 11th of March 1971 in Sofia, Bulgaria. In 1984 she joined the special school for mathematics and natural sciences in Sofia. From 1990 to 1995 she was a student in the Physics Faculty in the State University of Sofia. She graduated with a specialization in solid state physics. Her Master’s thesis was dedicated to microstructural studies of flame- and plasma-sprayed coatings made from Ni- and Fe-alloy metal powders. In this investigation techniques as SEM, metallographic methods and X-ray diffraction methods were used. From 1996 to 1998 she was employed in the Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences. There she studied the irradiation damage in nuclear reactor steels caused by fast neutrons. From 1999 till 2003 she was a PhD student at the Interfaculty Reactor Institute in Delft. This dissertation presents the results obtained during the latter period.
This dissertation describes the design and performance of an electrostatic variable energy positron beam. It is developed to perform Doppler-broadening measurements in the low mm range, positron lifetime measurements and transmission re-moderation experiments. The instrument has been built at Positron Centre Delft.