Electron Impact Ionization in EGSnrc

by

Leila Lukhumaidze

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Department of Physics

Carleton University

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Abstract

An accurate knowledge of the x-ray spectra from an x-ray tube enables system designers to predict patient dose accurately and develop better hardware and software systems to reduce patient dose. Also many radiological physics problems that can be solved by Monte Carlo simulation methods require an x-ray spectrum as input data. For these reasons it is important to assess the reliability of different cross sections implemented in EGSnrc.

The Monte Carlo calculations of x-ray spectra generated by 5-25 keV and 90-120 keV electron impact on thick targets of tungsten, molybdenum and titanium are done using the general-purpose EGSnrc BEAMnrc code with two different Electron Impact Ionization cross sections, one developed and implemented by Kawrakow¹ and another developed by Salvat² and referred to as the Penelope cross section.

The resulting spectra are compared with the corresponding experimentally measured x-ray spectra by Tian et. al³ and PTB⁴. The MC calculated low energy characteristic x-ray peaks generated using the Penelope cross section option and experimental ones are close to each other but still not satisfactory, whereas Kawrakow's cross section underestimates them. To assess the contribution from characteristic peaks, air kerma (kerma is a sum of initial kinetic energy of all ionizing particles liberated by uncharged ionising particles in a material of mass dm , and stands for kinetic energy released per unit mass) is calculated for each x-ray spectrum with and without the characteristic peaks. The contribution from high energy peaks is very small as expected, since the total fluence in these peaks is small compared to the fluence of bremsstrahlung photons. From the results it is clear that more theoretical research on EII cross sections is required to predict characteristic lines accurately.

Contents

1	Introduction	1
1.1	Overview	1
1.2	X-ray production mechanism, bremsstrahlung	2
1.3	X-ray production mechanism, characteristic radiation	4
1.4	Empirical parametrization of x-ray spectra	7
1.5	Semi-empirical model	7
1.6	Monte Carlo calculations	8
1.7	Discrepancies among x-ray spectra from different models	10
1.8	Purpose of current work	16
2	EGSnrc BEAM code	18
2.1	General overview of the code	18
3	Benchmark experimental spectra	21
3.1	Low energy experimental spectra of Tian et al.	21
3.2	High energy experimental spectra from tungsten target	23
3.3	Mammography energy x-ray spectra	26
4	Monte Carlo Simulation Methods	28
4.1	Monte Carlo simulations for low energy x-ray emmision	28

4.2	Monte Carlo simulations for high energy x-ray emmision from tungsten target	30
4.3	Monte Carlo simulations for mammography energy x-ray spectra	31
5	Results and discussion	32
5.1	Penelope Kawrakow peak ratios	32
5.2	Kerma	53
5.3	Characteristic peak ratios by different authors	58
6	Conclusions	61
	References	63

List of Figures

1.1	Bremsstrahlung x-ray production	3
1.2	Characteristic x-ray produciton	5
1.3	EII mechanism	6
1.4	Spectra from W target, TG 195	12
1.5	Spectra from Mo target, TG 195	13
1.6	Characteristic L lines in tungsten, EII	14
1.7	Characteristic K lines in tungsten, EII	15
2.1	The steps in the BEAMnrc system	20
3.1	Tian et. al experimental setup	22
3.2	The PTB experimental setup	25
3.3	Experimental set up for measuring x-ray spectra by Fewell	27
5.1	Spectra from a W target, Tian et. al	34
5.2	Spectra from a Mo target, Tian et. al	35
5.3	Spectra from a Ti target, Tian et. al	36
5.4	Characteristic peak ratios for W	37
5.5	Characteristic peak ratios for Mo	38
5.6	Characteristic peak ratios for Ti	39
5.7	Characteristic peak normalization	41

5.8	Normalized peak ratio for a W target	42
5.9	Normalized peak ratio for a Mo target	43
5.10	Normalized peak ratio for a Ti target	44
5.11	X-ray spectra from W(90keV), PTB	46
5.12	X-ray spectra from W(100keV), PTB	47
5.13	X-ray spectra from W(120keV), PTB	48
5.14	Normalized peak ratio for a W target, PTB	49
5.15	X-ray spectra from a W target, Fewell et.al	51
5.16	X-ray spectra from a Mo target, Fewell et.al	52
5.17	Normalized kerma for W, Mo and Ti.	55
5.18	Normalized kerma for a W target. K, L lines	56
5.19	Normalized kerma for a W target. K lines	57

Chapter 1

Introduction

1.1 Overview

Monte Carlo simulation is used to address a broad range of questions about the propagation of radiation in materials. It is the most suitable theoretical tool for taking into account all aspects of photon and electron transport through a heterogeneous medium. An example of it is the EGSnrc^{5,6,7} code system, which is well-suited for medical physics purposes, such as imaging a patient's anatomy using x-rays or delivering a prescribed radiation dose to a tumour while sparing healthy tissue. The EGSnrc code simulates Electron Impact Ionization (EII) using two different cross sections, one developed and implemented by Kawrakow¹ in 2008, and another developed by Salvat² and referred to as the Penelope cross section. Within the EGSnrc code system the Penelope cross section for EII was implemented in the EGSnrc code system by Mainegra Hing in 2010. These cross sections give different characteristic peak intensities in x-ray spectra, even for the same tube voltages and target materials. Since the EGSnrc code system is trusted by researchers worldwide for simulation accuracy and speed, it is worthwhile to assess the reliability of different cross sections implemented in it. The Monte Carlo calculated x-ray spectra generated by the impact of 5-120 keV electrons on tungsten, molybdenum and titanium targets with two different EII cross sections, one by Kawrakow and another by Penelope, are compared with the corresponding experimen-

tally measured x-ray spectra by Tian et. al³ and PTB⁴. The comparisons described in (Chapter 5) reveal that, compared to the Kawrakow cross sections, the Penelope cross sections yield a better, but not excellent agreement with the experimental data. The current study concludes by recommending the use of Penelope cross sections for EII in the EGSnrc code system, but for an accurate prediction of characteristic lines more theoretical research is required on EII cross sections.

