Imaging Applications and an Extension of the EGS4 Code System

A thesis submitted to the University of Surrey for the degree of Doctor of Philosophy

by

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Abstract

This thesis investigates the use of Monte Carlo methods to study several imaging applications. Studies are based on the EGS4 code system, and some of these used a low energy electron expansion for this software package that was developed during this work.

The code is firstly used to gain some insight into one-sided imaging techniques making use of megavoltage radiation. The method explored is based on induced positron annihilation. The dependence of annihilation yields on atomic number demonstrates that the technique is suitable for the inspection of high-Z inclusions in low-Z, less dense, matrices. Results obtained with the EGS4 code were found to be in good agreement with experimental data. Several applications have been considered via the simulation approach, showing that areas like civil engineering and nuclear material inspection can benefit from this novel inspection technique.

The limited accuracy of EGS4 in the simulation of X-ray tubes operating at diagnostic energies led to an expansion of the code to be developed. The enhanced code incorporates a generalized oscillator strength (GOS) model for electron atom inelastic collisions, where atomic bound effects are considered. An enhanced version of this model has been developed so that K-shell ionisation events could be reproduced realistically. The accuracy of low energy bremsstrahlung emissions has also been assessed, and an improved scheme for the angular sampling of newly created photons suggested.

The low energy electron expansion of EGS4 (the EGS4/GOS code) is described, and used to simulate photon spectra from diagnostic X-ray tubes. The results were compared with experimental data, showing an accuracy of the order of 15% near the Kα line.

Some X-ray tube design studies were carried out using the EGS4/GOS code. The importance of the different physical interactions was analysed. The results show that better fluorescence-to-bremsstrahlung ratios can be obtained with thinner targets, but a factor 2 increase in this ratio is achieved at the expense of a decrease of 40 times in efficiency. The need for low-Z substrates in thin-target applications is also discussed.
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Chapter 1

Introduction

This chapter introduces the overall organisation of the thesis and some of the fundamentals concerning the work carried out. Firstly, the subjects covered in each of the chapters and the organisation of this thesis is described. Then, the basic principles of the Monte Carlo technique, and its applications to simulation of the transport of radiation are introduced. The structure of the EGS4 code system and some imaging applications are then described. Some refinements of the technique and the need for possible enhancements in the EGS4 code are also discussed. Energy-momentum relations are described in Appendix A, and a general description of the semiconductor detectors used in experimental measurements is presented in Appendix B.

1.1 Layout of the thesis

This thesis is divided into 8 chapters. In this first chapter, the basic principles of the Monte Carlo method and its applications to the transport of radiation are described. Also, the EGS4 (Electron Gamma Shower, version 4) Monte Carlo code, and some imaging applications are presented. A one-sided imaging technique involving the use of megavoltage radiation and the detection of annihilation radiation is presented in Chapter 2. Experimental data and simulation results are compared, and the poten-
tial of the technique in different environments is discussed. In Chapter 3, the limited accuracy of EGS4 in the simulation X-ray tubes operating at diagnostic energies is discussed. Improved models for the inelastic collision of low energy electrons with atoms are presented in Chapter 4, while Chapter 5 discusses the schemes used to simulate bremsstrahlung emissions. A low energy expansion of EGS4 -the EGS4/GOS code-, and its suitability for simulation of photon production in X-ray tubes operated below 100 keV is presented in Chapter 6. The EGS4/GOS code was used in some design studies for diagnostic X-ray tubes operating in transmission geometry and the discussion is presented in Chapter 7. Finally, an overview of the studies and suggestions for future work are described in Chapter 8.

1.2 The Monte-Carlo Method

1.2.1 Historical introduction

The Monte Carlo Method is a technique often used in problems with a stochastic nature. The solution is built by random sampling the appropriate probability distributions, making use of a series of random numbers. The roots of this mathematical approach are usually associated with the French naturalist Buffon who, in the eighteenth century, introduced the "needle problem" [Rae76, Jam80] to calculate the value of $\pi$. In the late 1940's this technique was used to solve problems related to the transport of neutrons, with John von Neuman establishing the code name of "Monte-Carlo Method" for this approach.

In fact, Monte-Carlo calculations are nowadays associated with intensive computing, but the principles of random sampling seem to have been first investigated in 1777, with the formulation of the "Buffon's needle problem" [McC52]. In its simple guise, Buffon's calculation can be described in the following terms [Rae76]: if a needle of length $d$, is randomly thrown onto an array of equally spaced parallel lines, separated by a distance $D$ (where $D > d$), then what is the probability $P$
that the needle will intersect one of the lines? The solution for this problem yields $P = \frac{2d}{\pi D}$. By means of a simple “hit-or-miss” experiment, and after a large number of trials, $P$ can determined and used to estimate the value of $\pi$. This method turns out to be an inefficient approach for the calculation of $\pi$ as a slow convergence is expected [Jam 80], but the exercise is a good example of the application of random sampling techniques.

Some further work involving the use of random sampling techniques was carried out by Laplace and Lord Kelvin [Bri 97]. These involved not only the estimation of $\pi$, but also the evaluation of integrals used in the kinetic theory of gases. During the 1940’s scientists working on the development of nuclear weapons in Los Alamos National Laboratory (USA) used this approach in problems related to the transport of radiation. The collaborative work of Stan Ulam, John von Neuman and Nicholas Metropolis on techniques for statistical sampling (then based on the use of electromechanical devices) resulted in what is now widely known as the Monte-Carlo method. At the same time, Enrico Fermi devised an analog computer -the FERMIAC-, a “Monte Carlo Trolley” [Sei 96] capable of simulating neutron diffusion and multiplication, providing accurate predictions of experimental results [Bri 97].

The need for powerful machines that could apply the Monte-Carlo method to stochastical calculations requiring a “brute force approach” has triggered the development of increasingly faster computers. For this reason, these events are associated with the start of what is nowadays acknowledged to be the modern computer era [Bre 96]. Since then, computing power has constantly increased with a dramatic fall in cost. In the 1960’s, Gordon Moore of Intel came up with a now famous empirical law, stating that the computing power of transistors on a chip should quadruple more or less every 3 years. Data from the early 1990s [Nis 95] showed that microelectronics should continue to follow Moore’s law in the first decade of next century. However, it has recently been reported [Kel 98] that, by 2005, problems related to the aluminium-based signal propagation between transistors may well bring this exponential law to an end. This seems not to be the case at the moment. Indeed, a
recent timing benchmark [Bie 97b] shows that (for Intel processors) computing speed has in fact been doubling every 1.52 years.

The Monte-Carlo method is nowadays an increasingly popular approach and that is partially due to this technological revolution. The method can be used even in problems of a deterministic nature, such as integral calculations, constant evaluations [Jam 80], and all those rather complicated for classical approaches. As a result, a great deal of theoretical investigation and practical experience has been gained on Monte Carlo methods, which is now a common approach to the solution of a great variety of problems [Jam 80, Bie 97b].

1.2.2 Sampling techniques

In broad terms the Monte-Carlo method can be understood as a numerical technique, which uses random numbers to construct the solution of a physical or mathematical problem [Jam 80]. In the specific case of drawing random samples from a certain probability law, the technique can be presented in a rather simple form. Let $X$ be the stochastic variable with probability distribution $f(x)$, such that

$$
\int_{-\infty}^{+\infty} f(x) \, dx = 1. \tag{1.1}
$$

The basic idea behind the sampling of $f(x)$ is to build its cumulative probability distribution $F(x)$. This quantity represents the probability of picking values $X$, such that $X < x$. More simply

$$
F(x) = \text{Prob}(X < x) = \int_{-\infty}^{x} f(x') \, dx'. \tag{1.2}
$$

The distribution $f(x)$ can be sampled using $F(x)$, by using a set of random numbers with uniform distribution. In fact, if $x_i$ are samples from a uniform distribution in the interval $(0,1)$, the values $X_i$ calculated from

$$
x_i = \int_{0}^{x_i} f(x') \, dx'. \tag{1.3}
$$
are distributed according to \( f(x) \) [Lin65]. This method, often referred as “direct”, can only be used in situations where \( F(x) \) can be calculated and inverted. In failing to deliver this, more complex approaches have to be considered, such as the rejection technique or the “composition” method.

A simplified version of the rejection technique is graphically presented in fig. 1.1. Drawing samples distributed according to \( f(x) \), whose analytical form is assumed to be known, also requires the use of random numbers \( \xi \) uniformly distributed in the range \((0,1)\) and the process can be described in the following way. A random number \( \xi_1 \) is sampled from an uniform distribution in \((0,1)\), and used to determine a value \( x_i \) in the interval \((a,b)\) using the relation \( x_i = a + \xi_1 \times (b - a) \). A second random number \( \xi_2 \) is sampled, and \( x_i \) is accepted if \( \xi_2 < f(x_i)/y_{\text{max}} \).

Another sampling technique often used in Monte Carlo applications addresses
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more complex schemes. In fact, if a probability distribution function \( f(x) \) can be decomposed in the form

\[
f(x) = \sum_{i=1}^{n} \alpha_i h_i(x) g_i(x)
\]

such that \( h(x) \) can be sampled using the direct method as presented in eq. (1.3), \( 0 < g_i(x) < 1 \) and \( \alpha_i \) are all positive, the method goes in the following way. If \( \xi_i \) are random numbers sampled from uniform distributions in \((0,1)\) then [But61]:

1. Pick \( \xi_1 \) and determine \( i \) such that \( \sum_{j=1}^{i-1} \alpha_j < \xi_1 < \sum_{j=1}^{i} \alpha_j \).

2. Sample a value \( x \) from \( h_i(x) \) by solving \( \int_{-\infty}^{x} h_i(x') dx' = \xi_2 \).

3. Pick \( \xi_3 \), and accept the value \( x \) if \( \xi_3 < g_i(x) \).

This method is known as being a mixture of two techniques: "composition" and "rejection" [Ham64]. For \( g_i(x) = 1 \) then the pure "composition" method is used. For \( n = 1 \) the rejection technique is reproduced [Ham64]. The pictorial representation in fig. 1.1 reproduced with \( n = 1 \) and \( h_i(x) = 1 \).

1.2.3 Random number generation

In the discussion previously carried out, it was brought to light that numerical sampling from a given distribution (i.e. the Monte Carlo Method itself) requires sets of random numbers, with uniform distribution, to be available. The ability to exactly recreate a sampling procedure requires a reproducible random number sequence to be generated, preferably by means of a certain numerical algorithm. It is more or less intuitive that "truly" random numbers cannot be produced by means of deterministic algorithms [Pre92], something that was also realised by Von Neuman [Knu89]. In this context, the term "pseudorandom" is used to describe a series of numbers, produced by means of a computer algorithm (the generator), that mimics a random number sequence.
Although a considerable amount of research has been carried out on this topic, assessing the quality of a random number generator is still a rather difficult task [Jam 80, Jam 90]. An immediate question to be asked is the length of its period, i.e. how many different values can be generated using a certain scheme. But even very long sequences may fail other numerical tests, if they concern aspects like the uniformity or the correlation between samples [Mar 68, Knu 89]. So, it does seem more appropriate to take a pragmatic view and focus on the specific application for which the generator is intended to be used [Fer 92].

One of the random number generators most commonly used is based on the so-called "linear congruential method" (LC). Given a multiplier $a$, a starting value $\xi_0$ and a constant $C$, successive numbers $\xi_i$ are generated from

$$\xi_i = (a \xi_{i-1} + C) \mod M,$$

where $a \mod b$ represents the remainder of the (integer) division $a/b$. In order to maximise the period of the sequence $M$ should be chosen to be of the order of the maximum integer that can be represented in one computer word. Usually the sequence produced is machine-dependent and, on 32-bit machines, the period of the series generated is $\sim 10^9$.

Another type of random number generator is the so-called lagged Fibonacci [Jam 90, And 91]. As in the series with the same name, each value in the sequence is calculated by means of an arithmetic or logical operation between two numbers which have already occurred. Unlike the Fibonacci series, the operation does not involve the last two occurrences. The period of the lagged Fibonacci generator can be made as long as $10^{171}$ [Jam 90], and in most cases the series is portable (i.e. machine independent). An improved scheme for this kind of generator has been proposed by Lüscher [Lus 94], and recently made available in Fortran [Jam 94]. The basic idea is to throw away some of the numbers generated by a lagged Fibonacci series. In doing so, the generator is more likely to be in accordance with a wide variety of numerical tests [Knu 89, Vat 95].
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The choice of a suitable random number generator is the subject of a continuous debate. In a comprehensive review of random number generators [Jam 90], it has been strongly suggested that schemes based on lagged Fibonacci sequences should replace any methods based on the traditional LC. But on the other hand, it has been recently pointed out [And 91] that when simulating the response of ion chambers, LC methods seem to perform "as well" as any other scheme of random number generation. In addition to previous LC schemes, the lagged Fibonacci generator RANMAR [Jam 90], proposed by Marsaglia and Zeeman, has also been incorporated in the EGS4 code [Nel 84]. Its long period (∼10^{43}) and portability were the main reasons for its use in all the simulations described in this thesis.

1.2.4 Precision of the calculations

Assessing the uncertainties in Monte Carlo based simulations is a topic of considerable importance. This is because, as generally in experimental methods, results can only be analysed on the grounds of the associated uncertainties [Tay 82]. In Monte Carlo practice, uncertainties are usually divided in two categories [And 91, Bri 97]: one associated with the statistical nature of the method and another, more subjective, related to the overall formulation of the problem. In this section, only the first type of uncertainty is addressed and the formalism used is based on statistical methods widely applied in the treatment of experimental errors.

In broad terms, Monte Carlo results are obtained by scoring samples \( x_i \), representative of a certain measurable quantity \( X \). If this quantity is known to have a certain probability distribution function \( f(x) \), the expected value (or mean) of \( X \), \( E(X) \), is given by [Fel 50]

\[
E(X) = \int x' f(x') \, dx' \equiv \text{"true mean"}. \tag{1.6}
\]

On the other hand, the samples \( x_i \) obtained from the Monte Carlo process can be
used to estimate a mean value $\bar{x}$, from

$$\bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i,$$

where $N$ is the number of trials (briefly called histories) used in the calculation.

The relation between $E(x)$ and $\bar{x}$ is given by the Strong Law of Large Numbers [Fel50, Jam 80], which basically states that if $E(x)$ exists, then for large values of $N$, $\bar{x}$ will converge to $E(x)$. In other words, if a large number of histories is used, then average values can be used in the calculation of the expected value of a distribution.

Whereas the Law of Large Numbers states that estimates based on a large number of observations should reproduce expected mean values, it is also important to understand the convergence of the method. Or in other words, how to estimate the precision of a given result, if possible, by means of confidence intervals. This can be done using the Central Limit Theorem, which requires a few more parameters to be introduced.

The variance, $\sigma^2$, of the distribution $f(x)$ previously introduced, can be calculated from [Fel 50]

$$\sigma^2 = \int [(x - E(x))^2 f(x) dx = E(x^2) - [E(x)]^2$$

where $E(x^2)$ represents the mean value of $x^2$. The quantity $\sigma$, which is basically a measure of the spread of the distribution $f(x)$, can be estimated from the “set of measurements” $x_i$ through the calculation of the auxiliary quantity $S^2$. This is given by [Tay 82]

$$S^2 = \frac{1}{N-1} \sum_{i=1}^{N} (x_i - \bar{x})^2.$$

Similarly, $S$ represents a measure of the spread in the values $x_i$ and, provided that the quantity $E(x^2)$ exists and $N$ is large, can be used as reasonable estimation of $\sigma$. The variance, $S^2_{\bar{x}}$, of the calculated $\bar{x}$ is given by [Tay 82]

$$S^2_{\bar{x}} = \frac{S^2}{N}.$$
Keeping the notation previously introduced, the Central Limit Theorem states that, for a pair of arbitrary values $\alpha$ and $\beta$ (with $\beta > \alpha$), it is found that [Fel50]

$$\lim_{N \to \infty} \text{Prob} \left[ \alpha < \frac{E(x) - \bar{x}}{\sigma N^{-1/2}} < \beta \right] = \frac{1}{\sqrt{2\pi}} \int_\alpha^\beta e^{-t^2/2} dt \quad (1.11)$$

where $\text{Prob}[Z]$ means the probability of $Z$. Then, in the view of the expression (1.10) and for large values of $N$, as $S$ is expected to realistically reproduce $\sigma$, eq. (1.11) can be written in the form

$$\text{Prob} \left[ \alpha < \frac{E(x) - \bar{x}}{S_x} < \beta \right] \to \frac{1}{\sqrt{2\pi}} \int_\alpha^\beta e^{-t^2/2} dt. \quad (1.12)$$

The extreme importance of the Central Limit Theorem is now obvious. It points out that calculated averages $\bar{x}$ tend to be normally (i.e. Gaussian) distributed around the expected mean value of the original distribution $f(x)$. And also, that the width of the curve is characterised by the variance $S_x$. In other words, the convergence of $\bar{x}$ to the expected mean of the distribution $f(x)$ can be visualised in terms of a Gaussian distribution with variance $S_x$. This is interpretation was made under the assumption of "a large number of observations $N$". Following the discussion in [Tay82], this can be considered to happen when

$$\sqrt{\frac{N}{N - 1}} \sim 1. \quad (1.13)$$

The previous discussion can be summarised in the following way. Calculated averages $\bar{x}$ are a consistent estimation for mean values of probability distributions. Moreover, the convergence should basically follow a Gaussian distributions with a variance $S_x \propto 1/\sqrt{N}$.

In practical situations, a handy way of dealing with variances is by using normalised values. This leads to the definition of an estimated relative error, $R$, given by [Bri97]

$$R = \frac{S_x}{\bar{x}} \quad (1.14)$$

which may, unambiguously, be quoted to express the accuracy of a result. Following the definitions presented above, $R$ can be calculated from the set of values $x_i$ by
\[ R = \left[ \frac{\sum_{i=1}^{N} x_i^2}{\left( \frac{N}{\sum_{i=1}^{N} x_i} \right)^2} - \frac{1}{N} \right]^{1/2} \] (1.15)

It was reported [Bri97] that for applications in the field of radiation physics reliable results are generally obtained by means of Monte Carlo simulations when \( R < 0.05 \).

It should be stressed that the formalism presented to assess the accuracy of results obtained by means Monte Carlo techniques considered only the statistical uncertainties of the process itself. A wrong formulation of the problem, as well as other errors in the coding or the distributions in use, may result in systematic errors. These, classified by Andreo as “category A”, are more difficult to evaluate. Also, in situations where ratios are being estimated, it may be possible to obtain non-finite samples, in which case variances should be evaluated differently [Ma91]. These will not be considered in the scope of this work and, unless different a figure is presented, the results shown are such that \( R \leq 0.05 \).

1.2.5 Variance reduction techniques

Several techniques have been developed to make Monte Carlo calculations more efficient. In the light of eq. (1.10), the precision of a result is expected to vary with \( 1/\sqrt{N} \), so it is always possible to improve it by running more histories. But such improvements will be made at the cost of computing time (which should be proportional to \( N \)). So, the idea behind variance reduction techniques is to reduce the time it takes to calculate a result with a given precision [Bie88].

A reliable figure of merit which may be used to estimate gains in accuracy associated with a certain “variance reduction technique”, is the “efficiency”, \( \epsilon \), defined by [Bie88, Bri97]

\[ \epsilon = \frac{1}{TR^2} \] (1.16)
where $T$ is measure of the computing time (e.g. CPU time in seconds). This quantity may also used as a tally (i.e. a scored quantity) reliability indicator, in the sense that, for "well behaved" tallies, $c$ should be approximately constant. When using Monte Carlo methods to simulate the transport of radiation, improvements in efficiency are attainable, for example, by means of schemes such as forcing particles to interact, discarding those not contributing to evaluated tallies, or even further approximations in the transport physics. Comprehensive reviews of these variance reduction techniques can found in [Bie88, Bri97].

A variance reduction technique employed in the work hereby described was the so called particle splitting. This scheme addresses situations where the probability of a non-zero measurement is very low, which is to say that most of the $x_i$ are actually zero, so accounting for larger variances in the final result. This is, for example, the case in applications like the simulation of X-ray tubes operating at energies below 100 keV: the probability of producing bremsstrahlung and fluorescence photons is very small which results in very time consuming simulations. In these situations, assuming that only $n$ (out of $N$) histories contribute to non-zero identical scores $x$ (i.e. $x_i = x$, for $i = 1, \ldots, n$), and that $n \ll N$, then the relative error, $R$, from eq. (1.15) yields

$$R = \left[ \frac{nx^2}{n^2x^2} - \frac{1}{N} \right]^{1/2} \sim \frac{1}{\sqrt{n}},$$

that is to say, the relative error is mainly a function of the number events with non-zero scores. An efficient way of reducing $R$ is then to increase the $n$, especially if this is made at no significant increase of computing time.

In applications involving particle detection (as with X-ray tubes), the idea behind particle splitting is to emphasize the creation "interesting" of particles (i.e. those relevant in terms of the measured tally). When, the sampling algorithm selects one of these particles to be generated, then it can be assumed that $M$ of these events actually took place. A weight $1/M$ is then attributed to each of these particles so that the game is kept "fair", that is, on average, no laws are violated. This artefact results in the reduction of $R$, as it should result in more non-zero entries. On the other hand,
as these events have a very low probability of occurrence, no significant increase in the computing time should be observed, leading to more efficient simulations. This technique has been successfully used in the sampling of bremsstrahlung photons [Bie 89, Fad 90].

1.3 Radiation Transport using Monte Carlo Methods

The interaction of radiation with matter can be described as a statistical phenomenon where, at each step, particles can undergo one of a number of different interactions, each with a certain probability of occurrence. These probabilities are usually referred to as cross sections, \( \sigma_i \), and are expressed in units of an area. Denoting the total cross section by \( \sigma_T \) (i.e. \( \sigma_T = \sum \sigma_i \)), the distance \( s \) from a given position to the point of the next interaction is distributed according to the function \( p(s) \) given by [Rae 76, And 91]

\[
p(s) = N_{at} \sigma_T e^{-N_{at} \sigma_T s}
\]

(1.18)

where \( N_{at} \) represents the number of atoms per unit volume. This distribution can be sampled using the direct method as stated in eq. (1.3), using the relation

\[
s = \frac{-1}{\mu} \ln \xi^t
\]

(1.19)

where \( \mu = N_{at} \sigma_T \) represents the linear attenuation coefficient, and the random number \( \xi^t = 1 - \xi \) also has uniform distribution in (0,1).

Once the distance to the next point of interaction is determined, the algorithm has to select the type of interaction to occur. If the respective probabilities are numbered 1 to \( m \), this can be done by building the cumulative distribution \( F(i) \)

\[
F(i) = \frac{1}{\sigma_T} \sum_{j=1}^{i} \sigma_j
\]

(1.20)
with $\sigma_T = \sum_{j=1}^{m} \sigma_j$. Then, by using a random number $\xi$ from an uniform distribution in $(0,1)$, the interaction (labelled $k$) due to occur is selected from

$$F(k-1) < \xi < F(k).$$

(1.21)

The next step is then to work out the kinematics of the reaction, by randomly sampling the respective probability distribution functions.

The procedure just described has been implemented successfully to simulate the transport of particles like photons and neutrons [Rae 76, And 91, Bri 97]. Usually the total probability of interaction $\sigma_T$, and cumulative functions $F(i)$ are tabulated for different particle energies, thus reducing the computational effort during the simulation. In the case of photons with energies from 1 keV to several MeV, the interactions usually considered are [And 91] Rayleigh and Compton scattering, photoelectric collisions, pair production and, in some cases, nuclear reactions.

The same technique could, in principle, be applied to simulate the transport of electrons in matter. For energies from a few keV, the interactions to be considered are atomic excitation and ionisation, elastic scattering and bremsstrahlung emission. However, the very large number of interactions that charged particles undergo makes this kind of approach unrealistic in most situations, from the perspective of the computing time required. The orders of magnitude involved can be seen in fig. 1.2 where (total) electron and photon interaction cross sections in aluminium (Al) are plotted. To complement these data, it has been estimated that electrons slowing down from 500 keV to 1 keV in Al, may undergo $\sim 10^4$ collisions [And 91], while a photon will undergo about 30 Compton collisions as its energy decreases from 5 MeV to 1 keV [Rae 76].

