ELECTRON TRANSPORT MODELLING IN X-RAY TUBES

by

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Work carried out in collaboration between Philips Research, Hamburg in Germany and the Department of Physics, University of Surrey.

Submitted for the degree of Doctor of Philosophy to the University of Surrey 1997.
Dedicated to my wife Renate,

my daughter Julia

and the unborn baby.
Abstract

Although the discovery of cathode rays (fast moving electrons) dates back into the last century, a comprehensive study of fast moving electron transport in vacuum and condensed matter has never been done. In this thesis the tracks of fast moving electrons in condensed matter have been studied by using the Monte Carlo method. Also, the tracks of fast moving electrons in electric fields have been investigated by solving Laplace’s equation with the finite element method. The two techniques have been applied to a classical x-ray tube and a new development for a micro-focus x-ray tube. Also the general behaviour of reflected (back scattered) electrons has been studied and are presented in this thesis. Other areas of applications are proposed.
Acknowledgements

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1 Introduction

1.1 Purpose of this work

The task of this work is to study the behaviour of fast moving electrons in vacuum and in matter. The term 'fast moving electrons' is used for electrons with a kinetic energy in the range of interest, 10 to 250 keV.

Of special interest were the angular distributions of electrons 'reflected' from a plane surface for small incident angles, $\theta$ (see figure 1-1).

![Figure 1-1: Angular distribution of reflected electrons.](image)

The transport of fast moving electrons from vacuum into condensed matter and vice versa is important for several reasons.

i) Lack of data in literature

The transport of fast moving electrons in vacuum has widely been studied and published. However, little data is available concerning fast moving electrons in condensed matter in the x-ray energy region, say 10 to 250 keV.

In section 5 measured and simulated angular distributions of reflected electrons that were shot onto a plane surface are shown and compared.

ii) New idea for a micro-focus x-ray tube

One potential application is a new idea for a micro-focus x-ray tube, with the aim of producing a tube with a small high intensity focal spot (G. Harding [14]) by reducing the diameter of a pre-focused electron beam mechanically with a capillary (see figure 1-2). The
capillary has a conical hole that decreases in diameter to the desired diameter of the focal spot. The capillary acts like a funnel used for conveying liquids into a narrow-necked container. The idea also has much in common with an optical light pipe.

**figure 1-2: Principle of electron focusing using a capillary ('electron funnel').**

The advantages of such a capillary are firstly a mechanically defined focal spot size, independent of high voltage and beam current, and secondly (in contrast to a pinhole aperture) the capillary absorbs over a large area the energy of the electrons that do not get through the capillary. Therefore, cooling of the capillary becomes elementary.

The development of the capillary is given in section 6.

### iii) Combination of tools for electron transport in vacuum and matter

One important potential application is the combination electron transport in vacuum and in matter. Many simulation tools exist for fast moving electrons in vacuum, a few Monte Carlo simulation tools for electrons in matter, but the combination of the two simulation tools is novel. This work brings the two parts of electron transport together and outlines some applications (e.g. see §4.4).

### iv) Electron scatter in x-ray tubes (off-focus radiation)

In an x-ray tube the main electron current comes from an electron emitter, usually the filament, from where the electrons get accelerated until they reach the target (anode). However, some of the electrons that penetrate the target get scattered backward into the vacuum again. These back scattered electrons are still highly energetic and produce off-focus radiation. This effect has been studied by Roeck et al [30] and others.
However, there is still a lack of theoretical knowledge on off-focus radiation. A detailed theoretical study of back scattered electrons in x-ray tubes requires tools for electron transport in both vacuum and condensed matter. Both tools have been developed and are presented in this thesis (see §3 and §4).

Another important effect of back scattered electrons in x-ray tubes is the heat deposition outside the focal spot. This also may be investigated with the presented mechanisms to optimise cooling in high intensity x-ray tubes.

v) Non multiple scatter tools

While a fast moving electron 'walks' through condensed matter it undergoes a large number of scattering processes. The mean energy loss between two scattering processes is between 10 and 100 eV. Hence the number of scattering processes of a 150 keV electron that is followed down to 50 keV undergoes about 1,000 to 10,000 scattering processes. This value increases for higher energies.

Different multiple scattering theories were introduced which combine the angular distributions of many single scattering processes to a multiple scattering angular distribution (see §2.4). Two widely spread multiple scattering theories are from Molière [3] and Goudsmit and Saunderson [13].

Most available Monte Carlo simulation tools for electron transport use a multiple scattering theory. However, the multiple scattering theories of Molière and that of Goudsmit and Saunderson fail for the purposes of this work. They either become very complicated to calculate (in term of CPU-time and memory) or simply invalid. Another fact is that for some geometry (e.g. small incident angles) the number of elastic scattering processes reduces to one for a remarkable fraction of all electrons (see §2.4.3).

The Monte Carlo tool introduced in this thesis avoids using a multiple scattering theory and simulates all single scattering events. This incurs much computational time but leads to more accurate results.
1.2 Approach

The transport of electrons was studied under two headings: \textit{a)} in condensed matter and \textit{b)} in a vacuum. The approach for both media was to write a simulation tool, to benchmark it with measurements or other published simulation tools and then to do simulations for the desired applications.

There are two reasons for not using existing simulation tools:

One is: "Never trust a simulation tool unless you have put some errors into it yourself". All simulation tools are written for a special purpose; hence, it is always risky to use them for anything different from what they were created for.

The other reason is that writing a new simulation tool is a perfect way to get into the subject. Before any physical law concerning fast moving electrons is implemented in a computer program the physics behind it must be understood in depth.

The theory and the implementation of fast moving electrons in condensed matter are described in chapter 2 and chapter 3, respectively. The simulation of fast moving electrons in vacuum is described in chapter 4.

Chapter 5 describes some measurements on the angular distributions of reflected electrons that were performed at the Philips research laboratories in Hamburg.

Chapter 6 concentrates on the capillary design for a micro-focus x-ray tube; whereas chapter 7 shows further simulation results.
2 Theory

2.1 Model of the fast moving electron

Fast moving electrons can be described as particles or as waves. Depending on the effect to be described, one of the models is to be preferred. For the purpose of fast moving electrons in vacuum and condensed matter nearly all interactions can be described by the particle model. One exception is in the use of Fresnel’s law. This law is used to evaluate the fraction of electrons penetrating a boundary that are specularly reflected due to the effect of refraction (see §2.2.3). The treatment of electrons as particles is justified by their short wave length. The mean wave length is given by the DeBroglie equation

$$\lambda = \frac{h}{p}.$$  

The DeBroglie wave length for kinetic energies from 1 keV to 1 MeV is shown in figure 2-1.

![Figure 2-1: DeBroglie wave length of a fast moving electron versus its kinetic energy.](image)

Another exception where the wave model is preferred lies in the exact evaluation of the differential cross section for elastic scattering, $d\sigma/d\Omega$ (see §2.2 and §2.3.5). Here the wave length of the static potential field around an atomic nucleus has the same magnitude as the fast moving electron. However, the differential cross section (single scatter distribution) needs
only to be calculated once; the distributions may then be applied to electrons in the particle model.

The following two sections briefly describe the particle and the wave model.

2.1.1 Particle model

In the particle model fast moving electrons are described as point masses. The velocity of the particle, $v$, increases with its kinetic energy, $T$, although it never becomes faster than the speed of light in vacuum, $c$. The velocity of the particle of rest mass $m_0$ relative to the speed of light is expressed as $\beta$ which is related to the kinetic energy, $T$, by

$$\left( \frac{v}{c} \right)^2 = \beta^2 = 1 - \frac{1}{\left( 1 + \frac{T}{m_0 c^2} \right)^2}.$$ 

In table 2-1 the velocity of a fast moving electron relative to the speed of light in vacuum is listed for a number of kinetic energies. This work concentrates on kinetic energies from 10 to 250 keV. Hence, all kinetic equations must be derived for the relativistic case.

<table>
<thead>
<tr>
<th>kinetic energy $T$</th>
<th>relative velocity $\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 keV</td>
<td>0.062</td>
</tr>
<tr>
<td>10 keV</td>
<td>0.195</td>
</tr>
<tr>
<td>20 keV</td>
<td>0.272</td>
</tr>
<tr>
<td>50 keV</td>
<td>0.413</td>
</tr>
<tr>
<td>100 keV</td>
<td>0.548</td>
</tr>
<tr>
<td>250 keV</td>
<td>0.741</td>
</tr>
<tr>
<td>1 MeV</td>
<td>0.941</td>
</tr>
</tbody>
</table>

table 2-1: Particle velocity relative to the speed of light for different kinetic energies.

The mass of the particle, $m$, increases with its velocity due to relativistic effects. The electron has a rest mass, $m_0$, of $9.11 \times 10^{-31}$ kg. The more commonly used rest mass energy, $m_0 c^2$, is 511 keV. The mass of the electron at any kinetic energy is given by
\[ m = \frac{m_0}{\sqrt{1 - \beta^2}}. \]

In this thesis the non SI unit eV (electron Volt) is used for energy rather than the SI unit Joule (1 eV = 1.6*10^{-19} AsV = 1.6*10^{-19} Ws = 1.6*10^{-19} J). The energy range of interest is from 10 keV to 250 keV. In this energy range it is more convenient and more common to use the unit eV, which is therefore used throughout this paper.

2.1.2 Wave model

A moving particle may also be treated as a wave. If fast moving electrons (or, e.g., thermic neutrons) pass through a crystalline powder onto a screen they show concentric diffraction rings. This behaviour can only be explained by a wave model. As mentioned before, the wavelength, \( \lambda \), of any moving particle is given by the DeBroglie equation

\[ \lambda = \frac{h}{p} = \frac{h}{mv} \]

where \( h \) is Planck's constant and \( m, v \) and \( p \) are the relativistic mass, the velocity and the momentum of the moving particle, respectively.

The corresponding frequency, \( \nu \), is

\[ \nu = \frac{v}{\lambda} = \frac{p\nu}{h} = T \cdot \frac{1}{h} \cdot (1 + \sqrt{1 - \beta^2}). \]

where \( E \) and \( T \) are the total and kinetic energies of the particle \( (E = T + m_0c^2) \). The variable \( \beta \) is the velocity of the particle relative to the speed of light in vacuum.

2.2 Interactions of fast moving electrons

Fast moving electrons interact with matter in a variety of ways. Virtually all interactions are due to Coulomb forces between the fast moving electrons with electrons and protons in atoms. Some of the interactions only change the direction of the electron, not its energy; these are elastic scattering, refraction, specular reflection and diffraction. Other interactions lead to an
energy transfer; namely inelastic scattering. All these effects are explained in the following sections.

The probability by which an event takes place is measured in by its cross section, $\sigma$. With $N_E$ as the number of events, $N_I$ as the number of incident particles, $N$ the number of atoms per volume and $t$ the distance moved by the particles, the cross section, $\sigma$, is defined by

$$N_E = N_I \cdot N \cdot t \cdot \sigma \quad \text{or} \quad \sigma = \frac{N_E}{N_I \cdot N \cdot t}.$$ 

The cross section is measured in area units like barn and $\text{Å}^2$.

$$1 \text{Å} = 10^{-10} \text{m} \quad 1 \text{Å}^2 = 10^{-20} \text{m}^2 \quad 1 \text{barn} = 10^{-28} \text{m}^2$$

### 2.2.1 Elastic scattering

Once a fast moving electron has entered a medium, elastic scattering with the Coulomb field of nuclei is the predominant interaction; i.e. the elastic scattering has the largest cross section per atom. This means that there is a high chance for an electron to be scattered without losing energy. Nearly all electron scattering theories concentrate only on the Coulomb field around the nucleus and on the differential scattering cross section due to this Coulomb field. Section 2.3 will discuss the particulars of the scattering theories.

![figure 2-2: Trajectory of a moving electron passing an atomic nucleus.](image)

The elastic interaction of fast moving electrons with atomic electrons has only a very small cross section per atom. However, the atomic electrons have an influence on the Coulomb field surrounding the nucleus which is known as ‘shielding effects’. Different attempts were made to take this effect into account (see §2.3).
2.2.2 Inelastic scattering

For fast moving electrons in matter the second largest cross section is for the inelastic interaction with the atomic electrons. If an incident electron passes close to an atomic electron the latter leaves its atomic shell taking up some energy. The atomic electron either leaves the atom entirely (ionisation) or enters an outer shell which is a higher energy state (excitation). Hence the incident electron loses energy through collision with atomic electrons (collision loss). This happens mainly with the outer shell electrons.

![Inelastic scattering: collision loss](image)

In the energy region of x-rays, say 50 to 250 keV, the incident electrons lose about 99% of their kinetic energy by collision loss. This value increases for lower energies and decreases for higher energies.

Another inelastic effect is the interaction between electrons and the nuclear charge. If an electron gets close to the nucleus in a strong Coulomb field it emits a photon called *bremsstrahlung*.

![Inelastic scattering: bremsstrahlung](image)

The effect of bremsstrahlung takes up about 1% of the energy of the fast moving electron. The bremsstrahlung is the origin of the continuum spectrum from an x-ray tube anode. The energy loss that leads to radiation relative to the total energy loss is called the *radiation yield*. The radiation yield increases for higher energies and decreases with lower energies. This work
concentrates on the electron tracks; hence no further attention is given to the bremsstrahlung photons.

2.2.3 Refraction and specular reflection

The effects of refraction and specular reflection are only important when fast moving electrons enter a material almost parallel to the surface, say less than 1° for the angle $\theta$ between incident beam and surface. When the electron enters into the material it finds an mean inner potential, $\Phi$, of 5 to 20 Volts (see R.D. Heidenreich [15] appendix T). The mean inner potential is evaluated by integrating the potential over an exemplary volume element $V$ of the refracting medium. A detailed discussion can be found in the book by Z.G. Pinsker [26].

\[ \Phi = \frac{1}{V} \int \phi(r) d^3r \]

\[ \left( \frac{p}{p+\Delta p} \right) \mu = \frac{p+\Delta p}{p} = 1 + \frac{\Delta p}{p} \] (2-1)
The kinetic energy, \( T \), or the total energy of the electron, \( E \), increases by \( \Delta T \) which equals the charge of the electron times the mean inner potential that accelerates the electron, \( e\Phi \). It is useful to describe the increase of the momentum, \( \Delta p \), by the increase of energy, \( e\Phi \). This may be done by applying the relativistic energy-momentum relation:

\[
E^2 = p^2c^2 + m_0^2c^4
\]

\[
(E + e\Phi)^2 = (p + \Delta p)^2c^2 + m_0^2c^4
\]

\[
\frac{\Delta p}{p} = \sqrt{1 + \frac{2Ee\Phi}{p^2c^2} + \frac{(e\Phi)^2}{p^2c^2}} - 1
\]  \hspace{1cm} (2-2)

It is assumed, that the kinetic energy, \( T \), is large compared to the increase of energy, \( e\Phi \) (\( T \gg e\Phi \)). Hence, the last term in the square root of equation (2-2) can be neglected and the whole equation can be simplified.

\[
\frac{\Delta p}{p} \approx \sqrt{1 + \frac{2Ee\Phi}{p^2c^2}} - 1 \approx \frac{Ee\Phi}{p^2c^2} = \frac{e\Phi}{T} \left( \frac{T + m_0c^2}{T + 2m_0c^2} \right)
\]

The refractive index becomes

\[
\mu = 1 + \frac{\Delta p}{p} \approx 1 + \frac{e\Phi}{T} \left( \frac{T + m_0c^2}{T + 2m_0c^2} \right) \quad \text{for all kinetic energies,} \hspace{1cm} (2-3)
\]

\[
\mu \approx 1 + \frac{e\Phi}{2T} \quad \text{for non-relativistic energies, and}
\]

\[
\mu \approx 1 + \frac{e\Phi}{T} \quad \text{for extreme-relativistic energies.}
\]

All three equations are true for \( T \gg e\Phi \). The energy range of interest (10 to 250 keV) reaches close to the rest mass energy of electrons (511 keV). Thus, equation (2-3) is used for the simulation of fast moving electrons in matter.

Although fast moving electrons experience small acceleration towards condensed matter, some of the incident electrons are specularly reflected at the boundary from vacuum to condensed matter. This effect can only be described in the wave model (see §2.1.2).
To evaluate the intensity of the reflected electrons, Fresnel's law may be applied. Fresnel derived his equations for electromagnetic waves. However, the equations may also be applied to fast moving electrons if they are treated as waves. Following the treatment of Born and Wolf [4] §1.5.2:

\[ R_\parallel = \tan(\theta_r - \theta_i) \frac{A_i}{\tan(\theta_r + \theta_i)} \]

\[ R_\perp = -\frac{\sin(\theta_r - \theta_i)}{\sin(\theta_r + \theta_i)} A \]

where \( A \) and \( R \) are the amplitude of the electric vector of the incident and the reflected beam, respectively. The vectors are resolved into components parallel to (denoted by subscript \( \parallel \)) and perpendicular to (subscript \( \perp \)) the plane of incidence. The square of the reflected amplitude, which equals the intensity of the reflected beam, may be described by

\[ R^2 = R_\parallel^2 + R_\perp^2 = \frac{\tan^2(\theta_r - \theta_i)}{\tan^2(\theta_r + \theta_i)} A_i^2 + \frac{\sin^2(\theta_r - \theta_i)}{\sin^2(\theta_r + \theta_i)} A_\perp^2. \]

With \( A_i = A \cdot \cos \alpha \) and \( A_\perp = A \cdot \sin \alpha \) the equation can be written as:

\[ \frac{R^2}{A^2} = \frac{\tan^2(\theta_r - \theta_i)}{\tan^2(\theta_r + \theta_i)} \cos^2 \alpha + \frac{\sin^2(\theta_r - \theta_i)}{\sin^2(\theta_r + \theta_i)} \sin^2 \alpha. \]

If the incident beam is assumed not to be polarised, the equation can be integrated over \( 2\pi \) for all incident polarisation angles.

\[ \frac{R^2}{A^2} = \frac{1}{2\pi} \int_0^{2\pi} \left( \frac{\tan^2(\theta_r - \theta_i)}{\tan^2(\theta_r + \theta_i)} \cos^2 \alpha + \frac{\sin^2(\theta_r - \theta_i)}{\sin^2(\theta_r + \theta_i)} \sin^2 \alpha \right) d\alpha \]

\[ \frac{R^2}{A^2} = \frac{1}{2} \frac{\tan^2(\theta_r - \theta_i)}{\tan^2(\theta_r + \theta_i)} + \frac{1}{2} \frac{\sin^2(\theta_r - \theta_i)}{\sin^2(\theta_r + \theta_i)} \]

After some changes:

\[ \frac{R^2}{A^2} = \frac{1}{2} \left( \frac{\sin \theta_r \cos \theta_i - \cos \theta_i \sin \theta_i}{\sin \theta_i \cos \theta_i + \cos \theta_i \sin \theta_i} \right)^2 + \frac{1}{2} \left( \frac{\sin \theta_i \cos \theta_i - \cos \theta_i \sin \theta_r}{\sin \theta_i \cos \theta_i + \cos \theta_i \sin \theta_i} \right)^2 \]
Since the amplitude $R$ is the square root of the intensity, the right hand side of equation (2-4) gives directly the fraction of reflected beam.