1.2 X-ray production mechanism, bremsstrahlung

An accurate knowledge of the output x-ray spectra of an x-ray tube is essential in many areas of study. It forms the basis of almost all image quality simulations. It enables system designers to predict patient dose more accurately and hence aid in the development of better hardware and software systems to reduce patient dose. Many radiological physics problems that can be solved by Monte Carlo simulation methods require an x-ray spectrum as input data.

The impact of kilovolt electrons on a solid target generates an x-ray spectrum of photons, which consists of characteristic peaks superimposed on a continuous background. The discrete spectrum consists of characteristic x-rays, produced by electron impact ionization or bremsstrahlung photon absorption and scattering, whereas the continuous spectrum consists of bremsstrahlung photons produced by primary or secondary electrons. Bremsstrahlung photons can have any energies less than or equal to the incident electron energies.

When a charged particle is accelerated or decelerated, radiation is emitted. In matter, when an electron is attracted toward the positively charged nucleus (see figure 1.1), slows down and its path is deflected. Energy lost is emitted as an x-ray photon, which can have energy between zero and the energy of incoming electron.

This process is called bremsstrahlung from the German word braking radiation.

Figure 1.1: Schematic diagram of bremsstrahlung x-ray production. After deceleration an electron emits an x-ray photon in the field of positively charged nucleus.

1.3 X-ray production mechanism, characteristic radiation

An incident electron may create a vacancy in one of the inner shells which is filled by an outer shell electron, (see figure 1.2). In making such transitions, electrons emit photons of x-radiation with discrete energies given by the differences in energy states at the beginning and the end of the transition. The electron shells are labelled K, L, M, N, O, P and Q or $n = 1, 2, 3, 4, 5, 6$, and 7 going from the innermost shell outwards. The x-rays produced by transitions from the $n = 2$ to $n = 1$ levels are called K_α x-rays, and those transitions from the $n = 3, 4$ to $n = 1$ levels are called K_β , K_γ x-rays respectively. Each electron shell has sub-shells, for example the x-rays produced by transitions from the L_{III} (L sub-shell), L_{II} , M_{III} (M sub-shell) and $N_{II}N_{III}$ (N sub-shells) to K level are called $K_{\alpha 1}$, $K_{\alpha 2}$, $K_{\beta 1}$ and $K_{\beta 2}$ respectively.

Transitions to the $n=2$ or L-shell are designated as L x-rays (from the $n = 3$ to $n = 2$ is L_α , from the $n = 4$ to $n = 2$ is L_β , etc.). A transition from M_I (M sub-shell) to L_{III} (L sub-shell) is called L_1 . Because such x rays are distinctive for the particular element and transition, they are called characteristic x rays.

Electron Impact Ionization can be understood in the following way: first an electron creates a bremsstrahlung photon, which undergoes a photo-electric event with an inner shell electron in the same atom, the photo-electron escapes from the atom, leaving a vacancy in one of the inner shells, and this resulting vacancy leads to a fluorescence photon or an auger electron (see figure 1.3). If the bremsstrahlung photon escapes the atom and undergoes a photo-electric event in a different atom resulting in a fluorescence photon, then those characteristic lines are not from EII.

Figure 1.2: Schematic diagram of characteristic x-ray production by Electron Impact Ionization. A photon of x-radiation is emitted as an outer shell electron fills a vacancy in one of the inner shells.

Figure 1.3: Interpretation of characteristic x-ray production by Electron Impact Ionization. A vacancy created by a photo-electric event is filled by an outer shell electron, resulting in a fluorescence photon or auger electron.

1.4 Empirical parametrization of x-ray spectra

Determination of x-ray spectra can be divided into three main approaches: Empirical, semi-empirical and Monte Carlo calculations.

Empirical parametrizations use measured data to predict x-ray spectra. In 1932 Silberstein⁸ deduced x-ray spectra from attenuation data. Using Fewell's⁹ measured spectra, Boone et al.¹⁰ developed computer parametrizations using interpolating polynomials to generate x-ray spectra in the mammographic energy range from 18 kV to 40 kV from molybdenum (MASMIP), rhodium (RASMIP) and tungsten (TASMIP) targets. But these models are not able to calculate the x-ray spectra for different combinations of targets, filters and anode angles.

1.5 Semi-empirical model

Semi-empirical models calculate x-ray spectra using parameters from measured spectra in theoretical formulas to give good agreement with experimental data.

XCOMP is a computer program which calculates x-ray spectra, kerma, and half value layer (HVL) (half value layer is the thickness of a material, required to reduce the air kerma of an x-ray to half its original value) for eight different absorbing materials Al, Be, Cu, Pb, Sn, PMMA, oil and water with different thicknesses such as for various tube anode angle, kV and distance according to a model by Birch and Marshal¹¹.