Realising that simulating all the electron interactions would be rather unfeasible, Berger suggested that some interactions could actually be grouped and accounted for in terms of their “net” effect [Ber 63]. This pioneering approach urged the development of the so called “condensed history” method, where the grouping of physical interactions results in a “macroscopic” view of the transport process. The basic idea
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Figure 1.2: Atomic cross sections for electrons and photons in Al. The total photon cross section was calculated using the XCOM [Ber87] and includes Rayleigh and Compton scattering, photoelectric absorptions and pair production. Data for electrons is from the EEDL database [Per91] and includes atomic excitation and ionisation, elastic scattering and bremsstrahlung emission.

is to consider multiple collision models (e.g. the stopping power theory) instead of a comprehensive simulation of all the interactions. The step sizes should be chosen so that the number of steps is kept as small as possible (thus reducing computing time), but within the limits of the multiple scattering models [And91]. Grouping interactions means that stochastic events are represented by the average of a certain number of observations, which should itself be considered as an approach enclosing some level of approximation.

In his work, Berger suggested that the “condensed history” technique should be divided into two categories. One, Class 1, where all the interactions are grouped, and the step lengths are predetermined. Events involving energy losses can be considered
by means of the continuous slowing down approximation (CSDA) and elastic scattering by multiple scattering distributions. Step lengths can be either fixed or chosen so that, on average, the energy is reduced by a constant factor. The other category, Class II, follows a technique originally described in [Sch 59], where interactions associated with large energy losses ("catastrophic" or "hard" collisions) are excluded from the grouping scheme and explicitly considered. The step size is selected as the distance to the next catastrophic collision, with small energy losses (corresponding to "soft" collisions) considered in terms of their stopping power. Berger also suggested that in Class II algorithms, elastic collisions could be either all grouped or subject to a scheme where large angular deflections are separated and treated individually.

The performance of the two grouping schemes has been compared in Berger's initial paper [Ber 63], as well as in a recent review [And 91]. In these communications it was emphasised that Class II has the advantage that the initial state of secondary particles (knock-on electrons and bremsstrahlung photons) is unambiguously defined, and that angular deflections associated with energy losses are treated in a more realistic fashion. On the other hand, Class I offers the possibility of treating energy-loss straggling, a quantity that does not depend on a particular threshold for energy transfers.

1.4 The EGS4 code system

One of the publicly available codes to simulate the transport of electrons, positrons and photons in condensed media is EGS4 - the Electron Gamma Shower, version 4 [Nel 84]. The EGS system is a well organised and versatile software package that was originally developed to simulate the transport of radiation in high energy physics applications. Version 3 of the code [For 78] was designed to simulate electromagnetic cascades in different geometries, for energies ranging from several hundred keV up to a few thousand GeV [Nel 88]. The popularity of this general purpose code motivated
its extension to lower energies, resulting in the release of version 4 in 1984. The code has been extensively benchmarked [Nel97] and it is now acknowledged that realistic simulations can be carried out down to energies of the order of 1 keV for photons and 10 keV for electrons (and positrons). Several further improvements have been carried out since the 1984 release [Bie94, Nel97].

In terms of charged particle transport, the EGS4 code uses the condensed history technique with a Class II algorithm. Electron and positron inelastic collisions are treated in terms of their energy loss if below predefined values and fully simulated above those cuts. Elastic scattering from atomic nuclei and electrons is treated using the multiple scattering theory of Molière [Bet53]. Cross sections and other physical quantities to be used in the transport of particles are calculated using the material preprocessor PECS4. These general transport quantities are firstly determined and stored in a form for fast numerical evaluation, thus speeding up the EGS4 code. In addition, the PECS4 tool is written in a modular form so that it can be used for more general tasks, like evaluating physical quantities. The types of media (element, compound, mixture), their compositions and densities are defined in a simple input file to be used by PECS4. It is also in this input file that the thresholds for “catastrophic” interactions are defined. The variables that correspond to these energy cuts are $AE$ and $AP$, for the production of knock-on electrons and the bremsstrahlung photons, respectively.

The EGS4 code is basically a collection of routines that simulate the transport of particles, as well as the different interaction processes. The user should write a small program defining the geometry to be considered (subroutine HOWFAR) and the output tallies (subroutine AUSGAB). The code also offers the possibility of defining (kinetic) energy cuts below which the particles are considered to be locally deposited and no longer transported. These cuts should also be specified in the user code. All the original code was written in a structured language called Mortran3 [Coo82]. This code can be converted to standard Fortran using the compiler included in the standard distribution of EGS4.
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The way EGS4 is structured requires a certain level of expertise, so that a suitable user code can be produced. However, any initial difficulties are fully compensated for by the tremendous freedom in the choice of geometries and scoring tallies. The whole structure of EGS4 is carefully described in the user manual [Nel84], and aspects related to improvements in the code and benchmarks have been considered in several publications [Rog88, Bie94, Nel97, And91]. The next two sections concentrate only on the different interaction mechanisms that EGS4 simulates.

1.4.1 Photon interactions

The photon interactions considered in EGS4 are Rayleigh and Compton scattering, photoelectric collisions and electron-positron pair production. In broad terms, the total photon interaction cross section is determined, and the distance to the next interaction sampled using the techniques described in section 1.3. The geometry is “interrogated” and if a boundary between two different media is crossed, the transport is stopped so that the total cross section can be re-evaluated for the new material.

In terms of coherent (Rayleigh) scattering, the total cross section is evaluated using data from Storm and Israel [Sto70]. In the standard version of the code total cross sections are calculated as if all the atoms would act independently. The same assumption is made on the calculations of molecular form factors, where atomic data from [Hub79] is used. The realisation that this approximation was actually very crude when simulating low energy photon scattering, led to new molecular form factors for water to be incorporated in the code [Lei96]. In this update, data from [Mor82] is used and interference effects in water molecules are properly accounted for. After a suitable factorisation of the differential cross section (which is basically the Thompson cross section for a free electron multiplied by a form factor) the photon scattering angle is determined using the rejection technique.

Until very recently, Compton scattering events were considered with the assump-
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tion that atomic electrons were free and stationary particles. The kinematics of the collision was based on the Klein-Nishina differential cross section [Kno89], and the approach was considered to be accurate enough for most applications, especially at higher energies. A major improvement has also been introduced so that, at lower photon energies, bound electron effects can be considered properly. The total cross sections have been re-evaluated, the angular distributions modified and broadening introduced to account for the distribution of electron momenta. The enhanced code, LSCAT [Nam94], is publicly available and also incorporates the treatment for linearly-polarized photon scattering [Hir93]. With this low energy expansion, the treatment of Compton scattering with EGS4 is regarded as extremely accurate.

As for coherent scattering, the cross sections used for photoelectric events were taken from [Sto70]. In the original version, photoelectron creation and the possible emission of fluorescence photons were only considered for events involving the ionisation of the K-shell. Also, the photoelectron was considered to be emitted in the direction of the incident photon. An additional scheme for angular sampling of the photoelectrons has been developed [Bie86] and, more recently, the whole photoelectric treatment extended so that L-Shell fluorescence is also considered.

Electron-positron pair production in the EGS4 code follows the general treatment presented in Motz's review article [Mot69]. However, for photon energies below 50 MeV, the total cross section was calculated directly from [Sto70]. In these regimes, the energies of the created particles are determined using the unscreened Bethe-Heitler cross section [Hei60], while above 50 MeV the Coulomb corrected [Mot69] form of the same cross section is employed. In order to optimize the sampling algorithms, some approximations have been introduced. One is to consider that, for photon energies below 2.1 MeV, one of the particles is created at rest and the other given the rest of the available energy. Also, as the cross section for pair-production peaks at small angles the original version of the code employed a simplified scheme where one of the created particles is set in motion at a fixed angle. Situations where the electron-positron pair is measured before having the chance to
multiple scatter sufficiently, motivated an update to the angular sampling scheme to be introduced in EGS4 [Bie94b].

1.4.2 Electron/Positron interactions

As introduced above, the transport of electrons and positrons in EGS4 is based on a Class II condensed history algorithm. Interactions involving energy losses above certain thresholds are simulated fully, while small energy transfers are accounted for in terms of their stopping power (energy straggling is not considered in EGS4). This basically means that bremsstrahlung photons and secondary electrons, are only created if their kinetic energies are above the respective cut offs for "catastrophic" interactions.

The simulation of "hard" inelastic collisions of electrons and positrons with electrons in the medium are based on Möller and Bhabha differential cross sections [Jau76], respectively. After convenient factorisations, the energy transfers are sampled from the respective cross sections [Nel84] and subtracted from the incident particle's energy. No bound effects are considered, which is to say that the collision is assumed to occur between two free particles. The final state of secondary electrons is then fully specified from energy/momentum conservation laws. The (restricted) stopping powers associated with "soft" collisions are calculated using the Bethe-Bloch theory. The PECS4 preprocessor was updated [Dua89] so that collision stopping powers could be made compatible with those from ICRU Report-37. More recently, the density effect corrections as given in [Ste83] have also been introduced in the stopping power calculations [Hir95]. Treating target electrons as being free and at rest might not be a valid approximation for energies of the order of atomic binding energies. The relevance of this aspect for low electron energies is further analysed in chapters 3 and 4.

The treatment of bremsstrahlung emissions in EGS4 is based on the standard Bethe-Heitler cross section [Hei60, Jau76]. Below 50 MeV, the Coulomb corrections
applied were calculated from [Koc59], but the "Elewert factor" neglected. An updated scheme has been developed [Rog89] so that radiative stopping powers could be made compatible with those from ICRU-37/NBS. The realisation that, at high energies, the bremsstrahlung cross section is strongly peaked in the forward direction led to an approximate scheme being introduced in EGS4. This assumed that newly created photons emerge at a fixed angle with respect to the direction of the electron. An enhancement to deal with the angular distribution of bremsstrahlung photons, based on Koch and Motz's 2BS formula, has been developed [Bie89] and is currently available in the standard distribution of the code. The accuracy of the EGS4 code system in the simulation of bremsstrahlung emissions, at regimes below 100 keV, is analysed further in chapter 5.

In EGS4, elastic scattering from nuclei and electrons is simulated using the Molière theory of multiple scattering [Bet53]. When the particle is transported from one position to the point of the next interaction, the net effect of a certain number of elastic collisions is considered, and the particle deflected by a certain angle. This imposes a limit on the step size, as a minimum number of collisions ($W_0 > 20$ in Molière's formalism) should be considered. Also, the theory was developed under the small angle approximation and a correction factor has to be used in the treatment of large deflections [Ber63]. Some of the difficulties related to step size artefacts [Rog84], were solved with the release of PRESTA (Parameter Reduced Electron-Step Algorithm) [Bie87]. This powerful algorithm is also based on Molière's theory, but with the minimum number of collisions to be considered pushed down to $W_0 \geq \epsilon$ (the mathematical limit of the theory) [And91]. It also incorporates a path length correction, a lateral correlation algorithm as formulated in [Ber63], and a new boundary crossing algorithm (allowing larger steps to be taken away from boundaries). In a way, PRESTA can also be considered a variance reduction technique, as computing time may by reduced by means of improvements in the electron transport algorithm [Bie88]. The major constraints in electron transport, namely those related to the maximum energy loss per step, are due to be overcome with
the release of PRESTA-II [Bie97]. In the new scheme, near boundaries, multiple scattering is "switched off" and elastic collisions simulated fully [Bie96].

When simulating the transport of positrons, the process of two-photon annihilation with atomic electrons is also considered. Annihilation is considered to take place "in-flight" or when positrons come to a rest, i.e. when their kinetic energy falls below the pre-selected energy cuts. In the first case, the configuration of the final state is determined by Dirac's formula [Hei60], while annihilation at rest results in two 511-keV photons isotropically emitted in a back-to-back configuration. The annihilation is assumed to take place with stationary electrons, so effects like the binding energy and momentum distributions of annihilating electrons, are not considered.

### 1.5 Imaging applications

Simulations based on the use of Monte-Carlo methods, have been widely applied to the field of radiation imaging [Rae76, And91]. In areas like positron emission tomography (PET), radiography, tomography and photon scattering techniques, Monte Carlo techniques have played an important role in understanding the significance of the different steps involved in the formation of the images. As described in recent reviews [And91, Spe91], several imaging techniques and systems have been optimised using simulation-based studies.

One of the applications to be analysed further in this thesis is back-scatter imaging. This non-destructive approach is particularly suited to the examination of radiographically opaque objects, or in situations where access to the "other side" of the object is limited. The basic configuration of this kind of system is shown in fig. 1.3. In general, the interaction of an incident beam, $i$, within a certain volume element (voxel) $\Delta V$ results in a secondary form of radiation, $r$, that will form the measured signal. A now well established technique based on this principle is Compton Scatter
Imaging (CSI), where the characteristics of a medium are assessed by means of Compton scattered photons [Har97a]. Incident radiation usually comprises a collimated beam of X-rays with energies of a few hundred keV, and the output signal obtained via the detection of photons Compton scattered in the back direction. The technique is now widely used in industrial and medical applications [Har97a]. The high quality of images obtained using this approach has resulted in the development of the commercially available system ComScan [Har89].

As recently pointed out [Spe91], applications like CSI clearly benefit from suitable Monte Carlo simulations. Aspects like signal degradation due to multiple scattering events, attainable spatial resolution and maximum depth to be probed, can be determined by means of computer simulations. This was the case, for example, of some studies carried out recently (using EGS4) that aimed to understand the potential and limitations of CSI for the detection of cavities in sand [Ulm98].

Imaging systems employing X- or γ-rays, usually make use of X-ray tubes or radioactive sources, as primary radiation providers. The latter have the advantage
of (usually) producing monoenergetic radiation beams, an essential requirement in a wide variety of applications [Har 91, Spe 91]. However, their low intensity can represent a major drawback, in which case X-ray tubes represent a feasible alternative. Additionally, X-ray tubes are more controllable devices, although they have the big disadvantage of producing polychromatic photon beams. This may impose serious limitations on the overall performance of the system. This has led to some effort to be put on the development of “quasi-monoenergetic” tubes [Ale 86, Har 91]

Two simplified X-ray tube geometries are shown in fig. 1.4. In both cases, the photon flux produced via the interaction of electrons in the target is used directly as the primary source. For electron energies of the order of the target’s K-edge, the photon spectra produced consist of K-characteristic lines from the target superimposed on a broad bremsstrahlung background as shown, for example, in fig. 3.2. The

![Diagram of X-ray tubes in reflection and transmission geometries](image-url)
task of understanding the basic interactions that lead to the production of radiation in X-ray tubes, and its use in the optimisation of characteristic to continuous photon ratios, has received considerable attention over the last two decades [Dys 75, Har 91]. Some semiempirical models have been developed to study photon production in X-ray tubes [Sun 73, Tuc 91a, Tuc 91b]. This indicates that this area can also benefit from suitable Monte Carlo simulations.
Chapter 2

One-sided imaging using induced positron annihilation

2.1 Introduction

A one-sided imaging application involving the use of megavoltage radiation is considered in this chapter. Both experimental and EGS4-based studies are addressed in imaging studies that are based on the creation of positrons in condensed media, and the detection of radiation that is emitted in their annihilation. The technique is analysed from the point of view of the basic processes involved and through some experimental studies. The dependence of annihilation yield on the atomic number was determined, indicating that the technique can be used for substance identification. The benefits of one-sided imaging of high-Z inclusions in less dense, low-Z matrices, are discussed. The good agreement between experimental and simulation data allowed some potential applications to be considered through the simulation approach.
2.2 Induced positron annihilation as an imaging technique

The basic interactions behind induced positron annihilation are analysed now. The dependence of cross sections for positron production, the annihilation of these particles and the attenuation of the emitted quanta, are discussed separately. Furthermore, the overall combination of these effects for imaging purposes is debated.

2.2.1 Positron production

The interaction of photons with energies above the 1.022 MeV pair production threshold results, to some extent, in the creation of electron-positron pairs, in all materials. Near this zero-point threshold, the pair production cross section rises sharply with energy, and becomes the largest fraction of the total cross section at $\approx 5\text{ MeV}$ in high atomic number elements ($Z>70$) and at $\approx 20\text{ MeV}$ in low-$Z$ materials like aluminium (Al) [Har 97b].

The pair production cross section in Pb, is shown in fig. 2.1, for energies below $10^3\text{ MeV}$. In this plot, it is clear that after an abrupt increase near the threshold, much smaller variations are observed for the probability of creating electron-positron pairs, with this quantity reaching what seems to be a saturation level at higher energies [Hei 60]. As described below, the pair production cross section does have a strong dependence on the effective atomic number of the sample, but the general behaviour shown in fig. 2.1 is, to first order, material independent.

The production of electron-positron pairs occurs in the electric field of the nucleus as well as in that surrounding atomic electrons. This last contribution is zero for energies below $4m_0c^2$ (2044 keV), but for higher energy photons represents a fraction on the order of $C/Z$ of pair production in the nuclear field, where $C$ is a constant ($C \approx 0.7-0.8$) and $Z$ is the atomic number of the substance under consideration [Hei 60]. The nuclear and electron components of the pair production cross section...
Figure 2.1: Total pair production cross section in Pb ($\sigma_{pp}$). The data shown were calculated using XCOM [Ber87].

are shown in fig. 2.2. This plot shows that, in the case of Pb, the fraction of pair production events taking place in the field of atomic electrons never exceeds 2% of those occurring in the nuclear field. Moreover, for energies below $\approx 2.6$ MeV, it seems reasonable to neglect the electronic contribution.

In terms of atomic number dependence, the probability (per atom) for the production of electron-positron pairs ($e^-/e^+$) varies approximately with $Z(Z+C)$. The term $Z^2$ accounts for the production in the electric field of the nuclear protons, and $CZ$ (as previously introduced) for events taking place in the field of the atomic electrons [Hei60]. For photons of a given energy, the probability (per unit path length) of a pair production interaction can be calculated from the product of the respective cross section with the sample's atomic density (i.e. the number of atoms per unit volume). In elemental species, this last quantity is given by $\rho N_A/A$, where $N_A$ is
Ib

In the nuclear field

In the field of atomic electrons

Energy (MeV)

$\sigma_{pp}$ (barn/atom)

1.00E+02

1.00E+00

1.00E-02

1.00E-04

1

2

3

4

5

6

7

8

9

10

100

1000

Figure 2.2: Pair production cross section in Pb. Contributions from nuclear and electronic fields, as given by XCOM [Ber 87], are shown separately.

the Avogadro's number, $\rho$ the density, and $A$ the atomic weight of the sample. The ratio $Z/A$ varies only slowly for elements with $Z \geq 2$, so the electron-positron pair production varies approximately with $\rho Z$, hence the mass attenuation coefficient ($\text{cm}^2/\text{g}$) is proportional to $Z$. This is shown in fig. 2.3, where the mass attenuation coefficient for pair production in various elements, for 2.61 MeV photons, is plotted versus atomic number. As described below, $\gamma$-rays with this energy can be obtained from $^{232}\text{U}$ sources.

In the production of $e^-/e^+$ pairs, any excess kinetic energy above the threshold is in some way shared by the two created particles. For photon energies of the order of few MeV, it might seem reasonable to assume that the most probable outcome is that the newly created particles share the excess energy equally [Hei 60, Jan 76]. It should however be pointed out that the observed probability distribution that
describes the fraction of the excess kinetic energy carried by each particle is rather flat around the 0.5 centroid [Hei 60]. Therefore, a quasi-random distribution of the excess energy above the 1.022 MeV threshold for the created particles should be expected, especially for fractional shares in the range 0.2 to 0.7.

### 2.2.2 Positron annihilation

The positrons created via high energy photon interactions will eventually annihilate with an atomic electron. The cross section for this process, that results in the production of two photons, is given by [Hei 60, Jau 76],

\[
\sigma_{\text{ann}} = \pi r_o^2 \frac{1}{\beta^2 \gamma (\gamma + 1)} \left[ (\gamma + 4 + 1/\gamma) \ln \left( \gamma + \sqrt{\gamma^2 - 1} \right) - \beta (\gamma + 3) \right]
\]  

\[\tag{2.1}\]

\[
\beta = \frac{1}{\gamma + 1}
\]
where \( r_o \) denotes the classical electron radius, \( \beta \) the positron velocity (as a fraction of the speed of the light) and \( \gamma^{-2} = 1 - \beta^2 \). Annihilation processes involving the emission of three or, even, one photons may also occur (single photon annihilation is only possible in the presence of a third particle) but their yields are smaller than the two-photon process described by eq. (2.1), by two or more orders of magnitude [Hei 60, Jan 76].

The dependence of the cross section (2.1) on the positron velocity demonstrates that annihilation is more likely to occur for reduced kinetic energies. In addition, if the probability for annihilation is compared with those for other inelastic interactions, it can be shown that the former is several orders of magnitude smaller than the latter. This difference can be seen in fig. 2.4, where values calculated from eq. (2.1) are shown alongside the total electron cross sections for other events involving energy losses, in iron (Fe). Positrons and electrons interact differently in matter and this leads to small changes in cross sections and stopping powers for each particle type [Roh 54, Ber 84]. For this reason, the inelastic data set in fig. 2.4, should only be taken as representative of the orders of magnitude involved.

In the light of these data, it becomes clear that annihilation becomes significant, once the positron kinetic energy has been reduced through a number of inelastic interactions in the medium (excitation, ionisation and, possibly, radiative emissions). Depending on the nature of the atomic (or molecular) environment, annihilation may occur straightaway or via the formation of a metastable system (positronium), [Ber 77]. From their production until the moment that annihilation takes place, times of the order of hundreds of picoseconds are involved. If the annihilating particles are assumed to be initially at rest, then two 511 keV photons will be emitted in a back-to-back configuration (as required by the conservation of momentum).

Typical (CSDA) ranges for 1 MeV positrons are of the order 0.5 g cm\(^{-2}\) in C and 0.83 g cm\(^{-2}\) in Pb [Ber 84]. Hence, it may be concluded that this parameter is not strongly dependent on Z. For an atomic density of \( \approx 2.0 \) g cm\(^{-3}\) the distance travelled by a positron is typically of the order of 3 mm. Of course the mean distance, from
Chapter 2. One-sided imaging using induced positron annihilation

2.2.3 Interaction of annihilation photons with matter

It was discussed in section 2.2.2 that positrons (with energies up to a few MeV) are more likely to annihilate after losing most of their kinetic energy, and that the process will (in principle) give rise to the production of two photons. Neglecting any
residual energy of the particles before annihilation, this phenomenon should result in the emission of two 511 keV photons. Consequently, it is now worth considering how these photons interact in condensed media.

The total mass attenuation coefficient for 511 keV photons in various elements is plotted in fig 2.5. At this energy the dominant interaction process is Compton scattering in a wide variety of materials [Kno 89], which accounts for the slow change in the attenuation coefficient up to Z=50. For higher atomic number elements the values increase, reflecting the strong dependence of photoelectric cross section on the atomic number \( Z^n \), with \( n \) in the interval \([4,5]\) [Eva 82, Kno 89]. Indeed, as \( Z \) increases the photoelectric interaction assumes an increasing fraction of the total attenuation cross section. This is shown directly in fig. 2.6, where the ratio of photoelectric to Compton cross section as a function of \( Z \) (for 511 keV photons) is

![Graph showing mass attenuation coefficient vs. atomic number](image)

Figure 2.5: Mass attenuation coefficient for the absorption of 511 keV photons, as a function of atomic number. Values were calculated using XCOM [Ber 87].
plotted; at about $Z = 80$ this passes through unity, demonstrating the increasing importance of the photoelectric interaction in higher-$Z$ substances.

![Graph](image)

Figure 2.6: Ratio of photoelectric to Compton cross section (at 511 keV) as a function of atomic number $Z$. The values plotted were calculated using the XCOM database [Ber 87].

2.2.4 Method

Following on from the discussion presented in sections 2.2.1 to 2.2.3, it seems appropriate to use induced positron annihilation as the basis of an imaging technique that may be suitable for identifying samples according to their atomic number. The data presented in fig 2.3, shows that the interaction of high energy photons by means of electron-positron pair production is enhanced in condensed media with high atomic numbers. The subsequent annihilation of positrons with atomic electrons will result in the production of two 511 keV photons, which can then be used as information
carriers. Although fig. 2.5 makes clear that media with higher yields of positron production are also the more effective in the absorption of annihilations photons, high-Z materials can be expected to stand out in high contrast against less dense, low-Z backgrounds. This is shown in fig. 2.7 where the ratio between the linear attenuation coefficients for pair production over the ones for absorption of 511 keV photons, in different elements, is plotted. In situations where the distance travelled

![Graph showing the ratio of the attenuation coefficient for pair production (\(\mu_{pp}\)) with 2.61 MeV photons, to the total linear attenuation coefficient for the absorption of 511 keV radiation (\(\mu_T\)), as a function of atomic number. The values plotted were calculated using the XCOM database [Ber87].](image)

by positrons before their recombination with electrons is kept small, good spatial resolution may also be achieved.