The effect of refraction and the effect of reflection due to the refractive index are of great interest for incident electron beams almost parallel to the surface. The following three diagrams show the fraction of reflected electrons which penetrate from vacuum onto a plane surface with a mean inner potential of 15 V. The incident angle, $\theta$, in the three graphs is the angle between the incident beam and the surface, which is $\theta=90^\circ-\theta_i$ as defined in figure 2-5.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2-6.png}
\caption{Specularly reflected electrons as a function of incident angle on a lin-log scale.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2-7.png}
\caption{Specularly reflected electrons as a function of incident angle on a log-log scale.}
\end{figure}
2 Theory

Obviously, the reflection index ranges from zero to one. For incident angles much smaller than 90° and a reflection index much smaller than one, there are two proportional behaviour observed in the reflection index. Firstly, the reflection index is proportional to the inverse square of the incident energy (see figure 2-8), and secondly, the reflection index is proportional to the inverse incident angle to the power of four (see figure 2-7).

\[ \frac{R^2}{A^2} \propto \frac{1}{T^2} \quad \text{and} \quad \frac{R^2}{A^2} \propto \frac{1}{\theta^4} \]

Total reflection only takes place for electrons that come from condensed matter to the vacuum boundary. This is true since the mean inner potential, \( \Phi \), is always positive; hence, the refractive index is always greater than one.

2.2.4 Diffraction / coherent scattering

Electron waves are diffracted by atomic lattices in the same way as light and neutron waves. It was discovered independently by C.J. Davison and L.H. Germer and by G.P. Thomson, both in 1927. A short survey of electron diffraction is given by Mac Rae [18].

Electron, photon and neutron diffraction are all used for structure studies. The advantage of electron diffraction lies in the structural studies that involve small number of atoms. This is due to the strong interaction of fast moving electrons with matter. Thus, the principal area of
application of electron diffraction is for the study of thin films, surfaces, gases and small samples.

When fast moving electrons enter condensed matter, they strongly change their direction due to elastic scattering (see §2.2.1). However, to obtain a diffraction pattern, the incident and diffracted electrons should not have many elastic collisions so as to avoid changing their direction and blurring the diffraction pattern. Hence, a clear electron diffraction pattern can only be obtained for object sizes in the range of the mean free path of the fast moving electrons (see §2.6.1).

For thick objects the fast moving electrons greatly change their direction due to elastic scattering; some are even scattered backward. Therefore, even if the effect of diffraction has a large cross section, there are no diffraction peaks in the scattering cross section for thick objects.

This paper is mainly concerned in the reflection behaviour of fast moving electrons. Therefore no diffraction peaks are expected in the angular distribution of reflected electrons. The effect of diffraction has been neglected for all simulations in this paper and has not been implemented in the simulation tool ETraST (see §3.3). However, the angular distribution of reflected electrons for small incident angles and mono-crystalline reflectors may show some diffraction peaks. This may be a subject for further study.

2.3 Single scatter theory

2.3.1 Introduction

In principle the procedure to evaluate the elastic single scatter distribution of fast moving electrons in matter has two steps; the evaluation of the potential field and the scattering distribution.

The first step is to evaluate the charge distribution and the potential field, \( \varphi(r) \), around the nuclei of the scattering material. This may be done by solving Schrödinger's equation for the lowest energy \( E \) (see Messiah [20] §2.2.7). The nucleus is assumed to be a point charge with infinite mass.
$E\psi_e(r_1,...,r_z) = \left[ -\hbar^2 \sum_{i=1}^{z} \frac{\Delta_i}{2m} - \frac{Ze^2}{4\pi\varepsilon_0} \sum_{i=1}^{z} \frac{1}{|r_i|} + \frac{e^2}{4\pi\varepsilon_0} \sum_{i<j} \frac{1}{|r_i - r_j|} \right] \psi_e(r_1,...,r_z)$ \hspace{1cm} (2-5)

$E$ stands for the energy of the atom; $\Delta_i$ is Laplace's operator relative to $r_i$. The square of the eigen-function $\psi_e(r_1,...,r_z)$ gives the probability distribution of the atomic electrons, i.e. the charge distribution around the nucleus. There are different approaches to solve equation (2-5); one has been performed by Riley et al (see below). The charge distribution may be used to evaluate the potential field, $\varphi(r)$, around the nucleus.

The second step is to use the potential field, $\varphi(r)$, to evaluate the single scatter distribution. The standard deviation is taken from A. Messiah [20] §10.1.2. The way to evaluate the distribution for non-relativistic electrons is by using Schrödinger's equation again

$$E\psi(r) = \left[ -\frac{\hbar^2}{2m} \Delta + V(r) \right] \psi(r)$$ \hspace{1cm} (2-6)

where $V(r) = -e\varphi(r)$ for electrons.

It is assumed that the behaviour of fast moving electrons at greater distance from the atom is described by:

$$\psi = \psi_0 + \psi_s = \exp(ikr) + f(\Omega) \frac{\exp(ikr)}{r}$$ \hspace{1cm} (2-7)

The first term of the sum represents the incident wave, whereas the second term stands for the scattered wave. The scattering amplitude, $f(\Omega)$, leads to the single scatter distribution $\sigma$.

$$\sigma(\Omega) = |f(\Omega)|^2$$

Equation (2-6) can also be converted into integral form which is called the scattering integral solution:

$$\psi(r) = \exp(ikz) + \frac{-m}{2\pi\hbar^2} \int G(r,r') \cdot V(r') \cdot \psi(r') \, d^3r'$$ \hspace{1cm} (2-8)
In scattering experiments both the beam source and the detector for measuring the scatter distribution are far away from the potential field of the scattering atoms. In this case Green’s function yields to

\[ G(r, r') = \frac{-1}{4\pi} \frac{\exp(ikr)}{r} \cdot \exp(-ik \cdot r'). \]

Inserting this expression into equation (2-8) and comparing with equation (2-7) gives the expression for the scattering amplitude,

\[ f(\Omega) = \frac{-m}{2\pi \hbar^2} \int \exp(-i\mathbf{k} \cdot \mathbf{r'}) \cdot V(\mathbf{r'}) \cdot \psi(\mathbf{r'}) \, d^3\mathbf{r'}. \tag{2-9} \]

These are the two steps in evaluating the elastic single scatter distribution for non-relativistic electrons. For relativistic electrons the evaluation of the scatter distribution becomes more difficult. A more exact evaluation of the single scatter distribution has been performed by Riley et. al. (see §2.3.5).

For most cases equations (2-5) and (2-9) can not be solved analytically. The method to solve these equations is by approximations, numerically or by a combination of the two methods.

In section 2.3.2 the atoms of the scattering medium are treated as independent nuclei without the shielding atomic electrons. Section 2.3.3 gives some simple solutions for the potential around the nuclei (shielding approximations). The widely used Born approximation which is a solution of equation (2-6) is described in section 2.3.4 whereas section 2.3.5 refers to a more exact scatter distribution for the energy range in question (10 to 250 keV).

2.3.2 The unshielded atom and Rutherford scattering

At the beginning of this century Rutherford made the suggestion for the famous Geiger-Marsden scattering experiment [32]. In this experiment fast charged particles (\(\alpha\)-particles) were shot at a thin gold foil. A detector was positioned at various angles relative to the incident beam to measure the intensity as a function of the scattering angle. One completely unexpected effect was that some particles were scattered backward. From the measured distribution Rutherford derived his well-known scattering theory which laid the foundations of the nuclear atom model. His theory describes the intensity of scattered particles at any solid
angle. The appearance of the Rutherford scattering equation varies from publication to publication. One shall be shown here. With:

\( N_s \)  
number of scattered particles measured with the detector  

\( N_i \)  
number of incident particles  

\( N \)  
number of atoms per unit volume  

\( t \)  
path length of moving particle in scatter foil  

\( \frac{d\sigma}{d\Omega} \)  
differential cross section  

\( \theta \)  
scattering angle  

\( \Delta\Omega_d \)  
solid angle subtended by detector at the target  

\( Z \)  
charge number of foil nuclei  

\( z \)  
charge number of moving particle  

\( e \)  
elementary charge  

\( pv \)  
momentum and speed of moving particle

the Rutherford scattering formula is:

\[
N_s(\theta) = N_i N_t \cdot \frac{d\sigma}{d\Omega}(\theta) \cdot \Delta\Omega_d
\]  \hspace{1cm} (2-10)

\[
\frac{d\sigma}{d\Omega}(\theta) = \left( \frac{zZe^2}{8\pi\varepsilon_0 pv} \right)^2 \cdot \frac{1}{\sin^4(\theta)}
\]  \hspace{1cm} (2-11)

This formula is true in which the atomic electrons are ignored, and all atoms are independent of each other for the non-relativistic energy range. The same formula is applicable for fast moving electrons in the same approximation.

The first term on the right side of equation (2-11) is a measure of the total cross section, \( \sigma \). The energy of the incident particle is represented by the denominator of the first term in the form of the momentum-velocity product. For non-relativistic energies it equals the double kinetic energy (\( pv = 2T \)). This shows the strong dependency of the cross section on the incident energy (\( \sigma \sim 1/T^2 \)). The total cross section is also proportional to the square of atomic number and hence, to the square of the atomic charge (\( \sigma \sim Z^2 \)).

The second term on the right side of equation (2-11) shows the angular dependency of the cross section. For small angles there is a strong increase in the differential cross section. Since
the Rutherford scattering formula is derived for independent unshielded nuclei, the theoretical total cross section is of infinite size. Charged particles, that pass an unshielded nucleus at greater distance are still influenced by the potential of the nucleus and change their direction by a small fraction. This explains the increasing cross section for small scattering angles.

In the appendix (§A1) the Rutherford scattering formula has been derived in a pure particle model for the non-relativistic case.

2.3.3 Shielding approximations

Rutherford treated the atoms in the scattering material (e.g. gold foil) as independent unshielded nuclei. Hence, Rutherford’s scattering law is true only for an isolated nucleus with \( Z \) protons. However, the electrons of an atom have an influence on the Coulomb field around its nucleus. The negative Coulomb charge of the electrons ‘shields’ the positive Coulomb charge of the nuclear protons. From large enough distances (a few Å), the atom appears to be neutral. It is obvious that this shielding effect on the effective coulomb field has an influence on the scattering distribution derived by Rutherford as the incident particle traverses the electron cloud surrounding the nucleus.

Different attempts were made to take this shielding effect into account. Usually a correction function \( w(r') \) is added to the unshielded potential field around the nucleus (see Scott [35]).

\[
V(r) = \frac{Ze^2}{4\pi\varepsilon_0 r} w(r/r_0) = \frac{Ze^2}{4\pi\varepsilon_0 r} w(r')
\]

The constant \( r_0 \) is the shielding radius, usually taken to be the Thomas-Fermi radius

\[
r_0 = 0.885 a_0 Z^{1/3} = 0.468 \cdot Z^{1/3} \text{ Å}
\]

with \( a_0 \) as the Bohr radius (\( a_0 = h^2/\mu e^2 = 5.292 \cdot 10^{-9} \text{ cm} \)). This correction function leads to another correction function \( q(\theta) \) for Rutherford’s single scatter distribution (see Scott [35]).

\[
\sigma(\theta) = \sigma_{\text{R}}(\theta) \cdot q(\theta) = \left( \frac{Ze^2}{8\pi\varepsilon_0 p\nu} \right)^2 \cdot \frac{1}{\sin^4 \frac{\theta}{2}} \cdot q(\theta)
\]
The simplest way by which the shielding of the atomic electrons may be taken into account is by using an exponential factor.

\[ w(r') = \exp(\mu r') \]

The constant \( \mu \) is a correction factor of order unity that was used by Nigram, Sundaresan and Wu [25] to improve the resulting scatter distribution.

The Thomas-Fermi function (see [21] §14.2.5) assumes the atomic electrons as a continuum. An example of the Thomas-Fermi function is shown in figure 2-9. The variable \( x \) is proportional to the radius \( r \) and the function \( \chi \) is related to the potential \( V \). The function \( \chi \) is given by the following differential equation:

\[
\frac{d^2\chi}{dx^2} = \left\{ \begin{array}{ll}
x^{-1/2} \cdot \chi^{2/3} & \text{for } \chi > 0 \\
0 & \text{for } \chi < 0
\end{array} \right.
\]

with

\[
V(r) = \frac{Ze}{\sqrt{4\pi\varepsilon_0 r}} \quad \chi(r) = Z^{-1/3} bx \\
\quad b = \left( \frac{9}{128\pi} \right)^{1/2} \frac{h^2\varepsilon_0}{me^2}
\]

\[ \chi(x) \]

\[ \text{figure 2-9: Thomas-Fermi function } \chi(x): \chi''(x) = x^{-1/2} \cdot \chi^{2/3}, \chi(0)=1, \chi(\infty)=0 \]

In 1935 Rozental [31] gave a correction function which is a fit to the Thomas-Fermi distribution. It is valid for \( 1 \leq r' \leq 10 \).

\[ w(r') = 0.164\exp(-4.356r') + 0.581\exp(0.947r') + 0.255\exp(-0.246r') \]
Another fit was given by Molière [22] which is valid for $0 \leq r' \leq 6$:

$$w_r(r') = 0.10\exp(-6r') + 0.55\exp(1.2r') + 0.35\exp(-0.3r')$$

### 2.3.4 The Born approximation

This section was mainly taken from [12] §6.9 and [7] §1.5.2. If the amplitude of the scattered wave is small compared to the incident wave amplitude, the total wave amplitude, $\psi(r)$, in the integral of equation (2-9) may be replaced by $\psi_0(r)$, the incident wave amplitude as a first approximation. This is called the first Born approximation.

$$f_1(\Omega) = \frac{-m}{2\pi\hbar^2} \int \exp(-i\mathbf{k} \cdot \mathbf{r'})\psi_0(\mathbf{r'})d^3r'$$

In general this first approximation is very good for weakly scattering fields or objects. For stronger scattering further terms may be calculated in the Born series $\psi(r) = \psi_0(r) + \psi_1(r) + \psi_2(r) + \ldots$ by use of the recurrence relationship

$$f_n(\Omega) = \frac{-m}{2\pi\hbar^2} \int \exp(-i\mathbf{k} \cdot \mathbf{r'})\psi_{n-1}(\mathbf{r'})d^3r'.$$

However, the convergence of this Born series is usually poor if the first order approximation fails. The addition of the second order term improves the approximation over a rather limited range of scattering strengths and is sometimes useful in suggesting the nature of the modifications needed when the first order approximation fails. The higher order terms become rapidly more complicated and difficult to calculate and it is rarely useful to evaluate them.

### 2.3.5 More exact scatter distributions

It is not possible to calculate the differential cross section analytically for all elements. Even a numerical approach requires some approximation. However, numerical calculations for differential cross sections have been published which improve the comparison to measured data (see [29] and [33]).
Some differential cross sections were derived by Riley, MacCallum and Biggs [29]. These calculations were performed relativistically and include shielding effects. Examples for the single differential scatter distribution, $d\sigma/d\Omega(\theta)$, are given in figure 2-10 and figure 2-11.

**figure 2-10:** Single scatter distribution for 128 keV electrons on lead.

**figure 2-11:** Single scatter distribution for 4 keV electrons on uranium.

Riley et al. give the single scatter distributions for various elements and nine energies (1, 2, 4, 8, 16, 32, 64, 128 and 256 keV). They took these distributions and developed a twelve
parameter fit which gives the possibility to evaluate the differential cross section for any scattering angle. The twelve parameter fit is used in ETraST (see §3.3.4).

2.4 Multiple scattering of electrons

2.4.1 Introduction

Once a fast moving electron enters into condensed matter, it undergoes a large number of elastic scattering events. For example, the mean free path between successive elastic collisions for 100 keV electrons in aluminium is 64 nm; in gold it is 8 nm (evaluated with the total cross section of Riley et al [29] and equation (2-13) in section 2.6.1). The average energy loss between two elastic scattering processes for that energy is 55 eV in aluminium and 32 eV in gold (evaluated with the stopping power given in [2]). For example, if the computer simulation is to study the reflection behaviour of fast moving electrons that enter at normal incidence into a reflector, the mean number of elastic collisions per incident electron is about 1,000 to 10,000!

To reduce the computational labour that was above all important in the era of the early slow computers or even before the invention of computers, several multiple scattering theories were introduced. If the single scattering process has a defined scatter distribution, the related distribution after multiple scattering will also have a defined distribution. Some scatter distributions of 128 keV electrons in lead are shown in figure 2-12.

![Figure 2-12: Multiple scatter distributions of 128 keV electrons in lead.](image-url)
The relative intensity gives the probability that an electron is scattered by a given polar angle after a given number of successive scattering processes. The dashed line indicates the probability distribution for electrons with no predominant direction (1/4π). The numerically calculated distribution for one successive scatter event was taken from Riley et al [29]. Then a self written Monte Carlo tool was used to evaluate the multiple scattering distributions (see §3.2 and §3.3).

The multiple scatter theories usually give their distribution as a function of the distance travelled through the medium by the fast moving electrons. The number of elastic collisions for a given distance interval ds varies with a probability distribution that is taken into account.

2.4.2 Different multiple scattering theories

A survey of the ‘classical’ multiple scattering theories is given by Scott [35] and Bethe [3]. A more recent overview was published by Fernández-Vera et. al. [10] which includes aspects of the theories towards computational applications. The ‘classical’ four multiple scattering theories are from Molière [22][23], Snyder and Scott [38][34], Goudsmit and Saunderson [13], and Lewis [17]. They are all closely related mathematically and give accurate results if carefully evaluated. The first two immediately use the approximation of small scattering angles and then an expansion in Bessel functions. Goudsmit and Saunderson developed a theory valid for any angle by using an expansion in Legendre polynomials. Lewis starts from Legendre expansion and then moves over to the limit of small angles, thus establishing the connection between the first three methods. The theories of Molière [23][3] and Goudsmit and Saunderson [13] were studied in more detail in this present work.

In general it can be said that in all four theories the aim was to study the behaviour of high energy electrons in matter, say above 1 MeV. If applied to energies down to 10 keV they either become invalid or too complex for computational applications.

In his publication Molière [23] mentions the variable $B$ that is defined by the transcendental equation

$$\exp(B) = \frac{\Omega_b}{1.167}$$

where $\Omega_b$ is a measure of the number of scattering processes.
The multiple scattering theory of Molière is only valid for values of $B$ above or equal to $\approx 4.5$; that is a value of approximately 20 for $Q_b$. This limit is due to the small angle approximation underlying the multiple scattering theory. Below that value the multiple scattering distributions become less accurate. For the calculation of electron transport in condensed matter the electron track is subdivided into a number of distance step intervals. The lower limit of the variable $B$ leads to a minimum step size for the electron track. If the step size is large, the number of steps will become small and the simulation result will become less accurate. In the following table the minimum step size for fast moving electrons in lead is evaluated and compared with the mean energy loss over this distance.

<table>
<thead>
<tr>
<th>energy (keV)</th>
<th>velocity $\beta = v/c$</th>
<th>min. step size (mg/cm²)</th>
<th>stopping power (keV*cm²/mg)</th>
<th>energy loss (keV)</th>
<th>(%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>0.695</td>
<td>2.89</td>
<td>1.39</td>
<td>4.02</td>
<td>2.01</td>
</tr>
<tr>
<td>100</td>
<td>0.548</td>
<td>2.58</td>
<td>1.96</td>
<td>5.06</td>
<td>5.06</td>
</tr>
<tr>
<td>50</td>
<td>0.413</td>
<td>2.35</td>
<td>3.00</td>
<td>7.05</td>
<td>14.1</td>
</tr>
<tr>
<td>20</td>
<td>0.272</td>
<td>2.19</td>
<td>5.45</td>
<td>11.9</td>
<td>59.6</td>
</tr>
</tbody>
</table>

*table 2-2: Comparison of the min. step size with the mean energy loss for different energies.*

To remain within the valid limit of Molière's theory ($B \geq 4.5$), the energy steps become increasingly larger for smaller energies. A desirable relative energy step would be about 1 %. Since the energy range of interest reaches down to 10 keV, Molière's theory of multiple scattering of electrons is not applicable for the purpose of this work.