Tucker et al's.¹² model is a semi-empirical model which generates x-ray spectra from a molybdenum target, taking into account the fact that bremsstrahlung and char-

acteristic x-rays are produced at different depths in the target.

1.6 Monte Carlo calculations

When high-energy electrons and photons hit matter, they travel through the material and interact with atoms and their nuclei in many different ways which can be predicted by physics models.

In Monte Carlo calculations all particles are tracked and all interactions are simulated. Interaction rates and locations, secondary particle production, follow-on energies and angular deflections are calculated by statistical probability distributions derived from theoretical cross sections. Monte Carlo simulation is the most suitable theoretical tool for taking into account all aspects of photon and electron transport through a heterogeneous medium and calculating x-ray spectra, as long as the geometry is well known. Examples of such codes are the EGSnrc^{5,6,7}, Penelope¹³ and Geant^{14,15} code systems.

The EGS (Electron Gamma Shower)^{5,6,7} code system was developed to design detectors and do radiation protection calculations for high energy physics by two physicists: W. Ralph Nelson at Stanford Linear Accelerator Center(SLAC), and Richard Ford at the Hanson High Energy Physics Laboratory at Stanford University. Later they combined their work to produce the first complete version of EGS¹⁶ in 1978.

EGS3 the Electron Gamma Shower code system was designed to simulate the travel of electrons and photons through bulk media with energies ranging from an MeV to several thousand GeV, using knowledge of the probability distributions which govern the individual interactions of electrons and photons in materials to simulate the random trajectories of individual particles.

From the early 1980s several groups started developing EGS which lead to the current version of the code. The SLAC Radiation Physics Department began working with their counterpart at KEK in Japan(Hideo Hirayama), focusing on the design of future high-energy accelerators.

A low-energy benchmarking project, led by Dave Rogers started at the National Research Council of Canada (NRC) which adopted EGS as a theoretical tool in ionizing radiation standards to utilize it for radiotherapy and low-energy radiation protection (diagnostic x-ray). However applying EGS to solve low-energy problems had limitations, since radiotherapy treatments were changing from use of relatively low-energy Cobalt-60 gamma rays with energies around 1.25 MeV to the radiation produced by higher energy electron linear accelerators (4 - 50 MeV) and medical physicists needed a tool to predict the correct treatment dose.

For this reason a collaboration was formed among SLAC, KEK and NRCC which lead to the release of EGS4⁵ in 1985(written in Mortran3). An EGS4 extension, developed by Alex Bielajew and Dave Rogers, called the Parameter Reduced Electron Step Transport Algorithm (PRESTA)¹⁷, more accurately simulated low-energy electron transport and uses Monte Carlo simulations for coupled electron-photon transport with energies ranging from a few keV to several TeV in an arbitrary geometry.

The EGSnrc system was derived from EGS4 and contains many improvements in electron transport. Kawrakow and Bielajew¹⁸ developed a new electron transport algorithm called PRESTA- II. In addition to these advances, Kawrakow modelled Electron Impact Ionization and improved electron transport algorithm in EGS, which allows the code to calculate ion chamber response at the 0.1% level relative to its own cross sections¹⁹.

For a complete application of the original EGSnrc system, a user had to write a

user code which consists of a scoring routine called `ausgab` and two subroutines that provide EGSnrc with geometrical information via a well defined interface.

PENELOPE¹³ is another general purpose Monte Carlo code, which simulates coupled electron-photon transport with energies ranging from 50 eV to 1 GeV.

1.7 Discrepancies among x-ray spectra from different models

The x-ray spectra, calculated using different models do not have the same bremsstrahlung x-ray energy distribution and characteristic x-ray intensity, even for the same target angle and tube voltage. All these methods need to be validated by comparing to measured spectra. Usually the validation of Monte Carlo calculation codes is performed by doing simulations which reproduce an actual experiment and comparing the results to the experimental data. Ay et al²⁰. have compared x-ray spectra generated using different computational models to the measured spectra in diagnostic radiology and mammography.

The report of the AAPM's Task Group 195 provides a reference for benchmarking Monte Carlo simulations for four Monte Carlo codes against each other in different simulation scenarios²¹. Figure 1.4 shows a comparison of IPEM report 78 and Monte Carlo simulated photon fluence spectra per incident electron from a tungsten target irradiated by 100 keV electrons²¹. Differences among energy-discriminated fluences were around 10-20%, except for the very low-energy bins below approximately 12 keV for the W spectrum. Monte Carlo simulations were performed in vacuum, whereas IPEM x-ray spectra are in air. The MCNP code underestimates L characteristic x-ray line production and overestimates K_{β} characteristic line production.

Figure 1.5 shows a comparison of IPEM Report 78 and Monte Carlo simulated photon fluence spectra per incident electron from a molybdenum target irradiated by 30 keV electrons. As reported in TG 195's report, differences among simulated x-ray spectra were around 10-20 percent, except for the very low energies, less than about 3 keV. Monte Carlo simulations were done in vacuum whereas IPEM x-ray spectra are in air with some inherent filtration, which explains the difference among simulated and IPEM spectra. The discrepancies among the characteristic lines are mostly due to the different estimates in characteristic emission, as the calculations are sensitive to the electron impact ionization cross section.