When compared to imaging techniques based on Compton scattering [Har89] this method has some important advantages, especially for the inspection of ob-
jects that are accessible only from one side. On their return paths, annihilation photons have greater penetration than photons Compton scattered in the backward direction as (in practical situations) the energy of these is limited to a maximum of \( \approx 255 \text{ keV} \). Also, the isotropic emission of annihilation radiation overcomes the problem of reduced Compton backscatter probability as the energy of the inspecting radiation increases [Gil97]. In addition, it should be noticed that the \( Z^2 \) dependence of the pair production cross section should result in more sensitive variations with material properties, hence generating higher contrast than with Compton backscattering imaging (whose yield is proportional to \( Z \)).

The requirement for photon sources with radiation in excess of 1.022 MeV may present some experimental difficulties. The main alternatives are restricted to radionuclide sources or megavoltage bremsstrahlung radiation. In both cases, the use of penetrating radiation, requires a substantial amount of shielding to be used, in order to reduce the level of “cross-talk” between source and detector (for example suggested by the diagram in fig. 1.3)

Induced positron annihilation was first exploited in the early 1980’s by Sowerby and collaborators, to study the ash contents in mined coal [Sow81, Mil84]. Their set up included a \(^{60}\text{Co} \) source and a NaI(Tl) detector mounted in backscatter geometry. The success in the implementation of the method for the continuous analysis of coal on conveyor belts, led the same group to develop a similar scheme aimed at determining the iron content in iron ore fines [Ay187]. In this new application, 1.76 MeV \( \gamma \)-rays from a \(^{226}\text{Ra} \) source were used. Some other studies that have been carried out using a 20 MV bremsstrahlung spectrum from tungsten target to probe deep surfaces [Sil93].

However this concept has not received much attention over the last decade, and it was only recently that the potential of this technique for the inspection of civil engineering structures was assessed [Gil97]. Simulation and experimental studies of the technique have both been undertaken at the University of Surrey, Phillips Research (Hamburg) and Los Alamos National Laboratory [Har97b, Tav97] over the last con-
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ple of years, reviving the interest in this approach. Following Harding's suggestion [Har97b] the acronym PIPAR- Photon-Induced Positron Anihilation Radiation- has been adopted for this imaging technique.

2.3 Annihilation yields

For the purpose of assessing the potential of PIPAR, and following some initial simulation work at Surrey, some collaborative experimental studies were carried out using the facilities of the group NIS-6 at Los Alamos National Laboratory (New Mexico, USA). Since this technique is aimed at the location of high-Z inclusions in less dense, low-Z matrices, the Z-dependence of the backstreaming annihilation yield (i.e. those emitted in the direction of the incident surface) was evaluated. The same experimental set up was then simulated using the EGS4 code system, and the results compared.

2.3.1 Experimental system

The measurements were taken using the arrangement depicted in fig. 2.8. Both the interrogating source and the photon detector were housed in lead collimators; additional lead and tungsten carbide absorbers were positioned between the source and detector to further reduce any background emissions transmitted through the respective collimators.

A 2.615 MeV γ-ray from $^{232}$U was used as an interrogating source throughout the measurements. The decay chain of this isotope, illustrated in table 2.1, eventually leads to the formation of $^{208}$Tl, a β emitter that produces 2.615 MeV γ-rays. It is fortuitous that in the decay chain of $^{232}$U, the only γ-ray with energy above the pair-production threshold of 1.022 MeV is in fact the 2.615 MeV line. For the purpose of inducing pair production, $^{232}$U may be considered to be a monoenergetic source.
Secular equilibrium is established approximately 10 years after $^{232}\text{U}$ is purified, and $^{208}\text{Tl}$ behaves as a long-lived source with a 70-year half-life.

Two cylindrical $^{232}\text{U}$ sources (with a total activity of 397 mCi) were positioned inside a 20 cm long, 3 cm diameter lead collimator. The front surface of the source collimator was positioned (measured alongside its central axis) 28 cm from the sample surface and, as shown in fig 2.8, directed at an angle of 40° with respect to the detector axis. The beam spot of the incident photons at the sample was estimated to be an ellipse with approximate dimensions 11.3 cm by 7 cm, as determined by a light source shining through the collimator.

The coaxial geometry high-purity germanium detector (HPGe) used in the experiments comprised a 5.62 cm diameter Ge crystal that was collimated with a 5 cm long, 5.75 cm diameter lead collimator. The front surface of the collimator was positioned 48 cm away from the test object. The signals from the detector were shaped
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<table>
<thead>
<tr>
<th>Isotope</th>
<th>$T_{1/2}$</th>
<th>Main decay mode</th>
<th>Gamma rays emitted (keV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{232}$U</td>
<td>70 y</td>
<td>$\alpha$</td>
<td>58; 129</td>
</tr>
<tr>
<td>$\downarrow$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{228}$Th</td>
<td>1.91 y</td>
<td>$\alpha$</td>
<td>84; 116; 132</td>
</tr>
<tr>
<td>$\downarrow$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{224}$Ra</td>
<td>3.66d</td>
<td>$\alpha$</td>
<td>293; 646</td>
</tr>
<tr>
<td>$\downarrow$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{223}$Rn</td>
<td>55.6 s</td>
<td>$\alpha$</td>
<td>550</td>
</tr>
<tr>
<td>$\downarrow$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{216}$Po</td>
<td>0.15 s</td>
<td>$\alpha$</td>
<td>805</td>
</tr>
<tr>
<td>$\downarrow$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{212}$Pb</td>
<td>10.64 h</td>
<td>$\beta^-$</td>
<td>239; 300</td>
</tr>
<tr>
<td>$\downarrow$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{212}$Bi</td>
<td>60.6 min</td>
<td>$\beta^-$ (63.8%); $\alpha$ (36.2%)</td>
<td>727</td>
</tr>
<tr>
<td>$\downarrow$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{208}$Tl</td>
<td>3.1 min</td>
<td>$\beta^-$</td>
<td>227; 508; 511; 583; 860; 2615</td>
</tr>
</tbody>
</table>

Table 2.1: Decay chain of $^{232}$U. It should be pointed out that the $\beta^-$ decay of $^{212}$Bi leads to the formation of $^{212}$Po and this isotope also radiates 2.615 MeV $\gamma$-rays. The yield of this emission is however much smaller than the one from $^{208}$Tl.

and amplified, and then passed to a PC-based multichannel analyser that was used to determine the photon energy pulse-height distribution.

The pulse-height distributions obtained from copper (Cu) and lead (Pb) samples in $\approx 200$ s counting periods are presented in fig. 2.9-(a) and -(b), respectively. Fig. 2.9-(a) shows peaks corresponding to the 511 keV annihilation radiation, the singly-scattered Compton photons at $\approx 270$ keV, as well as some characteristic radiation produced from the Pb collimators (at $\approx 80$ keV). The peak at an energy of $\approx 200$ keV probably corresponds to multiply scattered photons that nevertheless enter the detector aperture. The pulse-height distribution for Pb, on the other hand,
shows a higher yield of annihilation photons and a substantial reduction in the number of Compton scattered photons, compared with Cu. The enhanced production of annihilation photons in Pb can be understood in the light of the discussion in section 2.2.1 while the suppression of lower energies and the appearance of intense characteristic X-rays from the lead sample reflect the increasing importance of the photoelectric interaction in high-Z materials.

![Graphs of Pulse height distributions for backstreaming photons.](image)

Figure 2.9: Pulse height distributions for backstreaming photons.

### 2.3.2 Simulation

The experimental results derived from the apparatus described in the previous section were simulated with a program based on the EGS4 code. The simulations were performed using the standard EGS4 code, together with the improvements of the PRESTA algorithm [Bie 87], the low-energy photon transport code LSCAT [Nam 94], the implementation of L-shell photoabsorption and L-shell X-ray fluorescence emissions [Hir 96], as well as the updated bremsstrahlung [Bie 89] and pair-production angular distributions [Bie 94b].
Chapter 2. One-sided imaging using induced positron annihilation

The signal of interest consisted of 511 keV photons, so the energy value below which photons were considered to be locally absorbed and consequently ignored was selected to be 510 keV. Positrons and electrons were transported down to kinetic energies of 80 keV and 1022 keV, respectively (above this value bremsstrahlung photons can still induce pair production). Although inefficient from the perspective of computational time, these values were chosen so that the accuracy of the results was not affected by neglecting the residual migration of positrons before annihilation. For the sake of accuracy, the value below which charged-particle interactions were treated in terms of their specific energy loss (EGS4 variables AE and AP) was selected to be 10 keV.

To realistically reproduce the experimental setup, the finite size of the radiation source, as well as the dimensions of its collimator, were modelled. As illustrated in fig. 2.10-(a), a disk-shaped photon emitter was considered to be positioned at the back of the 20 cm long collimator. For the sake of simplicity, the thickness of the source was neglected and its radius considered to be identical to the collimator. The detector was defined to be encapsulated within a collimator with dimensions shown in fig. 2.10-(b). In order to reduce the required computational time, the detector efficiency was considered to be 100% so that every photon emitted within the solid angle defined by the geometry was considered to be detected (in [Kno89], the full-energy peak intrinsic efficiency at 511 keV of an HPGe detector similar to that used is estimated to be of the order of 19% ). The size of the incident beam spot at the interrogated object was determined to be approximately 11 cm x 7.2 cm, values that agree well with the experimental values (11.3 cm x 7 cm).

### 2.3.3 Results

A list of the different samples measured, together with their thicknesses and the 511 keV photon yields, is presented in table 2.2. The experimental values correspond to the number of photons obtained over a 300-s counting period, with the background
Figure 2.10: Schematic representation of the collimators where source -(a) and detector-(b) were housed.

subtracted. Background was considered to be the number of photons obtained per 300 s with the sample removed, and determined to be of the order of 72 photons. The simulation results correspond to the number of detected annihilation photons per 40 million incident 2.615 MeV gamma rays.

Although the number of incident photons in the simulations was selected so that the 511 keV photon output was of the same order of magnitude as the experimental results, a direct comparison of simulated and experimental data can only be made after normalizing the data sets. This operation would not be necessary with the certainty that the number of incident γ-rays in the simulations matched the number that reached the samples during the 300-s counting period exactly, and if the detector response had been taken into account. It is reasonable to assume that the overall detection efficiency of the HPGe detector remained constant throughout the measurements. In this case, the two sets of data may be normalised by calculating the ratio of the number of photons used in the simulation to the number of photons that, on average, struck the samples during the 300-s counting period. This variable, C, can be determined by means of a least squares fit between the experimental data and C times the simulation data, for the different materials considered.
Using all the data points shown in table 2.2, the value of the constant C was found to be C = 0.747. However, the rather poor fit ($\chi^2/\nu = 14.2; r = 0.975$) motivated the exclusion of the data for cadmium and tungsten carbide, which clearly improved the fit ($\chi^2/\nu = 1.23; r = 0.999$, now with C = 0.835). The reason for excluding these two experimental points arises from the fact that the sample of cadmium used was not a solid block but an assembly of different sheets, and any gaps between the layers would result in a sample whose density is less than that of solid cadmium; in the case of tungsten carbide, neither the purity nor the density were known to a great degree of accuracy. Experimental and normalised simulation results are presented in fig. 2.11 where, for the sake of clarity, error bars are omitted. The agreement between the two sets of results is quite remarkable: the average difference obtained is approximately 5%, with a maximum value of 10% (in cadmium and tungsten carbide differences of the order of 25% are observed).
Figure 2.11: Annihilation photon yields from different samples: experimental (squares) and simulation (crosses) results.

2.4 Potential applications

The EGS4 code was used in a series of simulations aimed at understanding the suitability of this imaging technique in different environments. The geometries considered and results obtained are now discussed.

2.4.1 Structural inspection

The strength of concrete-based modern civil engineering structures is usually increased by incorporating steel reinforcing bars (rebars). These elements are placed within the concrete to protect them from the effects of external agents, thus ensuring the integrity of the whole structure. The condition of the rebars is sometimes
assessed by drilling holes in the structure, followed by visual inspection. This is a time consuming and potentially damaging procedure.

In order to overcome these limitations and those of related γ-ray methods, the use of PIPAR was evaluated for the in situ inspection of engineering structures. Typical materials used in reinforced structures are Portland concrete and iron (Fe). As presented in table 2.3, concrete is essentially composed of oxygen (O) and silicon (Si). This results in a material with an "effective" atomic number smaller than that of Fe (26). If the mass densities of concrete and iron are taken into account, the probability of inducing the formation of electron-positron pairs using 2.6 MeV photons is ≈ 8 times greater in Fe than in concrete. As the mean free path of 511 keV photons in concrete is of the order of 5.3 cm, the technique of induced positron annihilation should, in principle, be suitable to probe the condition and position of rebars up to depths of three mean free paths (i.e. ≈ 16 cm).

<table>
<thead>
<tr>
<th>Element</th>
<th>Fraction by weight (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1</td>
</tr>
<tr>
<td>O</td>
<td>52.9</td>
</tr>
<tr>
<td>Si</td>
<td>33.7</td>
</tr>
<tr>
<td>Al</td>
<td>3.4</td>
</tr>
<tr>
<td>Fe</td>
<td>1.4</td>
</tr>
<tr>
<td>Ca</td>
<td>4.4</td>
</tr>
<tr>
<td>Mg</td>
<td>0.2</td>
</tr>
<tr>
<td>C</td>
<td>0.1</td>
</tr>
<tr>
<td>Na</td>
<td>1.6</td>
</tr>
<tr>
<td>K</td>
<td>1.3</td>
</tr>
</tbody>
</table>

Table 2.3: Elemental composition of Portland concrete. For most applications its mass density can be considered to be 2.2 g cm⁻³.

The potential of PIPAR for one-sided imaging of civil engineering structures was evaluated using the EGS4 code system [Gil97]. The simulated geometries consisted
of Fe rebars positioned with their centres $\approx 35$ mm below the surface of concrete blocks (the kinetic energy cut-offs were chosen to be 10 keV). In the test runs, a pencil beam of 2.7 MeV photons was scanned across a test “phantom” and the total number of 511 keV photon backstreaming from the concrete surface was logged. The results are shown in figs. 2.12 and 2.13 for, respectively, a 25 mm diameter circular section rebar and a square shaped rebar of 19×19 mm.

![Graph showing number of backstreaming 511 keV photons](image)

**Figure 2.12:** Number of backstreaming 511 keV photons obtained in a line scan across a circular section rebar. The geometry considered is also shown.

The results for both these geometries indicate that the position of the rebar can be clearly identified by looking at the total yield of backstreaming annihilation photons. In addition, the shape of the measured “peak” shows an interesting correlation with the shape of the rebar. In the circular shaped rod, the increase in signal that is observed at the centre reflects the longer path length of the inspecting radiation along the rod diameter. In the case of the square section rebar, annihilation photons produced near the edges of the bar are attenuated less than those produced deeper
in the bar, since the fraction of their path in concrete is higher. This results in a slightly increased signal as the source moves from the centre of the bar to the iron-concrete interface.

The data presented in this section indicate that, for typical civil engineering structures, the position and condition of rebars may in principle be assessed using PIPAR. The kind of geometry considered is rather impractical as the “detector position” overlaps the incident beam, but the results are encouraging. This and other aspects of the potential of PIPAR as a one-sided imaging technique are analysed in detail in the, somewhat, pioneering work of Gilboy and collaborators [Gil97].
2.4.2 Nuclear materials verification

Some preliminary studies aimed at determining the feasibility of PIPAR for imaging special nuclear materials (SNM), against low-Z backgrounds were also carried out. Applications like protection and control of nuclear materials, as well as arms control and counter-terrorism, would clearly benefit from verification and assurance resulting from a one-sided imaging method. Existing methods, based on photon backscattering and tagged 14 MeV neutrons, tend to be large and complicated, and only allow limited penetration and specificity. The EGS4 code system was used to assess the potential of the PIPAR imaging technique in this kind of application.

Materials that are typically found in applications involving SNM and lower Z matrices, include uranium (Z=92, density = 18.9 g cm\(^{-3}\)) and HMX (empirical formula \(\text{H}_2\text{CN}_2\text{O}_2\), density = 1.9 g cm\(^{-3}\)). From the discussion presented in sections 2.2.1 and 2.2.3 it is anticipated that, for 2.6 MeV incident photons, the production (per unit length) of electron-positron pairs in uranium (U) may exceed that in HMX by two orders of magnitude. However, 511 keV photons are more likely to be self-absorbed in U than in HMX (fig. 2.5, together with the effect of mass density, lead to a factor of \(\approx 20\) difference in the total photon attenuation coefficient).

The first simulation study carried out investigated the dependence of the total yield of backstreaming photons on the thickness of U and HMX. The geometry used consisted of a pencil beam of 2.6 MeV photons incident on semi-infinite blocks of material, with varying thicknesses. The results obtained, in terms of the total backstreaming of annihilation photons per \(10^8\) incident particles, are shown in fig. 2.14, for both U and HMX. At first glance it can be seen that 511 keV yields seem to reach a certain level of "saturation" at specific thicknesses. This effect is primarily due to the increased attenuation of annihilation photons as they are produced deeper into the material (mean free paths are 6 cm in HMX and 0.3 cm in U). The growing attenuation of the incident flux at increasing thicknesses may also be of some importance (the mean free paths for 2.6 MeV photons in HMX and U are 13 cm and
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Figure 2.14: Annihilation photon yields as a function of sample thickness.

1.17 cm, respectively). Data in fig. 2.14 indicates that the maximum depth that can be probed is of the order of 12 cm in HMX and 2 cm in U (in which case the ratio of total yields of U to HMX is about 6.5).

The radial distributions of 511 keV photons back-emitted from samples of HMX and U were also evaluated. This was achieved by simulating a pencil beam incident on a semi-infinite block, with its thickness chosen so that 99% of incident photons interacted in the medium. The spatial distribution of backstreaming annihilation photons at the surface of the blocks are shown in fig. 2.15, where the fraction of the total backstreaming photons that lie a circle of radius R is plotted. In the case of HMX, 99% of the photons lie within a circle of radius $\approx 9$ cm, while in U the same fraction is enclosed in a circle of radius 0.5 cm. The differences observed in the spatial distributions can be understood in terms of the respective attenuation lengths. In U, 511 keV photons are more likely to interact in the medium that in HMX, and so longer paths are considerably more penalised. Annihilation tends to
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Figure 2.15: Radial distributions of 511 keV photon backstreaming, at the exit surface.

occur in the close vicinity to the incident beam axis, so larger radii correspond to longer paths for backstreaming photons. These effects result in a more "focused" beam in media with a high absorption coefficient.

Finally, two blocks, one of U and one of HMX, were considered to be side-by-side and a scan across the boundary was simulated. Thicknesses were once again selected so that transmission of the 2.6 MeV beam was less than 1%. The geometry and the results (a point-by-point image formed using total backstreaming 511 keV photons) are shown in fig. 2.16. The data plotted shows that the position of the boundary is accurately located. Also, it is clear that when approaching the boundary from the U direction, the number of backstreaming 511 keV photons increases. This localised effect is plotted in greater detail in fig. 2.17, and is due to the fact that a fraction of the photons produced in U actually come out through HMX, where the attenuation
is smaller. The opposite effect occurs when approaching the boundary from the HMX side: some of the HMX photons pass through U on their way out, where they are attenuated more strongly than in HMX, so causing a drop in the yield at the surface.

2.5 Conclusion

A one-sided imaging technique, PIPAR, based on the detection of 511 keV photons created via induced positron annihilation has been described. From the analysis of the different processes involved, it is clear that PIPAR is suited to the location of dense, high-Z, inclusions in lower-Z matrices. The experimental results for the dependence of the backstreaming photon yield shows nearly a factor of 20 increase
Figure 2.17: Scan across a U-HMX boundary: “transient” effect resulting from the different attenuation of annihilation photons on each side of the junction.

over the range $4 < Z < 82$. Hence, the measured signal shows strong dependence on the effective atomic number of the sample. Although relatively simple geometries have been considered, the feasibility studies carried out indicate that monitoring of engineering structures and nuclear materials inspection are two of the areas that may benefit from this method.

The results from the simulations carried out using EGS4 were found to be in good agreement with experimental data. This agreement, was expected since (as discussed in sections 1.4 ) the code is suited to the simulation of the transport of photons−electron/positrons with energies of the order of hundreds of keV upwards. Whether the generation and transport of positrons is sufficiently accurate in the current version of the code (especially if low energies are considered) should be the subject of further investigation.
Further improvements may be attainable in the imaging technique of induced positron annihilation. The information from Compton scattered photons and/or fluorescence photons may be combined with the annihilation signal, resulting in an enhanced one-sided imaging approach. Moreover, any residual energy of the electrons before annihilation takes place will result in a broadening of the 511 keV peak (the so-called “Doppler broadening”). This extra source of information is already used in the field of Positron Annihilation Spectroscopy (PAS) [Ber77, Dew88].

The EGS4 code has proved to be a useful tool in the simulation of PIPAR imaging systems. So, this versatile and powerful code, should be of great importance in the overall understanding and the optimisation of such systems. Further refinements of the technique, such as assessing the ultimate spatial resolution or PAS studies represent a challenge from the point of view of EGS4, as the code may not be accurate enough. This leaves room for some improvements to be incorporated, such as enhancements on energy and angular sampling schemes of newly created positrons and Doppler broadening effects in positron annihilation.

In broad terms, EGS4 is expected to produce reliable results in the simulation of imaging devices that operate at energies above a few hundred keV, especially if the signal measured does not have a strong dependence on the accuracy used in the transport of charged particles. However, a broad range of applications requires the use of radiation below 100 keV, with accurate electron transport being of great significance in these cases. The suitability of the code for simulation of X-ray tubes when operated below 100 keV is discussed in the next chapter.
Chapter 3

Low energy photon production: the breakdown of EGS4

3.1 Introduction

The EGS4 code has been shown to be effective in modelling the (high energy) imaging applications discussed in chapter 2. However it is important to evaluate how realistic the code is in simulating other devices, such as X-ray tubes operating at diagnostic energies (≤ 100 keV). As introduced in section 1.5, the use of M-C codes in low energy applications may have enormous potential. For example, in the case of X-ray tubes, important design parameters like the fluorescence-to-bremsstrahlung ratio can be analysed carefully, and this information used in the optimisation of the device. Alternatively, simulated photon spectra could be used to determine the quantitative accuracy of imaging systems and tomographic image reconstructions. This could lead to improvements in the performance of the overall imaging system.

In this chapter, the standard version of EGS4 is used to simulate the operation of a microfocal X-ray tube operating at 35 kVp in transmission geometry. The photon spectrum from a 2.75 μm thick silver target is evaluated and compared with experimental data.
3.2 X-ray spectra at diagnostic energies

The accuracy of EGS4 at predicting photon spectra from an X-ray tube operating at energies of a few tens of keV was evaluated by comparing simulated spectra against measured data. The experimental X-ray tube used the geometry depicted in fig. 3.1. The tube comprises a 2.75 \( \mu m \) thick silver (Ag) target (the site of photon production) deposited onto a 490 \( \mu m \) thick substrate of aluminium nitride (with a density \( \rho = 2.95 \text{ gcm}^{-3} \)). The electron beam is controlled using a grid electrode, and an electrostatic focussing arrangement is used to produce a small focal spot size (less than 8 \( \mu m \)) on the target surface [DeA95]. Photon energy spectra were measured using an uncollimated, coaxial geometry, high-purity germanium detector \( \approx 5 \) cm long and 2.48 cm in diameter. The detector was positioned 40 cm from the target of the X-ray tube with its axis 4 cm below the X-ray tube central axis.

![Figure 3.1: Schematic representation of the target and exit window of the microfocal X-ray tube used in the experiments.](image-url)
Chapter 3. Low energy photon production: the breakdown of EGS4

The photon spectrum obtained with the tube operated at 35 kVp is shown in fig. 3.2. Characteristic radiation from Ag, at energies of $\approx 22$ keV and $\approx 25$ keV (corresponding to the $K_{\alpha}$ and $K_{\beta}$ lines, respectively) can be clearly identified. An “escape” peak at $\approx 12$ keV, corresponding to events where K-fluorescence radiation from germanium (produced via the photoelectric absorption of 22.1 keV photons) is not successfully absorbed in the detector, can also be seen.