The multiple scattering theory of Goudsmit and Saunderson [13] remains accurate for all energies by using an expansion in Legendre polynomials. In general it is possible to apply their theory to any single scattering theory. However, two difficulties arose in trying to apply this theory to the single scattering theory from Riley et al. [29] (see §2.3.4). First, the polynomial series became extremely long for the energy range of interest (10 to 250 keV); and second, even the high precision floating point numbers of a typical computer (8 bytes long) were not accurate enough to evaluate the coefficients of the polynomials towards the end of the series. The problem arises when two numbers are to be added (one positive and one negative) where the sum is much smaller than the two numbers themselves. For example, for $a = -10^{50}$ and $b = 10^{50} + 1$ it is quite difficult for a computer to calculate the exact sum of $a$ and $b$. 


2.4.3 Reasons for not using a multiple scattering theory

There were two reasons for not implementing a multiple scattering theory in the simulation tool ETraST. The first reason is simple: all multiple scattering theories that were studied did not satisfy the requirements of the present application. Molière's theory is valid either for higher energies or for large energy steps; both are not desirable. The Legendre series of Goudsmit and Saunderson's theory become extremely long and difficult to evaluate. It would require much labour to implement this theory on a computer for the energy range of interest (10 to 250 keV). The second reason for not implementing a multiple scattering theory is that for many applications of interest, a large number of electrons leave the scattering medium after only a few elastic collisions. A typical application is the transmission of fast moving electrons through thin foils. Another application is to evaluate the distribution of reflected electrons that entered the reflector with an incident angle below 5° between incident beam and surface of the reflector. A simulation of the latter problem was performed for a gold reflector with 128 keV electrons and different incident angles (between incident beam and surface) using the simulation tool ETraST (see §3.3). The fraction of electrons that have left the target as a function of the number of elastic collisions is shown in figure 2-13. In the case of 0.1° incidence, 50% of the electrons left the reflector after only two elastic collisions. Any multiple scattering theory would produce an error in the distribution of the reflected electrons.

![Figure 2-13](image)

**Figure 2-13:** Fraction of electrons leaving gold reflector as function of the number of elastic collisions for different angles between incident beam and surface of reflector.
Many of the published multiple scattering theories were created in the age of slow computers. Today's computers are faster by a factor between ten and one thousand. While an old computer evaluated the angular distribution after 100 collisions by using a multiple scattering theory, a new computer does it in the same time by simulating all single scatter events. Of course, a faster simulation algorithm would allow simulation of a larger number of electrons in the same time. However, in all the performed simulations, no multiple scattering theory was used and the statistical error (which is due to a limited number of electrons) was acceptably small.

2.5 Stopping power

As a fast moving electron 'walks' through matter, it undergoes a large number of elastic and inelastic scattering events. Since the interest of this paper is rather in the tracks of the moving electrons than in the secondary particles, it is useful to collect all inelastic events into a continuous slowing down approximation (CSDA). Instead of evaluating every inelastic event, a continuous energy reduction is assumed (see figure 2-14).

![Figure 2-14: The continuous slowing down approximation for fast moving electrons.](image)

On a given step through the material the electron loses some energy $dE$ proportional to the step length $dx$. The ratio of energy loss and step length is the stopping power $dE/dx$ (which is the slope of the CSDA in figure 2-14). In the energy range of interest (10 - 250 keV) the main contribution to the stopping power ($\approx 99\%$) comes from excitation and ionisation of the atoms near the electron track $(dE/dx)_c$ (data from Berger and Seltzer [2]). A rather small
contribution (~ 1 %) comes from the energy loss due to production of radiation \((dE/dx)_r\). The subscript \(c\) stands for 'collision loss'; the subscript \(r\) stands for 'radiation loss'. The total stopping power is the sum of both:

\[
\frac{dE}{dx} = \left(\frac{dE}{dx}\right)_c + \left(\frac{dE}{dx}\right)_r,
\]

As mentioned before, the collision loss gives the main contribution to the energy loss of fast moving electrons in the energy region up to 250 keV. An expression for the collision loss has been derived by Bethe (see Knoll [16] §2.II.A):

\[
\left(\frac{dT}{dx}\right)_c = \frac{e^4 N Z}{m_0 c^2} \left(\ln \frac{m_0 c^2 T}{\gamma^2 (\gamma^2 - 1)} - \ln 2 \left[2 \sqrt{1 - \beta^2} - (1 - \beta^2) + (1 - \beta^2)^2 \right]\right)
\]

- \(e\) - elementary charge (1.6022*10^{-19} C)
- \(Z\) - atomic number of absorber
- \(N\) - atomic density of absorber
- \(m_0 c^2\) - rest mass energy of electron (511 keV = 8.18*10^{-14} J)
- \(\beta\) - velocity of electron relative to the speed of light
- \(\varepsilon_0\) - permittivity constant (8.85*10^{-12} C^2/N m^2)
- \(T\) - kinetic energy of electron
- \(I\) - mean excitation and ionisation energy of the absorber

This formula is strictly true if the SI-units are used. If all energies \((dT, m_0 c^2, T\) and \(I\)) are given in eV units then the exponent on the elementary charge \(e\) must be reduced from 4 to 2.

The mean excitation and ionisation energy is specific for each element. The values for \(I\) were taken from Berger and Seltzer [2]. They are 18.7 eV for hydrogen, 42 eV for helium, 38 eV for lithium, 60 eV for beryllium, 78 eV for carbon, 85 eV for nitrogen, 89 eV for oxygen, and 131 eV for neon. For elements with an atomic number greater than 12 there is an empirical relation between \(I\) and \(Z\) (Berger and Seltzer [2]).

\[
I = 9.76 \cdot Z + 58.8 \cdot Z^{-0.19} \quad (in\ eV)
\]
The following graph (figure 2-15) shows the stopping power for three elements in the energy range from 10 keV to 1 MeV. The stopping power is given relative to the density of the element; again, the data were taken from Berger and Seltzer [2].

![Graph showing stopping power for three elements](image)

**figure 2-15**: Stopping power for three elements. Solid lines indicate collision loss, \( (dE/dx)_c \); dashed line at high energy end shows total energy loss including radiation loss.

### 2.6 Free path of the electron between two interactions

The 'free path' is the distance moved by the electron between two collisions with nuclei. The atoms can be imagined to be randomly distributed in a given volume. If an electron enters into this volume it collides randomly with the atoms. The free path, which is the distance between two collisions, is therefore also random. The probability distribution of the free path length is an exponential function. The average distance travelled by the electron between successive collisions is called the 'mean free path' (see [12] §3.1). The probability distribution of the free path is given by

\[
p(x) = \frac{1}{x_{mf}} \cdot \exp \left( -\frac{x}{x_{mf}} \right) \quad (2-12)
\]

where the integrated probability from zero to infinity is one.
\[
\int_0^w p(x)dx = 1
\]

To estimate a random free path, a random number with a homogeneous probability distribution (see § 3.2.3) and the mean free path of the electron, \(x_{\text{mfp}}\), is needed.

### 2.6.1 The mean free path

To estimate the mean free path, \(x_{\text{mfp}}\), the total elastic scatter cross section, \(\sigma_{\text{tot}}\), and the number of atoms per unit volume, \(N\), are needed.

\[
x_{\text{mfp}}(T) = \frac{1}{N \cdot \sigma_{\text{tot}}(T)} = \frac{A}{N_A \cdot \rho \cdot \sigma_{\text{tot}}(T)}
\]  

(2-13)

- \(T\): kinetic energy of moving electron
- \(A\): relative atomic mass
- \(N_A\): Avogadro’s number \((6.022 \times 10^{23} \text{ mol}^{-1})\)
- \(\rho\): density

In figure 2-16, figure 2-17 and figure 2-18 the total cross section and the mean free path for fast moving electrons are plotted for aluminium, silver and tungsten, respectively. The data for the total cross section were taken from Riley et al [29].

*figure 2-16: Total cross section and mean free path for fast moving electrons in aluminium.*
2.6.2 The free path

A random free path with an exponential probability distribution is generated by using a homogeneously distributed random number, $r$ (see §3.2.3), and a mapping function (see §3.2.4). The homogeneously distributed random number, $r$, with a range of $0 \leq r < 1$ is used together with the mapping function, $m(r)$, to get directly the random free path $x_f$ with the desired distribution. The mapping function is generated in two steps.
Firstly the distribution $p(x)$ is integrated. The result is:

$$\int_{x_\text{mfp}}^{x_f} p(x)dx = \frac{1}{x_{\text{mfp}}} \cdot \int_{x_\text{mfp}}^{x_f} \exp\left(-\frac{x}{x_{\text{mfp}}}\right)dx = 1 - \exp\left(-\frac{x_f}{x_{\text{mfp}}}\right) = r$$

Secondly the formula needs to be inversed from $r(x_{fp})$ to $x_{fp}(r)=m(r)$:

$$x_{fp} = -x_{\text{mfp}} \cdot \ln(1-r) = m(r) \quad (2-14)$$
3 Simulation of fast moving electrons in condensed matter

3.1 Available simulation tools

Over the last 30 to 40 years a large number of Monte Carlo codes have been developed that simulate fast moving electrons in matter. An outstanding work was published by M.J. Berger some 35 years ago [1]. Usually the Monte Carlo codes are written for a specific purpose and care is needed when using it for another task. If an available code is used, all implemented formulas and theories should be studied carefully to avoid errors.

Out of the available simulation codes probably the most commonly used code EGS4 is studied in more detail here.

3.1.1 The EGS4 code

EGS4 stands for ‘Electron Gamma ray Shower 4’ and is often called ‘Eggs 4’ [24]. The original version, EGS3, was designed to simulate electromagnetic cascades in various geometries at energies up to a few thousand GeV and down to cut-off kinetic energies of 0.1 MeV for photons and 1 MeV for electrons (see [24] §1.2). This latest version, EGS4, claims extended low limit cut-off energies of 1 keV for photons and a few tens of keV for electrons (see [24] §1.3).

However, for the elastic scattering of fast moving electrons, EGS4 uses Molière’s multiple scattering theory (see §2.4.2). Molière himself gives limits for his theory which are exceeded for low energies (see table 2-1 in §2.4.2). It may be that the results from EGS4 in this low energy region are still correct but the code must be treated very carefully, especially for the angular distribution of electrons. The EGS4 code studied dated from 1995 (see [24]).

Since the energy of interest in this paper goes down to 10 keV the approach of simulating with EGS4 was rejected.
3.2 The Monte Carlo algorithm

3.2.1 Introduction

A significant part of this introduction are taken from [28] §7.6.

Monte Carlo is a numerical random process to solve integrals. Suppose $N$ random points $r_1, ..., r_N$, uniformly distributed in a multidimensional volume $V$. Then the basic theorem of Monte Carlo integration estimates the integral of a function $f(r)$ over the multidimensional volume $V$ by

$$\int f \, dV \approx V \cdot \langle f \rangle \pm V \sqrt{\frac{\langle f^2 \rangle - \langle f \rangle^2}{N}} \quad \text{with}$$

$$\langle f \rangle = \frac{1}{N} \sum_{i=1}^{N} f(r_i) \quad \langle f^2 \rangle = \frac{1}{N} \sum_{i=1}^{N} f^2(r_i)$$

The 'plus-or-minus' term is a single standard deviation error estimate for the integral.

Suppose we have a two-dimensional function $g(x, y)$ which needs to be integrated over a region $W$. To solve this integral with the Monte Carlo algorithm a simple shaped region $V$ is defined that encloses the region $W$ (e.g. see figure 3-1).

![figure 3-1: A simple Monte Carlo integration](image-url)
A function $f(x,y)$ is defined to be equal to $g(x,y)$ for points in the region $W$ and equal to zero for points outside. Now a large number of randomly distributed points in $f(x,y)$ in the region $V$ is summed up by the above equation to solve the integral of $g(x,y)$ in the region $W$.

The region $V$ should enclose $W$ as close as possible since the zero values of $f(x,y)$ will increase the error of the integral.

3.2.2 Monte Carlo algorithm to simulate electron tracks in matter

Once an electron enters matter it performs a random walk due to many single scatter events (see figure 3-2).

![figure 3-2: Random walk of electrons in matter](image)

The random walk of the electron is hard to evaluate on an analytical basis. The Monte Carlo technique is a useful instrument to solve this problem. The major events are nuclear scattering and energy loss due to ionisation, excitation and the production of bremsstrahlung. The procedure to simulate an electron track involves a loop with the following three steps:

1. **Move the electron by a random free path**
   The electron has a free path between two events. Although the free path is random it obeys an exponential probability distribution with a given mean free path (see § 2.6). If the electron leaves the absorber, the loop must be interrupted at this point.

2. **Evaluate the energy loss, e.g. continuous slowing down approximation (CSDA)**
   As the fast electron moves through the material it consistently loses energy (see §2.5). The different inelastic events are collected in the continuous slowing down approximation
(CSDA) leading to an average stopping power for the electron. If a fast moving electron reaches a lower energy limit it is counted as being absorbed.

3. Change direction of electron by a random scatter angle

Like the free path, the scatter angle of a single scatter event is truly random but obeys a probability distribution (see § 2.3). In this step a scattering angle is evaluated and the new direction of the electron is calculated.

Repeating these three steps again and again, the ‘random walk’ of an electron (electron track) is simulated (e.g. see figure 3-3). With a large number of electron tracks some new probability distributions can be evaluated. For example if a large number of electrons are fired normally onto a surface it is possible to calculate the angular and energy probability distribution of the back scattered electrons.

![Figure 3-3: Example of four random walks of 150 keV electrons in tungsten.](image)

Simulations with the Monte Carlo technique are not equivalent to analytical solutions; a statistical error always remains. Monte Carlo Simulations should be regarded as numerical experiments.

3.2.3 A homogeneously distributed random number generator

Random numbers are the heart of Monte Carlo algorithm. However, it would be a mistake to simply use and trust a built-in random number generator. Most of them do not meet the
requirements of a Monte Carlo algorithm. Hence some attention is paid to the random number generator in this section. A good overview of random number generators is given in reference [28] §7.1.

The first question that arises is: What is a good random number generator? This sounds almost like a philosophical question. Is there true coincidence? For a computer the answer is no. A random number generator always gives a sequence of reproductive numbers. Unlike true random numbers it is possible to predict the next number of such a generator. However, a good random number generator gives a sequence of calculated numbers which behave like true random numbers. Their statistical probability behaviour is equal at any time.

Beside this general statement there are some more specific criteria by which a random number generator should be examined:

A) The period of repetition
Some system supplied random generators give a sequence of numbers with a fairly short repetition period. If the number of required random numbers in one Monte Carlo simulation exceeds the repetition period of the random number generator then it will not achieve any further statistical enhancement.

B) Homogeneous distribution for multidimensional applications
A simple random number generator often has the disadvantage of sequential correlation on successive calls. If \( n \) random numbers at a time are used to plot points in an \( n \)-dimensional space the points tend to concentrate on \( (n-1) \)-dimensional planes. In [28] on page 277 an example of a wide spread random number generator is given were they found as few as 11 planes in a three-dimensional space.

C) Homogeneous distribution for higher and lower bits
If two low precision random numbers are needed they should not be drawn from one random number. Some random number generators have a good performance if the entire number is used. But if the low significance bits (LSBs) are evaluated by themselves, they give a rather poor performance.

A standard (linear congruential) random number generator is given by the following equation:
where $r_i$ is the random number and $a$, $c$ and $m$ are the constants for the generator. The modulo operator ensures that the random number does not exceed the upper limit of $m-1$. A good choice of the constants makes sure that the random number sequence repeats only after $m$ numbers. Some useful triplets are given in the following table. Although the resulting number is always smaller than $m$, the temporary result (before the modulo operation) might be larger. The fourth column gives the upper limit of the temporary result.

<table>
<thead>
<tr>
<th>$a$</th>
<th>$c$</th>
<th>$m$</th>
<th>lower than</th>
</tr>
</thead>
<tbody>
<tr>
<td>106</td>
<td>1283</td>
<td>6075</td>
<td>$2^{20}$</td>
</tr>
<tr>
<td>419</td>
<td>6173</td>
<td>29282</td>
<td>$2^{24}$</td>
</tr>
<tr>
<td>2041</td>
<td>25673</td>
<td>121500</td>
<td>$2^{28}$</td>
</tr>
<tr>
<td>4096</td>
<td>150889</td>
<td>714025</td>
<td>$2^{32}$</td>
</tr>
</tbody>
</table>

table 3-1: Some constants for the random number generator (3-1) taken from [28] page 285.

There is good evidence [28] that a simple multiplicative congruential algorithm

$$r_{i+1} = a \cdot r_i \pmod{m}$$

(3-2)

can be as good as the one given in (3-1) with $c \neq 0$. But the multiplier $a$ and the modulus $m$ must be chosen very carefully. Some possible choices of $a$ and $m$ are listed in the following table.

<table>
<thead>
<tr>
<th>$a$</th>
<th>$m$</th>
<th>lower than</th>
</tr>
</thead>
<tbody>
<tr>
<td>$7^5=16807$</td>
<td>$2^{31}-1=2147483647$</td>
<td>$2^{46}$</td>
</tr>
<tr>
<td>40014</td>
<td>2147483563</td>
<td>$2^{47}$</td>
</tr>
<tr>
<td>40692</td>
<td>2147483399</td>
<td>$2^{47}$</td>
</tr>
</tbody>
</table>

table 3-2: Some constants for the random number generator (3-2) taken from [28] page 278 and 281.
Although the random number $r_i$ is in the range of a 32-bit integer the temporary result (third column) can become very large and exceeds the capabilities of a 32-bit machine. A trick developed by Schrage [27], for multiplying two 32 bit integers with respect to a 32-bit modulus without using any intermediates larger then 32 bits (including a sign bit), is therefore extremely interesting. Schrage's algorithm is based on an approximate factorisation of $m$

$$m = ap + q \quad \text{with} \quad p = \lfloor m/a \rfloor \quad \text{and} \quad q = m \mod a,$$

the square brackets denoting the integer part. If $q$ is small, specifically $q<p$, it can be shown that both $a(r_i \mod p)$ and $q[r_i/p]$ lie in the range of $0 \ldots m-1$, and that

$$r_{i+1} = a r_i \mod m = \begin{cases} a(r_i \mod p) - q[r_i/p] & \text{when } \geq 0 \\ a(r_i \mod p) - q[r_i/p] + m & \text{otherwise} \end{cases}$$

(3-3)

In the following an example of a simple random number generator written in C is given. The computational environment is the same as for the ETraST code (see § 3.3.2). It uses the multiplicative congruential algorithm with Schrage's method.

```c
#include <stdio.h>
#include <stdlib.h>
#define RANO_M 2147483647 // range of integer random number: 0 ... M-1
#define RANO_A 16807 // multiplier of random number generator
#define RANO_Q 127773 // integer part of M/A
#define RANO_R 2836 // M modulo A

float ran0(long SetRi=0);

int main()
{
    int i;
    ran0(2); // set random number generator
    for(i=0; i<20; i++) // get and print 20 random numbers
        printf("%f\n", ran0());
}

float ran0(long SetRi)
{
    static long ri=1;
    long k;
    float number;
    if(SetRi!=0) ri=abs(SetRi); // Set start value.
    k = ri/RANO_Q; // Evaluate new random number
    ri = RANO_A*(ri-k*RANO_Q)-RANO_R*k; // by Schrage's method.
    if(ri<0) ri += RANO_M;
```
3 Simulation of fast moving electrons in condensed matter

number = ri*1.0/RAN0_M; // convert ri to float number
return number;

Figure 3-4: Source code of a simple random number generator.