Figures 1.6 and 1.7 show the importance of Electron Impact Ionization in x-ray spectra calculations using EGSnrc calculations to be described below.

Figure 1.6 shows a comparison of characteristic L lines of the spectrum obtained from tungsten irradiated by 100 keV electrons, calculated using two EII options (Kawrakow, Penelope) and EII off (characteristic photons are only from the photoelectric effect). For these L lines 84%, 90%, 88% and 88% of characteristic x-ray photons are generated with EII when using Kawrakow cross sections, whereas only 16%, 10%, 12% and 12% of characteristic x-ray photons are from photoelectric effects in L_1 , L_α , L_β and L_γ lines respectively. Using the Penelope cross sections 88%, 93%, 91% and 90% of characteristic x-ray photons are from EII and 12%, 7%, 9% and 10% from photoelectric effects.

Figure 1.7 shows the same comparison as figure 1.6 but for the characteristic K lines. Only 23%, 21%, 24% and 38% of characteristic x-ray photons are generated with EII by Kawrakow cross sections, whereas 77%, 79%, 76% and 62% of characteristic x-ray photons are from photoelectric effects in $K_{\alpha 2}$, $K_{\alpha 1}$, $K_{\beta 1}$ and $K_{\beta 2}$ lines respectively, and 25%, 28%, 28% and 44% of characteristic x-ray photons are from EII by Penelope and 75%, 72%, 72% and 56% from photoelectric effects.

Figure 1.4: Comparison among IPEM report 78's (theoretical x-ray spectra obtained from Spectrum Processor of the Institute of Physics and Engineering in Medicine's Report 78) photon fluence spectrum per initial electron for 100 keV electrons on a W target and various Monte Carlo simulations reported in AAPM's TG 195. The IPEM data included inherent filtration and air, whereas the Monte Carlo calculations have no filtration and are in vacuum.

Figure 1.5: Comparison among IPEM report 78's(theoretical x-ray spectra obtained from Spectrum Processor of the Institute of Physics and Engineering in Medicine's Report 78) photon fluence spectrum per initial electron for 30 keV electrons on a Mo target and various Monte Carlo simulations reported in AAPM's TG 195. The IPEM data included inherent filtration and air, whereas the Monte Carlo calculations have no filtration and are in vacuum.

Figure 1.6: X-ray spectrum from tungsten target at 45° irradiated by 100 keV electrons showing a comparison among EII off and on with Kawrakow or Penelope options.

Figure 1.7: X-ray spectrum from tungsten target at 45° irradiated by 100 keV electrons showing a comparison among EII off and on with Kawrakow or Penelope options.

1.8 Purpose of current work

Ay et. al.²⁰ showed that there is no significant discrepancy in the calculation of absorbed dose when using different computational models for generating x-ray spectra. Nevertheless given the limited flexibility of the empirical and semi-empirical models, the spectra obtained through Monte Carlo simulation offer several advantages by providing detailed information about the interactions in the target and filters, which is relevant for the design of new target and filter combinations and optimization of radiological imaging protocols.

The aim of this study is to assess the reliability of different cross sections implemented in EGSnrc. For this reason x-ray spectra emitted from different target materials (W, MO and Ti) are calculated using the general-purpose EGSnrc BEAM code with two different Electron Impact Ionization cross sections, one developed by Kawrakow and another developed by Salvat and referred to as the Penelope cross section. They are compared to published experimental data in which experimental conditions were sufficiently described.

In the EGSnrc BEAMnrc code, the Penelope option for the EII cross section combines the relativistic plane-wave Born approximation (PWBA) with a semirelativistic version of the distorted-wave Born approximation (DWBA)², whereas the EII cross section derived by Kawrakow and implemented in EGSnrc BEAM code calculates EII cross sections using a PWBA¹. The PWBA accurately describes the ionization process only for electrons and positrons with kinetic energy E higher than 30 times the ionization energy of the active shell. In the relativistic version of the PWBA the projectile wave functions are approximated by Dirac plane waves, and the distortion caused by the field of the target atom is neglected. A more accurate theoretical description of triple differential cross sections is obtained from the relativistic distorted-wave Born

approximation, which accounts for the effects of distortion and electron exchange. In the limit where the distorting potential vanishes, the distorted waves reduce to plane waves and, therefore, the DWBA reduces to the PWBA. Thus, in principle the EII cross sections used in the Penelope option are more accurate. The goal of this work is to see if this is correct and how accurately the cross sections reproduce physical reality.

Chapter 2

EGSnrc BEAM code

2.1 General overview of the code

The BEAM code²² is a general purpose Monte Carlo transport package which is capable of simulating the radiation beams from any radiotherapy source, such as low-energy x-rays, ^{60}Co units and electrons and photon beams from accelerators.

BEAMnrc is based on the EGSnrc Monte Carlo system for simulating radiation transport. The BEAMnrc code produces a phase-space output file, which includes the energy, position, direction, charge and history tag for each particle at step in the model. The phase-space file can be re-used by the BEAMnrc code as an input file to the patient dose computation algorithm.

The BEAMnrc code consists of a series of component modules, each of which operate independently of the other component modules. Each component module(CM) occupies a slab perpendicular to the beam axis, and deals with a specific class of geometric shapes within the horizontal band. This allows the user to simulate different designs of machines.