![Photon spectrum](image)

Figure 3.2: Photon spectrum obtained with a 35 keV electron beam, as measured with a HPGe detector.

The geometry presented in fig. 3.1 was modelled using EGS4. The simulations were carried out using the standard version of the code, with the PRESTA algorithm [Bie 87], the ICRU/NBS radiative stopping powers [Rog 89] and the LSCAT extension [Nam 94]. The angular sampling of bremsstrahlung photons in this series of simulations was based on the algorithm presented in [Bie 89], and the features described correspond to the “state of the art” of low energy physics publicly available for EGS4. The thresholds $AE$ and $AP$ were considered to be $\approx 0.512$ MeV and 0.001 MeV, respectively. In this geometry, less than 1% of the photons with
an energy below 7 keV were transmitted through the AlN substrate. Therefore, the (kinetic) energy cuts in these simulations were selected to be 7.5 keV. For the sake of simplicity, no particle transport was performed beyond the tube front window. The fraction of photons reaching the detector was assumed to be that geometrically accepted within the solid angle defined by the detector. The glass window was considered to be SiO₂ with a density \( \rho = 2.2 \text{ gcm}^{-3} \) and the plastic layer a polyester with chemical composition \( \text{C}_{10}\text{H}_{18}\text{O}_{4} \) and density \( \rho = 1.38 \text{ gcm}^{-3} \). Since the spot size of the electron beam onto the target was less than 8\( \mu \text{m} \), the simulation assumed an incoming electron beam infinitely narrow and perpendicular to the target surface.

As discussed in section B.2.1 the efficiency of the detector used in the energy range 5 keV → 40 keV is close to unity and its full-width-at-half-maximum (FWHM) was found to vary with energy according to

\[
(FWHM)^2 = (2.35)^2 (1.28 + 0.29E) \times 10^{-2} \tag{3.1}
\]

where both the photon energy \( E \) and (FWHM) are expressed in keV. For ease of comparison with experimental data, the simulated spectrum has been convolved with eq. (3.1), and the result obtained is presented in fig. 3.3.

The experimental data presented in fig. 3.2 were not matched by the simulated data. This indicates that EGS4 is not suitable for the modelling of X-ray production in X-ray tubes. In fact, by looking at the relative intensities of the fluorescence peak and the bremsstrahlung tail at the \( K_\alpha \) line, it becomes clear that the production of fluorescence photons is not realistically modelled in the present version of EGS4. This is because, as discussed in section 1.4, during electron-electron collisions, EGS4 treats the target electron as a free particle. Thus, there is no information concerning the ionised shell and so the emission of fluorescence photons can not be modelled accurately. The characteristic photons observed in fig. 3.3 are all produced through the photoelectric absorption of bremsstrahlung photons that have created vacancies in the K-shell (this process is analysed further in chapter 7). The use of ICRU/NBS radiative stopping powers from [Rog89] should ensure reasonable esti-
Chapter 3. Low energy photon production: the breakdown of EGS4

Figure 3.3: Simulated spectrum of an X-ray tube, obtained using the current version of EGS4. The geometry considered is given in fig. 3.1, with the tube operated at 35 kVp, and $2.4 \times 10^8$ incident electrons composing a pencil beam. The data set was convolved with eq. (3.1) to consider the effect of the HPGe detector.

mation of bremsstrahlung yields. However, the accuracy of the angular distribution of bremsstrahlung photons is debatable. Hence, also for this reason the fluorescence to bremsstrahlung ratio may not be simulated accurately.

3.3 Conclusion

The data presented in this chapter make it clear that EGS4 can not be used in the simulation of X-ray tubes operating at energies near the K-edge. The assumption that target electrons are free turns to be a very restrictive approximation in low energy applications. Moreover, the accuracy of inelastic cross sections calculated under the "free and at rest" approximation may also be questionable at these energies. The shape of the bremsstrahlung part of the spectrum presented in fig. 3.3 seems to
broadly reproduce the experimental data. However, the accuracy in the treatment of bremsstrahlung emissions should also be the subject of further investigation, as inappropriate models for this interaction may also affect the measured spectra.

The need for a suitable simulation package, preferably based on the EGS4 code system, that could help in optimising imaging devices like the X-ray tube just described, motivated the development of an enhanced version of the code. More realistic models for electron-atom inelastic collisions and bremsstrahlung emissions are described in the next two chapters.
Chapter 4

Low energy electron-atom inelastic collisions: the GOS model

4.1 Introduction

The results presented in section 3.2 indicate that the standard version of EGS4 cannot accurately predict spectra from X-ray tubes operating near a shell threshold. As discussed previously, the assumption that target electrons are free leads not only to cross sections and stopping powers being estimated poorly, but even more importantly, the lack of information concerning the ionised shell makes the emission of fluorescence photons impossible to calculate. Hence realistic X-ray tube spectra cannot be reproduced.

To overcome this limitation of EGS4, a model that deals with electron atom inelastic collisions beyond the "free and at rest" assumption is described. Indeed, by using the concept of a generalized oscillator strength (GOS), and a simple representation of this important quantity, accurate cross sections and stopping powers down to sub-keV energies can be reproduced. An enhanced version of this model that accurately accounts for the ionisation of the K-shell together with a discussion of the suitability of this approach for simulating the transport of electrons in condensed
media (and X-ray tubes in particular), are both presented in this chapter.

4.2 Electron-atom inelastic collisions

As in other probabilistic phenomena, quite apart from just a measure of the probability of occurrence, the collision cross section, provides a reasonable understanding of the process as a whole. The atomic differential cross section (DCS) for the inelastic collisions of (fast but non-relativistic) electrons with an isolated atom containing $Z$ electrons, involving an transfer of energy $W$, can be written, to the first Born approximation and disregarding exchange effects, as \[ \frac{d^2\sigma}{dQdW} = \frac{2\pi e^4}{m_0 v^2} \frac{1}{W Q} \frac{df(Q,W)}{dW} \] 

where $e$, $m_0$ and $v$ are (respectively) the electron charge, mass and velocity; $Q$ (also referred to as the “recoil energy”) is related to the momentum transferred $\mathbf{q}$ by

\[ Q = \mathbf{q}^2 / 2m_0. \]

The function $\frac{df(Q,W)}{dW}$ is called the generalized oscillator strength (GOS) and reflects the dynamics of the target atom, i.e. it specifies the atomic (internal) response to transfers of $Q$ and $W$. This term can also be identified with an inelastic form factor \[ \text{[Ino 71, Fan 63]} \] a term widely used when treating the interaction of photons with matter. The GOS can be conveniently visualised as a surface (the “Bethe surface”) spanning over the axis $(Q,W)$ and, based on classical arguments \[ \text{[Woo 72, Bir 58]} \] may be heuristically regarded as the effective number of atomic electrons actually taking part in the inelastic interaction. In agreement with this view, the Bethe sum rule

\[ \int_0^\infty \frac{df(Q,W)}{dW} dW = Z \]

is satisfied, for any value of $Q$. In the limit $Q \to 0$, the GOS reproduces the optical oscillator strength (OOS) density $df(W)/dW$, a quantity often used to describe the
absorption of electromagnetic radiation by a free atom, within the dipole approximation [Sta82]. In other words, by denoting \( \sigma_{pho}(E) \) as the cross section for the absorption of a photon with energy \( E = \hbar \omega \) then [Fan68, Sta82]

\[
\sigma_{pho}(E) \propto \frac{df(\omega)}{d\omega}
\]

such that [Ino71, Bon93]

\[
\lim_{Q \to 0} \frac{df(Q, \omega)}{d\omega} = \frac{df(\omega)}{d\omega}.
\]

An alternative way of treating this interaction is to use Linhard's dielectric theory [Rit59]. In this case the inelastic DCS may be written as [Rit59]

\[
\frac{d^2\sigma}{dQdW} = \frac{2\pi e^4}{m_0 v^2} \frac{1}{WQ} \frac{2W}{\pi \Omega_p^2} Z \text{Im} \left( \frac{1}{\epsilon(Q, W)} \right)
\]

where \( \Omega_p^2 \) is the plasmon energy of a free electron gas, that, for a density of \( N_e \) atoms per unit volume, can be calculated from [Woo72]

\[
\Omega_p^2 = 4\pi e^4 \hbar^2 N_e Z/m_0.
\]

The quantity \( \epsilon(Q, W) \) is the complex dielectric constant of the condensed medium. It is often used to describe phenomena like polarization, reflection and energy absorption in media exposed to electromagnetic fields [Woo72]. This property is usually written as \( \epsilon(\vec{K}, \omega) \), where the wavelength vector \( \vec{K} \) and frequency \( \omega \) are can be related to the quantities introduced in (4.1) through [Ino71, FVa96]

\[
Q = \hbar^2 K^2/2m_0 \quad \quad W = \hbar \omega.
\]

In the form \( \epsilon(\vec{K}, \omega) \), the dielectric function can be understood (through the application of the classical electromagnetic theory) as a property of condensed media, that relates polarization charge densities to perturbing electric field potentials [Rit59], when these quantities are expressed in terms of their spatial and temporal Fourier components [Rit59, Woo72]. The rate at which energy from an electromagnetic field is dissipated in condensed media is proportional to \( \text{Im} (-1/\epsilon(Q, W)) \) [Woo72], so this term is often classified as the material's "energy loss function" [FVa96].
The absorption of photons can also be treated in terms of the dielectric constant just introduced. In this case, an optical oscillator strength can be defined as \[ \frac{dW}{dW} = \frac{2W}{\pi\Omega_p^2\epsilon} \text{Im} (\epsilon(W)) \] \hspace{1cm} (4.9)

Recalling equations (4.5) and (4.6) and since \[ \text{Im} \left( -\frac{1}{\epsilon} \right) = \frac{\text{Im}(\epsilon)}{|\epsilon|^2} \] \hspace{1cm} (4.10)
is clear that for small momentum transfers, the optical oscillator strength from (4.9) will only be reproduced from \( \text{Im}(-1/\epsilon) \) in the limit \( |\epsilon|^2 \rightarrow 1 \). For aluminium and gold this occurs at energies above \( \approx 20 \text{ eV} \) \cite{Ehr63} and \( \approx 60 \text{ eV} \) \cite{Coo65}, respectively.

Both theories presented describe the same kind of physical interaction hence they must, somehow, be connected. The cross sections (4.1) and (4.6) become trivially identical if
\[ \frac{dW}{dW} = \frac{2W}{\pi\Omega_p^2\epsilon} \text{Im} \left( -\frac{1}{\epsilon(Q,W)} \right) \] \hspace{1cm} (4.11)
a relation that, as it has been pointed out \cite{FVa96}, alters and extends the concept of the GOS, so that it includes effects not explicitly considered in Bethe's theory, like polarization and collective excitations in the scattering medium. As a result, the concept of the "Bethe surface" can be extended to deal with electron inelastic scattering in condensed media. The optical oscillator strength can also be taken as the limit of the GOS when \( Q \rightarrow 0 \), provided that \( |\epsilon|^2 \approx 1 \), an approximation that seems valid for applications involving electron energies \( \geq 100 \text{ eV} \).

As discussed above, the GOS function introduced in (4.1), or equivalently the dielectric function \( \epsilon \), plays a highly important role in electron-atom inelastic collisions. Exact analytical expressions could be used for the calculation (after suitable integration over \( Q \) and \( W \)) of inelastic mean free paths, collision stopping powers and energy straggling parameters. Moreover, a good understanding of the role of each kinematic variable involved in the overall process could be achieved. However, this key quantity is known only for relatively simple systems such as the hydrogen atom \cite{Ino71} and the free electron gas \cite{Ash88}, and even in these cases its form
is rather complicated for simulation purposes. A variety of models that mimic the fundamental properties of the "Bethe surface" have been developed over the last 15 years [Lil83, FVa92, FVa93]. Being simpler and so more attractive from the modelling point of view, these approximate representations of the GOS have been used successfully to simulate the transport of electrons and positrons in condensed media [Lil85, Bar95, FVa96].

4.3 Modelling the GOS by means of delta functions

In a comprehensive "topographic" analysis of the "Bethe surface", Inokuti [Ino71] demonstrated conspicuous features that, underlying the basic ideas presented in Bethe’s pioneering work [Lan68], motivated electron-atom inelastic collisions to be understood from a different perspective. In his studies, Inokuti concluded that, for atoms in their ground state, the GOS is always positive and non-vanishing only for small values of $Q$ and also along the line $Q = W$ (named by Inokuti "the Bethe ridge"). When $Q \rightarrow 0$, the interaction has a "resonant-like" character where the incident electron basically interacts with the oscillator density structure of the atom, with $W$ being of the order of the atomic resonance energies. In the high-$Q$ region the collisions exhibit a "binary" nature, where target electrons behave as if they were essentially free and at rest, and the relation $Q \approx W$ holds. In classical terms [Bir58, Gol80] collisions involving small energy transfers are associated with large impact parameters, so resonant interactions are usually classified as distant and binary-like as close.

Based on the properties of the GOS just presented, Liljequist [Lil83] proposed a simple model where the response of the target atom is represented by a limited set of $M$ oscillators (or excitations). Denoting the strength and characteristic energy of
each oscillator by $f_i$ and $W_i$ respectively, the Liljequist GOS is written as

$$\frac{df(Q, W)}{dW} = \sum_{i=1}^{M} f_i F(W_i, Q, W)$$

(4.12)

with the “spectrum” of the $i$th oscillator, $F(W_i, Q, W)$, given by

$$F(W_i, Q, W) = \delta(W - W_i)\theta(W - Q) + \delta(W - Q)\theta(Q - W)$$

(4.13)

where $\theta(x)$ denotes the Heaviside step function and $\delta(x)$ the Dirac delta function. The “Bethe sum rule” (4.3) and the mean ionisation energy $I$ - the geometrical mean of all the ionisation and excitation modes of the target atom [Bir 58] - are then reproduced from

$$\sum_{i=1}^{M} f_i = Z \quad \sum_{i=1}^{M} f_i \ln W_i = Z \ln I.$$  

(4.14)

From (4.12) and (4.13) it can be seen that the corresponding OOS reduces to a set of $\delta$-oscillators, namely

$$\frac{df(Q = 0, W)}{dW} = \sum_{i=1}^{M} f_i \delta(W - W_i).$$

(4.15)

This results in a spectrum with the same analytical form as the one used by the Sternheimer in the calculation of density effect corrections [Ste52]. For high-$Q$ transfers the, relation $Q = W$ is the key feature.

Further specifications of the GOS model presented in (4.12) require the definition of the $2M$ parameters involved, i.e. the resonance energies $W_1...W_M$ and the oscillator strengths $f_1...f_M$, by means of physically motivated arguments. In his communication, Liljequist suggests that each oscillator should be associated with the specific excitation spectrum of a shell, sub-shell or band. In its most simplistic version, as Sternheimer had suggested [Ste52], the oscillator strength (per atom) may be associated with the number of electrons $Z_i$ in that group by simply setting $f_i = Z_i$. For inner shells, studies based on the photoelectric theory [Bet57], revealed that the optical oscillator strength density varies with energy as

$$\frac{df(W)}{dW} \propto W^{-c}$$

(4.16)
where $c$ is a number in the ranging from 2.5 to 3.5 [Bet 57]. Based on this argument, Liljequist proposed the characteristic energy of each oscillator, $W_i$, calculated from

\[ W_i = a U_i \]  

(4.17)

where $U_i$ is the corresponding ionisation energy and the factor $a$ can, to a good approximation, be considered to be the same for all inner shells. It can be shown [Lil 83, Lil 85], that $a$ is related to the constant $c$ introduced in (4.16), by means of

\[ c = \exp \left[ \frac{1}{a - 1} \right] \]

(4.18)

and, in practical cases, lies in the interval $1.5 \rightarrow 3$. If accurate inelastic mean free paths/stopping powers are not required below 100 eV, a representation of the GOS model has been suggested [Sal 92] where valence electrons are accounted for by means of a single oscillator, which is associated with characteristic plasmon excitations. Their strength ($f_v$) and resonant energy, $W_v$, can be estimated from optical functions or energy loss spectra [FVa 92, FVa 93]. When such data is not available, $f_v$ can be taken as the number of electrons in the atom with binding energies less than a few tens of eV, and $W_v$ can be calculated from

\[ W_v = b \Omega_p \left( \frac{f c}{Z} \right)^{1/2} \]

(4.19)

where $b$ is a parameter of the order of unity [Lil 83] and $\Omega_p$ the plasmon energy introduced in (4.7).

By substituting (4.17) in (4.14), it is then possible to calculate the semiempirical constant $a$ from

\[ \ln a = (Z - f_v)^{-1} \left[ Z \ln \Gamma - f_v \ln W_v - \sum f_i \ln U_i \right]. \]

(4.20)

If experimental information is not available, $b$ can be set to unity or adjusted so that the value of $a$ calculated from (4.20) is found to be in the interval $1.5 \rightarrow 3$.

The energy loss DCS, $d\sigma/d\Omega$, and other important quantities such as the inelastic mean free path, $\lambda_i$ and the corresponding collision stopping power, $S_e$, can then
be calculated from the GOS model discussed, by integrating (4.1) over the kinematically allowed recoil energies, $Q$. For the inelastic collision of an incident electron with kinetic energy $E$ that transfers an energy $W$ to a target atom, $d\sigma/dW$ can be conveniently split into the contributions of close and distant excitations,

$$\frac{d\sigma}{dW} = \int_{Q_-}^{Q_+} \frac{d^2\sigma}{dWdQ} = \frac{2\pi e^4}{m_0v^2} \left( \frac{d\sigma_c}{dW} + \frac{d\sigma_d}{dW} \right) \tag{4.21}$$

where, as shown in Appendix A, the minimum and maximum and values of $Q$ (denoted $Q_-$ and $Q_+$) are given by

$$Q_{\pm} = \left\{ E_0^2 + \left[ (E + 2E_0)^{-1/2} - (E - W)(E - W + 2E_0)^{-1/2} \right]^2 \right\}^{1/2} - E_0. \tag{4.22}$$

The cross sections shown in eq. (4.21) can be written as [Lil83, Sal92]

$$\frac{d\sigma_c}{dW} = \sum_{i=1}^{M} \frac{f_i}{W^2} \theta(W - W_i) \quad \frac{d\sigma_d}{dW} = \sum_{i=1}^{M} \left( \frac{f_i}{W} \right) \ln \left( \frac{W_i}{Q_-} \right) \delta(W - W_i). \tag{4.23}$$

The extension of the model beyond the limit of first Born approximation requires some relativistic corrections to be introduced [Sal92]. In terms of close collisions, it was recognised that the Rutherford cross section $1/W^2$ should be replaced by the Møller and Bhabha formulae [Jau76] for electrons and positrons (respectively). The relativistic form of the DCS for close collisions is then given by

$$\frac{d\sigma_c}{dW} = \sum_{i=1}^{M} \frac{f_i}{W^2} F^{(\pm)}(E,W) \times \theta(W - W_i) \theta(W_{\text{max}} - W) \tag{4.24}$$

where the functions $F^{(\pm)}(k)$ are the ratios of the Møller and Bhabha DCSs to the Rutherford DCS, calculated from [Sal92]

$$F^{-}(k) = 1 + \left( \frac{k}{1-k} \right)^2 - k \frac{\gamma - 1}{1-k} \left( \frac{1}{\gamma} - \frac{1}{\gamma - 1} \right) \left( \frac{k^2 + k}{1-k} \right) \tag{4.25}$$

for electrons, and

$$F^{+}(k) = 1 - \left( \frac{\gamma - 1}{\gamma} \right)^2 - \left\{ \frac{2(\gamma - 1)^2 - 1}{\gamma^2 - 1} - k \frac{k^2}{(\gamma + 1)^2} \right\} \left[ 3(\gamma + 1)^2 \right. \left. + 1 - 2\gamma(\gamma - 1)k + (\gamma - 1)^2k^2 \right] \tag{4.26}$$
for positrons, and the reduced energy loss given by \( k = W/E \). The maximum energy loss is \( W_{\text{max}} = E \) in the case of positrons while for electrons, due to indistinguishability of incident and target electrons, \( W_{\text{max}} = E/2 \) [Jau76]. Following Fano’s treatment [Fan63], Salvat suggested that the DCS for distant collisions could be calculated from [Sal92]

\[
\frac{d\sigma_d}{dW} = \sum_{i=1}^{M} \frac{f_i}{W_i} \left[ \ln \left( \frac{W_i Q_+ + 2m_0c^2}{Q_- W_i + 2m_0c^2} \right) \right. \\
+ \ln \left( \frac{1}{1 - \beta^2} \right) - \beta^2 - \delta \right] \delta(W - W_i) \tag{4.27}
\]

where the density effect correction \( \delta \) was introduced to account for the polarization of the medium by the incident charged particle [Ber84], and \( Q_- \) is calculated from eq. (4.22) with \( W = W_i \).

In summary, the GOS model initially introduced by Liljequist and the high-energy corrections suggested by Salvat, allowed the energy-loss DCS to be written according to (4.21) using (4.24) and (4.27). If no experimental data is available to help in the estimation of the effective number of electrons per shell, \( f_i \), and their resonance energies, \( W_i \), these quantities can be set, for inner-shells, as the number of electrons in the shell and the values calculated from (4.17), respectively. Valence electrons can be represented by a single oscillator with a strength equal to the number of electrons bound with energies less than a few tens of eV and resonant energy calculated from (4.19). With \( N \) atoms per unit volume, inelastic mean free paths and collision stopping powers for electrons with kinetic energy \( E \) can then be calculated from

\[
\lambda_i^{-1}(E) = N \int \frac{d\sigma}{dW} dW \quad S_i(E) = N \int W \frac{d\sigma}{dW} dW. \tag{4.28}
\]

The maximum energy loss \( (W_{\text{max}}) \) is equal to \( E \) for distant excitations and \( E/2 \) for close collisions. In the light of (4.24) and (4.27) these quantities may be written as a sum where each term is associated with an atomic shell. This approach is well suited to implementation in simulation codes where the emission of secondary
electrons and the particles emitted in the “relaxation” of ions with inner shell vacancies (fluorescence photons and/or Auger electrons) must be modelled. The standard version of the EGS4 code does not realistically model these processes and so significant improvements can be achieved if the electron transport is extended to use the GOS model. It should be noted that this GOS model constitutes the “bulk” of electron-atom physics in the PENELOPE code [Bar 95].

4.4 Predicted inelastic cross sections and collision stopping powers

For the kind of applications where the GOS model should be applied, it is important to assess how accurately electron inelastic mean free paths and associated stopping powers can be estimated. Such analysis was carried out through a comprehensive comparison of the results calculated from (4.28) with other theoretical and experimental data for low, intermediate and high-Z elements. The summary of this exhaustive study, is presented in figs 4.1 to 4.4 for beryllium (Be), aluminium (Al), copper (Cu) and gold (Au). In this calculation binding energies were taken from [Bea 67] and the density effect correction calculated from [Ste 83]. Oscillator strengths of inner shells were set to the occupation numbers, \( Z_i \), for all elements but aluminium (data for Al is shown in table 4.1). Further parameters used are presented in table 4.2 where, for Al and Au \( W_{cb} \) was obtained from [Sal 92], and calculated from eq. (4.19) with \( b = 1 \) for the remaining elements.

From the data shown here, it is possible to conclude that, above \( \approx 100 \) eV, predictions based on the GOS model presented in section 4.3 are in good agreement with other published data, even for materials like Cu that do not exhibit well defined plasmon lines [Pal 85, FVa 92]. It is clear from equations (4.24) and (4.27) that this GOS model can not be used at energies below \( W_{cb} \), and Liljequist pointed out the fact that below \( \approx 2W_{cb} \) the predicted cross sections/stopping powers may be
somewhat crude. Considering table 4.2, it is seen that these limitations hardly apply above 100 eV, and satisfactory estimates are obtained. From figs. 4.1 to 4.4 it is also possible to conclude that the Bethe-Bloch formula “breaks down” at low energies (especially in intermediate/high-Z elements). In agreement with the extension suggested by Salvat et al. [Sal92], the high-energy Bethe-Bloch stopping powers from ICRU-37 [Ber84], are reproduced accurately.
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<table>
<thead>
<tr>
<th>Shell</th>
<th>Z</th>
<th>( f_i )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1s_{1/2}</td>
<td>2</td>
<td>1.65</td>
</tr>
<tr>
<td>2s_{1/2}</td>
<td>2</td>
<td>2.05</td>
</tr>
<tr>
<td>2p_{1/2}</td>
<td>6</td>
<td>6.2</td>
</tr>
<tr>
<td>c.b.</td>
<td>3</td>
<td>3.1</td>
</tr>
</tbody>
</table>

Table 4.1: Oscillator strengths for aluminium as determined in [Shi 80] from optical data.