A shuffling procedure may be used to break up sequential correlation of a simple standard generator (see figure 3-5). An array with N elements is filled with random numbers. The previous random number ‘ran’ is used to choose a random number from the array (1. step). The chosen random number is taken from the array to the output of the generator (2. step). Finally, the gap in the array is refilled by a new standard random number.

Figure 3-5: Shuffling procedure to break up sequential correlation.

Of course, this shuffling procedure takes up more memory and, even worse, more computational time. However, it is worth it to obtain better random numbers.

If a longer sequence of random numbers is needed, as the one given in the example, two different random number generators may be combined. The new period is then the least common multiple of the two single periods. The principle is to add two random numbers of two independent generators and then to modulo the modulus of either of the generators. The prerequisite is that the value of the two moduli of the two generators $m_1$ and $m_2$ are close together.

For example two generators with the 2\textsuperscript{nd} and 3\textsuperscript{rd} constant set from table 3-2 are assumed. Two random numbers $r_a$ and $r_b$ are generated in the range of 1...$m_1$ and 1...$m_2$ respectively. In order not to exceed the range of a 32 bit integer at any time it is convenient to subtract the two random numbers $r_a$-$r_b$ and then to add $m_2$-1 if the result is zero or smaller. The period of this
generator is extremely long. The two single periods \(m_1 = 2^631\times 81031\) and \(m_2 = 2^2\times 19\times 31\times 1019\times 1789\) share only the factor 2, so the period of the combined generator is \(= 2.3\times 10^{18}\).

For the calculations in this paper a rather complicated and (unfortunately) slower random generator was implemented. This generator uses two simple random number generators as given in (3.2). The first flow of random numbers is shuffled in an array with 50 elements to break up sequential correlation (see figure 3.5). Then to every shuffled random number a second random number is added, as described in the previous paragraphs, to increase the period of repetition. In [28] on page 281 this generator is described as 'perfect' with $1000 offered to the first reader who finds the generator to fail in a nontrivial way.

### 3.2.4 A random number generator with a given probability distribution

A key for effective Monte Carlo computation lies in random number generators with a given probability distribution (see [28] §7.2). A desired probability distribution is achieved by a homogeneously distributed random number generator and a mapping function (figure 3.6).

![figure 3-6: Mapping function to generate a random number with a desired distribution.](image)

The mapping function is generated in two steps. The first step is to integrate the desired distribution; the second step is to evaluate the inverse of the integrated function. As an example the mapping function for a sine half wave distribution shall be evaluated. The probability distribution must not be smaller than zero at any point in the range of definition. Also, the integral in the range of definition must be one. For the sine half wave the cosine
function in the range from \(-\pi/2\) to \(\pi/2\) was chosen. The integral of the raw cosine function in the range of definition is 2; hence a factor of 0.5 must be included to the probability distribution function to reduce the area to 1.

\[
p(x) = \frac{1}{2} \cos x
\]

The desired distribution is shown in figure 3-7.

**figure 3-7: Example of a desired probability distribution.**

Now the first step is to integrate the distribution function from the minimum range on.

\[
\int_{x_{min}}^{x} p(x') dx' = \frac{1}{2} \int_{-\pi/2}^{\pi/2} \cos(x') dx' = \frac{1}{2} [1 + \sin x]
\]

The result is a function that increases from zero at the minimum range to one at the maximum range. The slope is always greater or equal zero. The integrated probability distribution of a sine half wave is shown in figure 3-8.
The second step is to inverse the integrated probability distribution. This equals the exchange of the axes of the coordinate system. In the case of the sine half wave the integrated function

\[ x = \frac{1}{2} [1 + \sin(M(x))] \]

becomes

\[ M(x) = \arcsin(2x - 1). \]

The example of the mapping function, \( M(x) \), of a sine half wave is shown in figure 3-9.
For computing on a machine this function might be evaluated either analytically or numerically. For a simple distribution like the sine half wave or an exponential distribution the analytical way may be preferred. For more complicated distributions the numerical evaluation is a simple way to generate the mapping function. Attention must be paid to the resolution of the mapping function.

3.3 The simulation tool ETraST

Why is it necessary to write yet another Monte Carlo simulation tool? There are two reasons to write this simulation tool. Firstly all available codes which were studied use a multiple scattering theory, mainly that of Molière. They are good for high energies and a large number of single scatter events. ETraST does not use any multiple scattering theory since some electron tracks have as few as one (or even zero) scatter events. Secondly, even if a simulation tool exists which is useful for the tasks in this paper, writing a new one is a perfect way to get into the subject. For example, it took several months before the limits of Molière’s theory were appreciated and that approach was rejected. The details of a Monte Carlo simulation tool must be studied carefully to avoid errors in the simulation results.

3.3.1 The task of ETraST

ETraST (Electron Trac \textit{k} Simulation Tool) is written for energies between 5 and 250 keV. The aim is to follow the track of primary electrons; hence all secondary electrons or photons are neglected. Great attention was paid to the angular and energy distributions of back scattered electrons. In particular small incident angles (relative to the scatterer surface) were of great interest (see §7.1).

3.3.2 Environment

The ETraST code was written on and for a Pentium, IBM compatible personal computer (133 MHz) with the Microsoft Windows95\textsuperscript{TM} system. The Object Windows Library of the Borland C++ 5.01 compiler was used. ETraST is a mixed on-line and batch controlled tool.

The simulation times of the results performed for this work varied from a few seconds to a week. The simulation time is proportional to the number of elastic scatterings calculated.
during run time. Hence, the simulation time increases with number of electrons, range between incident and low limit energy, number of data sets etc.

A useful procedure is to perform a pre-run with, say, 1000 electrons per set, and then to use the simulation time (which is always stored at the end of each output file) to estimate an appropriate number of electrons. Since the time for the preparation of the simulation is always a few seconds, independent of the number of electrons, it is neglected in the stored simulation time.

### 3.3.3 Structure

ETraST is structured around the physical behaviour of fast moving electrons in matter. The various computational steps are all implemented in separate blocks (C++ objects). The different blocks are:

- RefractionClass (including specular reflection)
- FreePathClass (between successive scatter events)
- ScatterClass (all elastic events except refraction)
- EnergyClass (all inelastic events)
- UserFileClass (to read the user files)

The last block is a tool to read the user files and give messages if there are any errors. The five blocks are collected in the ‘ToolClass’ block which provides all required tools for the simulation block ‘SimulationClass’. The simulation is controlled by the ‘EtrastClass’ block.

The random number generator is implemented in an extra block ‘Ran2’ since it is fairly complicated (see 3.2.3). It also has the ability to store and restore itself at any time. This is important for interrupting a simulation and still getting results which can be reproduced.

An overview of all classes is given in figure 3-10.
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3.3.4 Implementation

The ETraST source code is organised in a Borland C++ project containing different files. The sum of all ASCII source file sizes is 146 KB which is 4000 lines of code. It is not the aim of this chapter to show exactly how every routine of ETraST is implemented or even to give the source code. The aim is to give references to all physical data which are required for the simulation and how to use them. Special attention is given to the four blocks 'RefractionClass', 'FreePathClass', 'ScatterClass' and 'EnergyClass' which describe the physical behaviour of fast moving electrons. So far scattering in seven elements, namely aluminium, copper, silver, tungsten, gold, lead and uranium has been implemented in ETraST.

Refraction of fast moving electrons 'RefractionClass'

This block contains only one function. This function covers both the case fast moving electrons which enter the material and fast moving electrons which leave the material. For the calculation three parameters are needed: the direction of the incident electron, its energy, and the mean inner potential of the material. The energy and the mean inner potential is needed to evaluate the refractive index from vacuum into the material. The incident angle is required to calculate the transmission angle and to evaluate the reflection coefficient with Fresnel's law.
The equations are given in chapter 2.2.3. It is important to use the square of the reflection amplitude to evaluate the reflection coefficient \((R^2/A^2)\). The reflection coefficient is in the range between zero and one and can be compared with a homogeneously distributed random number to decide whether or not an electron is reflected.

**Free path between two elastic collisions 'FreePathClass'**

The mathematics for the free path calculation is described in § 2.6. The probability distribution always obeys an exponential function. What needs to be calculated is the mean free path for any energy in a given material.

\[
x_{\text{mfp}}(T) = \frac{A}{N_A \cdot \rho \cdot \sigma_{\text{tot}}(T)}
\]

The atomic weight \(A\), Avogadro’s number \(N_A\) and the density \(\rho\) are the well known constants. The total cross section \(\sigma_{\text{tot}}(T)\) was taken from Riley et al [29]. In this article the cross sections are listed for the energies 1, 2, 4, 8, 16, 32, 64, 128 and 256 keV. During preparation ‘PrepareFreePath’ the mean free path is calculated for energies from 0 to 256 keV in 1 keV steps and stored in an array with 257 elements. Since the mean free path gives nearly a straight line on a log-log scale, the interpolation between the given mean free path has been done using the function

\[
x_{\text{mfp}}(T) = b \cdot T^m
\]

where \(m\) and \(b\) are two constants given by the two neighbouring values for the mean free path. For any energy of the fast moving electron the mean free path becomes

\[
x_{\text{mfp}}(T) = x_{\text{mfp}1} \cdot \exp \left( \frac{\ln x_{\text{mfp}2}}{\ln \frac{T_2}{T_1}} \cdot \ln \frac{T}{T_1} \right)
\]

where \(T_1\) and \(T_2\) stands for the given energies below and above the energy of interest and \(x_{\text{mfp}1}\) and \(x_{\text{mfp}2}\) are the two mean free paths respectively.
Elastic scattering of fast moving electrons 'ScatterClass'

For the single scatter distribution a 12 parameter fit from Riley et al [29] was used to provide the input data. The fit function is

\[
\sigma(\theta) = \sum_{m=1}^{4} A_m (1 - \cos \theta + 2B)^m + \sum_{n=0}^{6} C_n P_n(\cos \theta)
\]

where \(A_1, \ldots, A_4, B)\) and \(C_0, \ldots, C_6\) are the constants taken from the Riley tables and \(P_0\) to \(P_6\) are the well known Legendre polynomials. The constants are listed for 80 elements for energies of 1, 2, 4, 8, 16, 32, 64, 128 and 256 keV.

Out of these distributions mapping functions are evaluated on a numerical basis (see § 3.2.4). For the temporary calculations an array with 10,000 elements was used. The final mapping functions are stored in arrays with 1,800 elements.

Firstly a procedure was implemented which evaluates the absolute scatter cross section for any angle by using the 12 parameter fit. The normal procedure to generate the mapping function would be to normalize the distribution to an area of unity and then to integrate and finally inverse the function. However, in order to save CPU time the absolute distribution is integrated immediately. The last value of the integration array is at the same time the normalisation factor. All elements of the integration array must be divided by the last element to normalize the function. The final step is to inverse the integrated normalized function into the final array of the mapping function. The mapping functions are evaluated for seven energies (4, 8, 16, 32, 64, 128 and 256 keV).

During runtime the scatter cross section between two points in the mapping function is linearly interpolated; the scatter cross section between two energies is interpolated with an exponential function.

In their article Riley et al gave the differential scatter cross section in two different sets of tables. The first set is for 22 selected elements and gives the absolute values of the differential cross sections for various angles. The second set is a 12 parameter fit for as many as 80 elements. During this work it was found that the second set of tables has an error which is constant over the angle but varies with energy and atomic number. The fitted cross sections of
the second set of tables were integrated to the total cross sections and then compared with the total cross sections of the first set of tables. With \( \sigma_{\text{tot}1} \) and \( \sigma_{\text{tot}2} \) as the total cross sections from the first and second set of tables the following equation has been derived:

\[
\sigma_{\text{tot}1} = 2.827 \cdot 10^{-9} \cdot Z^2 \cdot \frac{1 - \beta^2}{\beta^4} \cdot \sigma_{\text{tot}2}
\]

with \( \beta \) being the velocity of the fast moving electron relative to the speed of light and \( Z \) the atomic number of the element. With this equation the total cross sections for the elements which have not been listed in the first table can be evaluated.

**Energy loss of fast moving electrons ‘EnergyClass’**

In ETraST the energy loss of a fast moving electron is calculated by the stopping power in the continuous slowing down approximation CSDA (see § 2.5). The stopping power data \( dT/dx \) were taken from Berger and Seltzer [2]. They are listed for many elements and some compounds; the energy range is from 10 keV to 1 GeV. From 10 to 100 keV the stopping power is listed in 5 keV steps; from 100 to 1000 keV in 50 keV steps.

During preparation of the simulation ETraST stores the stopping power in a 50 element array for the energies 5 to 250 keV. On a log-log scale the stopping power variation with energy gives almost a straight line; hence the interpolation to get the missing values above 100 keV is done using the equation

\[
F_{sp}(T) = b \cdot T^m
\]

where \( m \) and \( b \) are two constants given by the two neighbouring points of the stopping power. For any energy of fast moving electrons between two given values, the stopping power becomes

\[
F_{sp}(T) = F_{sp1} \cdot \exp \left( \ln \frac{F_{sp2}}{F_{sp1}} \cdot \frac{\ln \frac{T}{T_1}}{\ln \frac{T_2}{T_1}} \right)
\]

where \( T_1 \) and \( T_2 \) stand for the given energies below and above the energy of interest and \( F_{sp1} \) and \( F_{sp2} \) are the two stopping powers respectively. The missing stopping power for 5 keV was evaluated by the expression given in § 2.5.
During simulation the stopping power between two values of the 50 element array are linearly interpolated.

### 3.3.5 How to use ETraST

First of all an input file for ETraST must be created. The input file contains information about the simulation type, the number of data sets, the incident energy and so on. There are five different simulation types implemented in ETraST. They are listed in the appendix together with the syntax of the input file.

In this section the usage of ETraST is shown in an example. The energy and angular distribution of back-scattered electrons from a semi-infinite reflector is investigated. The incident energies are 100 and 200 keV. The incident angles between incident electrons and the surface of the reflector are 5 and 10 degrees. An input data file with the following content is created:

<table>
<thead>
<tr>
<th>Reflection</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>10</td>
</tr>
<tr>
<td>100</td>
<td>10</td>
</tr>
<tr>
<td>200</td>
<td>20</td>
</tr>
<tr>
<td>200</td>
<td>20</td>
</tr>
</tbody>
</table>

*figure 3-11: An example input data set.*

It is assumed, that the executable ETraST code is installed on a Pentium computer under the Windows95 system. After the tool has been started it presents itself as in figure 3-12.

*figure 3-12: ETraST just after it is started.*

Now three things need to be done before the simulation may be started.
The first step is the choice of element for the reflector. The second menu item <Element> contains all seven available elements, namely aluminium, copper, silver, tungsten, gold, lead and uranium. This may be done either by mouse click or the keyboard using the <Alt> button and the underlined letter in the menu (see figure 3-13).

![Figure 3-13: ETraST: The choice of an element.](image)

The second step is to load the input file. The first menu item <Control> pops up a second menu of which the first line <Input file> opens the input dialogue box (see figure 3-14). This is the standard file open dialogue box of Windows95. After choosing an input file and pressing the open button the ETraST window shows the name and the path of the chosen file.

![Figure 3-14: ETraST: Choice of an input file.](image)
Thirdly the number of electron histories to be simulated is entered. This is the number of electrons per data set. The second line <Number of electrons> in the <Control> pop up menu opens the dialogue box to enter the number of electrons (see figure 3-15). This number must be between 1 and 1,000,000,000.

![Figure 3-15: ETraST: Entering the number of electron histories to be simulated.](image)

Now the simulation may be started. This happens by selecting the third line <Start simulation> in the <Control> pop up menu (see figure 3-16).

![Figure 3-16: ETraST: How to start the simulation.](image)

After the simulation process has been started, ETraST does some preparation for the main simulation procedure. The status (fourth line in the ETraST window) changes from ‘Doing nothing ...’ to ‘Preparation ...’ (see figure 3-17). This part takes only a few seconds.
3 Simulation of fast moving electrons in condensed matter

figure 3-17: ETrasT: The preparation process (only a few seconds).

After all preparations are completed, the main simulation process begins. The status line (fourth line) shows which data set is currently simulated; the gauge bar shows how far the current data set has been simulated (see figure 3-18). The simulation time depends on the number of electron histories and on the simulation set-up. For example, if electrons enter a surface at a very small angle it is likely that some of them leave the surface after only a few collisions; hence only a small calculation time is needed.

figure 3-18: ETrasT: The simulation runs!

Depending on the simulation type various output files are generated. In this example four output files are generated, one file for each data set. A summary of the first file is shown below:
### Simulation of fast moving electrons in condensed matter

- **material**: W
- **incident angle**: 5 deg
- **incident energy**: 100 keV
- **minimum energy**: 10 keV
- **total number**: 10000
- **table**: energy; polar angle; azimuth angle
- **units**: keV; rad; rad

<table>
<thead>
<tr>
<th>Energy</th>
<th>Polar Angle</th>
<th>Azimuth Angle</th>
</tr>
</thead>
<tbody>
<tr>
<td>93.3621</td>
<td>2.43949</td>
<td>0.392004</td>
</tr>
<tr>
<td>63.7552</td>
<td>1.95116</td>
<td>7.86869</td>
</tr>
<tr>
<td>88.7503</td>
<td>2.47809</td>
<td>0.502839</td>
</tr>
<tr>
<td>68.913</td>
<td>2.58596</td>
<td>-6.71013</td>
</tr>
</tbody>
</table>

...  
...  
...  
99.4065 1.72545 0.226025  
37.5323 2.47354 -8.41416  

**Simulation time**: 0:03:58.06 (238.06 s)

---

**Figure 3-19: Summary of the first output data set.**

The first ten lines give some general information about the simulation set-up. The sixth and the seventh line show the structure of the following table. The three numbers stand for energy, polar angle and azimuth angle; the units are keV for the energy and radians for the two angles. A polar angle of zero represents an electron which arrives normal to the surface. All back scattered electrons must have a polar angle in the range from $\pi/2$ to $\pi$. The azimuth angle is the direction of the electron around the axis normal to the surface. The zero azimuth angle lies on the plane of incidence in the forward direction.

The last line of the output file gives the simulation time for this data set. It is helpful to estimate the simulation time of larger data sets in advance of a run.

The output files may be evaluated with some simple programs written in any language. The output files are in ASCII format; the simulation output data always start at the eleventh line. The numbers in one line are separated by a TAB character; the last line may be recognised by the 's' of 'simulation time' in the first column.
3.4 Benchmarking

For benchmarking, two transmission curves in aluminium were simulated and compared with published data. The transmission curve is the fraction of transmitted electrons through a foil as a function of the foil thickness (see figure 3-20).

\[ \text{aluminium foil} \]
\[ \text{incident electron beam} \quad \rightarrow \quad \text{transmitted electrons} \]
\[ \text{foil thickness} \]

Figure 3-20: The principal set-up to evaluate the transmission curve.