Modelling a particular machine starts by selecting the required component modules in order, and assigning unique names so that each particular CM can be used more than

once. After the machine is specified, a script pulls together all the relevant source codes and compiles the code. Figure 2.1 shows the overall structure of the BEAMnrc system and the steps involved in using it.

In the model of a machine there can be scoring planes at the back plane of an arbitrary number of component modules. These are perpendicular to the z-axis which is taken as the beam axis. Phase-space data can be created at each plane. Besides using standard source routines such as pencil beam, point source, circular or rectangular beams it is possible to use a phase-space data file as an input in the simulation. In this way it is possible to simulate the head of an accelerator down to the applicator and then reuse the same data with a variety of different applicators in place.

An in-house program BEAMDP(BEAM Data Processor), which is developed for the OMEGA (Ottawa Madison Electron Gamma Algorithm) project can be used to analyse phase-space files generated using the BEAMnrc code and to derive data such as spectral distribution of particles, scored on the scoring planes by the BEAMnrc code.

As mentioned above, the BEAMnrc code is written as a series of independent component modules, contained between two planes which are perpendicular to the z-axis (beam axis). For each component module all the physical dimensions and materials are set by the user. The outer boundary for each CM is constant and set separately, any gaps between them are filled with air or other default medium.

Two component modules: SLABS and XTUBE are used in the current study. The component module SLABS models parallel slabs in the x-y plane. The SLABS can have different materials and thickness and their outer boundary is square.

The second CM XTUBE used in this study models an x-ray tube as the photon source. It simulates an x-ray target in air or vacuum. The target angle is fixed by the target surface and z-axis, and can be chosen by a user. The user has options among

incident rectangular or circular electron beams coming in normal to the z-axis, which allows the simulation of an x-ray tube.

Figure 2.1: The steps in the BEAMnrc code²², it starts by defining an ordered set of component modules. In the next step, all source codes are gathered and the code is compiled. In the simulation part, the BEAMnrc reads cross section data and input file, which contains information about geometry, incident beam, output and simulation control parameters. From ref²², used with permission.

Chapter 3

Benchmark experimental spectra

3.1 Low energy experimental spectra of Tian et al.

Measured spectra provide the gold standard for comparing computer-generated spectra. A major problem is knowing the actual geometric set up since "inherent filtration" is a vague term and surface roughness and deprecation from the target on window all can have significant effects. Three sets of measured spectra are used in this work for comparing Monte Carlo generated x-ray spectra.

The first set of benchmarks are published measurements by Tian et. al³ of bremsstrahlung spectra generated by 5-25 keV electron impact on thick targets of titanium, molybdenum and tungsten. The details of the experimental set-up are as follows:

The mono-energetic electron beams from near threshold to several tens of keV are provided by an electron gun and adjusted in accordance with x-ray counting rates. The electron beam is collected by a deep Faraday cup and then is fed into an digital current integrator. The digital current integrator has an accuracy of better than 1 % for the charge measurements. The direction of the incident electron beam is perpendicular to the direction of a Si(Li) detector (see figure 3.1), and the target is tilted 45° with respect to the direction of the incident electron beam. The x-ray detector is placed horizontally, so the x-ray emission angle is 90° with respect to the incident electron beam direction.

The distance from the detector to the target is 6.124 cm and the measurements are done in vacuum.

Figure 3.1: Schematic diagram of the experimental setup by Tian et.al used in the measurements of low energy x-ray spectra³. Measurements were done in vacuum.

The x-rays emitted from the thick targets are recorded by a Si(Li) detector, with the intrinsic detection efficiency of 5 %. The parameters of the detector are 12.7 μm Be-window thickness, 38.6 $\mu\text{g}/\text{cm}^2$ Au contact layer, 0.1 μm Si dead-layer and 4.21 mm thick detector sensitive layer.

3.2 High energy experimental spectra from tungsten target

The published experimental measurements by Ankerhold et al.⁴ from the PTB are a second set of experimental data used in the present work, to compare to Monte Carlo calculated data. The measurements for the ISO (The International Organisation for Standardization) photon reference radiations labelled N-10 to N-120 are performed at two different x-ray units of the Individual Dosimetry Section of the PTB German Standards lab in Braunschweig. A 120 kV facility with a type MB 121/1 tube from the firm AEG is used for the radiation qualities labelled N-10 to N-80, and a 420 kV facility with a type MB 420/1 AEG tube is used for the radiation qualities labelled N-100 to N-120. Both x ray tubes have a tungsten anode with a 20° angle. A PTW monitor chamber (model No 786) is installed behind both x ray tubes. The chamber has three Kapton foils, two of which serve as entrance and exit windows and the third one is a central electrode. So the inherent filtration of the 120 kV x-ray facility is a 1 mm thick Be window of the x-ray tube and a 250 μm Kapton monitor chamber. The inherent filtration of the 420 kV facility is given by the window of the x-ray tube of 7 mm Be and a 250 μm Kapton monitor chamber.

The pulse height spectra are measured with a commercial ORTEC Ge spectrometer, which has a planar high purity Ge crystal and 250 μm thick Be entrance window. A

schematic view of the experimental set-up for the pulse height spectra measurements is shown in figure 3.2. Before and behind the monitor there is a diaphragm pair, which collimates the x-ray beam to a diameter of 3.5 cm at a 1 m distance from the focus and of 8.8 cm at 2.5 m distance. The spectrometer crystal is surrounded by a lead shield and in front of the Ge crystal, a lead collimator with an aperture is installed, which reduces the number of photons entering the detector and eliminates edge effects and the influence of stray radiation. The thickness of the lead cylinder and the thickness of the front of the lead collimator allows radiation to only pass through the aperture and not through the walls.