<table>
<thead>
<tr>
<th>Element</th>
<th>Z</th>
<th>( f_{cb} )</th>
<th>( W_{cb} ) (eV)</th>
<th>( a )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Be</td>
<td>4</td>
<td>2</td>
<td>18.5</td>
<td>1.97</td>
</tr>
<tr>
<td>Al</td>
<td>13</td>
<td>3.1</td>
<td>15.0</td>
<td>2.62</td>
</tr>
<tr>
<td>Cu</td>
<td>14</td>
<td>11</td>
<td>38.0</td>
<td>2.91</td>
</tr>
<tr>
<td>Au</td>
<td>79</td>
<td>11</td>
<td>40.0</td>
<td>1.83</td>
</tr>
</tbody>
</table>

Table 4.2: Generalized oscillator strength parameters used in the calculation of the data presented in figs 4.1 to 4.4. The adjustment factor \( a \) was calculated from eq. (4.20).

4.5 K-shell ionisation cross section

Although the results presented have indicated that (total) inelastic mean free paths and stopping powers can be reasonably estimated using the GOS model, the same does not apply to partial ionisation cross sections, especially near the shell thresholds. It can be seen from equations (4.24) and (4.27) that the inelastic cross section predicted by this model is null for energies below \( W_i \). Since the factor \( a \) is of the order of 2 (table 4.2) this implies that for an atomic shell with binding energy \( U_i \), the present version of the model can not be used in the estimation of ionisation cross sections for energies below \( \approx 2U_i \). This is clear in fig 4.5 where the K-shell ionisation cross section for Ag, as calculated from the GOS model, is compared with other data. The estimated cross section is null in the range 25 keV \( \rightarrow \approx 45 \) keV, while the “blip” at \( \approx 90 \) keV corresponds to the threshold for close collisions.
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Figure 4.2: Inelastic mean free path ($\lambda_i$) and collision stopping power ($S_e$) in Al, calculated using the GOS model (solid lines). Experimental data from Tracy [Sea 73] (solid squares), Al-Ahmad [AIA 83] (solid triangles), and theoretical calculations from Tanuma et al. [Tan 91] (circles) and EEDL [Per 91] (stars). The dotted line was calculated using the Bethe-Bloch formula from ICRU-37 [Ber 84].

The need for a more realistic description of events involving K-shell ionisation by electron impact, when the incident electron possesses an energy close to the shell threshold, motivated the introduction of some improvements in the model discussed from equations (4.12) to (4.27). In order to keep the simple representation of the Bethe surface described above, an idea introduced by Liljequist [Lil 85] for obtaining more accurate estimations of energy loss spectra, was explored further. This avoided the use of more complex alternative approaches [May 90, Gry 65]. In this enhanced version of the GOS model, an inner-shell $j$ is represented by a set of $M_j$ oscillators, with resonant energies $W_{j,n}$ that are distributed according to the relation

$$W_{j,n} = W_{j,1} + (n - 1)\Delta W, \quad n = 1, 2, ..., M_j$$

(4.29)
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Figure 4.3: Inelastic mean free path ($\lambda_i$) and collision stopping power ($S_i$) in Cu, calculated using the GOS model (solid lines). Experimental data from Burke et al. [Bur82] (solid squares) and Al-Ahmad [AlA83] (solid triangles). Theoretical calculations are from Penn [Pen87] (triangles), Tanuma et al. [Tan91] (circles) and EEDL [Per91](stars). The dotted line corresponds to the Bethe-Bloch formula.

Based on photoelectric theory [Bet57], and as introduced in (4.16), oscillator strengths may be written as

$$f_{j,n} \propto W_{jn}^{-c}$$  \hspace{1cm} (4.30)

with $c$ given by [Lil83]

$$c = 1 - [\ln (W_j/U_j)]^{-1}.$$  \hspace{1cm} (4.31)

As discussed by Liljequist, $W_{j,1}$ should be of the order of the binding energy $U_j$ and the spacing between oscillators should be $\Delta W \ll U_j$. However, the particular values of these quantities are not important, as long as the relations

$$\sum_{n=1}^{M_j} f_{j,n} = f_j \quad \sum_{n=1}^{M_j} f_{j,n} \ln W_{jn} = f_j \ln W_j$$  \hspace{1cm} (4.32)
Figure 4.4: Inelastic mean free path ($\lambda_i$) and collision stopping power ($S_e$) in Au, calculated using the GOS model (solid lines). Experimental data is from Henke [Hen72] (solid square), Baer et al. [Bae74] (solid triangle) and Al-Ahmad [AlA83] (solid circles). Theoretical calculations are from Love's model [Lov78] (crosses), Ashley [Ash88] (circles) and EEDL [Per91](stars). The dotted line corresponds to the Bethe-Bloch formula.

are satisfied. Realistic electron energy loss spectra for aluminium, iron and copper were obtained with inner shells represented by sets of 20 to 30 oscillators [Lil85].

It was therefore necessary to investigate whether more accurate K-shell ionisation cross sections could be obtained using this enhanced version of the GOS model. Accordingly, the threshold $W_{K,1}$ was set to be equal to the K-edge energy, $U_K$, and the total strength, $f_K$, calculated using photoelectric absorption data. The motivation for using photoelectric absorption data to calculate $f_K$ in this rather novel approach was the close relation between the GOS and the interpretation of quanta absorption in terms of a OOS, discussed in section 4.2. Denoting the photoelectric
cross section (in barns), at a given energy $E$, by $\sigma_{\text{pho}}(E)$, the strength $f_K$ can be calculated using the relation [Fan68, Sta82, FVa93]

$$f_K = \frac{1}{109.8} \int_{\epsilon_K}^{\infty} \sigma_{\text{pho}}(E) \, dE$$

(4.33)

where the energy integration is done in units of eV.

The oscillator strengths $f_K$ that were used in the enhanced version of the GOS model were calculated using the "C" version of subroutine MUCAL [Boy96], by means of a numerical integration. The authors of MUCAL (a fit to the photon absorption data published by McMaster et al. in 1969 [McM69]) give no warranty on their program, but MUCAL was found to agree to within 10% with the XCOM program [Ber87]. Although data is very limited for elements with $Z>83$ and not avail-
Figure 4.6: Total oscillator strength for the K-shell, calculated from eq. (4.33) using photoelectric absorption data.

able at all for \( Z < 11 \), this routine was preferred to XCOM and the EEDL database [Cul 97] because of the availability of its source code. By carrying out the integration of (4.33) using the extended trapezoidal rule [Pre 92], the total strength, \( f_K \), was estimated for several elements and the results are shown in fig. 4.6. In the case of Al, the value of \( f_K \) calculated from eq. (4.33) is \( f_K = 1.67 \), an estimation that agrees well with the experimental measurement of \( f_K = 1.65 \) determined by Shiles and collaborators [Shi 80].

In spite of the significant improvements obtained by Liljequist when inner shells were represented by sets of \( \approx 30 \) oscillators, the dependence of the K-shell ionisation cross section on this parameter was also evaluated. Atomic binding energies were once again obtained from [Bea 67] and the density effect corrections were calculated according to [Ste 83]. An example of the results obtained for two materials is dis-
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Figure 4.7: Dependence of the K-shell ionisation cross section for aluminium ($\sigma_K$) on the number of oscillators used, $M_j$. The solid line was obtained with 100 oscillators, the dashed line with 50 oscillators and the dotted line with $M_j = 10$.

played in figs. 4.7 and 4.8, where the K-shell ionisation cross sections for Al and Ag are plotted: noticeable variations (in magnitude and “shape”) for less than 50 oscillators can be found while above this value the dependence is not so strong. The use of a higher density of oscillators (i.e. a larger number of oscillators) would obviously lead to more accurate values. However, since this model is intended to be used for simulation purposes, it is necessary to balance calculation time against the limited improvements in accuracy obtained for large oscillator numbers. Therefore, for the purpose of simulating the transport of electrons, a version of the GOS model is used where the K-shell is represented by a set of 70 oscillators. The K-shell ionisation cross sections for Ag, Al and Au (as determined under these conditions) are shown in figs. 4.9 and 4.10, where for comparison purposes the values obtained from the
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Figure 4.8: Variation of the K-shell ionisation cross section for silver ($\sigma_K$) with the number of oscillators used, $M_j$. The solid line was obtained with $M_j = 100$, the dashed line with $M_j = 50$ and the dotted line with $M_j = 10$.

Kolbenvest model [Kol67] (used in ETRAN [Sel91] and the ITS series [Hab92]), the Gryzinski model (recently introduced in EGS4 [Nam97]), the EEDL database and other experimental data are also plotted. The significant improvement achieved in the model is clear when figs. 4.5 and 4.9 are compared.

Except in the case of aluminium where data concerning the "effective number of electrons" in each shell is available from [Shi80], a small correction has to be introduced in this enhanced model, so that the fundamental relations given by (4.14) are still satisfied. This means that it is necessary to somehow distribute the "strength" ($2-f_K$) among the outermost shells, making sure that the mean ionisation energy $I$ is still reproduced. This re-distribution was made numerically rather than by using other physically motivated arguments, by finding a new oscillator strength dis-
Figure 4.9: K-shell ionisation cross section ($\sigma_K$) for Ag calculated from the enhanced GOS model (solid line) with $M_j = 70$ and $f_K$ estimated from eq. (4.33). Symbols represent the same as data plotted in fig. 4.5. Theoretical data is shown for the Kolbenstved model [Kol67] (dashed line), the Gryziński model [Gry65] (dotted line) and the EEDL database [Per91] (stars).

For low Z materials, the strength to be re-distributed among other shells is small ($f_K$ approaches 2 as shown in fig 4.6, as discussed in [Com48]). For higher Z elements, the number of shells is large, and so this correction requires only minor changes to the initial model. It should however be pointed out that, although this approach does not strictly describe the “transfer of strength” from inner to outer shells [Bet57, Com48, Shi80], it does allow the maintenance of the fundamental properties of the GOS that were the “building blocks” of the model described in section 4.3. The data shown in fig 4.11 is representative of the accuracy obtained in the prediction of electron inelastic mean free paths and collision stopping powers,
Figure 4.10: K-shell ionisation cross section ($\sigma_K$) for Al and Au ($\times 10^3$) calculated from the enhanced GOS model (solid line) with $M_j = 70$ and $f_K$ estimated from eq. (4.33). Experimental data is from Hink et al. [Hin66] (solid circles), Davis et al. [Dav72] (solid squares), and Rester et al. [Res66] (solid triangles). Theoretical data is shown for the Kolbenstved model [Kol67] (dashed line), the Gryziński model [Gry65] (dotted line) and the EEDL database [Per91] (stars).

with this version of the GOS model where. As previously, a good agreement with several other sources can be observed.

4.6 Conclusion

In summary, a model for electron-atom inelastic collisions at energies where bound effects can not be neglected has been described. From the results that have been presented, it can be concluded that accurate cross section and stopping powers can be determined down to energies of the order 100 eV. On the other hand, the relativistic
corrections introduced allow the model to be used over a range considerably wider than other approaches. Other ways of modelling electron-atom inelastic collisions at relatively low energies have been developed over the last few years, each with their strengths and weaknesses [F Va96, F Va92]. However, as Salvat and collaborators have pointed out [Sal92], the simplicity of the model together with its reasonable accuracy in predicting the inelastic parameters relevant to electron transport algorithms, and the ability to model the emission of secondary particles by means of relatively simple algorithms, make this model well suited for Monte-Carlo purposes. The enhanced version of the GOS model that has been developed for the K-shell,
combines the simplicity and suitability of the original model with a more realistic description of events involving the ionisation of the K-shell near its threshold. Therefore this approach is expected to suit the kind of applications discussed in chapter 3, that the standard version of EGS4 failed to reproduce accurately. Towards this goal, the next chapter addresses the accuracy of the bremsstrahlung models currently in use, and leads to the development of a new scheme for the angular sampling of radiated photons.
Chapter 5

Bremsstrahlung emissions

5.1 Introduction

As discussed in chapter 3, realistic X-ray tube simulations require both accurate models for the production of characteristic radiation, and appropriate treatment of bremsstrahlung emissions. The accuracy of the standard release of EGS4 for modelling low energy bremsstrahlung emissions is carefully assessed, and the motivation for a new scheme for the angular sampling of newly created photons is analysed. This analysis has led to an updated algorithm being employed, that is more accurate at energies below a few hundred keV, to be introduced in EGS4. The implementation and timing performance of the new scheme are also discussed below.

5.2 Radiative emissions in the original EGS4 code

The modelling of bremsstrahlung emissions in the EGS4 code is based on the standard Bethe-Heitler cross sections taken from Koch and Motz's review article [Koc59]. At moderate and high energies the bremsstrahlung photon angular distribution cross section is strongly peaked in the forward direction. Therefore, in radiative events, the emission angles tend to be small when compared with the angular deviations
that result from multiple scattering. This argument has led to the introduction of a simple scheme in EGS4 where bremsstrahlung photons are considered to emerge at a fixed angle (an estimation of mean value of the angular distribution) relative to the direction of the primary electron (whose direction remains unchanged).

The "Elwert factor", a nonrelativistic Coulomb correction to be applied to the bremsstrahlung cross sections from Koch and Motz, was not introduced in the original version of EGS4. This factor, $f_E$, can be written as \[\text{[Koc 59, Sel 85]}\]

\[
f_E = \frac{\beta_0}{\beta_1} \frac{1 - \exp\left[\frac{2\pi Z}{(137/\beta_0)}\right]}{1 - \exp\left[\frac{2\pi Z}{(137/\beta_1)}\right]}
\]

where $\beta_0$ and $\beta_1$ are the velocities of the incoming and outgoing electron (respectively) in units of the speed of the light, and $Z$ the atomic number of the element under consideration. As an example, fig. 5.1, shows $f_E$ for 35 keV ele-

![Figure 5.1: Elwert factor $f_E$ in Ag for 35 keV incident electrons for different photon energies, corresponding to the value of $\beta_1$ in eq. (5.1).](image-url)
trons in silver (Ag). The result of neglecting $f_E$ is an underestimation low energy bremsstrahlung cross sections. Although it is strongly recommended to use the $f_E$ correction at energies below 2 MeV [Koc59], the realization that, at these energies, only a small fraction of the electron energy is lost in radiative emissions, means that $f_E$ was not incorporated in the original version of EGS4.

From this summary, it is clear that the original algorithms are not very accurate in the estimation of low energy radiative emissions and/or “thin target” bremsstrahlung applications. In order to overcome these limitations, it has been necessary to develop some extensions to the original code, as described in the following sections.

### 5.3 Improved radiative stopping powers

The corrections applied below 2 MeV in the bremsstrahlung cross section used in EGS4 (factor $A'(Z, E_0)$ in equation (2.77) of [Nel84] and briefly called APRIM) are calculated for 5 values of $Z$ and 13 different energies using data from [Koc59]. Since these correction factors are crude, an upgrade was introduced [Rog89] in order to cause the radiative stopping powers in EGS4 to match those in ICRU Report 37 [Ber84]. The new multiplicative correction factors applied to the bremsstrahlung cross sections are calculated using the data from [Sel86] and can be used by setting the option IAPRIM=1 in PEGS4 input files. The data presented in fig. 5.2 shows the (unrestricted) radiative stopping power in Ag (normalized to the data from ICRU-37) for both the original Koch and Motz corrections and the new APRIM values. From this plot it is evident that the original version of EGS4 underestimates the production of low energy bremsstrahlung photons, a realisation that can be understood, for example, from data given in fig. 5.1.

As it has been pointed out [Rog89], the new APRIM values (being a function of $Z$ and electron energy only), are introduced so that the mean radiative energy loss equals the one in ICRU-37. The cross sections themselves are not the same as
Chapter 5. Bremsstrahlung emissions

Figure 5.2: Radiative stopping power in Ag, calculated from PEGS4 using Koch and Motz corrections (triangles) and the new APRIM values (squares) from [Rog 89]. Data sets have been normalised ICRU Report 37 [Ber 84] values (solid line with value 1).

those given by [Sel 86], since different differential cross sections are actually used. It is however worth noticing the remarkable improvement in accuracy obtained when the new APRIM values are used. This is clear in fig. 5.3 where the bremsstrahlung differential cross section (differential in photon energy) in Ag for an electron kinetic energy of 35 keV is plotted, after being normalized to the values published by Pratt, Tseng and collaborators [Pra 77]. This work is the basis of Seltzer and Berger data [Sel 86] below 2 MeV.

In the light of data presented in figs. 5.2 and 5.3, it is clear that for energies of the order of several tens of keV, realistic bremsstrahlung stopping powers and (total+partial) cross sections can only be obtained when the ICRU-37/NBS stopping...
Figure 5.3: Bremsstrahlung cross section, differential in photon energy, in Ag for an electron (kinetic) energy of 35 keV. Data sets were calculated with PEGS4 using Koch and Motz corrections (triangles) and the new APRIM [Rog 89] values (squares) and have been normalized to the values of Pratt and collaborators [Pra 77] (solid line with value 1).

powers (i.e. the new values of APRIM) are in use.

### 5.4 Angular distribution of radiated photons

It has already been discussed that in the original version of EGS4, the angular sampling of bremsstrahlung photons is based on an simplified algorithm where newly created photons are assumed to be emitted at a fixed angle with respect to the direction of the radiating electron. For an electron with total energy \( E \) (in units of the electron rest mass) this angle (in radians) has the the form \( \Theta = 1/E \) and represents
an estimate of the average emission angle. The observation that this simplification was crude, even in the estimation of bremsstrahlung emission in thick targets, motivated Bielajew and co-workers [Bie89] to introduce a new angular sampling scheme in EGS4.

The formula used in the updated angular sampling routine is 2BS of Koch and Motz [Koc59], which is a bremsstrahlung cross section differential in photon energy and angle. Only the angular part of 2BS was used, and it was pointed out [Bie89] that the small angle approximation and the relativistic regimes for which this cross section was derived, could limit the usage of this formula to energies above a few MeV. The time degradation introduced by the new algorithm was found to be of the order of 20%–30% in “thin-target” applications and 13% in the estimation of “thick-target” bremsstrahlung. The figures presented were obtained using a code where electrons were forced to radiate and were not actually transported. For standard applications where electron transport is in effect the most time consuming operation, the timing degradation should be much smaller.

Although accurate at energies of the order of a few MeV [Koc59], it is necessary to evaluate how suitable 2BS is in the estimation of photon angular distributions in regimes below 100 keV. This was made by comparing the photon angular dependence of this bremsstrahlung cross section with the data published by Kissel et al. [Kis83]. The Kissel data is a theoretical prediction calculated using the theory of Tseng and Pratt [Pra77, Tse79], and has shown to be in good agreement with experimental results [Amb91a, Amb91b]. The angular dependence of the bremsstrahlung double differential cross section (differential in photon energy and angle) in Ag for an electron energy of 50 keV, and photon energies of 10 keV ($k/T = 0.2$) and 35 keV ($k/T = 0.7$), are shown in figs. 5.4 and 5.5 while fig. 5.6 shows the same kind of data for an electron energy of 500 keV and a photon energy of 250 keV. Each plot shows Kissel’s data (from [Kis83]) and the predictions obtained using formulas 2BS and 2BN (taken from [Koc59]), where in each graph all the curves have been normalized to the same area.
Figure 5.4: Bremsstrahlung cross section, differential in photon energy and angle (DDCS), in Ag for an electron (kinetic) energy of 50 keV and a photon energy of 10 keV ($k/T = 0.2$). Data plotted is from Kissel et al. [Kis 83] (solid squares), Koch and Motz’s 2BS (circles) and 2BN formulas (triangles). Curves are normalised to the same total area.

It becomes clear from figures 5.4 and 5.5 that for lower energies, much better estimates are obtained if 2BN is used for angular sampling of bremsstrahlung photons than with 2BS. For electron energies on the order of several hundred keV, fig. 5.6 indicates that the three curves tend to overlap. The same kind of dependence was also found in a comprehensive study where lower and higher Z elements like helium and uranium were considered. Therefore, for the overall goal of improving the current version of EGS4 for lower electron energies, it was decided to incorporate 2BN into the code’s bremsstrahlung angular sampling algorithm.

The 2BN bremsstrahlung cross section differential in photon angle and energy is basically an integration of the nonscreened “Bethe-Heitler formula” [Hei 60, Jau 76]
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Figure 5.5: Bremsstrahlung double differential cross section (photon energy and angle) in Ag for an electron energy of 50 keV and $k/T = 0.7$ (photon energy $\equiv 35$ keV). Data shown is from Kissel et al. (solid squares) and Koch and Motz's 2BS (circles) and 2BN formulas (triangles). Curves are normalised to the same total area.

(used in the ETRAN/ITS series) over all electron scattering angles. According to Koch and Motz's review paper, for a material with atomic number $Z$, this double-differential cross section derived under the first Born approximation, can be written in the form

$$
\frac{d\sigma_{\delta,\theta}}{d\Omega_{\delta}} = \frac{Z^2 r_0^2}{8\pi 137} \frac{dk}{k} \frac{p}{p_0} \frac{d\Omega_k}{d\Omega_{\delta}} \left\{ \frac{8\sin^2 \theta (2E_0^2 + 1)}{p_0^2 \Delta_0^2} - \frac{2(5E_0^2 + 2EE_0 + 3)}{p_0^2 \Delta_0^2} \right\} 
$$

$$
\quad - \frac{2(p_0^2 - k^2)}{Q^2 \Delta_0^2} + \frac{4E}{p_0^2 \Delta_0} + \frac{L}{pp_0} \left[ \frac{4E_0 \sin^2 \theta (3k - p_0^2 E)}{p_0^2 \Delta_0^2} + \frac{4E_0^2 (E_0^2 + E^2)}{p_0^2 \Delta_0^2} \right] 
$$

$$
\quad + \frac{2 - 2(7E_0^2 - 3EE_0 + E^2)}{p_0^2 \Delta_0^2} + \frac{2k(E_0^2 + E_0^2 - 1)}{p_0^2 \Delta_0} \right\} - \left( \frac{4\epsilon}{p\Delta_0} \right)
$$
Figure 5.6: Bremsstrahlung double differential cross section (photon energy and angle) in Ag for an electron energy of 500 keV and k/T = 0.5 (photon energy ≈ 250 keV). Data shown is from Kissel et al. (solid squares) and Koch and Motz's 2BS (circles) and 2BN formulas (triangles). Curves are normalised to the same total area.

\[
\left(\frac{e^2}{pQ}\right) \left[ \frac{4}{\Delta_0^2} \Delta_0 - \frac{6k}{\Delta_0} - \frac{2k(p_0^2 - k^2)}{Q^2\Delta_0} \right]
\]

(5.2)

where \( r_0 \) is the classical electron radius, \( k \) the photon energy, \( \theta \) the emission angle (in radians, with respect to the direction of the incident electron) and the pairs \((E_0, p_0)\) and \((E, p)\) are the total (energy, momentum) of the electron before and after the radiative emission, respectively. The energies \( k, E_0 \) and \( E \) are in units of the electron rest mass, the momenta in units of \( m_0c \) (\( c \) is the speed of light in vacuum) and the auxiliary quantities \( L, \Delta_0, \epsilon, Q \) and \( e^2 \) correspond to

\[
L = \ln \left[ \frac{EE_0 - 1 + pp_0}{EE_0 - 1 - pp_0} \right]; \quad \Delta_0 = E_0 - p_0 \cos \theta; \quad \epsilon = \ln \left[ \frac{E + p}{E - p} \right]
\]
\[ Q^2 = p_0^2 + k^2 - 2p_0 k \cos \theta; \quad e^\varphi = \ln \left[ \frac{Q + p}{Q - p} \right] \]

In EGS4, the sampling of 2BS is made by using a mixed procedure [Nel84]. No analytical (or mixed) methods have so far been developed for sampling 2BN, and so this is currently done using the rejection technique introduced in section 1.2.2. Here, the energy of the emitted photon is determined by EGS4's "run time" differential cross section and then with \( E_0, k \) and \( E [\equiv (E_0 - k)] \) known, the maximum value of eq. (5.2) is determined using the "golden section search" described in [Pre92]. Only the angular part of 2BN is relevant in the calculation, and so with the maximum of the function determined and its analytical form known, the sampling of the photon emission angle is then a straightforward operation (as suggested in fig. 1.1). The only approximation introduced during this sampling has to do with the fact that eq. (5.2) diverges when the photon energy is equal to the electron's initial kinetic energy \( (T_0) \). In this case, the angular sampling algorithm assumes that the photon energy is \( 0.999 \times T_0 \) (but does not change the photon energy itself).