It is usual to write the foil thickness, \( z \), relative to the mean range of the fast moving electrons, \( r_0 \), which is the total path length moved by the electron in the continuous slowing down approximation (CSDA). The mean range in aluminium is 21.1 and 68.9 \( \mu \)m for 50 and 100 keV respectively. For comparison the measurements of Dupouy et al [8] and the transmission curves from Seltzer and Berger [37] were used. The Seltzer and Berger curves were also evaluated on a theoretical basis, but they collected a number of measured data and found their transmission curves to be in good agreement with the measured points. The following graphs show the transmission curves for aluminium with incident energies of 50 and 100 keV. For each transmission curve 500,000 electrons were simulated.

Both transmission curves evaluated with ETraST are in good agreement with the simulation results from Seltzer and Berger and the measurements taken by Dupouy et al. The remaining errors may have different sources: One is the input data for the simulation tool. The mean free path, the angular distribution for elastic scattering and the stopping power may contain inaccuracy that influence the simulation result. E.g., a greater stopping power would shift the transmission curve to the left, closer to the measured points in the 50 keV graph.
Another source of error might be due to the fact that the simulation tool ETraST neglects all secondary rays. For example, for very thin foils, say less than 5% of the mean range, the transmitted electron flux is stronger than the incident electron flux due to secondary electrons (see the top left end of the 100 keV graph). However, this effect becomes more important for higher energies (see Seltzer and Berger [37]).

Finally, and this might be a major error source, the measured data from Dupouy et al [8] may contain some inaccuracy. From the experiments described in section 5 it is known how difficult it can be to normalize measured results.

The overall agreement is very satisfying and gives confidence in the other simulation results. Another benchmark was established with our own experimental measurements. These measurements and the comparison with the simulated data are shown in section 5.
4 Electron trajectories in an electric field in vacuum

The aim of this work is to study the behaviour of fast moving electrons in vacuum and in matter. Although the evaluation of fast moving electron tracks in vacuum with an external electric field has been studied and widely investigated (e.g. [5][36]), it is the combination of electron tracks in vacuum and in matter which is of interest in this thesis. For the purpose of completeness the evaluation of electron tracks in vacuum is shown in this chapter.

Although there exist several simulation tools that evaluate electron tracks in vacuum, the theory described in this section has been implemented into a computer program. This is justified by the aim to combine the evaluation of electron tracks in vacuum (this section) and in matter (see §3).

Since this thesis is only concerned with low current electron beams, the effect of space charge is neglected. With this assumption the evaluation of the electric field and of the electron tracks in this field can be divided into two independent steps. The first step is the evaluation of the electric field (see §4.1); the second step is to calculate the electron track within the electric field (see §4.2).

4.1 The electric field

4.1.1 Laplace's equation

To derive Laplace's equation Maxwell's third equation is used:

\[ \oint_{\text{surface}} \mathbf{D} \cdot d\mathbf{A} = \iiint_{\text{volume}} \mathbf{\rho} \cdot d\mathbf{V} \]

Following the treatment of [5] §9-2 this equation may be applied to an elemental volume \( \Delta V = \Delta x \Delta y \Delta z \) as shown in figure 4-1.
The electric flux vector $\mathbf{D}$ is resolved into the rectangular components $x$, $y$ and $z$. For the elemental volume $\Delta V$ Maxwell's third equation becomes

$$
\iint_{\text{surface}} \mathbf{D} \cdot d\mathbf{A} = \frac{\partial D_x}{\partial x} \Delta V + \frac{\partial D_y}{\partial y} \Delta V + \frac{\partial D_z}{\partial z} \Delta V = \rho_v \cdot \Delta V
$$

which is Gauss's law.

In the limit as $\Delta V$ approaches zero:

$$
\frac{\partial D_x}{\partial x} + \frac{\partial D_y}{\partial y} + \frac{\partial D_z}{\partial z} = \rho_v.
$$

With $D_x = E_x \varepsilon$ and $E_x = -\frac{\partial \phi}{\partial x}$ for the $x$ component and for the $y$ and $z$ components likewise, the previous equation may be written as

$$
\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} = -\frac{\rho_v}{\varepsilon}
$$
which is Poisson’s equation that relates the potential field to the charge distribution.

In an x-ray tube with negligible space charge between the conductors \((\rho_V = 0)\), Poisson’s equation reduces to Laplace’s equation

\[
\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} = 0.
\]

To solve Laplace’s equation with a computer on a numerical basis, a three-dimensional lattice must first be constructed. This lattice contains a large number of cubes with the edges \(\Delta x\), \(\Delta y\) and \(\Delta z\). Each point \((i, j, k)\) has a potential, \(\varphi_{i,j,k}\). The six neighbouring coordinates are \(\varphi_{i-1,j,k}\), \(\varphi_{i+1,j,k}\), \(\varphi_{i,j-1,k}\), \(\varphi_{i,j+1,k}\), \(\varphi_{i,j,k+1}\) and \(\varphi_{i,j,k-1}\). Substituting into Laplace’s equation this becomes

\[
\frac{\varphi_{i-1,j,k} - 2\varphi_{i,j,k} + \varphi_{i+1,j,k}}{(\Delta x)^2} + \frac{\varphi_{i,j-1,k} - 2\varphi_{i,j,k} + \varphi_{i,j+1,k}}{(\Delta y)^2} + \frac{\varphi_{i,j,k-1} - 2\varphi_{i,j,k} + \varphi_{i,j,k+1}}{(\Delta z)^2} = 0.
\]

If the lattice is constructed in such a way that \(\Delta x\), \(\Delta y\) and \(\Delta z\) are equal, the previous equation reduces to a single common denominator and can be written as

\[
\varphi_{i,j,k} = \frac{\varphi_{i-1,j,k} + \varphi_{i+1,j,k} + \varphi_{i,j-1,k} + \varphi_{i,j+1,k} + \varphi_{i,j,k+1} + \varphi_{i,j,k-1}}{6}. \tag{4.1}
\]

This equation is the basis for all further calculations.

4.1.2 The potential field

The numerical evaluation of the potential field is a standard theory (e.g. [36]). To calculate the potential field of an x-ray tube (or any other charged object) a lattice consisting of variable and fixed potential coordinates is needed. The fixed coordinates are for the boundary conditions of the potential field, i.e. the walls of the x-ray tube. These coordinates have a fixed potential and require no further calculations. The variable coordinates are the potentials that need to be calculated, i.e. inside the vacuum in an x-ray tube.

In figure 4-2 a typical x-ray tube for industrial applications is shown. In many cases the three-dimensional potential field can be reduced to two dimensions. In this example the potential
field distribution does not change in the third dimension, hence a two-dimensional lattice is sufficient to evaluate the potential field.

![Figure 4-2: Geometry of the Philips industrial x-ray tube MCN 225.](image)

In figure 4-3 to figure 4-5 the true geometry of the x-ray tube is replaced by a lattice with fixed and variable mesh points. The fixed points are indicated by dots. The black and grey dots indicate zero and high negative voltage on the anode and cathode respectively. Since the x-ray tube is vertically symmetrical, it is sufficient to evaluate the potential field only for one half of the tube.

![Figure 4-3: Top half of the Philips MCN 225 x-ray tube.](image)
Establishing values between zero and one \((0 \leq \varphi \leq 1)\) simplifies the calculations. To find the absolute potential, the evaluated relative values must be multiplied by the maximum voltage.

For the calculations equation (4-1) must be reduced to two dimensions:

\[
\varphi_{i,j} = \frac{\varphi_{i-1,j} + \varphi_{i+1,j} + \varphi_{i,j-1} + \varphi_{i,j+1}}{4} \tag{4-2}
\]

This is the key equation to evaluate a potential field which is constant in its third dimension.

There are two ways to evaluate the potential field with equation (4-2). One is the direct solution the other one is the relaxation method. The first method evaluates directly the potentials of the mesh points and is in many situations faster but requires a lot of memory and
is more complicated to implement. The latter method is a iterative approach, requiring only little extra memory, is very easy to implement but may have a long calculation time. Both methods are discussed by Seitelman [36]. However, he concentrates on meshes with only about 10 elements on the edges, whereas the edges of the meshes described in this section are of the order 100 and higher.

Both methods, direct solution and relaxation, were implemented and compared. The resulting potential fields that were used to compare the methods were equal for both methods within the normal computational error. Only the last digit of a double precision number (15 digits) differed sometimes by one or two. However, all calculations presented in this section were done by the relaxation method. This is due to different reasons: The first one is simple, since the relaxation method is easy to apply, it was implemented first. Secondly, for the lattice sizes used in this section, the direct solution method needed the same magnitude of calculation time as the relaxation method. Thirdly, in relaxation method the potential field approaches its final value step by step. It is possible to interrupt the procedure and to use the potential field for further calculations with only a small error.

Since both methods are well described in the literature (see [5] and [36]), only the simple relaxation method shall be described here.

The procedure is to apply equation (4-2) to all variable mesh points \( \phi_{i,j} \) until they reach a final value. This means for a given variable mesh coordinate, the new value is evaluated by adding the values of the four neighbouring coordinates \( \phi_{i-1,j}, \phi_{i+1,j}, \phi_{i,j-1} \) and \( \phi_{i,j+1} \) and then dividing the sum by four. Repeating this process for all variable mesh coordinates forms the first iteration to evaluate the potential field. This iteration must be repeated until the potentials approach a constant value.

The order in which the mesh points are evaluated has no influence on the result but it is still worth considering to speed up the iteration process.

4.1.3 From the potential field to the electric field

The two-dimensional potential field is stored in a two-dimensional array. The potentials between the points may be approximated by linear interpolation. The negative gradient of the potential field is equal to the electric field.
\[ E = -\nabla V \]

In further calculations, the potential and electric fields are separated into their x- and y-components.

\[ E_x = -\nabla V_x = -\frac{\partial V}{\partial x} \quad \text{and} \quad E_y = -\nabla V_y = -\frac{\partial V}{\partial y} \]

Part of a potential field lattice with some representations is shown in figure 4-6. The aim at this stage is to evaluate the potential and the electric field at any position \((x, y)\). The variables \(x_f\) and \(y_f\) are the distances from the point of interest to the next lower mesh in the evaluated potential field relative to the mesh size \(\Delta x\) and \(\Delta y\), respectively (\(0 \leq x_f < 1\) and \(0 \leq y_f < 1\)).

\[ \begin{align*}
\varphi_{x,y} &= (1-x_f)(1-y_f)\varphi_{i,j} + (1-x_f)y_f\varphi_{i,j+1} + x_f(1-y_f)\varphi_{i+1,j} + x_f y_f\varphi_{i+1,j+1} \\
E_x &= \frac{1}{\Delta x} \left[ \varphi_{i,j} - \varphi_{i+1,j} + \left( \varphi_{i+1,j} + \varphi_{i,j+1} - \varphi_{i,j} - \varphi_{i+1,j+1} \right) \cdot y_f \right] \\
E_y &= \frac{1}{\Delta y} \left[ \varphi_{i,j} - \varphi_{i,j+1} + \left( \varphi_{i+1,j} + \varphi_{i,j+1} - \varphi_{i,j} - \varphi_{i+1,j+1} \right) \cdot x_f \right]
\end{align*} \]

*figure 4-6: Part of a potential lattice.*

For the graphical representations in figure 4-6, the following equations give the linear interpolation for the potential and the x- and y-components of the electric field at any point.
4 Electron trajectories in an electric field in vacuum

4.2 Electron trajectories

The following sub-section is an overview of the calculation method for the electron trajectories in vacuum. This includes all necessary equations for the simulation of the electron pathways. In sub-sections 4.2.2, 4.2.3 and 4.2.4 the justification of the calculation method is given.

4.2.1 Overview

Electrons with defined start conditions (position, velocity and direction) in an electrostatic field in vacuum move on precisely defined trajectories. The dynamic state of an electron is fully described by the momentum vector $\mathbf{p}$ and the position vector $\mathbf{r}$. The momentum and the position of the electrons change continually along their path.

While a charged particle moves through an electric field it is subject to a force that is proportional to the charge of the particle and to the strength of the electric field. Assuming that the effect of the charged particle on the electric field is negligible, it is possible to evaluate the electric field and the accelerating force on the electron at any position.

$$\mathbf{F} = E \cdot e$$

This force leads to a change in momentum $\mathbf{p}$.

$$\mathbf{F} = \dot{\mathbf{p}} = \frac{d\mathbf{p}}{dt} \quad \text{or} \quad d\mathbf{p} = \mathbf{F} \cdot dt.$$ 

It is convenient to split up the electron trajectory into equally spaced time intervals, $\Delta t$ (see §4.2.3). The momentum after a time step becomes then

$$\mathbf{p}_{n+1} = \mathbf{p}_n + \Delta \mathbf{p} = \mathbf{p}_n + E \cdot e \cdot \Delta t$$

(4.3)

with $\mathbf{p}_n$ and $\mathbf{p}_{n+1}$ being the momentum of the electron at the beginning and end of the time interval $\Delta t$. This equation holds for a constant electric field, $E$, over the time step $\Delta t$. If the electric field changes strongly within a time interval, the step size must be reduced. The position of the electron $\mathbf{r}_{n+1}$ after an interval $\Delta t$ may be expressed in terms of the velocity of the electron.
It is more convenient to separate equations (4-3) and (4-4) into their $x$, $y$ and $z$ components. These equations were used to evaluate the electron paths in vacuum.

### 4.2.2 Choice of the parameter

To describe completely the dynamics of a point mass in a three-dimensional space, six parameters are needed. These parameters should be chosen carefully to ensure good results over a wide range of energy. This point is particularly worth considering for calculations on a computer, due to their limited precision in floating point calculations.

The **absolute** and the **relative velocity** of an electron, $v$ and $\beta$, are useful only for kinetic energies below the rest mass energy of the electron. For higher energies the two quantities approach a maximum value ($v_{\text{max}}=3 \times 10^8 \text{ m/s}$ and $\beta_{\text{max}}=1$). The change of energy then results only in a change of the very last digits (e.g. $\beta(71 GeV)=0.99999997$ and $\beta(72 GeV)=0.99999997$). Hence, the calculations become less exact, if not insignificant.

The **total energy**, $E$, (kinetic energy plus rest mass energy) is useful only for energies above the rest mass energy of the electron. For small kinetic energies the total energy approaches the rest mass energy (e.g. $E(T=1 GeV)=511.004 \text{ keV}$ and $E(T=2 GeV)=511.005 \text{ keV}$).

The **kinetic energy**, $T$, itself is a useful parameter for the whole energy range. However, in trying to keep the calculations as simple as possible it turns out to be more complicated.

Finally, the **momentum**, $p$, is a useful parameter for the whole kinetic energy range. The equations to calculate the electron tracks then become fairly simple.
4.2.3 Choice of the interval unit

The electron trajectory can not be calculated in one go with one set of equations. The electron’s path is divided into many steps. Each of these steps is taken to be linear, i.e. the path is straight and the electric field strength is constant. There are various ways to divide up the electron trajectory. Three different kinds of interval units were compared, namely time, energy and distance. In all cases constant step size divisions were used.

For small kinetic energies the relative change of momentum, \( \Delta p/p \), for a given distance step interval \( ds \) is larger than for high energies. Hence, the refractive index, \( \mu \), is also large (see equation (2-1) in section 2.2.3) which leads to an increasing curvature of the electron track. The low energy region of the electron track should therefore be calculated in more detail than the high energy region. This is not the case if the track is divided into equal sized energy or distance intervals. With equal time intervals the distance travelled by the electron per step decreases as its energy falls (for energies not much greater than the rest mass energy).

There is another reason for using equal time intervals. For some borderline cases the other two interval units fail. If at one step the kinetic energy is zero the distance interval unit fails since it would lead to an infinite time value. Also, if over one step the electric field is zero the energy interval unit would fail since this again would lead to an infinite time value.

As already shown in equation (4-3) and (4-4) the time interval unit is used for all further calculations.

4.2.4 Choice of the calculation method

Three methods to calculate the electron tracks were compared, namely by energy, by acceleration and by momentum of the electron.

For the energy method, the potential in the electric field before and after each step is used to calculate the energy change. This is very simple but the evaluation of the new direction is more complicated. A number of trigonometric functions are needed which cost valuable CPU-time during evaluation of the electron track.
The method by acceleration of the electron seems to be simple, but is only true for non-relativistic energies. The second Newtonian axiom fails for kinetic energies near and above the rest mass energy of the electron. The numerical result would be such that the electrons reach the target with a higher energy than the potential difference through which they are accelerated.

\[ F = m \cdot a = \frac{m_0 \cdot a}{\sqrt{1 - \beta^2}} \quad \text{for high energies} \]

Finally, the method by change of momentum was examined. It was found that for all energies, the change in momentum with corresponding change in time equals the force of attraction acting on the electron:

\[ F = \dot{p} = \frac{dp}{dt} \]

This method is described in § 4.2.1 and was used for all further calculations.

### 4.3 Selected simulation results - benchmarking

For benchmarking purposes the industrial x-ray tube MCN 225 from Philips was examined (see figure 4-2). The small dot in the middle of the cathode is a cross section through the filament. The figure represents a two-dimensional cut through the x-ray tube. The outer form of the tube is cylindrical, hence the electric and potential fields in the outer region have cylindrical symmetry. However, the filament is a cylinder into the plane of figure 4-2. Furthermore, the cathode does not change in its third dimension in the region around the filament (parallel to the filament). Hence the potential field is also constant over the third dimension in the region around the electron beam.

To generate large lattices, a simple computer routine was written. This routine can be called with any absolute point in the x-ray tube (x- and y-position). It returns the type of this point (fixed or variable) and for fixed points the voltage (usually zero or one). With this routine it is quite easy to generate a large input data set.
The evaluation of the potential field was done in four steps. First of all a lattice was put over the whole geometry of the x-ray tube with a mesh size of 100 µm. For this rather large lattice (780*400 elements) equation (4-2) was applied until no further changes could be found.

A second lattice was then generated which covered only the region around the electron beam with a resolution of 50 µm. The boundary conditions due to the tube walls were taken from the computer routine. The other boundary conditions were taken from the previous lattice. Again, equation (4-2) was applied until no further changes could be found.

Two more lattices were generated in the same way. The third lattice is for the first =5 % of the electron path. It has a resolution of 10 µm. The fourth lattice is a close up of the filament with a resolution of 2 µm.

All four data sets have their valid region. If a point is in the valid region of more than one data set (e.g. close to the filament all four data sets are valid) the data set with the highest resolution is chosen for the calculations.

The following three figures show the calculated electron trajectories. In figure 4-7 a scaled overview of the electron tracks is given. A close-up view of the filament with the beginning of the electron tracks is shown in figure 4-8. Finally the vertically stretched electron paths are shown in figure 4-9.

\[ \text{figure 4-7: Electron tracks in the MCN 225 x-ray tube; 225 keV (large focus)} \]
Since the x-ray tube is vertically symmetrical, for all electron trajectories that reach the x-axis from the top another electron path crosses the axis from the bottom. Hence for the calculation of the trajectories, the x-axis can be assumed to be a perfect mirror.

The calculated focal spot size can be found on the right hand side in figure 4-9. The highest electron track ends at the vertical position of \( y = 1.1 \text{ mm} \). Since this is only the upper half of the electron trajectories, this value must be doubled. The resulting focal spot size of 2.2 mm is well in accordance with measured focal spots. In figure 4-10 a photo of an MCN 225 focal
spot is shown. A vertical section through the spot is comparable with the simulated data which suggests that the model is valid.

\[ 2.2 \text{ mm} \]
\[ 1 \text{ mm} \]

**figure 4-10:** Photo of the actual focal spot of an MCN 225 x-ray tube.

With the simulated data it is also possible to bring the final position of the electrons on the target into relationship with their start position on the filament. The final position of the electrons is shown as a function of the start position in figure 4-11.