This experimental set-up detects only those photons that move from the focus of the x ray tube through the collimator to the Ge crystal. The photons which could reach the Ge crystal without the collimator are not detected. The fraction of those photons which would reach the detector if there were no the collimator is less than 0.3 % of those photons which reach the detector without any scattering.

The pulse height spectra measurements were performed at 1.0 m and 2.5 m distance between the Ge spectrometer and the focus of the x ray tube with a small statistical uncertainty. In order to prevent the pile-up events in the pulse height spectra the current of the x ray tube during the measurements was 0.1 mA. A background spectrum with small statistical uncertainty was subtracted from each pulse height spectrum.

Figure 3.2: The PTB⁴ experimental setup for the measurements of the pulse height spectra of the radiation qualities of the ISO narrow spectrum series N-10 to N-120. The target is a tungsten anode with a 20° angle. The inherent filtrations of the 420 kV and 120 kV x-ray facilities are $250\ \mu\text{m}$ Kapton monitor chamber and the window of the x-ray tube of 7 mm and 1 mm Be respectively located at 0.75 cm from the target. the Ge detector has a Be foil $250\ \mu\text{m}$ thick serving as entrance window, which was modelled in MC calculations. The region downstream of the tube window is air.

3.3 Mammography energy x-ray spectra

The third set of experimental mammography energy x ray spectra (acquired by personal communication from Jennings) from Mo, Rh and W targets were measured by Fewell and colleagues in the spectroscopic laboratories of the Center for Devices in Radiological Health. A high frequency inverter x-ray generator was used to power the two different x-ray tubes which were used during the experimental measurements. Each x-ray tube had approximately 0.5 mm of beryllium window as the x-ray tube window and no other added filtration was used. The rhodium x-ray spectra were generated by a GE Senographe DMR x-ray tube (tube housing model: Statorix M52, x-ray tube model: GS412-49), the geometry for the DMR tube is shown in figure 3.3. The molybdenum anode and tungsten anode x-ray tubes are both manufactured by Eureka x-ray tube. The spectra are produced from 18 kV to 42 kV at even kV settings for molybdenum, rhodium and tungsten anodes of the x-ray tube. The measurements are done in air and the spectra are standardized to constant mAs. A high purity germanium detector coupled to a multichannel analyser for detecting x-ray spectra was placed 2.6 cm from the chest wall position which is considered to be at 90^0 to the incident electrons. For the molybdenum and the tungsten anodes, the measured x-ray spectra were rebinned into 500 eV intervals starting at 0.5 kV. For the rhodium anode x-ray tube, spectra are rebinned into 500 eV intervals and bins started at 0.2 keV.

Figure 3.3: The experimental set up for spectral measurements by Fewell and colleagues⁹. The inherent filtration is Be window of about 0.5 mm at 2 cm distance from the target. Measurements are done in air.

Chapter 4

Monte Carlo Simulation Methods

4.1 Monte Carlo simulations for low energy x-ray emission

The energy distribution of emitted x-rays from W, Mo and Ti targets irradiated by 5-25 keV electrons are simulated using the Monte Carlo simulation EGSnrc BEAMnrc code, with two different options for Electron Impact Ionization cross sections, one developed and implemented by Kawrakow¹ and another developed by Salvat² referred to as the Penelope cross section. The electron beam is simulated as a 0.15 cm diameter parallel circular beam incident on the target from the side. The targets were simulated using the XTUBE component module of the BEAMnrc code. The XTUBE component module simulates an x-ray target backed by a target holder, either in air or vacuum. The simulation geometry from the exit window of the XTUBE through to the detector is the same as the experimental set-up, shown in figure 3.1, i.e., the incident electrons impact vertically and the 2.0 cm thick targets are tilted by 45° angle. The region downstream of the target is simulated as vacuum according to the experimental set-up.

Fluence is scored in a 2.2 cm² square region of a scoring plane (this is the largest area which gives the best statistics without changing the fluence) which is at the back plane of a SLABS component module of 6 * 10⁻⁶ cm vacuum, 6.124 cm from the center of the target and perpendicular to the photon beam axis. The width of the energy bins

is 0.125 keV, sufficiently small to allow rebinning without adding significantly to the uncertainty in the comparison.

Simulation transport parameters included electron lower energy cut-offs ECUT and AE of 0.512 MeV, and photon lower energy cut-offs PCUT and AP of 0.001 MeV, with boundary crossing algorithm set to EXACT and the electron-step algorithm set to PRESTA-II, where AE is the low energy threshold in MeV for discrete electron collision losses, i.e., kinetic energy plus rest mass energy of the electron, AP is the low energy threshold in MeV for discrete electron radiation creation (bremsstrahlung radiation), ECUT is the total electron cut-off energy in MeV, i.e., kinetic energy plus rest mass energy of the electron (energy is deposited locally below this value), PCUT is the photon cut-off energy in MeV (energy is deposited locally below this value).