Sampling a strongly peaked function like the one shown in figs 5.4 to 5.6 is quite inefficient from the computational point of view. To benchmark the timing degradation introduced when 2BN is used to calculate the angular distribution of bremsstrahlung photons, the emission of (50 million) photons was simulated (by repeatedly calling subroutine BREMS in the EGS4 code) for an electron energy of 35 keV incident on a Ag target. The timing performance of the 3 algorithms now available in EGS4 (normalised to the time taken by the original "fixed angle" scheme) is shown in table 5.1. Here it is clear that the 2BN sampling method is the least efficient. As discussed previously, however, actually transporting the electron is the most time consuming part of electron/photon simulation. This means that the timing degradation introduced by the 2BN sampling method in terms of the overall simulation time will not be as dramatic as the data shown in table 5.1 indicates at first glance.

When compared to 2BS, sampling the 2BN distribution is rather inefficient, and
Table 5.1: Calculation time required by the different sampling algorithms when normalized to that for the “fixed angle” scheme.

is clear from fig. 5.6 that very little improvement is obtained by using 2BN at energies above a few hundred keV. For this reason, when coding expression (5.2) into the EGS4 code, an energy cut (to be chosen by the user) was introduced, above which 2BS is used.

5.5 Conclusion

The accuracy of EGS4 in modelling bremsstrahlung emissions below a few hundred keV was analysed. The rather crude scheme used in the angular sampling of newly created photons motivated the introduction of an additional algorithm based on formula 2BN from Koch and Motz that, although computationally less efficient, is more accurate than other approaches. Overall, the data presented here suggests that, when using the new APRIM correction factors and 2BN angular sampling, fairly realistic simulations of radiative emission, at energies of the order of several tens of keV, can be performed. The relevance of this approach in the determination of photon spectra from X-ray tubes is discussed in the next chapter, where a low energy electron expansion of EGS4 (especially suited for the estimation of photon production in X-ray tube targets) is described.
Chapter 6

Low energy electron transport: the EGS4/GOS code

6.1 Introduction

An enhanced version of the EGS4 code, where electron inelastic collisions and bremsstrahlung emissions are treated using the models discussed in chapters 4 and 5, is now introduced. The scheme employed for the “run-time” interpolation of cross sections/stopping powers is assessed and the algorithms used in the kinematics of inelastic collisions described. The code is then used to estimate photon spectra from X-ray tubes and its accuracy tested by validating against experimental data. The improvements achieved with the new code are also analysed.

6.2 Interpolation of cross section and stopping powers

In the EGS4 code system, cross sections and (restricted) stopping power are interpolated using a logarithmic-linear technique. More precisely, the logarithm of the
particle's kinetic energy is used to provide an integer index into tables of interaction
probabilities, using a linear relationship. That is, for a particle with kinetic energy
$E$, in a particular medium $med$, an index $l$ (variable $l_{ke}$ in the code) is calculated
from
\[ l = \text{int} \left[ e_{ke1}(med) \ln(E) + e_{ke0}(med) \right], \tag{6.1} \]
where $\text{int}[x]$ denotes the integer part of the real number $x$. The constants $e_{ke1}$ and
$e_{ke0}$ in eq. (6.1) are chosen so that the errors associated with the interpolation
scheme are minimised (PEGS4 targets an error of the order of 1% over the con-
sidered energy range). Expression (6.1) basically defines an “energy grid”, dividing
$E$ into a set $M$ intervals that are distributed according to
\[ E_i = \exp \left( \frac{(l - e_{ke0})/e_{ke1}}{l = 1, \ldots, M}. \tag{6.2} \]
General transport quantities $\sigma(E)$ are then estimated by means of their interpolated
values $\sigma_{int}(E)$, of the form
\[ \sigma_{int}(E) = t_{sig1}(l, med) \ln(E) + t_{sig0}(l, med), \tag{6.3} \]
In each interval $E_i \rightarrow E_{i+1}$ the constants $t_{sig1}$ and $t_{sig0}$ are calculated by means of
a linear interpolation of $\sigma$ vs $\ln(E)$ using 200 equally spaced points.

In order to keep new and old codes compatible, the same technique was used in
the interpolation of electron cross sections and stopping powers given by the GOS
model (described in chapter 4). The energy grid used was the one selected by PEGS4
and, in each interval, the linear interpolation was performed (as in PEGS4) using 200
points equally spaced in $\ln(E)$. This is a relatively straightforward operation. In
each interval $E_i \rightarrow E_{i+1}$ [calculated from eq. (6.2) using $e_{ke1}$ and $e_{ke1}$ as selected
by PEGS4] the variables $t_{sig1}(l, med)$ and $t_{sig0}(l, med)$ can be determined from
[Pre92]
\[ t_{sig1}(l, med) = \frac{\left( \sum_{j=1}^{200} X_j Y_j \right) \left( \sum_{j=1}^{200} Y_j \right) - \left( \sum_{j=1}^{200} X_j \right) \left( \sum_{j=1}^{200} Y_j \right)}{\text{det}} \tag{6.4} \]
and

\[ tsig0(t, med) = \frac{\sum_{j=1}^{200} X_j^2 \left( \sum_{j=1}^{200} Y_j \right) - \left( \sum_{j=1}^{200} X_j Y_j \right) \left( \sum_{j=1}^{200} X_j \right)}{\text{det}} \]  

(6.5)

where \( X_j \) is related to the kinetic energy \( E \) through \( X_j = \ln E_j \) and \( Y_j \) is the function to be interpolated [from equation (6.3) \( Y_j = \sigma(E_j) \)]. The auxiliary quantity \( \text{det} \) is the determinant of the set of equations derived from a least-squares fit, as defined by

\[ \text{det} = \left( \sum_{j=1}^{200} X_j^2 \right) \left( \sum_{j=1}^{200} Y_j^2 \right) - \left( \sum_{j=1}^{200} X_j Y_j \right)^2 . \]  

(6.6)

Although accurate when used with the standard version of EGS4, it is important to understand how suitable this interpolation scheme is for the tabulation of data from the GOS model described in chapter 4. In fact, the definition of the energy intervals in PEGS4, i.e. \( e_{keV} \) and \( e_{keV} \) in eq. (6.1), is made so that the errors introduced are of the order of 1%, but this optimisation scheme was not introduced in the interpolation of the GOS cross sections/stopping powers. Thus, an exhaustive evaluation of the interpolation algorithm was carried out, by determining the differences between interpolated and true values (as given by the original functions). This study was performed in the range \( 1 \text{ keV} \rightarrow 60 \text{ keV} \), for 15 million randomly selected entries. Results of this benchmarking are presented in figs. 6.1 and 6.2. Figure 6.1 shows the distributions of the magnitude of error, while fig. 6.2 shows the dependence of the mean error on the (kinetic) energy considered. This data corresponds to cross sections estimated for inelastic collisions, as given in (4.21), that involve energy transfers above 1 keV.

The data shown in figs. 6.1 and 6.2 make it clear that cross sections and stopping powers can be interpolated using the "standard" technique developed for EGS4. By looking at fig. 6.2, it is clear that some optimisations could be carried out so that the selected energy intervals could, in some way, match the oscillator strength structure more accurately. This kind of procedure is already in use in PEGS4 when interpolating photon cross sections, where the energy grid is chosen by considering
Figure 6.1: Distribution of the errors introduced by the interpolation scheme in the estimation of cross section for close collisions. The energy range considered was 1 keV to 60 keV. In this histogram, 99% of the entries lie in the interval [-0.5%, 0.5%].

shell thresholds. Yet, this analysis shows that the inaccuracies introduced are not significant, and even look smaller than the uncertainty associated with the original quantities calculated from the GOS model (as data presented in sections 4.4 and 4.5 seems to indicate).

6.3 Transport Algorithm

As stated in section 1.4, EGS4 treats inelastic interactions of electrons (and positrons) using the condensed history technique and a “class II” algorithm. Electron-electron collisions and radiative emissions are simulated fully when the energy of the created particles are above pre-selected thresholds (variables AE and AP for electrons and
photon absorptions (and subsequent emission of fluorescence photons, respectively) while below these values, interactions are treated in terms of their stopping powers (straggling is not taken into account).

In this enhanced version of the code, electron inelastic cross sections and corresponding (restricted) stopping powers are calculated using the model described in sections 4.3 and 4.5. The emission of fluorescence photons in events involving the ionisation of the K-shell is highly relevant for the kind of studies that were described in chapter 3, therefore, distant collisions with the K-shell were treated as "catastrophic" and not in terms of their stopping power. For both close and distant collisions, tables of cumulative probability distributions are built from eq. (4.28). These are then used in the "selection" of the interacting target oscillator \( i \) which, from eq. (4.13), is associated with a particular shell of binding energy \( U_i \). Thus, a
simple but fairly realistic model for atomic ionisation [Sal 92] is to assume that, for a
certain energy transfer $W$, an electron (or “delta ray”) with energy $W - U_i$ is emitted
in the direction of the momentum transfer $\vec{q}$ (as presented in fig. A.1). When
a vacancy in the K-shell is created, branching ratio data from LSCAT [Nam 94] are
used to model the possible emission of fluorescence photons.

Other features were included in the EGS4/GOS code so that realistic simula-
tions of low energy electron transport in matter could be achieved. Electron elastic
scattering is described in terms of the PRESTA algorithm developed by Bielajew
and Rogers [Bie 87] while-photon transport is modelled using the general algorithms
described in the EGS4 manual [Nel 84]. To ensure accurate simulation of photon in-
teractions, the LSCAT extension code (that accounts for the bound Compton effect
and Doppler broadening) [Nam 94] and the implementation of L-Shell photoelectron
production and L X-ray production [Hir 96] were also incorporated.

Another option included in the new code is the possibility of treating the emission
of K-lines even when EGS4’s original electron inelastic cross sections are in use. In
this case, when an electron-atom inelastic collision occurs, the probability of ionising
the K-shell is evaluated using the GOS model as described in section 4.5, and the
possible emission of fluorescence photons is modelled accordingly. This treatment is
similar to the one of Namito and Hirayama [Nam 96, Nam 97], but with K ionisation
cross sections evaluated differently.

To deal with the small probability of producing a fluorescence photon, the variance
reducing technique of particle splitting (similar to one introduced by Bielajew
and collaborators [Bie 89] for the treatment of bremsstrahlung emissions) was also
incorporated in the code. Following the description in section 1.2.5, each time a
vacancy is created in the K-shell the probability of emitting a fluorescence photon is
evaluated $N$ times, with the “weight” of the created photons adjusted to a fraction
$1/N$ relative to the electron’s initial weight.

Electron bremsstrahlung is accounted for by using the models described in chap-
Chapter 6. Low energy electron transport: the EGS4/GOS code

6. The angular sampling of radiated photons can be performed using the original “fixed angle scheme”, or in a more realistic approach, using formulas 2BS or 2BN from Koch and Motz. Given the discussion in section 5.3, at energies of the order of several tens of keV, accurate cross sections can only be reproduced when the ICRU/NBS radiative stopping powers are in use.

An algorithm that accounts for the variation of discrete electron interaction cross section with energy has been developed for the EGS4 code system [Ma92]. This corrects the original code for the fact that, especially at energies below 10 keV, the cross sections for discrete interaction decreases with energy and so the distance travelled by the electron may be overestimated. Although this updated scheme was optimised for the electron cross sections in use at the time (and not the ones given by the GOS model) no changes have, so far, been carried out.

In summary, in this enhanced version of the code the user has the choice to use either the electron cross sections and stopping powers as calculated using the standard PEGS4 preprocessor or, alternatively, the ones calculated by the GOS model as described in section 4.3. In this case, distant collisions with the K-shell are simulated fully, and the possible emission of K-photons treated. Even when using the original EGS4 electron-electron inelastic cross sections, a flag can be set so that the emission of fluorescence photons after the ionisation of the K-shell can be evaluated. A further option introduced is the possibility of using Koch and Motz’s 2BN formula for newly created bremsstrahlung photons.

6.4 Kinematics of inelastic collisions

Inelastic collisions of electrons with atoms are treated in terms of the models described in section 4.3. This means that energy transfers and scattering angles for “hard” interactions (i.e. those with energy transfers above a threshold $W_c$) must now be determined using the cross sections given by equations (4.24) and (4.27).
6.4.1 Close collisions

In terms of close collisions, the probability distribution function (PDF) for energy transfers $W$ is given by eq. (4.24). For an incident electron with kinetic energy $E$ interacting with $i$th oscillator, this equation can be written in terms of the reduced energy loss $k = W/E$ as [Sal92]

$$ P_{\text{ee}}^{(-)}(k) = k^{-2} F^{(-)}(k) \theta(k - k_c) \theta(1/2 - k) $$

(6.7)

where for an electron kinetic energy $E$, if $\max(x, y)$ is function that returns the higher of two real numbers $x$ and $y$, then $k_c = \max(W_i, W_e)/E$. A distribution $\Phi^{(-)}(k)$ can be defined [Sal92] such that

$$ \Phi^{(-)}(k) = (k^{-2} + 5a) F^{(-)}(k) \theta(k - k_c) \theta(1/2 - k) $$

(6.8)

with $a \equiv (1 - 1/\gamma)^2$. In the interval $(k_c, 1/2)$, $\Phi^{(-)}(k) > P_{\text{ee}}^{(-)}(k)$, therefore the energy loss $k$ can be sampled from eq. (6.7) with trial values sampled from eq. (6.8) and acceptance probability $P_{\text{ee}}^{(-)}(k)/\Phi^{(-)}(k)$.

Random sampling from the PDF $\Phi^{(-)}(k)$ can be performed, when the following decomposition (normalised to 1 in the interval $k_c \to 1/2$) is considered

$$ \Phi_{\text{norm}}^{(-)}(k) = \frac{1}{1 + 5ak_c/2} [p_1(k) + (5ak_c/2) p_2(k)] $$

(6.9)

with

$$ p_1(k) = \frac{k_c}{1 - 2k_c} k^{-2} \quad \text{and} \quad p_2(k) = \frac{2}{1 - 2k_c} $$

(6.10)

The distribution (6.9) can be sampled using the composition method introduced in section 1.2.2, with the (normalised) distributions $p_1(k)$ and $p_2(k)$ sampled using the direct method. As discussed in sections 4.2 and 4.3, this kind of interaction has a binary character where the relation $Q = W$ holds, so with all the kinematic variables selected, the scattering angle $\theta$ can be determined from relations (A.5) to (A.7).
6.4.2 Distant collisions

It was discussed in chapter 4 that distant collisions have a resonant character, where the incident particle mainly interacts with the oscillator structure of the target atom. In the collision with the $i$th atomic oscillator energy transfers are, on average, of the order of its resonant energy $W_i$ [Fan63]. However, the complete specification of the scattering event requires that the recoil energy $Q$ is also determined. Following the detailed studies carried out by Fano [Fan63], Salvat suggested that the (unnormalized) PDF for $Q$ could, to a good approximation, be calculated from [Sal92]

$$P_d(Q) = \frac{1}{Q(Q + 2Q_E^i)}, \quad \text{for } Q_- < Q < W_i.$$  \hspace{1cm} (6.11)

It is straightforward to integrate this equation in the interval $(Q_-, W_i)$. After a convenient normalization, sampling values of $Q$ that are distributed according to (6.11) using the direct method turns out to be a rather simple operation. Then, with $Q$ and $W$ determined, scattering angles and energies that fully specify the configuration of the final state can be calculated.

6.5 Results

In all the following simulations, the threshold below which interactions were treated in terms of their stopping power was 1 keV (i.e. $AE \approx 0.512$ and $AP = 0.001$). The bremsstrahlung cross sections were calculated as described in section 5.3, using the corrections calculated from ICRU37/NBS radiative stopping powers by setting $IAPRIM = 1$ in the PEGS4 input files. The bremsstrahlung splitting macro described in [Bie89] and the equivalent incorporated in the code to deal with the creation of vacancies in the K-shell were also used, with $N = 200$. 
6.5.1 Placios’ experiment

The first set up considered was the one described by Placios in 1967 [Pla67], that is presented schematically in fig. 6.3. In his experiment, a 100 keV electron beam is normally incident on a 29.1 mg/cm² thick tin (Sn) target. Photons emitted from the target were counted using a NaI(Tl) scintillation detector. Energy spectra were recorded at 70° (and 110°) with respect to direction of the incident electron. The detector was positioned 19.6 cm from the target. This arrangement was simulated using the EGS4/G0S code, in which the (kinetic) energy below which particles were no longer transported was selected to be 4 keV. As in section 3.2, the photon spectra at the detector were calculated by selecting those photons which entered the relevant solid angle. The simulated photon spectrum was then convolved with the detector response (the FWHM at 25 keV was considered to be 8 keV), and since the Placios experimental data has been corrected for detection efficiency, there was no need to make any other correction on the simulated data.

The results obtained, in terms of the number of photons per unit solid angle per MeV per incident electron at 70°, and for 50 million incident electrons (composing an infinitely narrow beam), are shown in fig. 6.4. The three simulated spectra shown correspond to the data obtained with the standard EGS4 code, the standard version of EGS4 plus the treatment of K-shell fluorescence using the GOS model (EGS4+K) and a version of the code where (as described in section 6.3) the treatment of electron-atom inelastic collisions was based on the GOS model (EGS4/G0S); for the three codes the angular sampling of bremsstrahung photons was based on Koch and Motz’s 2BN formula.

As pointed out in previous work [Nam96, Tav96, Nam97], it is clear from this set of results that the standard version of EGS4 is unsuitable for simulating experiments where the emission of K fluorescence photons following electron impact ionisations has to be modelled accurately. It can also be seen that the EGS4/G0S code results in a more accurate estimation of the bremsstrahlung part of the spectrum. As
Chapter 6. Low energy electron transport: the EGS4/GOS code

Figure 6.3: Schematic representation of the experiment used by Placious [Pla67] to measure the photon spectra produced by 100 keV electrons incident on a Sn target.

is also the case in Compton scattering, the assumption that target electrons are free leads to an overestimation of the cross section and, in relative terms, a reduction of the bremsstrahlung yield. Although $\approx 30\%$ slower than the other two codes, the improvement in accuracy to $\approx 15\%$ at the $K_\alpha$ energy, together with its resonably good estimate of the bremmstrahlung tail, clearly shows the suitability of the EGS4/GOS code in the simulation of this kind of experiment.

The relevance of the modified bremsstrahlung angular scheme in use was also assessed for this kind of set up. The EGS4/GOS code was used in two other runs where the only parameter modified was the algorithm used to sample the direction of radiated photons (i.e. “fixed angle” and 2BS). The differences obtained between the three methods were found to be no greater than 4%. This result shows that in
Figure 6.4: Photon spectrum emerging at 70° (with respect to the 100 keV incident electron beam) from a Sn target. Experimental data corresponds to the results obtained by Placious (squares), and simulation to the spectra obtained with EGS4/GOS (solid line), EGS4+K (dashed line) standard EGS4 (dotted line) codes.

situations where the electron scatters considerably before radiating, realistic results are obtained using the “fixed angle” approach, even for low energy incident electrons. The timing benchmarks (table 6.1) for this data show that the code runs 11% and 80% slower than the fixed angle approach when the 2BS and 2BN angular distributions, respectively, are used. In view of the data presented in table 5.1, it is worth noticing that the timing degradation in the actual code is far less dramatic than the figures shown for the angular sampling of bremsstrahlung photons alone.
### Table 6.1: Time performance of the EGS4/GOS code in simulation of Placios’ experiment (normalized to the “fixed angle” scheme).

<table>
<thead>
<tr>
<th>Sampling Scheme</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>“Fixed angle”</td>
<td>1.00</td>
</tr>
<tr>
<td>2BS</td>
<td>1.11</td>
</tr>
<tr>
<td>2BN</td>
<td>1.80</td>
</tr>
</tbody>
</table>

6.5.2 Simulation of a micro focal X-ray tube

The EGS4/GOS code was also used to simulate the photon spectrum obtained from the microfocal X-ray tube presented in section 3.2, with basically the same settings. Simulated spectra obtained using the enhanced code and the corresponding experimental data for tube voltages of 35 kVp and 30 kVp are shown in figs. 6.5 and 6.6. For comparison purposes, data simulated with the standard version of EGS4 are also shown.

The agreement between the EGS4/GOS code and experimental data, over all the energy range considered, is quite good. Near the $K_{\alpha}$ line, for both tube voltages, the agreement was found to be of the order of 11%, and once again the bremsstrahlung tails are modelled accurately. The peak at $\approx 12$ keV on the experimental spectra is, as discussed in section 3.2, the “escape line” of the germanium detector and is not reproduced in the simulations because no photon or electron transport was performed in the detector region. The geometry used is quite inefficient from the computational point of view (only 0.25% of the photons emitted from the tube reach the detector). This leads to rather long run times for each tube voltage. Therefore, the suitability of schemes based on the “fixed angle” and 2BS formula to model bremsstrahlung angular distributions was not evaluated for this set up.

A further geometry was also simulated that was similar to that presented in fig. 3.1. In this case, a 40 nm thick Ag target was deposited onto a 680 $\mu$m thick AlN substrate. Photon spectra were measured using a liquid nitrogen cooled Si(Li)
Figure 6.5: Photon spectra obtained with the X-ray tube operated at 35 kV_p. Simulated data is presented in the form of histograms for EGS4/GOS code (solid line) and the EGS4 code (dotted line), for the same number of incident electrons. Experimental data (line) was normalised to the same total number of photons obtained with the EGS4/GOS code.

detector that was positioned 14 cm away from the X-ray tube front window. The center of the detector was aligned with the X-ray tube axis. Experimental results and simulation data for this geometry, using a tube voltage of 35 kV_p, are shown in fig. 6.7. The simulation data was corrected to account for the efficiency and energy response of the detector, that is analysed in section B.3.1. The two sets of simulation data shown correspond to simulations carried out using angular sampling schemes based on Koch and Motz's 2BN and 2BS formulas. The same number of incident electrons were used in each case. The experimental data were normalised so that the area under the curve matched that for the 2BN data.

Figure 6.7 shows that 2BS is clearly overestimating the number of bremsstrahlung...
Figure 6.6: Simulated and experimental spectra obtained for a tube voltage of 30 kVp. Simulated data is presented in the form of histograms for EGS4/GOS code (solid line) and the EGS4 code (dotted line). Experimental data (line) was normalised to the same total number of photons obtained with the EGS4/GOS code, and both sets of simulated data correspond the same number of incident electrons.

Photons emitted at small angles, as evidenced by the fluorescence-bremsstrahlung ratio in the two sets of simulation data. This is expected (based on the cross-section data presented in figures 5.4 and 5.5), even though there is obviously some bremsstrahlung production in the AIN substrate (as further analysed in section 7.5). Once again the agreement between the EGS4/GOS code and experimental data is quite good. The use of the 2BN sampling method resulted in a 10% increase in simulation time. This small increase is due to the fact that the majority of the electron transport is carried out in the AIN substrate where (being a lower-Z material) the bremsstrahlung yield is smaller. Although these simulations are close to the limit of validity of the PRESTA algorithm, this is not so relevant when considering the
production of photons. Therefore, the forthcoming PRESTA-II [Bie97] algorithm has not been incorporated in these particular simulations.

6.6 Conclusion

An enhanced version of the EGS4 code where electron-atom inelastic collisions are modelled considering atomic bound effects was described. The code also includes an updated angular scheme for bremsstrahlung photons based on Koch and Motz's 2BN formula. The accuracy of this new algorithm was tested by simulating photon production in X-ray tubes, and the results compared with experimental data.
Good agreement was obtained in the modelling of fluorescence and bremsstrahlung photons, showing that the new code is better suited for this kind of experiments than previous approaches [Tav.98].

The software package presented overcomes the low energy limitations of EGS4, identified in chapter 3. Indeed, realistic simulations of X-ray tubes operating at diagnostic energies can now be performed using the EGS4/GOS in both thin and thick-target applications. The new code may now be used to gain some insight into the physics that constrains the performance of X-ray tubes. As an example of a range of applications where EGS4/GOS may be applied, some design studies for X-ray tubes in transmission geometry are discussed in chapter 7.
Chapter 7

X-Ray tube design studies using the EGS4/GOS code

7.1 Introduction

Models for electron-atom inelastic collisions and bremsstrahlung emissions for energies below 100 keV have been discussed in chapters 4 and 5 (respectively). In chapter 6, the incorporation of these models in EGS4 was presented, and the code was used in simulations concerning photon production in X-ray tubes. The accuracy of the code was tested using experimental data, showing a good agreement between the two approaches. Thus, with the aim of obtaining a better understanding of X-ray tubes, it is worth using this updated code to gain some insight into the processes responsible for the conversion of the electron’s energy into measured photon spectra.