**figure 4-11:** Final position of the electrons on the target as a function of the start position; MCN225 x-ray tube; 225 keV; polynomial fit.

The shape of the graph is typical for this design of the cathode. The graph can be used to qualify the electron optics of an x-ray tube. It shows that all electrons that originate from \( \pm135^\circ \) of the filament surface reach the anode whereas electrons from outside that region get
lost elsewhere. This is in agreement with figure 4-8 where the electrons from the rear side of the filament are absorbed within the cathode. Another interesting fact is that the number of maxima and minima between any angle and zero in the graph equals the number of maxima and minima of the electron trajectory at the same angle (compare with figure 4-8).

If any parameter of the cathode (and anode) design is changed this type of diagram gives a good impression of the influence on the focal spot and hence is a good basis for further changes.

4.4 Conclusion

The procedure of evaluating the potential and electric field in x-ray tubes was shown and performed on an industrial x-ray tube. The electron tracks were calculated and found to be in good agreement with measured results.

The simulation of primary electron tracks in x-ray tubes as shown in this section covers only a narrow range of applications. In combination with the simulation tool ETraST (see §3.3) it opens the possibility to simulate electron tracks for a number of applications. For example further studies could be done on the simulation of off-focal radiation in x-ray tubes (see Roeck et. al. [30]). The fast moving electrons reach the target (anode) and may be simulated with ETraST to calculate the angular and energy distribution of the back scattered electrons. These electrons must then be followed in the vacuum again until they reach another point on the anode or the tube walls. The ETraST program must then be used again to calculate the electron track in condensed matter. This should continue until the electrons are finally absorbed. The same procedure may be used to evaluate the heat deposition on the output window.

Another interesting area of research would be the focus spot shape and the heat deposition within the focal spot in x-ray tubes (see Fraenkel [11]).
5 Measurement of reflected electrons

5.1 Introduction

The aim was to validate some ETraST simulations (see §3) by measuring the angular
distribution of fast moving electrons that were reflected from a plane semi-infinite reflector
(see figure 5-1).

![Diagram of incident beam and reflected electrons]

*figure 5-1: Angular distribution of reflected electrons.*

To get a complete picture of the reflected electrons for one incident angle, $\theta$, the intensity of
the reflected electrons must be measured as a function of their polar and azimuth direction and
of their energy. Such a measurement would be expensive and time consuming. The
measurements in this chapter are thus limited to the intensity as a function of the angle in one
dimension. The variation of intensity in the other direction and the energy distribution of the
reflected electrons were not analysed.

Related measurements were done by McMullan [19] who also gave a brief survey over other
related measurements. All these measurements either concentrate on the energy distribution of
the reflected electrons or they give only a very rough estimate of the angular distribution. The
measurements in this section concentrate on the angular distribution. The angular resolution is
about $0.5^\circ$ to $1^\circ$.

An electron trap was constructed which allows measurement of the electron flux in a well-
defined area. All electrons outside the sensitive area are screened out. All electrons inside the
area are captured so that they cannot escape, which otherwise may have an adverse effect on
the results. A cross section through the electron trap is shown in figure 5-2.
5 Measurement of reflected electrons

The electron trap is made out of two concentric hollow cylinders. Both cylinders have a slit that forms the sensitive area of the electron trap. The outer cylinder has the task to screen off all electrons outside the sensitive area. Once an electron enters the trap, it is the task of the inner cylinder to keep the electron inside until it is absorbed. Hence this contributes to the measured current. The slit of the inner cylinder is slightly wider to avoid incident electrons hitting the outer surface of the inner cylinder.

The electron intensity distribution concerned in this case was along the plane of incidence (see figure 5-3).

The electron intensity distribution rectangular to the plane of incidence is integrated over a defined angular range due to the length of the slit in the electron trap.

5.2 The set-up

All measurements were done with an experimental x-ray tube (see figure 5-4). The x-ray tube is made of a 16 cm diameter vertical cylinder welded together with a horizontal 10 cm
diameter cylinder for the cathode (on the back side in figure 5-4). The large vertical cylinder has a removable cover for operating the set-up on the inside of the x-ray tube. The electron trap is fixed on the cover and can be turned by a hand wheel around the centre of the cylinder. On the front side an electrical connector is welded into the large vertical cylinder. This connector is used for the current measurements. A turbo vacuum pump is connected to the 10 cm horizontal cylinder.

![Diagram of the experimental x-ray tube](image)

*figure 5-4: The outside view of the experimental x-ray tube.*

The cathode originates from a Philips industrial x-ray tube and has two different sized filaments. Only one filament can be used at once; they generate two focal spots with the sizes 2 mm (‘large focus’) and 0.6 mm (‘small focus’). During the experiments the filament for the small focus burned, hence, after that happened, all measurements were done with the large focus. However, the electron beam is mechanically defined by the apertures so both filaments could be used in the same way for the experiments.

The electric current that leaves the filament was kept constant by the control unit of the experimental x-ray tube. All measured currents in the set-up were also found to be constant (better than 1%) except for a 20 kHz signal on all currents which was due to the electronics that controls the temperature of the filament. In fact, this signal was as large as 10 % or even
20% relative to the measured currents. However, this 20 kHz signal was eliminated by a first order low pass filter with a cut off frequency of 170 Hz. The long term stability was good; the results could be reproduced at any time.

The set-up on the inside of the experimental x-ray tube is shown in figure 5-5. The incident electron beam coming from the cathode is collimated by two vertical slits, the first and second apertures. The sizes of the slits are variable from 0 to 2 mm. The two apertures are 60 mm apart.

![Figure 5-5: Set-up for the measurements of reflected electrons (top view into the tube).](image)

After the electrons have passed through the apertures they reach the reflector. The centre of the reflector is 28 mm behind the second aperture. The reflector can be rotated around its centre from zero (parallel to the incident beam) to 90 degrees (normal to the incident beam).

Some of the reflected electrons enter and are absorbed in the electron trap. The electron trap can be rotated around the reflector by a hand wheel on the outside of the x-ray tube. The entrance slit of the electron trap is always at a distance of 53.5 mm from the centre of the
The solid angle subtended by the electron trap varies with the slit width in the electron trap; the slit length is always 40 mm. A slit width of 1 mm corresponds to a fixed solid angle of about $6.7 \times 10^{-3}$ steradian.

The two apertures and the reflector are installed together on a ground plane. It is possible to shift this ground plane horizontally, perpendicular to the incident electron beam (vertical in figure 5-5). By doing so, an optimal position within the incident electron beam can be found.

The above set-up makes it possible to choose any incident angle, $\theta$, and to measure the electron flux at any reflection angle, $\varphi$ (see figure 5-1).

### 5.3 The incident electron beam

Firstly, the cross section of the incident electron beam was studied. The following two graphs represent different aspects of the fast moving electrons coming from the cathode. Regarding the graph in figure 5-6, the first aperture was adjusted to a 1 mm slit and the second aperture was removed. The whole set-up was then shifted horizontally to find the optimal orientation for the set-up. To estimate the electron flux behind the apertures, the electric current in the reflector was measured with a reflector angle of 90° (the incident beam normal to the surface). In this arrangement, the electron trap is covered by the reflector. The measured current does not represent the absolute electron flux since a fraction of the incident electrons get scattered out of the reflector again. However, since the fraction of back scattered electrons is constant due to constant energy of the incident electrons, the measured reflector current represents the relative electron flux of the incident beam on the reflector. The factor between relative and absolute electron flux remains constant.

The horizontal position for all further measurements was chosen at the maximum of the small focus (horizontal position -1.5 mm).
figure 5-6: Electron beam cross section; measured by shifting the whole set-up horizontally.

Before taking the readings plotted in figure 5-7 the first and the second aperture were adjusted to a 1 mm slit width. The reflector was removed, and the shape of the focus was measured with the electron trap situated \(\approx 80\) mm behind the second aperture (see figure 5-5).

figure 5-7: Cross section of incident electron beam measured with electron trap.

The size and the divergence of the electron beam are limited by the first and second aperture. Once an electron has passed the first aperture it enters a field free area, hence the electron
trajectories can then be assumed be straight. With a slit width of 1 mm for the first and second apertures the maximum angular divergence becomes ±1° deg. The size of the focal spot 80 mm behind the second aperture is geometrically limited to 3.7 mm (see figure 5-8). The measured spot size in figure 5-7 is 1 mm larger due to the 1 mm slit width in the electron trap.

**figure 5-8: Mechanical limits for the focal spot size 80 mm behind the second aperture.**

### 5.4 Angular distribution of reflected electrons

The angular distributions of reflected electrons were measured and compared with simulated results. In both cases fast moving electrons were shot onto a plane gold surface at different incident angles, \( \theta \). The following three diagrams show the reflection distribution for the incident angles 20°, 10° and 5° deg, respectively. The incident energy was 100 keV. The measured reflection intensity at each point is an average over ±22.5° rectangular to the plane of incidence due to the size of the electron trap (see also figure 5-3). In order to compare the measured and simulated data, the theoretically calculated reflected electrons were also averaged over the same angular range of ±22.5°.

All three angular distributions were measured and simulated. The measured curves are normalized relative to the incident current, whereas the simulated curves are normalized to the number of incident electrons. Therefore the unit for the relative intensity is the reciprocal of steradian and contains no units for the electric current or the number of electrons. Therefore, the measured and simulated curves can directly be compared.
For the simulated curves, 2,000,000 electrons have been simulated per graph; they were followed down to a cut-off energy of 10 keV. All electrons with an energy less than 10 keV were assumed to be absorbed.

**Figure 5-9:** Angular reflection distribution, 100 keV electrons, gold reflector, 20° incident angle, averaged over a 45° azimuth angular interval (i.e. ±22.5° on either side of the plane of incidence).

**Figure 5-10:** Angular reflection distribution, 100 keV electrons, gold reflector, 10° incident angle, averaged over a 45° azimuth angular interval.
All three graphs (figure 5-9, figure 5-10 and figure 5-11) clearly show a higher intensity for the simulated distribution than for the measured one. This may be due to some simulation errors, but a much more likely source of error is the normalisation of the measured data. There was no exact experimental information available about the incident electron current hitting the surface of the reflector. For the normalisation, the electron flux was estimated from the cross section of the incident beam (small focus) shown in figure 5-7. This is only a rough estimate and is one source for the difference between the curves.

An interesting characteristic in figure 5-11 is that the simulated curve falls below the measured curve for angles above 50°. This is most probably due to surface roughness of the reflector that was used for the measurements. For the simulated curve, an ideal surface was assumed that has no roughness at all. The reflection distribution from a rough surface has less intensity within the main reflection peak, but a higher intensity at large reflection angles. The following section deals with surface roughness and its influence on the angular reflection distribution.
5.5 Reflectors with different surface roughness

Two reflectors with different surface roughness were compared. Both reflectors were made of brass with a 15 μm gold electroplated layer. In figure 5-12 microscopic pictures of the two reflectors are shown. The left photo was taken of a reflector just after the plating process. The surface roughness is a few microns. The microscope photo on the right shows a reflector that was polished simply with a cloth and grinding paste. There are still some discontinuities but the mean surface roughness is far less than 1 μm.

![Microscopic pictures of reflectors](image)

*figure 5-12: An unpolished and a polished gold reflector layer.*

Both reflectors were used to measure the angular distribution of reflected electrons as described in section 5.4. The incident electrons had an energy of 100 keV; the incident angle was 5°. For both curves a 6 μm aluminium filter was inserted in front of the electron trap to screen all low energy electrons. This filter mainly changes the overall intensity, this is the reason for less intensity relative to the 5° curve in figure 5-11. The two measured angular distributions are plotted in figure 5-13. Both measured curves were normalized in the same way as the measured curves in the previous section.
5 Measurement of reflected electrons

figure 5-13: Angular reflection distribution, 100keV electrons, gold reflector, 5° incident angle, averaged over a 45° slice.

The difference between the two curves is extremely great. The result suggests that, for any application, great attention should be paid to the roughness of the surface of the reflector.

One question that arises is what the angular distribution of the reflected electrons would look like with a reflector surface smoother than the one used in this experiment. This question could of course be answered by another experiment including a reflector with a better surface. If a further enhancement of the reflector surface does not change the angular distribution of the reflected electrons, then the distribution represents that for a perfect surface.

Another way of investigating the influence of surface roughness is by repeating the experiment with the same two given reflectors but for different angles, say 10° and 20° deg. This could give more information about the principle behaviour of a rough surface reflector. Hence, it might help in answering the question of the behaviour of a perfect surface.

5.6 Conclusion from the measurements

The angular distributions of reflected electrons were measured and simulated for different incident angles on a gold reflector. The simulated distributions were found to be in good agreement with the measured results except for the overall intensity which was about 10%
Measurement of reflected electrons

different. This may be due to errors during the normalisation procedures for the measured
curves. With the present set-up it was impossible to directly measure the incident current on
the reflector and hence, to accurately normalize the measured data. Other sources of error lie
in the simulation tool ETraST. The input data for the program, especially the stopping power
and the total scattering cross section might not be accurate enough for the applications in this
experiment. However, the predicted shape of the reflected electron curve is a good match to
the experimental data.

A further experiment could be carried out to measure the current of the incident electron beam
more precisely to limit the overall error of the measured distributions. This would require a
larger electron trap that measures the whole incident electron beam at once. This measurement
needs to be taken only one time for each slit widths of the apertures.

It would also be worth considering improving the quality of the mechanics of the electron
trap. A smaller slit and a more precise mechanic for the hand wheel that turns the electron trap
would improve the angular resolution. Hence, the angular distribution of reflected electrons
with incident angles of 1° and less could be measured more readily.

A smaller slit in the electron trap would lead to smaller electric currents and would require an
increasing sensitivity of the electronics. For the measurements in this section the electric
currents were approximately between 0.1 and 100 µA. These currents were fairly simple to
measure with a current-voltage converter. However, the exact measurement of lower currents
need an improvement in the electronics.

In its present state the simulation tool ETraST copes only with perfect surfaces. It would be
interesting to implement surface roughness into ETraST and then to compare simulated and
measured data again. The shape of the reflected electron distribution might even be used to
study the surface roughness of materials.
6 Capillary for a micro-focus x-ray tube

6.1 Introduction

The discovery of x-rays was made by Röntgen on 9 November 1895 and attempts were made at once to explore their use in microscopy. A good survey over x-ray microscopy was done by Cosslett and Nixon [6]. The main distinguishing characteristics of x-rays have special value for microscopy. Their short wavelength compared with visible radiation offers a correspondingly higher resolution than that of the optical microscope. Their relatively great penetration into matter gives the possibility of investigating internal structure, in both biological and inorganic specimens. Some good techniques exist to study the microscopic surface structure of an object. Some of these are the classic optical microscope, the electron microscope and the scanning tunnelling microscope. But if a three-dimensional object is to be studied internally, the above mentioned techniques fail. With x-rays it is possible to study the inside of an object without destroying it (i.e. non-destructively). For typical applications a spatial resolution of a few 10 μm is desirable.

There are two simple ways to achieve high resolution:

The first principle is to use an x-ray emitter with a normal focal spot size, say 1 mm. The transmitted x-rays are detected with a high resolution screen, say a few 10 μm. The object must be close to the screen and far away from the focal spot to gain the maximum resolution (see figure 6-1).

![figure 6-1: High resolution imaging using a high resolution detector screen.](image)

This technique is useful if high resolution screens are available. The classical x-ray films have a fairly high resolution, but on-line electronic detector screens still have a limited resolution
(see Yaffe and Rowlands [40]). 'On-line' in this case means that the time between taking the image and displaying it on the screen is less than one or even 0.1 seconds.

The second principle to achieve high resolution is by using a micro-focus x-ray emitter and a normal resolution screen. Then the best resolution can be achieved by shifting the object as close to the emitter as possible and placing the detector screen at a substantially large distance to form a highly magnified x-ray shadow image (see figure 6-2).

![figure 6-2: High resolution imaging using a micro-focus x-ray emitter.](image)

A desirable micro-focus x-ray tube has a minimal focus size coupled with a reasonably strong intensity. Hence, the aim is to form the electron beam in an x-ray tube to be as narrow as possible and with a high electron flux at the anode.

A micro-focus x-ray tube may be used in combination with an on-line detector system for on-line microscopy [39]. A typical application is die bonding tests on power semiconductors [9].

### 6.2 Standard micro-focus techniques

The standard technique is to use a small electron emitter and then to accelerate and form the thermal electrons into a narrow electron beam. A typical electron emitter is a heated tungsten 'hair pin'. The thermal electrons leave the hot wire with a given position, energy and direction. The electrons are accelerated by an electric field and formed into a converging pencil beam by electric and magnetic lenses.

When electrons leave the emitter they vary in three ways, namely the start position, energy and direction. The energy and the direction can be combined to one quantity which is the tangential momentum. However, the emitted electrons still vary in two ways, position and tangential momentum. From classical optics it is known that it is impossible to focus thermal electrons emitted from a surface to a point (e.g. see [4]). If the electrons would vary only in
one quantity, it would be possible to focus all electrons onto one point. Or, in other words, it is always possible to eliminate one of the two sources that enlarge the focal spot. But since the variation is in two quantities, the focus achievable is always a compromise between the two.

The typical way of handling this problem is by reducing the size of the electron emitter to a minimum and hence reducing the variation of the start position. However, this leads to another problem: if the emitter size is reduced to a minimum, the temperature must be increased to get the same electron flux. A higher temperature of the filament reduces its lifetime. Hence, decreasing the diameter of the focal spot by reducing the size of the filament must be paid for by a reduced lifetime. A practical solution is an unsealed tube with an exchangeable filament. This means the x-ray tube must be equipped with a high vacuum pump that adds complexity and expense.

The classical technique contains other weaknesses. Further control potentials are required in addition to the tube high voltage for the electron optics. These potentials must be varied together with the high voltage and anode current (which are always variable). This requires much electronics and adjustment for a single x-ray tube.

Another aspect of the same problem is the sensitivity to a change in high voltage or anode current. Although the optics are corrected for each chosen setting, the focus shape varies with high voltage and anode current.

A novel technique to generate a small electron focal spot with a high electron flux is described in the following section.

### 6.3 Electron capillary x-ray tube

At Philips Research laboratories in Hamburg, Germany a new technique has been developed to focus an electron beam down to a small diameter with a high electron flux (see Harding [14]). The principle is to reduce the diameter of a pre-collimated electron beam with a mechanical capillary (see figure 6-3). The capillary is a funnel that collimates the electron beam on a mechanical basis by quasi-specular reflection.
The capillary combines two effects: one being that some of the electrons that hit the wall of the capillary are reflected into the output hole (this effect is studied and described in the following two sections (§6.4 and §6.5)), and the other such that the energy which does not get through the output hole is deposited over a large area on the capillary walls. The cooling of a pinhole aperture becomes difficult for high electron intensities, whereas it is relatively easy to remove the deposited energy from the large surface area of the funnel-like capillary.

The capillary has three advantages:
Firstly, with a capillary it is possible to reduce the focus size without reducing the size of the filament. This leads to a **longer lifetime** of the filament. Hence the x-ray tube may be a sealed tube design which has only one filament for its whole lifetime.

Secondly, **high intensities** on the output of the capillary can be achieved simply by shooting more electrons into the capillary since its transmission efficiency is largely unaffected by the power involved over a useful range.