Straight simulation is very inefficient for describing the emission of characteristic x-rays and bremsstrahlung photons. In order to improve the simulation efficiency, we apply the directional bremsstrahlung splitting technique of Kawrakow et al.²³. The photon splitting region was defined at 6 cm from the target with radius of 5 cm. and splitting number 10,000 which gives the maximum efficiency for low energy x-ray calculations²⁴.

Two sets of simulations of the experimental benchmarks are done for tungsten, molybdenum and titanium materials. Option set 1 uses the above mentioned transport parameters and cross sections by Kawrakow for Electron Impact Ionization, which is the default for the EGSnrc code. Option set 2 uses the Penelope cross sections option by Salvat for Electron Impact Ionization.

4.2 Monte Carlo simulations for high energy x-ray emission from tungsten target

For the simulation of unfiltered x-ray spectra from a tungsten target irradiated by 90-120 keV electrons the general purpose Monte Carlo EGSnrc BEAM code is used (similar to the section 4.1). The simulation geometry is similar to the experimental set-up of the 120 kV facility described in section 3.2 and shown in figure 3.2, i.e., 90-120 keV electrons incident normally on a tungsten anode of an x-ray tube. The generated x-ray spectrum then passes through the tube's inherent filtration of 1.0 mm Be and monitor chamber of total thickness of 250 μm of Kapton. According to the experimental conditions the region downstream of the target is simulated as air. The lead collimator is not modelled as it is part of the experimental analyses.

Fluence is scored in a 10.0 cm^2 region of a scoring plane which is perpendicular to the photon beam and 1.0 m from the upstream surface of the target. The width of the energy bins are 0.125 keV.

Simulation transport parameters are the same as those described in section 4.1 and the variance reduction technique of directional bremsstrahlung splitting is used.

Two sets of simulations of the experimental benchmarks are done for x-ray spectra from the tungsten target. Option set 1 uses the transport parameters described in section 4.1 and Electron Impact Ionization cross section by Kawrakow. Option set 2 used Penelope cross sections option by Salvat.

4.3 Monte Carlo simulations for mammography energy x-ray spectra

Mammography x-ray energy spectra were generated using the EGSnrc BEAM code with the same component modules and transport parameters as those used in sections 4.1 and 4.2. The simulation geometry is similar to the experimental set-up described in figure 3.3, i.e., the targets are tilted by 22.5° angle, generated x-ray spectrum passes through the tube's inherent filtration of the Be window. According to the experimental conditions the region downstream of the target is simulated as air.

Fluence is scored in a 10.0 cm^2 region of a scoring plane which is perpendicular to the photon beam and 60.0 cm from the upstream surface of the target. The width of the energy bins is 0.125 keV.

Because of not having information about the exact thickness of the tube's Be window, several simulations are done with different Be window thicknesses and 2.0 mm of Be window is chosen, which gives better agreement with the experimental bremsstrahlung x-ray energy distribution.

Similar to the sections 4.1 and 4.2, two sets of calculations are done for x-ray spectra from tungsten and molybdenum targets with the different options for EII.

Chapter 5

Results and discussion

5.1 Penelope Kawrakow peak ratios

Three sets of x-ray spectra simulations of the experimental benchmarks were done to assess the effect of different cross sections for Electron Impact Ionization in the EGSnrc code. To account for the energy resolution of the detector, simulated spectra were convoluted with a Gaussian distribution with an energy-dependent full width at half maximum, using "c++" code I wrote. The variation of the FWHM with the photon energy was estimated from measured x-ray spectra from W, Mo and Ti targets. The experimental spectra are rescaled by dividing them by a constant so as to have the same bremsstrahlung shape as the corresponding simulated spectra. Both calculated spectra are absolute.

In figures [5.1](#), [5.2](#) and [5.3](#) we compare simulated and measured x-ray spectra generated by 25 keV electrons impinging on thick W, Mo and Ti targets [3.1](#).

Figure [5.1](#) compares experimental x-ray spectra (from Tian et. al^{[3](#)}) from a W target irradiated by 25 keV electrons to the two sets of spectra simulated using the EGSnrc BEAM code. Above 3 keV there is a good agreement of the bremsstrahlung x-ray energy distribution of the experimental and both simulated spectra. The L characteristic lines with Electron Impact Ionization cross section by Penelope overlay the experimental

ones, whereas the EII cross section by Kawrakow underestimates the L characteristic peaks. As to the simulated M characteristic lines, both MC codes underestimate the experimental measurements, although in practice this would not be important as the air and inherent filtration will remove the 2 keV lines (mean free path is 1.6 cm in air).

Figure 5.2 shows x-ray spectra produced from a Mo thick target by 25 keV electron impact. Above 3 keV energy, agreement between experimental and simulated bremsstrahlung spectra is also satisfactory. Also, we see good agreement in L characteristic lines between experimental and two sets of simulated spectra (EII cross section by Kawrakow and Penelope). EII cross section by Penelope shows better agreement with experiment for the K characteristic peaks, but Kawrakow's option underestimates the K characteristic x-ray production as in the case of W spectra for L peaks.

Figure 5.3 shows the experimental spectra from a Ti target irradiated by 25 keV electrons. In the low energy region, there are some peaks that possibly come from impurities in the Ti target. Except for small discrepancies for K_α and K_β simulated characteristic peaks between 4 to 6 keV, which have a slight systematic shift in energy, experimental spectra agree well with the two sets of simulated spectra with different options for the Electron Impact Ionization.