This chapter starts by addressing the physical interactions behind the creation of photons in X-ray tubes operating at diagnostic energies. The dependence of the cross sections for electron impact ionisation of the K-shell and bremsstrahlung emission on the energy of incident electrons is discussed, together with the angular dependence of emitted radiation. Then the EGS4/GOS code is used to study the production of photons at different target depths. The relevance of target thickness to the
performance of such devices (in terms of their efficiency and spectral composition) is then considered. Finally, the need for low-Z substrates in thin target applications is discussed, as a way of reducing the amount of bremsstrahlung radiation.

7.2 Analysis of the relevant interactions

With the aim of optimising X-ray tubes similar to the ones discussed in section 6.5.2, a good starting point is to understand the production of bremsstrahlung and fluorescence radiation in the tube target. Of special interest is how the probability of generating photons changes as electrons travel deeper inside the target. In other words, as the incident particle penetrates in the material, its energy is degraded by means of collisions with other electrons and through radiative emission. This reduction in the electron kinetic energy affects the probability of ionising the K shell and of radiating bremsstrahlung photons. So, the explicit dependence of these probabilities on the electron kinetic energy will in some way determine the relative yields of fluorescence and bremsstrahlung photons in the final spectrum.

The two processes (bremsstrahlung and fluorescence) that lead to the generation of photons in X-ray tube targets, when operating at energies of a few tens of keV are analysed now. As discussed previously, the dependence of the cross sections for these interactions on the kinetic energy of the electron should be considered. Also, in situations where the direction of the incident electrons does not change significantly before radiative events, the angular distribution of newly created bremsstrahlung photons may, in some way, determine the shape and intensity of the continuum tail, and so this topic will also be discussed.

7.2.1 Bremsstrahlung radiation

In materials like Ag, and for electron energies of the order of a few tens of keV, the bremsstrahlung cross section decreases with electron energy. This is shown
in fig. 7.1 where the total bremsstrahlung cross section, as given in [Per91], is plotted. It should, however, be noticed that from the point of view of the energy lost by incident electrons, this interaction becomes more significant for higher electron energies. In fact, the ratio of bremsstrahlung to excitation and ionisation increases with electron energy. This means that the higher the electron energy, the more likely it becomes for the electron to lose energy via radiative emission. Moreover, at these energies, the radiative stopping power increases with energy [Ber84], showing that the process of emitting bremsstrahlung photons becomes a more significant energy loss mechanism at higher electron energies.

Figure 7.1: Bremsstrahlung cross section in Ag, for electron energies up to 40 keV, as given in the EEDL database [Per91].

Quite apart from the total probability of an electron radiating, it is important to understand the relative contributions of high and low energy bremsstrahlung photons. For the sake of simplicity, these can be defined as photons with energies above and below the $K_\alpha$ line ($\approx 22.1$ keV in Ag), respectively. The material
pre-processor PEGS4 was used to estimate the bremsstrahlung cross sections corresponding to emission of photons with energies from 1 keV to 22.1 keV ("low energy" bremsstrahlung, $\sigma_{LBr}$) as well as emissions above this threshold, $\sigma_{HBr}$. The result is shown in fig. 7.2, from where it can be seen that increased electron energies favour the emission of photons with higher energies.

Figure 7.2: Bremsstrahlung cross section in Ag, corresponding to the emission of photons with energies above 22.1 keV ($\sigma_{HBr}$) and between 1 keV and 22.1 keV ($\sigma_{LBr}$). Data sets were calculated using PEGS4.

In the applications discussed herein, the intensity of bremsstrahlung radiation has a considerable angular dependence. Indeed, low energy photons tend to be emitted in the direction of motion of the incident particle, while for photons with energies approaching the kinetic energy of the incoming electron, the emission intensity peaks at substantially larger angles. This behaviour is shown in fig. 7.3 where the angular dependence of the bremsstrahlung double differential cross section for 35 keV electrons at different photon energies (in Ag) is plotted. These distributions,
representing the average number of photons emitted at a certain angle (per unit solid angle), were calculated using formula 2BN from Koch and Motz [Koc59]. A more

![Diagram](image)

**Figure 7.3:** Angular dependence of bremsstrahlung photon intensity, for 35 keV electrons in Ag. Calculations were based on the double differential cross section 2BN from Koch and Motz [Koc59].

pictorial view of this diagram is plotted in fig. 7.4 where, for the sake of clarity, fewer photons energies are displayed.

Data presented in figs. 7.3 and 7.4 show that the angular distribution of bremsstrahlung photons has a noticeable dependence on the energy of the radiated particle. However this may not be observed for the photon flux emitted from the X-ray tube target. In fact, if the incident electron scatters significantly before radiating, or the radiating particle is a secondary electron, its direction may be very weakly correlated to that of particles incident onto the target material. These angular deviations will act to “blur” the intensities predicted in fig. 7.3. Also, photon
absorption at the site of production may alter the energy distribution of photons transmitted from the target. This can have a greater effect than the anisotropy of the emissions themselves. Electron scattering and self-absorption can be minimised if thin targets are used, in which case bremsstrahlung intensities are expected to vary according to figs. 7.3 and 7.4. The relevance of electron scattering in terms of the characteristics of measured spectra is analysed further in section 7.4.

7.2.2 Fluorescence emissions

The emission of K-fluorescence radiation is one of the processes that follows the creation of vacancies in the K-shell. In this case, an electron from an outer shell fills the position available in the K-shell and a photon is emitted, balancing the change
in the electron’s binding energies. The ion with a vacancy in the K-shell may follow other forms of “relaxation” such as the emission of Auger/Coster-Kronning electrons [Kno89], which (in Ag) have $\approx 30\%$ chance of taking place. Or to put it more simply, the probability for a Ag atom with a K-vacancy to give rise to a K characteristic photon (the so called “branching ratio”) is $\approx 70\%$ [Hir96].

Ionisation of the K-shell may take place by means of electron impact ionisation events or photoelectric absorption. When the electron energy is just above the K-edge, electron impact ionisation is more likely to occur from incident electrons than through secondary $\delta$-rays. On the other hand, photoionisation of the K-shell requires first the production of bremsstrahlung photons with energies above $\approx 26$ keV which are then absorbed in the target, through excitation of the K-shell (the mean free path of 27 keV photons in Ag is $\approx 20$ $\mu$m).

From the data presented in fig. 4.9 it is anticipated that, for electron energies in the range 25 keV to $\approx 90$ keV, the production of fluorescence photons (via electron impact ionisation) in Ag will increase sharply with energy. The production of bremsstrahlung photons with energies above 26 keV also increases with electron energy, and these radiative events are likely to occur almost as often as electron ionisation of the K-shell (as suggested by data in fig. 7.5). It should however be emphasized, that this does not imply that the two processes will contribute with similar weights to the total fluorescence observed. This is because fluorescence induced by high energy bremsstrahlung photons also relies on the successful absorption in the material by means of ionisation of the K-shell.

To a good approximation, fluorescence radiation can be treated as being emitted isotropically. At an atomic scale, the change in the electron’s angular momentum when the transition takes place, leads to some degree of anisotropy in the emission [Sie65]. However, the atoms in X-ray tube targets may be considered to be randomly oriented. For this reason, the overall fluorescence is expected to be isotropic.
7.2.3 Relative yields

In the previous two sections, the dependence of bremsstrahlung and K-shell ionisation cross section on electron energy have been analysed separately. Since both quantities contribute to the total probability of interaction at any given step, it is interesting to inspect how their ratio changes with electron energy. This leads to the definition of a factor $F(E)$, whose variation with the electron energy $E$ may, in some way, mimic the dependence of the relative yield of characteristic radiation over bremsstrahlung emissions. In a rather simplistic form, by denoting $\sigma_{Br}(E)$ and $\sigma_K(E)$ as the cross sections for bremsstrahlung emission and ionisation of the K-shell
by electron impact, a factor $F(E)$ may be defined as

$$F(E) = \frac{\sigma_K(E)}{\sigma_{Br}(E)}. \quad (7.1)$$

This factor $F(E)$, was calculated using data shown previously in figs. 7.1 and 4.9. The result is shown in fig. 7.6. This kind of energy dependence was more or less expected, as $\sigma_K(E)$ increases with energy, while $\sigma_{Br}$ decreases with energy. From this plot it becomes clear that higher electron energies favour the production of fluorescence photons relative to bremsstrahlung emissions, with the ratio varying by nearly a factor of 10 in the range 25 keV to 40 keV. Thus, it is expected that as electrons travel into the target, the reduction in their energy should actually enhance the number of photons in the bremsstrahlung tail over the observed fluorescence intensity.

Figure 7.6: Ratio of the K-shell ionisation cross section by electron impact to the bremsstrahlung cross section, as defined in eq. (7.1), in Ag.

Following the analysis carried out in section 7.2.1, it is now worth splitting the
Chapter 7. X-Ray tube design studies using the EGS4/GOS code

bremsstrahlung cross section into its high and low energy contributions, and to inspect their variation relative to the K-shell ionisation cross section. In agreement with the factor $F(E)$ introduced in eq. (7.1), two other quantities, $F_H(E)$ and $F_L(E)$, can now be introduced so that high and low energy bremsstrahlung can be considered separately. These are given by

$$F_L(E) = \frac{\sigma_K(E)}{\sigma_{LBr}}, \quad F_H(E) = \frac{\sigma_K(E)}{\sigma_{HBr}},$$

(7.2)

where $\sigma_{LBr}$ and $\sigma_{HBr}$ are the cross sections for the emissions of photons with energies below and above 22.1 keV (as stated previously). The factors $F_L(E)$ and $F_H(E)$ are shown in fig. 7.7. Once again, given the data in fig. 7.2, the behaviour $F_L(E)$ could be more or less anticipated. However, the plot shows that, in spite of the increase of $\sigma_{HBr}$ with energy, its variations are dominated by those in $\sigma_K(E)$.

![Graph](image_url)

Figure 7.7: The quantities plotted, $F_L(E)$ and $F_H(E)$, are the ratios of the K-shell ionisation cross section to the cross sections for the production of low and high energy bremsstrahlung photons, respectively.

In summary, due to the sharp increase of the K-shell ionisation cross section
at energies near the K-edge, the production of fluorescence photons, relative to bremsstrahlung emission, will also increase with energy. The data presented in fig. 7.7 show that this happens for both bremsstrahlung photons with energies above and below 22.1 keV. This study only concerned average probabilities, and no self attenuation was considered. However, since electrons continuously lose energy while travelling through the target material, more bremsstrahlung than fluorescence radiation should be produced at depth.

### 7.3 Photon production in the target

The investigation carried out in section 7.2 provides relevant information, towards the understanding of photon production in X-ray tube targets. However, this analysis provides limited insight about the processes taking place in the target material. For this reason, more detailed studies aimed at investigating features like the site of production of photons in the target, as well as their angular distribution, were carried out using the EGS4/GOS code. The geometry used is representative of a broader range of applications, and is depicted in fig. 7.8. Essentially it comprised Ag targets (with thickness up to $\approx 50 \, \mu m$) and electron beams with energies of the order of 35 keV. Although only a simple case is considered, mapping of photon production at different depths and assessment of the significance of electron scattering before bremsstrahlung emissions should, together, provide important information for a wide variety of devices.

#### 7.3.1 Depth dependence

The number of fluorescence and bremsstrahlung photons produced by 150 million incident electrons (comprising a pencil beam), at different target depths, is shown in fig. 7.9. In this run all bremsstrahlung photons with energies above 1 keV have been considered. At first glance, this picture shows that bremsstrahlung production
Figure 7.8: Geometry considered in the studies concerning X-ray tube photon production.

occurs in a region that extends to a depth of 2.0 \( \mu m \) (where 99\% of the production takes place), while K-shell fluorescence seems to occur much closer to the entrance surface.

The data presented in fig. 7.9 for the production of fluorescence photons included emissions induced by electron impact ionisation and photoelectric absorption. The two contributions are plotted separately in fig 7.10 - (a) and - (b) and it is clear that events involving the ionisation of the K-shell by electron impact occur close to the beam entry point (98\% of the production occurs within 1 \( \mu m \)). On the other hand, photoelectric absorption of high energy bremsstrahlung photons is more probable at substantially increased depths. Considering the exponential law governing photon absorption in matter, this could be more or less expected (at \( \approx 40 \mu m \) the production is found to be less than 1\% of its maximum).

In terms of bremsstrahlung production, data in fig. 7.9 can be deconvolved so that photons with energies below and above 22.1 keV (referred as “low” and “high” energy bremsstrahlung) are considered separately. The result is shown in fig. 7.11,
Figure 7.9: Number of photons produced at different depths. Data sets correspond to the number of particles created, per million incident electron. Fluorescence production has also been multiplied by 20.

From where is clear that bremsstrahlung photons with higher energies are more likely to be produced nearer the incident surface where the electron's energy is still high. As incident particles travel deeper and deeper into the target, the reduction in their kinetic energy enhances the emission of bremsstrahlung photons with lower energies. This result is consistent with the analysis carried out in section 7.2.1.

Following from the discussion in section 7.2.3, it is now interesting to inspect how the relative production of fluorescence over bremsstrahlung radiation varies with depth. This can be done, using the data presented in fig. 7.9, by simply calculating the ratio of curves, as a function of target depth. The result is shown in fig. 7.12, and the dependence found is consistent with the results shown in figs. 7.9 and 7.10. The decrease in the ratio of fluorescence to bremsstrahlung as a function of depth is seen to be a direct consequence of the decrease of the energy of the propagating particles. The "turning point" in this behaviour, that occurs at a depth
of about 1.3 \mu m, is due to the considerable reduction in bremsstrahlung production at increased depths, and the continuing emission of characteristic radiation following photoelectric absorptions.

To summarise, characteristic radiation induced by electron impact ionisation and high energy bremsstrahlung photons are more likely to be produced at depths smaller than one micron. On the other hand, generation of lower energy bremsstrahlung occurs up to depths of the order of 2 \mu m. Virtually all the fluorescence induced by electron impact ionisation events occurs within the first 1.5 \mu m while that generated via photoelectric absorption extends up to depths of 40 \mu m.

### 7.3.2 Radial distributions

The radial distributions of the events resulting in the creation of bremsstrahlung and fluorescence photons has also been analysed. From fig. 7.13, where the fraction of the total production within circles of radii \( R \) is plotted, it is possible to conclude that
Figure 7.11: Production of low and high energy bremsstrahlung photons as a function of target depth. The data sets correspond to the number of photons per million electron, and the high energy component has been multiplied by 20.

\[ \approx 90\% \text{ of the bremsstrahlung is produced for radii smaller than } 1 \mu m. \] For fluorescence emissions, a large fraction is produced for small radii, but a second component extends over radial distances of nearly 100 \( \mu m \). These two components are actually those corresponding to emission following electron and photon induced ionisation, respectively. This is shown in figs. 7.14-(a) and (b) where the two quantities are plotted separately. Most of the fluorescence induced by electron impact ionisation occurs within \( \approx 0.8 \mu m \), while events relying on photoabsorption of bremsstrahlung photons extend over radii of \( \approx 100 \mu m \) (where the production is less than 1\% of its maximum).
Chapter 7. X-Ray tube design studies using the EGS4/GOS code

7.3.3 Angular distributions

The angular dependence of bremsstrahlung intensity was also evaluated. The data, in the form of intensity versus angular position (with respect to the electron’s incident direction) is shown in fig. 7.15. The two distributions correspond to photons with energies in intervals of width 0.1 keV that were centered at 10 keV and 30 keV. Comparing with the predicted intensities shown in fig. 7.3, it can be noticed that shapes are similar but the variations tend to be much smaller. These flatter distributions are a consequence of angular deviations that electrons have suffered before radiating that, in a way, “mix-up” the angular distributions of bremsstrahlung photons.

How much the electrons change their direction, in targets of different thicknesses, before emitting bremsstrahlung photons is shown in fig. 7.16. In this graph, the curve represents the fraction of electrons with angular deflections greater that θ. It can be seen that for a 2.2 μm thick target, half of the radiating electrons have changed
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Figure 7.13: Radial distribution of photons produced in a Ag target.

Figure 7.14: Radial distribution of fluorescence photons produced in a Ag target, after (a) electron impact ionisation and (b) photoelectric absorptions. Note the different scales on the radial axis.
Figure 7.15: Angular dependence of bremsstrahlung radiation intensity for two different photon energies.

their direction by more than 70°. For 300 nm and 100 nm thick targets, the figures are not so dramatic, and for the thinner target, nearly 40% of the particles suffer no significant change in their direction, with a negligible fraction of electrons being deflected by more than 70°, before radiating.

7.3.4 Electron backscattering

The relevance of electron backscattering for this kind of application was also evaluated. The study measured the number of electrons and their energy, as they were back-emitted from the incident surface. The result, in terms of an electron energy distribution is plotted in fig. 7.17, with data normalised to 100 incident electrons. As it has been suggested [Bie97], the maximum fractional energy loss per step in
Figure 7.16: Significance of electron scattering before radiative emissions, in targets of different thicknesses. At a given angle $\theta$, the curves represent the fraction of electrons that deviated more than $\theta$ before a bremsstrahlung emission.

This simulation was selected to be 1% (variable ESTEP in the code). From this plot, several results can be inferred. First, the curve peaks at energies close to that of the incident particles. This indicates that most of them are actually primary electrons that are elastically scattered and so lose very little of their initial energy. This data can be used to calculate the energy that, on average, is backscattered. Normalising this quantity to the number of incident 35 keV electrons, leads to value of 20.1 keV. In other words, a fraction of $\approx 57\%$ of the incident energy is backscattered, resulting in a rather inefficient process. For the purpose of generating X-rays (and especially K-characteristic radiation) only electrons with energies above 25 keV should be considered. This accounts for a fraction of about 45% of incident electrons.

In applications where tube efficiency is a critical parameter, a loss of the order of 50% might not be tolerable. In this case, studies should be carried out towards an optimized geometry where backscattered electrons can be re-absorbed. Although more complex from the operational point of view, the improvements in efficiency
may well justify the approach. This aspect will not be addressed in the following sections, but the EGS4/GOS code may in principle be used in such studies.

### 7.4 Dependence of transmitted spectra on target thickness

From the results discussed in sections 7.3.1 and 7.3.3 it is anticipated that target thickness plays an important role in terms of the characteristics of measured spectra. This is because, the production of photons is extended over a considerable region, and reduced scattering in thinner targets may lead to observable anisotropies in the angular distribution of bremsstrahlung radiation.

In fact, if thinner targets are considered, not only will the electrons be less likely to change their initial direction before radiating, but the overall photon production
will also be suppressed. Two simulated transmission spectra, measured in the direction of the incident beam, for target thicknesses of 40 nm and 2.2 \( \mu \text{m} \) are shown in fig 7.18. Both spectra are normalized to the same number of fluorescence photons. In these simulations an overall increase in the bremsstrahlung tail is seen for the thicker target (particles with energies below 10 keV were considered to be locally absorbed). This realisation is, in a way, a consequence of reduced electron scattering in thinner targets, that results in high energy photons being emitted off-axis. Also, more bremsstrahlung photons are produced in thicker targets, especially at lower energies.

![Figure 7.18: Simulated photon spectra from targets with different thicknesses. Measurements were made at 0°. Both sets of data were normalized to the same number of fluorescence photons, and convolved with the energy response of a HPGe detector.](image)

Broadly speaking, data in fig. 7.18 suggests that, in geometries where measurements are made along the beam axis, a good reduction in the bremsstrahlung component can be achieved by using thin targets. This means that higher fluorescence-to-bremsstrahlung ratios are attainable for reduced target thicknesses. Such improve-
ment is, however, achieved at the expense of efficiency. Reduced electron scattering and suppression of low energy bremsstrahlung production occurs when there is a low probability of the electron interacting in the target, but this also affects the fluorescence yield. To put it more simply, fig. 7.9 shows that for targets only a few nm thick, a substantial part of the overall fluorescence is also suppressed.

Since the fluorescence to bremsstrahlung ratio and efficiency vary with target thickness, it is interesting to study this relationship. This variation for spectra measured at 0° is shown in table 7.1, where absolute values for efficiency and fluorescence-to-bremsstrahlung ratios are presented. A more informative plot is presented in fig. 7.19, where the data sets have been normalized to the efficiency of the 40 nm thick target and the fluorescence-to-bremsstrahlung ratio of the 2.2 μm target. The performance of X-ray tubes with targets of different thicknesses may then be assessed in the following way: a 40 nm thick target is ≈ 37 times less efficient than a 2.2 μm thick one, but exhibits a factor ≈ 2.1 increase in fluorescence-to-bremsstrahlung ratio.

<table>
<thead>
<tr>
<th>Target thickness (nm)</th>
<th>Efficiency</th>
<th>F/B</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>40.89</td>
<td>0.172</td>
</tr>
<tr>
<td>100</td>
<td>112.29</td>
<td>0.152</td>
</tr>
<tr>
<td>300</td>
<td>473.04</td>
<td>0.133</td>
</tr>
<tr>
<td>475</td>
<td>842.28</td>
<td>0.118</td>
</tr>
<tr>
<td>650</td>
<td>1101.78</td>
<td>0.108</td>
</tr>
<tr>
<td>2200</td>
<td>1519.71</td>
<td>0.081</td>
</tr>
</tbody>
</table>

Table 7.1: Characteristics of photon spectra emerging at 0° from targets of different thicknesses. Efficiency is calculated as the number of fluorescence photons at 0° per unit solid angle per incident mC, and the fluorescence-to-bremsstrahlung ratio (F/B) as the number of characteristic photons over the total number of bremsstrahlung photons with energies above 10 keV.
Figure 7.19: Fluorescence-to-bremsstrahlung ratio versus efficiency for different target thicknesses. Data shown is presented in table 7.1.

7.5 Bremsstrahlung production in the target substrate

The analysis carried out in the previous section only concerned the production of photons in the tube target. However, when considering a more practical geometry (such as the one in fig. 3.1), it is quite reasonable to assume that some bremsstrahlung will be produced in the target substrate. This will be particularly important if thin targets are considered, as the electrons with higher energies are more likely to be transmitted from the target to the substrate. A straightforward comparison between the spectra presented in fig 7.18 (where only the production in a 40 nm Ag target is considered) the data in fig. 6.7 (that includes the substrate), shows that there is an obvious increase in the bremsstrahlung yield.

In order to gain a more quantitative view on the impact of the substrate, a set up
consisting of a 40 nm Ag target deposited onto a 680 μm AlN substrate (as shown in fig 7.20) was considered. The bremsstrahlung production in both target and substrate, due to a 35 keV incident electron beam was evaluated using the EGS4/GOS code and the result is presented in fig. 7.21. This shows that, for spectral

![Diagram](image)

**Figure 7.20:** Set up considered the significance of bremsstrahlung production in the target substrate.

measurements at 0°, the contribution of radiative events taking place in AlN is considerably higher than those due to emission from the Ag target. It was determined that 99% of the electrons incident on the Ag film are transmitted to the AlN with energies above 34 keV. In this way, for the purpose of understanding bremsstrahlung production in substrates, it can be considered that a "quasi-monoenergetic" 35 keV electron beam is incident on the substrate.

If thin-target applications are to be considered, fig. 7.21 suggests that bremsstrahlung photons produced in the target substrate may seriously degrade the performance of tube. Indeed, considering the whole set up, figures shown in table 7.1 for F/B in thinner targets can be reduced by an order of magnitude, with this being counter-productive from the operational point of view. To overcome this problem
(at least partially) alternative solutions can be based on the use of substrates with lower atomic numbers. A feasible choice is to employ boron \((Z=5, \rho = 2.34 \text{ gcm}^{-3})\) instead of AlN. Although more challenging from the experimental point of view, lithium \((Z=3, \rho = 0.53 \text{ gcm}^{-3})\) may also represent a further option, so these two materials have been considered in this study. The bremsstrahlung yield (in the form of a ratio of the bremsstrahlung cross section to the total cross section for interactions involving energy losses) in lithium (Li), boron (B) and AlN have been calculated using the EEDL database [Per91]. The results are shown in fig. 7.22, for electron energies of a few tens of keV. This data indicates that substantial reductions in the bremsstrahlung yield may be obtained if Li or B, rather than AlN, are used as substrates.