Finally, the **focus** size and shape are **mechanically defined** and hence insensitive of changes in high voltage or anode current. The only quantity that may change with high voltage is the intensity of the electron beam at the output, that is behind the capillary. The intensity can, however, always be adjusted with the anode current.

The effect of the capillary was studied in theory by simulation and experimentally with selected measurements. In the following section a one-dimensional capillary (which collimates the electron beam in one dimension) was investigated by simulation and by measurements (see §6.4).

A two-dimensional capillary was studied by simulation only (see §6.5).
6.4 One-dimensional capillary

To start with, a one-dimensional capillary was studied. One-dimensional means that the incident electron beam is collimated only in one dimension. The investigation was carried out both by simulation and by experiment. The examination focuses on the reflection behaviour of electrons in a capillary. The energy deposition in the capillary has not been studied in detail.

6.4.1 Simulation

For the simulation of the one-dimensional capillary the incident electron beam was assumed to be mono-energetic, parallel (no divergence) and homogeneous. A gold capillary, 50 mm long was assumed with a 1 mm input slit. The output slit was varied from 30 \( \mu \text{m} \) to 1 mm (see figure 6-4).

![Figure 6-4: Simulation set-up for the one-dimensional capillary.](image)

The incident electrons were assumed to be parallel with an energy of 100 keV. For each output slit width 20,000 electrons were tracked down to 50 keV. Once an electron within the capillary had an energy of less than 50 keV, it was assumed to be absorbed since this large degree of energy loss implies a large number of scattering events and it is very unlikely that such an electron will reach the output hole at all. Also, even if a low energy electron reaches the target, it has a lower radiation yield (see §2.2.2) and produces only x-rays below its remaining kinetic energy; hence its contribution to the x-ray spectrum is of less importance. The results of the simulations by ETrAST are shown in figure 6-5.
Figure 6-5: Fraction of transmitted electrons of a gold 1d-capillary (100 keV electrons).

The fine dashed line indicates the direct electrons that passed through the capillary without any interactions with the capillary. It is obviously a diagonal line through the chart, since it is proportional to the ratio of the output and input slit widths. The dash-dot line indicates all electrons that got through the capillary. Some of the transmitted electrons passed through the capillary due to scattering at the gold surface of the capillary. The scattered (reflected) fraction is indicated by the coarse dashed line. Finally, the solid line indicates the ratio of the scattered and the directly transmitted electrons, which is the enhancement of the transmitted flux due to scattered electrons.

The maximum absolute enhancement of the electron flux due to reflected electrons occurs at medium slit widths. However, a maximum relative enhancement of ≈80% (concentration factor of 1.8) may be achieved with a small output slit.

The enhancement may be further increased by changing other parameters of the capillary. For example if the input and output slits are given fixed values, the length of the capillary may be optimised for maximum electron flux on the output of the capillary (see §6.5.2 for the two-dimensional capillary).

Another approach to optimise the enhancement is to vary the principle shape of the capillary. A two-dimensional parabolic capillary is discussed in section 6.5.2.
6.4.2 Measurements

For the measurements with a one-dimensional capillary the same experimental x-ray tube as described in section 5 was used (see figure 5-4). Only the inside set-up of the tube was different (figure 6-6).

![Diagram of x-ray tube set-up]

**figure 6-6: Set-up for measurements with the one-dimensional capillary.**

A primary aperture with a 1 mm slit limits the electron beam to a horizontal size of 1 mm. The vertical size of the beam is given by the cathode optic which is about 3 mm. Behind the primary aperture there are two movable reflector jaws made of brass with a gold layer on the electron side. Finally, the target is copper and has two insulated tungsten apertures (left and right) in front of it. The two apertures are useful to gain information about the incident electron beam divergence.

The thickness of the gold layer was chosen under following considerations: The mean range of 120 keV electrons in gold, which is the mean distance travelled by the electrons, is about 22 μm. This value also represents the maximum penetration depth of the electron. The maximum penetration depth of a reflected electron is half of this value, since it has to travel into and out of the material. Now, it is very unlikely, that an electron travels straight into the
material then makes a 180° turn within one scattering and comes out on a straight line again. In fact, only the electrons that enter and leave the reflector jaws under very small angles relative to the reflector surface will have a chance to reach the target. Finally, only the electrons with little energy loss, say less than 20 %, are of interest to contribute to the x-ray bremsstrahlung spectrum. Hence, most of the electrons of interest will have a penetration depth of less than 1 μm. For the measurements the thickness of the gold layer was chosen to be about 1 μm.

With the given set-up it was possible to measure four separate electric currents. The four currents are from the reflector jaws, the target, the left and the right aperture. The four currents were measured as a function of the reflector angle. In figure 6-7 the reflector angle is shown in terms of the output slit width. Since the input slit is constantly 1mm, the reflector jaws are parallel for an output slit of 1 mm. The left and the right aperture were 1mm apart. They are in line with the reflector jaws for an output slit of 1 mm (as shown in figure 6-6).

In figure 6-7 all four measured currents are plotted as a function of the output slit width. Also the sum of the four currents is shown which is equal to the current that gets through the primary aperture into the capillary. The high voltage was 120 kV; the anode current before the primary aperture was 200 μA.

*figure 6-7: Measured currents on a one-dimensional capillary. 200 μA incident current before the primary aperture; 1 mm input slit of the capillary; 120 keV electrons; gold reflector.*
The sum of the four currents is almost constant; hence it can be assumed that no electric current gets lost in the set-up. To compare the measured results with the simulated data, all measured values were normalized to the sum of the four currents. For each position of the reflector the four currents were divided by the sum of the four currents. The resulting relative values are plotted in figure 6-8. The sum of relative values of target and apertures is also plotted in the graph. The sum of the relative values of target, apertures and reflector jaws is unity (100 %) for any reflector angle.

\[ \text{figure 6-8: Measured currents on a one-dimensional capillary. The currents are normalized to the sum of all currents. 1 mm input slit of the capillary; 120 keV electrons; gold reflector.} \]

The diagram is best understood by starting to analyse it from the left. In the region with an output slit below 0.8 mm, the two tungsten apertures are covered by the reflector jaws. From mechanical considerations, all incident electrons that got through the capillary directly hit the target and cannot reach the apertures. However, the two apertures function as a simple electron trap and catch some of the secondary electrons that were scattered backward from the target (see figure 6-9). The fraction of the aperture current relative to the target current is \( \approx 40 \% \) (20 \% for each aperture). Therefore the target current must be corrected by a factor 1.4 to gain a more realistic value.
6 Capillary for a micro-focus x-ray tube

figure 6-9: The aperture in front of the target traps most of the back scattered electrons.

For the case of parallel reflector jaws (1 mm output slit width), the sum current of target and apertures is only \( \approx 55 \% \) of the total current. If the trajectories of the incident electrons were parallel, all incident electrons would reach the target. The reduced sum current of target and apertures must be due to a strong angular divergence of the incident electron beam. This angular divergence makes it difficult, but not impossible to evaluate an enhancement value for the capillary.

Even when the reflector jaws are parallel, some incident electrons hit the reflector and some of them are reflected onto the target. The measured sum current of target and apertures is the sum of the direct and some scattered electrons. The fraction of direct electrons for parallel reflector jaws may be deduced from the case where the reflector jaws are opened further. If the reflector jaws are opened to an output slit greater than 1 mm, some of the electrons that were scattered onto the target now reach one of the apertures in front of the target directly (see figure 6-10). This explains the decreasing target current for an increasing output slit above 1 mm. With an output slit of 4 mm the target current falls below 35 \%. This value must be multiplied by the factor 1.4, which was derived from the 0 \( \ldots \) 0.8 mm output slit region to take the back-scattered electron into account. This leads to a fraction of direct electrons of 47 \% relative to the incident current for an output slit not smaller than 1 mm. For smaller output slits the fraction of direct electrons on the target decreases proportional to the output slit width.

figure 6-10: Enhancement for parallel reflector jaws due to scattered electrons.
In figure 6-11 the fraction of the direct electrons on the target is indicated by a fine dashed line. The dashed dotted line shows the sum current of the target and the apertures relative to the incident current (taken from figure 6-8). This current is the sum of direct and scattered (reflected) electrons. The difference between this current and the direct component gives the fraction of scattered (reflected) electrons on the target (coarse dashed line). The ratio of the scattered to the direct electrons is the enhancement factor of the capillary. For very small output slits the enhancement factor tends to a final value of 70 % (concentration factor of 1.7).

![Graph showing scattered and direct electrons](image)

**Figure 6-11: Evaluation of the enhancement factor (scattered divided by direct fraction).**

### 6.4.3 Comparison of simulated and measured results

The overall agreement of simulated and measured results is satisfactory. The main difference between the two experiments (Monte Carlo simulation is often described as a 'numerical experiment') lies in the incident electron beam. With open reflector jaws in the measurement set-up, less than 50 % of the diverging beam of incident electrons directly reach the target. More than half of the electrons leave the parallel beam path before they reach the target and are absorbed in the secondary aperture.

This is due to two effects: Firstly, for the measurements the incident angles of the electrons on the reflector are larger than those assumed in the simulation. The larger the incident angle, the less is the intensity of the reflected electrons in the forward direction. Secondly, when the
incident electrons hit the reflector they are further away from the output slit than in the simulation. Hence for the reflected electrons the output slit appears to be narrower and they have a smaller probability of passing through the output slit and second aperture.

Both effects lead to a reduced fraction of scattered electrons reaching the target. On the other hand, an incident beam with no angular divergence exists only in theory; the incident beam used in the experiment comes much closer to a real electron beam in an x-ray tube. It may be worth repeating the simulations assuming an incident beam with a given angular divergence.

### 6.5 Two-dimensional capillary

A two-dimensional capillary collimates an incident electron beam in two dimensions. The capillary examined in this section acts like a funnel. It has a relatively large input hole, say 1 mm, and a smaller output hole, say 30 μm. The walls of the capillary are cone shaped. A sketch of a two-dimensional capillary is shown in figure 6-12.

![Sketch of a two-dimensional capillary](image)

*figure 6-12: Sketch of a two-dimensional capillary.*

For the purpose of the micro-focus x-ray tube practicable diameters for the input and output holes would be 1 mm and 30 μm respectively. The capillary was examined by simulation only. Experimental measurements would be difficult and expensive since a new capillary must be produced for any change in mechanical parameters. Once a design has been optimised by simulation, real capillaries can be machined for practical tests.
6.5.1 Two-dimensional capillary with variable output diameter

For the first simulation (‘numerical experiment’) the capillary was chosen to be 50 mm long with a 1 mm input hole. The output hole was varied from 30 μm to 1 mm. The material was gold with a perfect surface. The incident electrons were parallel and homogeneously distributed over the input hole. The incident energy was 100 keV; the electrons were followed down to 50 keV as before. 40,000 incident electrons were simulated for every diameter of the output hole. The results are shown in figure 6-13.

![Diagram](image)

**Figure 6-13: Evaluation of the enhancement for a two-dimensional capillary.**

The simulated data are shown in the diagram in the same way as for the one-dimensional capillary: The fine dashed line indicates the fraction of the incident electrons that get directly through the capillary. The dash dot line indicates all electrons that get through the capillary. The fraction that gets through the capillary after experiencing at least one collision with the capillary walls is indicated by the coarse dashed line. Finally, the solid line indicates the enhancement defined as the scattered fraction divided by the direct fraction. For example, a capillary with a 30 μm output hole has an enhancement of 93% which is a concentration factor of 1.93.

It is interesting that the enhancement for the two-dimensional capillary is very similar to that for the one-dimensional capillary. The enhancement increases approximately linear with
decreasing output diameter. The limiting value for zero diameter is only slightly above the enhancement for the one-dimensional capillary.

6.5.2 Optimisation of the two-dimensional capillary

Until now the only parameter that was investigated for maximum electron flux at the output was the size of the output slit or output hole for a one- or two-dimensional capillary, respectively. Two other aspects shall be discussed here. One is the length of the capillary, the other, more general, is the shape of the capillary.

Firstly the optimal length of the capillary shall be studied by simulating capillaries with different lengths but equal input and output holes. For this experiment the input and output diameter were chosen to be 1 mm and 30 μm respectively. The length of the capillary was varied from 1 to 100 mm. Again, the material was gold with a perfect surface. The incident electrons were parallel and homogeneously distributed over the input hole. The energy of the incident electrons was 100 keV; the electrons were followed down to 50 keV. 50,000 incident electrons were simulated for every length of the capillary. The resulting data are shown in figure 6-14.

![Figure 6-14: Optimisation of the two-dimensional capillary length for maximum enhancement.](image)
In the diagram the thick line shows the enhancement due to scattered electrons with an energy of 50 to 100 keV. The electrons with a high energy after scattering are of more interest since the radiation yield decreases with lower energies (see §2.2.2). The diagram shows that most of the scattered (reflected) electrons still have a high energy; the thin line just below the thick line indicates the enhancement due to electrons with final energy between 90 and 100 keV. The electrons emerging with energy below 90 keV give only a small contribution to the overall enhancement.

The optimal length for the overall enhancement in this case is \( \approx 5 \) mm. For the maximum enhancement of the high energy electron throughput the optimal length is slightly longer, about 7 mm. For a 7 mm capillary the calculated overall enhancement is 195 \% which is a concentration factor of 2.95.

For an aluminium capillary the optimal length is approximately 10 mm with an enhancement of 205 \% corresponding to a concentration factor of 3.05. The choice of material for the capillary differs from that for the target. The reflection behaviour of an element must be studied to decide whether it leads to an improved capillary enhancement factor. A large total elastic scatter cross section together with a small stopping power is desirable.

The enhancement could be further increased by varying the shape of the capillary. Using a cone shaped capillary like the one studied in this section, the output hole of the capillary as seen by the reflected electrons always lies beside the maximum intensity of the reflected electrons (see the following figure).

*figure 6-15: Output hole of a capillary as seen by the reflected electrons.*
The following figure shows a two-dimensional angular distribution of reflected electrons with an incident energy of 100 keV and an incident angle of 2° between incident beam and surface of reflector. It is taken from figure 7-4 and is described in more detail in section 7.1. The darker the region, the higher the intensity of the reflected electrons. The small circle exemplary indicates the output hole as seen by reflected electrons in a typical capillary.

The output hole (as seen by reflected electrons) could be shifted to the maximum intensity by using a parabolic capillary (see figure 6-16). The maximum intensity is approximately where a specularly reflected beam would be, i.e. in the plane of incidence where the reflection angle equals the incident angle. The parabola is the function that reflects parallel incident beams into one point. It is estimated that a parabolic capillary would improve the enhancement of the capillary still further by a factor of 2 to 4.

Although a parabolic capillary would support the requirements of micro-focus x-ray tubes, it is very difficult to produce in practice. Until now, there was no technique found by which a hole can be produced, 10 mm deep, 1 mm to 30 μm in diameter, of parabolic shape and with a good surface.

Another point is that even with an enhancement factor of 10 only 1 % of the incident electrons get through a capillary with input and output holes of 1 mm and 30 μm respectively; 99 % of the electrons are lost on the capillary walls. To get 50 W into the focal spot some 5 kW must be shot into the capillary!

One alternative is to use a smaller pre-focused electron beam, say 100 μm in diameter. The capillary is then used for two purposes: One is a small enhancement in the 30 μm spot (presumably less than 100 %). Secondly, in comparison to a pinhole aperture the electrons deposit their energy over a larger area and cooling is then less of a problem.
7 Other simulation results

The simulation tool ETraST has been used for various applications. Two other simulation results are presented in this chapter.

7.1 Reflection of fast moving electrons

In section 5 the behaviour of reflected electrons was studied only in one dimension. In this section two-dimensional distributions of reflected electrons are investigated by simulation using the simulation tool ETraST (see §3.3).

A large number of electrons were shot onto a plane surface that acts like a reflector. 'Reflector' does not mean that most of the electrons are specularly reflected like visible light from a mirror. The electrons usually enter into the surface layers of the reflector material and are scattered, resulting in a fraction of them leaving the reflector again. Only for very small angles and for perfectly plane surfaces does the effect of specular reflection exist (see §2.2.3). The electrons that are reflected by scattering come out of the reflector with an arbitrary direction; but they obey a defined probability distribution. Some of these distributions have been estimated by the following simulations.

The principle set-up for the simulations is shown in figure 7-1. A large number of electrons with different incident angles were shot onto a plane gold surface. All electrons that emerged from the reflector were stored separately and were analysed later. Ten million electrons with an energy of 100 keV were simulated as the incident beam; they were followed down to an energy of 50 keV. All electrons with an energy less than 50 keV that had not left the reflector were assumed to be absorbed.

\[\text{figure 7-1: Principle set-up for the two-dimensional reflection simulation.}\]
The following graphs show the two-dimensional angular distributions of reflected electrons with incident angles of 10°, 5°, 2° and 1° deg. The intensity is the number of electrons per electron and per steradian. This means that the intensity taken from the diagram multiplied by the solid angle of interest (in steradian) is the fraction of the incident electrons that are reflected into the solid angle of interest.

*figure 7-2: Two-dimensional reflection distribution of 100 keV electrons with 10° incidence.*

*figure 7-3: Two-dimensional reflection distribution of 100 keV electrons with 5° incidence.*
7 Other simulation results

Figure 7-4: Two-dimensional reflection distribution of 100 keV electrons with 2° incidence.

Figure 7-5: Two-dimensional reflection distribution of 100 keV electrons with 1° incidence.

The diagrams look very similar; they vary mainly in scale and intensity. The maximum intensity is in all cases slightly below the point where a specularly reflected beam would be expected. Since the set-up is symmetrical around the plane of incidence, the resulting probability distribution is symmetrical around the zero azimuth angle.
The mean energies of reflected electrons increases for lower incident angles. Generally it can be said: The less an electron changes its direction the higher the average kinetic energy after reflection. Hence, the larger the incident angle, the less is the mean energy of the reflected electrons. Also, the mean energy of reflected electrons increases for smaller reflection angles. E.g., for an incident angle of 10° the electrons that are reflected with a (polar) angle of 5° have a higher mean energy than the electrons that are reflected with an angle of 15°.

The following graph (figure 7-6) shows the angular distribution of reflected electrons along the plane of incidence for different incident angles. The 10° curve compares with the two-dimensional graph in figure 7-2. The reflection angle in figure 7-6 is the polar angle in figure 7-2. The only difference is in the incident energy, which is 150 keV for the following graph. The values in figure 7-6 are the mean intensity over a strip along the plane of incidence (as an illustration see also figure 5-3). The width of the strip is twice the incident angle, e.g. for an incident angle of 10° the strip width is ±10° in azimuthal direction. The total number of simulated 150 keV electrons was 500,000 per graph; the cut-off energy was chosen to be 100 keV. All electrons with an remaining energy below this value were assumed to be absorbed and did not contribute to the angular distribution of the reflected electrons.

\[ \text{figure 7-6: Angular distribution of reflected electrons along the plane of incidence for different incident angles; gold reflector, 150 keV incident energy; 100 keV cut off energy.} \]
reflector materials. A parameter fit could also be developed that gives the angular distribution for a range of incident angles and energies. However since this was not the main task of this work it has not been followed to that extent.