The geometry shown in fig 7.20 was then considered in two different configurations, with 1 mm thick substrates of Li and B (respectively) replacing AlN. The
fraction of bremsstrahlung radiation produced in the new substrates was evaluated using the EGS4/GOS code and the result is shown in fig. 7.23. This data shows that the contribution of bremsstrahlung corresponding to radiative emissions that take place in the substrate can be significantly reduced if Li or B are used to replace AlN. The enhancement of the tails at lower energies reflects the reduction in self-attenuation in B and Li. In fact, low-Z media where bremsstrahlung interactions are less likely to occur, also turn to be more transparent especially at lower photon energies. This is shown in fig. 7.24, where photon transmission through the 3 substrates considered is plotted.

In summary, applications that require the use of thin Ag targets can benefit if the metal film is deposited on a B or Li substrate, rather than on AlN. This is because of the considerable reduction in the bremsstrahlung yield in lower Z media. However, AlN seems rather appropriate for the purpose of filtering spectra from Ag targets, as
it combines a high photon transparency at 22.1 keV with a strong absorption below 10 keV. Therefore, in practical situations where B or Li are to be used as substrates, an additional AlN wafer should be employed as a filter, thus reducing the number of low energy photons being emitted from the tube.

7.6 Conclusion

The basic principles involved in the generation of photons in X-ray tubes operating at diagnostic energies, have been analysed. The dependence of the cross sections for the ionisation of the K-shell (by electron impact) and bremsstrahlung indicated that, just above the Ag K-edge, higher electron energies favour the emission of characteristic radiation over the generation of bremsstrahlung. The angular distribution
Chapter 7. X-Ray tube design studies using the EGS4/GOS code

Figure 7.24: Photon transmission through the 3 substrates considered. Data has been calculated using the XCOM program [Ber87].

of bremsstrahlung radiated has also been considered, showing anisotropies highly dependent on photon energy.

The EGS4/GOS code was then used in a series of simulations aimed at understanding the production of photons in Ag targets. The production of photons as a function of target thickness and the significance of electron scattering on the angular distribution of bremsstrahlung radiation was analysed. Underlying the previous discussion concerning the mechanisms involved, it has been shown that the characteristics of transmitted spectra (measured along the beam line) may have a strong dependence on target thickness. Indeed, it has been determined that with thinner targets, better fluorescence to bremsstrahlung ratios are attainable. This improvement is, however, obtained at the expense of efficiency. It has also been shown that in thin-target applications, a considerable amount of bremsstrahlung may be generated in the substrate. For this reason, low-Z materials like B or Li (rather than AlN),

---

Energy (keV)

Transmission (\%)

1 mm Li

1 mm B

680 \mu m AlN

0 5 10 15 20 25 30 35 40

0 20 40 60 80 100

0 5 10 15 20 25 30 35 40
where this interaction is less likely to take place, should be employed.

The applications discussed in this chapter are representative of a wide range of studies where the EGS4/GOS code may be used. In fact, the benchmarks carried out in chapter 6 have demonstrated that this package may be used accurately at energies of the order a few tens of keV. These regimes can be associated with several imaging systems. Issues like suitable filtering systems or novel configurations that further improve the fluorescence to bremsstrahlung ratios can now be addressed from the simulation point of view. Complete radiographic and/or tomographic systems may also be simulated, so helping to understand the ultimate performance of these systems. For these reasons, it is expected that, in the near future, the EGS4/GOS package will successfully be used in the field of radiation imaging.
Chapter 8

Conclusions and future work

The work carried out over the last three years, basically concerned the use of the EGS4 code system in imaging applications. Each chapter contains some concluding remarks where the relevance of the results presented in that chapter and future developments were discussed. This final chapter summarizes the overall research undertaken and suggests directions for further research.

Firstly, a one-sided imaging technique based on induced positron annihilation (PIPAR), was described. The yield of annihilation photons was experimentally determined, and showed a strong increase with the atomic number of the sample. This property makes the PIPAR approach suitable for substance identification. The results obtained with EGS4 were found to be in good agreement with experimental data, emphasizing the suitability of this code in the simulation of megavoltage systems. A few other applications like the inspection of civil engineering structures and nuclear verification were the addressed via the simulation approach.

The PIPAR technique may itself be the subject of further investigation, as more information can in principle be obtained at very little cost. In fact, if spectroscopy studies are to be carried out, Compton scattered photons and characteristic radiation from high-Z materials should be understood as extra measurable signals to be used in elemental identification. In this kind of study, EGS4 may be used as an important
Chapter 8. Conclusions and future work

development tool, as it realistically reproduces the relevant physical processes of PIPAR systems.

A direction that can also be further explored is the Doppler broadening of annihilation peaks. This technique is often used in studies aimed at probing electron momentum distributions in condensed media. In this way, it might be possible to extract some extra elemental information in PIPAR systems. The present version of EGS4 would not be suitable for these kind of studies, as the modelling of annihilation “at rest” is made under the assumption that atomic electrons are stationary particles. But this leaves room for improvements in the code. The physics beyond two-photon annihilation is well known and data concerning electron momentum distributions is available, so this is one of the areas where the EGS code could be improved. Then, more accurate models for positron annihilation, would certainly widen the range of applications of EGS4, as it would be suitable for systems where bound annihilation physics plays a major role.

The limitations identified in the EGS4 code system, when used to simulate low energy photon production, motivated the consideration of some new approaches. The approximations in the models for electron-atom inelastic collisions and bremsstrahlung emissions were debated, leading to some alternative schemes being suggested. These consisted of the treatment of electron inelastic collisions by means of a generalized oscillator strength (GOS) model where the atomic structure of target atoms is explicitly considered. The cross sections for low energy bremsstrahlung production were also evaluated, resulting in the development of a new scheme to model the angular distribution of newly created photons.

In the review carried out it was shown that electron inelastic mean free paths and stopping powers predicted from the GOS model were fairly accurate down to energies of the order of a few hundred eV. Treating atomic electrons as free particles was seen to be a crude approximation for energies below a few keV (especially in high Z materials), with the GOS formulation being an appealing solution. However, partial cross sections were roughly estimated from the GOS model, especially near
the shell threshold. This motivated the development of an improved version of the GOS model to deal with K-shell ionisation events. The new scheme combined the simplicity of the original GOS formulation with realistic K-shell ionisation cross sections. These are fundamental requirements for applications like the simulation of X-ray tubes operated at diagnostic energies.

The extension of this model to energies below 100 eV requires important improvements to be introduced. Indeed, more realistic models to deal with the excitations of valence electrons should be considered, as this represents the dominant inelastic process. The same happens if accurate modeling of L-shell ionisation events are to be considered. An approach similar to that used for the K-shell can be considered, but it might prove difficult to validate, since experimental data for L-shell ionisation cross sections are scarce.

Generally speaking, realistic modelling of low energy bremsstrahlung emissions can be obtained with EGS4 when the ICRU/NBS cross sections are in use. However, applications like thin-target bremsstrahlung production also require realistic schemes for the angular distribution of created photons. The current algorithms may fail in this respect, making it necessary to use a new scheme developed here, computationally inefficient. In the future, the development of improved numerical or analytical sampling techniques will result in a more efficient approach to the treatment of low energy bremsstrahlung emission.

The EGS4/GOS code, which basically incorporates the low energy extensions for electron inelastic collisions and bremsstrahlung emissions in EGS4, was then used to simulate the production low energy photons. Experimental data has shown that spectra from thin and thick target applications can be reproduced realistically using the new code, with accuracies of the order of 15% near the Kα peak. This major improvement in the simulation approach allowed some studies of photon production in X-ray tubes to be carried out. The analysis addressed aspects that affect the characteristics of transmission target X-ray spectra. From the practical point of view, the important conclusion is that higher ratios of fluorescence to bremsstrahlung
radiation are achieved with thinner targets, but such improvement is obtained at the expense of a dramatic fall in efficiency.

So far, only one application of the EGS4/GOS code has been considered, and so its physics is still to be explored fully. It will be particularly interesting to assess the relevance of the improved electron transport schemes in applications that deal directly with energy deposition in small volumes. Areas like solid state detectors and microdosimetry are amongst those to be considered, as experimental data are commonly available. Another "natural" application of this code is the simulation of X-ray tubes in reflection geometry. In this case the level of accuracy obtained in transmission tube simulations should be reproduced.

Realistic simulations of X-ray tubes operating at diagnostic energies are then expected to have enormous potential, with immediate benefits in the field of radiation imaging. Indeed, several aspects, like achieving the best configuration, the choice of suitable filtering systems, and even the complete simulation of an imaging system can be formulated with the EGS4/GOS code. The ability to reproduce complete imaging applications by means of Monte Carlo simulations, should result in a better understanding of the systems themselves. These advances are then expected to allow several optimisations to be carried out.

In broad terms, the use of Monte Carlo methods to simulate the transport of radiation should continue to expand amongst the physics community. Computing power increases exponentially and the fall in cost make these machines available to more and more people; extensive databases and more accurate particle transport algorithms are constantly being developed. These two aspects seem to benefit from each other, projecting the use of Monte Carlo simulations further and further. Realistic modelling at relatively low cost, makes it almost inevitable that Monte Carlo applications will be considered the first step in the establishment of new experiments.
Appendix A

Energy – momentum transfers in inelastic collisions

The linear momentum, $\vec{p}$, of an electron moving with a velocity $\vec{v}$ is defined as

$$\vec{p} = \gamma m_0 \vec{v}$$  \hspace{1cm} (A.1)

where $m_0$ denotes the particle mass and $\gamma^{-2} = 1 - \beta^2$, with $\beta$ the velocity $v$ in units of the speed of light ($c$). This relation can be used in classical and relativistic regimes [Gri87]. From this point, it is possible to obtain a relation between the particle's kinetic energy $E$ and its momentum, namely

$$(cp)^2 = E \left( E + 2m_0c^2 \right)$$ \hspace{1cm} (A.2)

from which $E$ can be determined as

$$E = \left[ m_0^2c^4 + (cp)^2 \right]^{1/2} - m_0c^2.$$ \hspace{1cm} (A.3)

Inelastic collisions are usually treated in terms of the scattering angle $\theta$ and energy loss $W$. If $\vec{p}$ and $E$ are the momentum and kinetic energy of the incident
electron, the corresponding quantities after the collision are $p'$ and $E' = E - W$, as shown in fig A.1. The conservation of momentum implies that

$$q^2 = p^2 + p'^2 - 2pp' \cos \theta. \quad (A.4)$$

In general, equation (A.4) is written in terms of the recoil energy $Q$ that is defined as the kinetic energy of a free electron with a linear momentum $\vec{q}$ [Fan 63]. Using the result from (A.2), momentum conservation leads to

$$Q \left( Q + 2m_0c^2 \right) = (cq)^2 = c^2 \left( p^2 + p'^2 - 2pp' \cos \theta \right) \quad (A.5)$$

Using equation (A.2) to replace momenta by the associated kinetic energies, (A.5) becomes

$$Q \left( Q + 2m_0c^2 \right) = E(E + 2E_0) + (E - W)(E - W + 2E_0)$$

$$-2 \left[ E(E + 2E_0)(E - W)(E - W + 2E_0) \right]^{1/2} \cos \theta \quad (A.6)$$
Appendix A. Energy – momentum transfers in inelastic collisions

with $E_0 = m_0 c^2$. Using (A.3), $Q$ can finally be determined as

$$Q = \left[ E_0^2 + E(E + 2E_0) + (E - W)(E - W + 2E_0) \right]$$

$$- 2 \left[ E(E + 2E_0)(E - W)(E - W + 2E_0) \right]^{1/2} \cos \theta}^{1/2} - E_0. \quad (A.7)$$

The minimum and maximum values of $Q$ — denoted $Q_-$ and $Q_+$ — correspond to scattering angles of $\theta = 0^\circ$ and $\theta = 180^\circ$, and can be calculated from the associated quantities $q_-$ and $q_+$. From (A.4) these last can be determined from

$$q_+^2 = (p + p')^2 \quad (A.8)$$

in which case $Q_+$ is given by

$$Q_+ = \sqrt{E_0^2 + c^2 (p + p')^2} - E_0. \quad (A.9)$$

In terms of initial and final kinetic energies (A.9) becomes [Sal 92]

$$Q_+ = \left\{ E_0^2 + \left[ E(E + 2E_0) \right]^{1/2} \mp \left[ (E - W)(E - W + 2E_0) \right]^{1/2} \right\}^{1/2} - E_0 \quad (A.10)$$

These lengthy equations become much easier to handle in the non-relativistic limit (where the kinetic energy is much smaller than the electron rest mass). Kinetic energy and momentum are related by means of

$$E = \frac{p^2}{2m_0} \quad (A.11)$$

and the equation relating the recoil energy $Q$ and the scattering angle $\theta$ is simply

$$Q = 2E - W + 2\sqrt{E(E - W)} \cos \theta. \quad (A.12)$$

The minimum value of $Q$ can, in this case, be calculated from [Lil 83]

$$Q_- = \left[ \sqrt{E - W} - \sqrt{E} \right]^2 \quad (A.13)$$
Appendix B

Semiconductor detectors

B.1 General description

Crystalline materials where atoms are arranged in a periodic lattice exhibit energy bands for electrons, a property that, itself, reflects the periodicity of the potential energy in the medium [Sze81]. The energy of electrons in the material is confined to one of these bands, which are separated by regions (or gaps) where electron states cannot exist. The upper bands are called the conduction band and correspond to states where electrons are free to migrate through the material. In contrast, electrons in the lower bands (the so called valence band) are strongly bound to the atomic structure and take part in the interatomic forces within the crystal. The energy separation between these two bands is called the band gap, \( E_g \), which is an important parameter in the characterisation of semiconductor materials [Sze81].

The fundamental electrical properties of solids are related to the number of electrons in the conduction band that, free to move through the crystal, will contribute to the electrical conductivity of the medium. In both insulators and semiconductors, the number of electrons in the solid is just enough to fill all available sites in the valence band while in metals the highest occupied energy level lies in the conduction band. For this reason, metals exhibit high electrical conductivities while in semicon-
Appendix B. Semiconductor detectors

In semiconductors and insulators, electrical conduction becomes significant only in the presence of (external) excitation processes that are able to transfer electrons from the valence to the conduction band. The band gaps in insulators are usually of the order of 5 eV, whereas for semiconductors the band gap is considerably less: 1.115 eV in silicon (Si) and 0.665 eV in germanium (Ge), at 300K [Kno89].

Electrical conduction in semiconductors depends not only on the presence of electrons in the conduction band, but also on vacancies created by excitation processes. Conductivity can be enhanced through the addition of dopants. In fact, the transition of electrons to the conduction band due, for example, to thermal excitation creates vacancies in the valence band (so called holes). These, representing a net positive charge, will also move under an electric field and their motion contributes to the total electrical conductivity [Kno89]. In this way, any excess of charge carriers (electrons or holes) results in an enhancement in the materials' electrical conductivity. In the case of tetravalent elements like Si and Ge, conductivity may be affected by doping with pentavalent elements like phosphorus (P) or trivalent elements like boron (B), that increase the concentration of electrons or holes, respectively. Materials where receptor impurities dominate are usually referred to as p-type, while materials with an excess of electrons due to donor impurities are usually classified as n-type. A pure material, where electron and hole concentrations are the same, is briefly referred to as intrinsic.

The properties created near the junction between n- and p-type materials are of great importance not only for radiation detectors but also, more generally, in modern electronics [Sze81]. The gradient in the concentration of charge carriers promotes the diffusion of holes from the p to the n side of the junction, and of electrons in the opposite direction. An equilibrium situation is eventually reached, where the electric field created by the charge build up compensates for the tendency of further diffusion. The region over which the charge imbalance exists is called the depletion region, and its extension over both sides of the junction is strongly determined by the initial doping profiles [Sze81]. This depletion region can act as a radiation detector.
where electron-hole pairs created due to the absorption of incoming radiation migrate under the influence of the spontaneous contact potential formed across the junction.

In terms of its application in a radiation detector, the properties of a $p-n$ junction can be improved further when reverse biased. Indeed, if the device is polarised in a way such that the voltage applied to the $n-$side is higher than the one applied to the $p-$side, the size of the depletion region is increased, resulting in a higher sensitive volume [Kno89]. Moreover, since the resistivity of the depletion region is higher than that of the $p-$ and $n-$type materials, virtually all the voltage applied to the crystal appears across it. This improves the collection of electron-hole pairs that were, otherwise, more exposed to trapping and recombination phenomena [Kno89]. In this condition the depletion region performs much as a gas detector. The charges created by the absorption of radiation move under the influence of an applied electric field. In the case of semiconductor detectors, electron and holes often have similar mobilities and they can both contribute to the measured signal.

Semiconductor based radiation detectors combine reasonable X-ray detection efficiency with good energy resolution. The relatively small energy required to create a charged carrier pair in a semiconductor ($\approx 3$ eV, against $\approx 20$ eV in gas detectors) results in good statistical accuracy, while their solid densities make them more effective than gases at stopping photons. Some of the major limitations of these devices are known to be their small volumes and the need for cooling systems, so that thermal excitation can be reduced [Kno89].

The width, $\sigma^2$, of a typical peak in the spectrum due to the detection of monoenergetic radiation can be written as [Kno89]

$$\sigma^2 = \sigma_D^2 + \sigma_X^2 + \sigma_E^2$$  \hspace{1cm} (B.1)

where $\sigma_X^2$ and $\sigma_E^2$ are the noise terms associated with incomplete charge collection and the effects of the electronic components used, respectively. At a given energy, $E$, the inherent statistical fluctuation in the creation of electron-hole pairs, $\sigma_D^2$, is
usually written as [Kno 89]

$$\sigma_D^2 = F \varepsilon E$$  \hspace{1cm} (B.2)

where $F$ is the Fano factor and $\varepsilon$ the energy necessary to create an electron-hole pair.

The performance of the semiconductor detectors that were used in this thesis is analysed (from the user point of view) in the next two sections. Detailed descriptions of semiconductor devices and their application in the detection of ionising radiations can be found, respectively, in [Sze 81] and [Kno 89].

## B.2 Hyper-pure Germanium detector

The closed-ended coaxial geometry high-purity Germanium (HPGe) detector used in the measurement of X-ray tube spectra is schematically presented in fig. B.1. This detector comprises a Ge disk 2.48 cm in diameter and $\approx 3$ mm thick, where the absorption of radiation takes place. A $\approx 0.3$ mm beryllium (Be) window protects the crystal from exposure to visible light. The system is housed in a liquid nitrogen (LN$_2$) cooled cryostat.

Although less efficient than scintillation detectors like NaI or BGO [Kno 89], the configuration presented in fig. B.1 is remarkably effective at detecting photons with energies below 50 keV. The total linear attenuation coefficient for the absorption of radiation in Ge was evaluated using the XCOM database [Ber 87] and the result is plotted in fig B.2. In the light of this data it can be seen that at 50 keV, 99.5% of the incident photons should interact and (most likely) be absorbed, in the detector. For this reason, it is acceptable to consider that photons with energies below 50 keV are fully absorbed in the HPGe detector presented in fig. B.1. On the other hand, at energies of the order of 8 keV more than 95% of the photons are transmitted through the Be window. Thus, for practical considerations, the Ge detector presented in fig. B.1, may be considered to have efficiency of unity for
Appendix B. Semiconductor detectors

B.2.1 Operating characteristics

According to the manufacturer's datasheets, the nitrogen cooled HPGe detector should be operated at bias voltage of 1000 V. This parameter was the subject of further analysis but no significant changes in the performance of the system were observed for voltages in range 950V to 1000V. Below 950 V no pulses were obtained from the detector output, which indicates that no charge can be collected in these regimes. At a bias voltage of 1000 V, the operating current was found to be of the order of 0.95 nA.

The preamplifier output was passed through an Ortec-570 shaping amplifier and so to a Nucleus Inc. PCAII multi-channel analyser (MCA). The time constant of the shaping amplifier was optimised so that the best possible energy resolution
could be achieved. The results of this study are shown in fig. B.3, where is clear that the best performance is obtained for a time constant of $10 \, \mu s$. The energy resolution was calculated by means of gaussian fits to the observed peaks, using the Levenberg-Marquardt method formulated in [Pre92] to minimize the $\chi^2$ of the fit (no background subtractions were performed). An energy spectrum obtained under these optimised conditions (operating voltage $1000\,V$ and shaping time $10 \, \mu s$) is shown in fig. B.4, where peaks corresponding to characteristic radiation from different elements are shown.

The need to convolve simulated data with the detector response requires this function to be fully specified, preferably by means of analytical expressions. It was discussed in section B.2 that for energies below $50 \, \text{keV}$ the efficiency of the
Figure B.3: Performance of the HPGe-based detection system for different shaping times of the CR-RC filter.

The HPGe detector may be considered to be 100%. No detailed information concerning the other noise sources was available so, from eq. (B.1), an expression of the form

$$\sigma^2 = mE + b$$

(B.3)

was used to mimic the dependence of the system’s noise response with energy. The constants $m$ and $b$ were calculated by means of a linear fit to experimental data. The $FWHM$ of the detector was then found to vary with energy according to

$$(FWHM)^2 = (2.35)^2 (1.28 + 0.29E) \times 10^{-2},$$

(B.4)

with both $FWHM$ and $E$ expressed in units of keV. The data points used in this fit, as well as experimental and calculated energy resolutions, are presented numerically in table B.1. Although eq. (B.3) represents a rather simplistic version of eq. (B.1), the difference between experimental and predicted values does not exceed 6%. This
Figure B.4: Photon spectrum obtained with the HPGe detectors in use.

makes eq. (B.4) suitable for the determination of the statistical fluctuations in the HPGe-based detection system.

<table>
<thead>
<tr>
<th>Element</th>
<th>Characteristic line</th>
<th>Energy (keV)</th>
<th>Resolution(%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rb</td>
<td>K(_\alpha)</td>
<td>13.4</td>
<td>4.18</td>
</tr>
<tr>
<td>Ag</td>
<td>K(_\alpha)</td>
<td>22.1</td>
<td>2.80</td>
</tr>
<tr>
<td>Ba</td>
<td>K(_\alpha)</td>
<td>32.2</td>
<td>2.45</td>
</tr>
</tbody>
</table>

Table B.1: Energy resolution of the HPGe-based detection system. Calculated values were determined from eq. (B.4).

B.3 Lithium-drifted silicon detector

The configuration of the silicon detector used in some of the experiments carried out, is shown in fig B.5. This comprises a p-i-n diode where the compensated region, \(i\), is
established by means of an ion drifting process. In the specific case of this detector, lithium (Li) ions have been used, and this kind of configuration is widely known as Si(Li).

![Diagram of Si(Li) detector](image)

Figure B.5: Schematic representation of the Si(Li) used in the measurements.

To a good approximation, the Si(Li) detector used comprises a 4.5 mm thick block of Si with a 0.2 mm thick layer of aluminium (Al) in front of it. The detection efficiency of this kind of detector is shown in fig B.6. For energies below $\approx 22$ keV the detection efficiency is mainly regulated by the transmission through the Al window, while above this value, it is the absorption in the silicon crystal that determines the performance of the detector.

### B.3.1 Operating characteristics

The Si(Li) detector and the preamplifier's FET were both kept at a temperature of 77 K, using liquid nitrogen. The system was operated at a bias voltage of 400V and,
in these conditions, the current through the crystal was observed to be of the order of 1 nA. Signals from the preamplifier were formatted in a Link Systems-2010 pulse processor, and then fed into a Nucleus Inc. PCAII multi-channel analyser (MCA). A photon spectrum obtained from the MCA, using the configuration just described is presented in fig. B.7.

As with the HPGe detector, the statistical fluctuations in this system were associated with the incident photon energy by means of a linear relationship. Using the procedure described in section B.2.1, this relation was now found to be

\[(FWMH)^2 = (2.35)^2(-3.9 + 0.46E) \times 10^{-2},\]  \hspace{1cm} (B.5)

with both \(FWMH\) and \(E\) expressed in keV. The data points used in the determination of eq. (B.5) presented in table B.2, show a good agreement between measured
Appendix B. Semiconductor detectors

Figure B.7: Photon spectrum recorded using with the Si(Li) detector.

Table B.2: Energy resolution of the Si(Li) detection system. Calculated values were determined using eq. (B.5).
Bibliography


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