### 7.2 Energy deposition profile

Another important application for the simulation tool ETraST (see §3.3) is the evaluation of the energy deposition of fast moving electrons in matter. A large number of electrons were simulated to enter normally into an absorber of effective infinite thickness (thickness greater than maximum range). Along their track through the absorber the electrons continually lose energy. The major inelastic events are collisions with atomic electrons that lead to excitation or ionisation. Radiations from these secondary events are mainly of low energy and hence have a very small range before their energy is converted into thermal energy. It is assumed that the place, where the incident electron loses its energy, is the place where that energy is converted into thermal energy.

500,000 electrons with an energy of 200 keV were normally incident on a gold absorber of effective infinite thickness. The electrons were followed down to 5 keV; the remaining energy was considered to be absorbed at the last position of the electron. The resulting energy deposition profile is shown in figure 7-7.

![Energy deposition profile of 200 keV electrons in gold.](image)

*figure 7-7: Energy deposition profile of 200 keV electrons in gold.*
The y-axis in the diagram gives the energy deposition per electron and per μm of absorber thickness in keV/μm. The area beneath the graph represents the deposited energy per electron. The total deposited energy is always less than the incident energy since some electrons get reflected with a remaining kinetic energy. The deposited energy is the incident energy (200 keV) multiplied by an energy absorption coefficient.

The maximum energy deposition is not at the surface but 2-3 μm below. The first explanation for this effect might be that this maximum energy deposition below the surface is due to the Bragg peak in the Bragg curve. The Bragg curve represents the deposited energy as a function of the distance moved by the electron. It equals the stopping power not as a function of the electron kinetic energy but again as a function of the distance moved by the electron. The Bragg curve of a 200 keV electron in gold has been plotted in figure 7-8 using Bethe's stopping power equation for collisional loss (see §2.5). For the calculation of the Bragg curve the electron trajectory is assumed to be straight.

![Bragg curve](image)

*Figure 7-8: Bragg curve for 200 keV electrons in gold.*

The Bragg peak is at 48μm depth, whereas the maximum energy deposition of 200 keV electrons in gold is only 2-3 μm underneath the surface of the absorber. In fact, the maximum energy deposition has nothing to do the maximum stopping power for low energy electrons. The following diagram shows an artificial energy deposition curve assuming a constant stopping power of 5 keV/μm over all kinetic electron energies. 50,000 electrons with an energy of 200 keV were normally incident on a gold absorber of effective infinite thickness.
The electrons were followed down to 5 keV; the remaining energy was counted to be absorbed at the last position of the electron.

![Figure 7-9: Artificial energy deposition curve for a constant stopping power of 5 keV/\mu m.](image)

The reason for the maximum energy deposition below the surface of the absorber has much to do with the angular broadening of the fast moving electrons after a number of scatter events. For the first few microns the electrons maintain their direction before their angular distribution becomes almost homogeneously distributed. A simplified sketch of this behaviour is shown in the following figure. In this picture the position of the maximum energy deposition depends mainly on the ratio of stopping power and angular broadening of the electron beam.

![Simplified sketch of the electron tracks in an absorber.](image)

From this maximum on, the energy deposition decreases for deeper layers in the absorber. The energy deposition due to fast moving electrons becomes zero at a finite depth.
The absorber of interest in an x-ray tube is the target where some of the electron energy is converted into x-rays mainly by the effect of bremsstrahlung (see §2.2.2). Fast moving electrons inside matter occasionally produce bremsstrahlung quanta. The energy of the quanta ranges from zero to the incident energy of the electron. After an electron has migrated some distance through the target it has lost much of its incident energy. Such an electron can only produce bremsstrahlung of limited energy. Thus, only the high energy electrons can produce high energy bremsstrahlung.

The question that arose is, at which depth the high energy bremsstrahlung is produced. To answer this question the electron path was divided into three parts. The first part is where the electron has an energy between 200 and 180 keV (the first 10 %). The second region has an electron energy between 180 and 100 keV (the next 40 %). Finally the third segment is where the electrons have an energy between 100 and zero keV (which is 50 %). For each part of the path the energy deposition was stored in a separate array. As in figure 7-7 the total number of incident electrons was 500,000 per graph. The electrons were followed down to a cut-off energy of 5 keV; the remaining energy was counted to be absorbed at the last position of the electron. The simulated energy deposition curves are shown in figure 7-11.

\[\text{figure 7-11: Energy deposition profile of 200 keV electrons in gold. The electron path is divided into three energy parts.}\]
The area beneath the curves does not represent the energy range of the fast moving electrons but that of the energy deposited by the given energy ranges. The difference is due to reflected electrons with a rest kinetic energy.

The high energy electrons lose 10% of their energy over the first 6 μm. Hence the bremsstrahlung with an energy above 180 keV is produced within the first 6 μm of the target. The electrons that have already lost substantial energy have also moved a distance through the target. They are thus spread out throughout the target volume and produce low energy bremsstrahlung over a wider depth range in the target.

It is possible to shape the bremsstrahlung spectrum by varying the thickness of the target. For example, a low Z substrate could be used together with a high Z layer on the incident surface.

\[\text{figure 7-12: Thin target layer to shape the bremsstrahlung spectrum.}\]

The radiation yield (the fraction of the absorbed energy that is converted into x-rays) increases for high Z elements. E.g. the radiation yield of 200 keV electrons in aluminium is 0.28 %, whereas in tungsten it is 2.4 %. Thus, if electrons get through the high Z layer into the low Z substrate they will produce very few low energy x-ray photons.

Therefore, if the high Z layer is made thinner, relatively less low energy x-ray photons will be produced and the resulting output x-ray spectrum will be hardened. There will still be low energy photons produced, but their fraction decreases for thinner high Z layers. The simulation tool ETraST may be used to tailor the design to produce the required spectral distribution.
8 Conclusion

The simulation tools presented in this thesis open the possibility to model electron transport in both, vacuum and condensed matter. Although a large number of electron transport Monte Carlo codes have been published in the past, no investigated Monte Carlo codes are capable to simulate fast moving electrons in condensed matter in the x-ray energy region, 10 to 250 keV. Even more, the combination of simulation tools for fast moving electrons in electric fields in vacuum and in condensed matter is novel and has not been found in the literature.

The physical background of the Monte Carlo simulation tool for fast moving electrons in condensed matter has been described in detail (section 2 and 3). The reliability of the simulation output has been benchmarked with transmission curves (section 3.4) and measured angular distributions of reflected electrons (section 5).

To evaluate electron trajectories in vacuum, a finite element tool has been written to calculate the potential field distribution by solving Laplace's equation numerically (section 4). Some electron trajectories in an x-ray tube have been calculated; the resulting focal spot has been compared with measured results (section 4.3).

These two simulation tools offer a wide range of applications. Some of these applications have been shown in this thesis: The behaviour of reflected electrons have been studied by measurements (section 5) and simulation (section 5 and 7.1). A capillary for a micro-focus x-ray tube has been investigated again by both, measurements (section 6.4.2) and simulation (section 6.4.1 and 6.5). Finally an energy deposition profile has been studied using the simulation tool ETraST (section 7.2). Other applications have been mentioned in the introduction (see §1.1).

8.1 Further work

In section 7.1 only a few examples of two-dimensional electron reflection distributions are given. It is still very time consuming to evaluate the reflection behaviour of fast moving electrons. Hence it would be useful to develop an effective fit for the angular and energy distribution of reflected electrons as a function of incident angle and energy for different materials.
For the capillary it would be worth repeating some of the simulations including a realistic angular divergence of the incident electron beam. It seems likely that the simulated and measured results will converge for realistic incident beams.

It would be good to construct a large electron trap to measure the total incident current before measuring the angular distribution of reflected electrons (section 5). This would help to normalize the measured curves and in comparing it with simulated results.

Although the two simulation tools for fast moving electrons in vacuum and in condensed matter have been developed in this work, they have not been combined into one tool. The combination of the two simulation tools would enlarge the field of applications.

The off-focal radiation in x-ray tubes is still an area which has not been studied in detail yet. The off-focal radiation could be simulated in one go if the two simulation tools were combined.

A related application is the off-focal energy deposition in x-ray tubes. Of special interest is the deposition in the beryllium output window in high power tubes (>1kW).

Another field for further work is to either write or use an existing Monte Carlo tool that takes more physical effects into account. This is to simulate more specific cases and to improve the accuracy of the simulation results. Some physical effects of interest are secondary electrons, bremsstrahlung, photo electric effect, photon transport, electron diffraction etc. Also, the implementation of surface roughness would be interesting to improve the comparison with measured distributions of reflected electrons (see section 5.5).

With these extensions, the optimal thickness for a high Z material of a layered target can be evaluated for a desired photon spectrum.
Appendix 1: Derivation of the Rutherford formula

The Rutherford scattering formula has been described and derived in different ways in many textbooks, e.g. by A. Messiah [20] §6.1.5 and §11.2.2. On the following pages Rutherford’s scattering law is derived by treating electrons as particles (like planets around the sun). All relativistic effects are neglected.

The scattering formula describes only the probability distribution of the polar scattering angle. The scattering nuclei are treated to be spherically symmetrical and all polarisation effects are neglected. Therefore the azimuth scattering angle is of homogeneous distribution and needs no further explanation.

To derive Rutherford’s scattering equation it is useful to split the velocity of the moving particle into its radial and tangential components

\[ \mathbf{v} = (v_r, v_\phi) = (\dot{r}, r\dot{\phi}) \]

with \( \dot{r} \) being \( r \) differentiated with respect to time. The centre of all coordinates is the atomic nuclei (\( R_{\text{nuclei}} = 0 \)). The angular momentum of the moving particle is

\[ L = mrv_\phi = mr^2\dot{\phi} \]

The kinetic energy at any point is

\[ W_{\text{kin}} = \frac{1}{2}mv^2 = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\phi}^2) . \]

To become independent of time, the two previous equations are brought together

\[ W_{\text{kin}} = \frac{1}{2}m[(r'\dot{\phi})^2 + (r\dot{\phi})^2] = \frac{1}{2}m[(r' L/mr^2)^2 + (r L/mr^2)^2] = \frac{L^2}{2m}\left(\frac{r'^2}{r^4} + \frac{1}{r^2}\right) \]

with \( r' \) being \( r \) differentiated with respect to angle \( \phi \).

With \( V \) as the potential energy the previous equation can be written more generally as
Appendix 1: Derivation of the Rutherford formula

\[ W = \frac{L^2}{2m} \left( \frac{r'^2}{r^4} + \frac{1}{r^2} \right) + V(r) \]

which is the total energy of the moving particle.

This equation describes the path of a charged moving particle that passes a spherically symmetrical Coulomb field.

The potential energy of charged particles around a free nucleus is:

\[ V(r) = \frac{zZe^2}{4\pi\varepsilon_0 r} \]

with \( z \) being the charge number of the moving particle (for electrons -1, for positrons and protons 1, and for alphas 2). The shape of \( r \), which satisfies the differential equation for the total energy, \( W \), is a conic section:

\[ r = \frac{k}{1 - \gamma \cos \phi} \]

and

\[ r' = \frac{-ky\sin \phi}{(1 - \gamma \cos \phi)^2} = \frac{-r^2\gamma\sin \phi}{k} \]

with \( k \) and \( \gamma \) being the cone parameters. These two equations may be combined to

\[ \frac{r'^2}{r^4} = \frac{\gamma^2 \sin^2 \phi}{k^2} = \frac{\gamma^2 (1 - \cos^2 \phi)}{k^2} = \frac{\gamma^2}{k^2} + \frac{2}{kr} - \frac{1}{r^2} \]

With this expression the total energy of the moving electron becomes

\[ W = \frac{L^2}{2m} \left( \frac{\gamma^2}{k^2} + \frac{2}{kr} \right) + \frac{zZe^2}{4\pi\varepsilon_0 r} \]

Since the total energy is constant over \( r \) the sum of all terms which include radius \( r \) must become zero. Hence two new equations can be defined:
Appendix 1: Derivation of the Rutherford formula

\[
W = \frac{L^2 \gamma^2 - 1}{2mk^2}
\]

\[
V(r) = \frac{zZe^2}{4\pi\varepsilon_0 r} = -\frac{L^2}{mkr} \quad \text{and} \quad k = -\frac{4\pi\varepsilon_0 L^2}{zZe^2}
\]

Inserting this expression into the previous one the total energy becomes:

\[
W = \frac{(zZe^2)^2}{2m(4\pi\varepsilon_0 L)^2} (\gamma^2 - 1)
\]

The angular momentum of the electron is constant (Johannes Kepler's second law); hence

\[
L = mvr = mvd_0 = pd_0
\]

with v and p being velocity and momentum of the moving particle at large distance from the nucleus and \(d_0\) the distance between nucleus and electron trajectory without a potential field (see the following figure).

![Figure Al-1: Definition of the constant \(d_0\).](image)

The next step is to insert the constant angular momentum, \(L\), into the expression for the total energy, \(W\); then to divide both sides by \(W = W_{\text{kin}} = \frac{mv_0^2}{2}\), the kinetic energy at greater distance from the nuclei (\(r \to \infty, V \to 0\)). Hence, the following two expressions can be derived.

\[
\gamma^2 = 1 + \left(\frac{4\pi\varepsilon_0 pv}{zZe^2}\right)^2 d_0^2 \quad \text{and}
\]

\[
d_0^2 = \left(\frac{zZe^2}{4\pi\varepsilon_0 pv}\right)^2 (\gamma^2 - 1).
\]

The first equation shows that the trajectory of the moving particle is always of a hyperbolic shape, since \(\gamma\) is always larger than one. It also shows that the trajectory shape is the same for
positive and negative charge of both, moving particle and nuclei. The only difference lies in the azimuth component of the scattering angle. However, since the azimuth component is homogeneously distributed, the final scattering distribution will not differ at all.

The relationship of the polar scattering angle, $\theta$, and the cone parameter $\gamma$ can be drawn from the equation for the cone. The angle between the poles, $\theta$, may be expressed by

$$\theta = 2 \arcsin \frac{1}{\gamma} \quad \text{or} \quad \gamma = \frac{1}{\sin \frac{\theta}{2}}$$

with $\theta$ being the scattering angle relative to the straight trajectory.

Inserting the right hand equation into the previous one, the distance $d_0$ becomes

$$d_0 = c \sqrt{\frac{1}{\sin^2 \frac{\theta}{2}} - 1} \quad \text{with} \quad c = \frac{zZe^2}{4\pi\varepsilon_0 pv}.$$ 

Now, the differential cross section becomes:

$$\frac{d\sigma}{d\Omega}(\theta) = \frac{1}{2\pi \sin \theta} \frac{d\sigma}{d\theta} = -\frac{d_0}{\sin \theta} \frac{dd_0}{d\theta} = \frac{c^2}{2 \sin \theta} \frac{\cos \frac{\theta}{2}}{\sin^3 \frac{\theta}{2}} = \frac{c^2}{4} \frac{1}{\sin^4 \frac{\theta}{2}}$$

And finally

$$\frac{d\sigma}{d\Omega}(\theta) = \left( \frac{zZe^2}{8\pi\varepsilon_0 pv} \right)^2 \cdot \frac{1}{\sin^{4} \frac{\theta}{2}}$$

which is Rutherford's scattering law.
Appendix 2: Input files for ETraST

The Electron Track Simulation Tool ETraST is mainly controlled by an input file. The content of the input file is described in this section.

In the first line of the input file is a single word which classifies the simulation type. The different possibilities are:

- Reflection
- Measure
- Transmission
- Transmission_distribution
- Foil

The following lines (from line two on) are different for the various simulation types. They are briefly explained in the following sections.

**A2.1 Simulation type 'Reflection'**

Electrons are incident on a semi-infinite large reflector. Each reflected electron is stored separately in an output file. The output file name is ‘REFL[element][number].OUT’ where [element] is the short name of the element (e.g. AL for aluminium) and [number] is the number of the data set starting with zero. For example ‘REFLPB06.OUT’ is the 7th data set of reflected electrons in lead.

In the second line of the input file ETraST expects an integer number for the number of data sets. This number must be between one and 100.

From the third line on for each data set one line with three floating point numbers is expected. The three numbers are

1. incident energy (in keV),
2. low limit energy (in keV) and
3. incident angle (in deg).

A possible input data set could be:
Appendix 2: Input files for ETraST

Reflection
4
100 10 5
100 10 10
200 20 5
200 20 10

A2.2 Simulation type ‘Measure’

This simulation type equals the Reflection type but includes an incident angle divergence. Electrons are incident on a semi-infinite large reflector. Each reflected electron is stored separately in an output file. The output file name is ‘MEAS[element][number].OUT’ where [element] is the short name of the element (e.g. AU for Gold) and [number] is the number of the data set starting with zero. For example ‘MEASW02.OUT’ is the 3rd data set of reflected electrons in tungsten. In the second line of the input file ETraST expects an integer number for the number of data sets. This number must be between one and 100.

From the third line on for each data set one line with four floating point numbers is expected. The four numbers are

1. incident energy (in keV),
2. low limit energy (in keV) and
3. incident angle (in deg).

The fourth floating point number stands for a maximum (positive and negative) angular divergence. A triangular probability distribution is assumed.

A possible input data set could be:
Appendix 2: Input files for ETraST

Measure
4
100 10 1 .955
100 10 2 .955
100 10 5 .955
100 10 10 .955

A2.3 Simulation type ‘Transmission’

Calculates the transmission curve for electrons incident normal on a foil. The output file name is ‘TRAN[element][number].OUT’ where [element] is the short name of the element (e.g. AL for aluminium) and [number] is the number of the data set starting with zero. For example ‘TRANCU08.OUT’ is the 9th transmission curve in copper.

In the second line of the input file ETraST expects an integer number for the number of transmission curves. This number must be between one and 100.

From the third line on for each transmission curve one line with three floating point numbers is expected. The three numbers are

1. the incident energy (in keV),
2. the low limit energy (in keV) and
3. the foil thickness (in µm).

A possible input data set could be:

Transmission
4
50 10 4
100 10 8
150 20 12
200 20 16

A2.4 Simulation type ‘Transmission_distribution’

This simulation type equals the ‘Transmission’ type with the only difference that the angular distribution in the forward direction for each layer is added in the output file. The output file
name is ‘DIST[element][number].OUT’ where [element] is the short name of the element (e.g. AL for aluminium) and [number] is the number of the data set starting with zero. For example ‘DISTAG01.OUT’ is the 2nd transmission curve with the angular distribution in silver.

In the second line of the input file ETraST expects an integer number for the number of data sets to be simulated. This number must be between one and 100.

From the third line on for each data set one line with three floating point numbers is expected. The three numbers are

1. the incident energy (in keV),
2. the low limit energy (in keV) and
3. the foil thickness (in μm). A possible input data set could be:

```
Transmission_distribution
4
50 10 4
100 10 8
150 20 12
200 20 16
```

**A2.5 Simulation type ‘Foil’**

Calculates six coefficients for fast electrons on foils. The six coefficients are:

- number reflection coefficient
- number absorption coefficient
- number transmission coefficient
- energy reflection coefficient
- energy absorption coefficient
- energy transmission coefficient

The output file names are ‘FOIL[element][number].OUT’ where [element] is the short name of the element (e.g. AL for aluminium) and [number] is the number of the data set starting with zero. For example ‘FOILAu03.OUT’ is the 4th coefficient set in Gold.
In the second line of the input file ETraST expects an integer number for the number of coefficient sets. This number must be between one and 100.

From the third line on for each coefficient set one line with three floating point numbers is expected. The three numbers are

1. the incident energy (in keV),
2. the low limit energy (in keV) and
3. the foil thickness (in μm). A possible input data set could be:

```
Foil
4
50 5 2
100 10 4
150 15 6
200 20 8
```
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