Figures 5.4, 5.5 and 5.6 show the ratio between characteristic peaks generated from W, Mo and Ti targets using the two options for Electron Impact Ionization (error bars are calculated using error propagation, taking into account statistics on the counts in the region of interest). From these figures, we can see that the intensity of characteristic peaks simulated using EII cross section with the Penelope option for W and Mo is higher compared to those with the Kawrakow, whereas characteristic peaks from Ti simulated using the EII option by Kawrakow have higher intensity compared to Penelope option when electron the beam has energies 20 keV and 25 keV and has lower intensity for an electron beam with energy 10 keV.

Figure 5.1: Comparison between experimental and simulated x-ray spectra from a W target irradiated by electrons with energies of 25 keV using Kawrakow and Penelope cross sections. Experimental data are from Tian et. al³ (section 3.1). Measurements are done in vacuum.

Figure 5.2: Same as figure 5.1 except for a Mo target.

Figure 5.3: Same as figures 5.1 and 5.2 except for a Ti target.

Figure 5.4: Ratios of area of characteristic peaks with the Penelope cross section vs those with the Kawrakow cross section for MC calculated x-ray spectra from a W target.

Figure 5.5: Same as figure 5.4 except for a Mo target and including 10 keV incident electrons.

Figure 5.6: Same as figures 5.4 and 5.5 except for a Ti target.

Comparison of simulation results with experimental spectra is made here in relative terms, by normalizing the measured x-ray spectrum to the same energy region of the bremsstrahlung spectrum as the Monte Carlo result. The process is explained in figure 5.7. We normalized simulated and calculated characteristic peaks of x-ray spectra on the bremsstrahlung background, by dividing the area of each peak to the area of a fixed energy region of the bremsstrahlung spectra. The actual differences would be larger if the background was subtracted from each of the peak's areas, but this would introduce considerable uncertainty due to the difficulty in specifying the background in some cases. The present technique still accurately reflects which cross section option is closer to experiment. Figures 5.8, 5.9 and 5.10 show ratios of normalized characteristic peaks obtained by using Penelope and Kawrakow cross sections to the normalized experimental characteristic peaks, that are produced by 10-25 keV electrons on thick targets of W, Mo and Ti.

Figure 5.8 shows the difference between normalized characteristic L lines from the W target generated by using Penelope and Kawrakow cross sections for electrons impinging with energies 20-25 keV. From the figure we can see that the deviation from the experiment is higher when using Kawrakow's cross section i.e., normalized simulated/experimental ratios (error bars are obtained using error propagation) for all L lines and energies is closer to 1.0 when using the Penelope cross section, than when using Kawrakow's.

Figure 5.9 is the same as figure 5.8, but for a Mo target. In the case of the Mo target, Penelope cross sections for Electron Impact Ionisation give better agreement to the experimental results as was the case for W target.

Similar to the W and Mo targets, figure 5.9 proves better agreement for K characteristic x-ray lines from Ti target generated by Penelope cross sections, as the ratios are closer to unity.

$$\begin{aligned}
 L1(\text{normalized.M.C}) &= \frac{A}{E} \\
 L\alpha(\text{normalized.M.C}) &= \frac{B}{E} \\
 L\beta(\text{normalized.M.C}) &= \frac{C}{E} \\
 L\gamma(\text{normalized.M.C}) &= \frac{D}{E}
 \end{aligned}$$

$$L1(\text{norm}) = \frac{L1(\text{normalized.M.C})}{L1(\text{normalized.exp})} \quad L\alpha(\text{norm}) = \frac{L\alpha(\text{normalized.M.C})}{L\alpha(\text{normalized.exp})} \quad L\beta(\text{norm}) = \frac{L\beta(\text{normalized.M.C})}{L\beta(\text{normalized.exp})} \quad L\gamma(\text{norm}) = \frac{L\gamma(\text{normalized.M.C})}{L\gamma(\text{normalized.exp})}$$

Figure 5.7: Characteristic peaks of x-ray spectra are normalized on the bremsstrahlung background by dividing the area under each peak to the area of a fixed energy region of the bremsstrahlung background.

Figure 5.8: Normalized peak ratios for a W target for two EII cross sections. All experimental and MC calculated peaks are normalized on the background i.e., area under each characteristic peak is divided by the area of bremsstrahlung spectra corresponding to a fixed energy region (from 12.5 keV to 15.5 keV), the ratios of MC calculated spectra are then divided by the corresponding ratios of experimental spectra (experimental spectra from Tian et al.).

Figure 5.9: Same as figure 5.8 except for a Mo target. Bremsstrahlung energy region is from 5 keV to 8 keV.

Figure 5.10: Same as figures 5.8 and 5.9 except for a Ti target. Bremsstrahlung energy region is from 6 keV to 9 keV.

Figures 5.11, 5.12 and 5.13 compare simulated and PTB measured x-ray spectra generated by 90-120 keV electrons impinging on a thick W target. In order to compare the relative shapes of experimental and simulated the x-ray spectra, the experimental spectra are multiplied by a scaling factor so as to match the simulated results in the bremsstrahlung region. Good agreement can be observed between the two sets of bremsstrahlung x-ray spectra produced by 90 to 120 keV electrons on the W target and using Penelope or Kawrakow cross sections. While the simulated characteristic K lines have lower intensity in both simulation results, L characteristic lines agree well with the experimental ones.

Figure 5.14 shows the difference between normalized characteristic L and K lines from W target irradiated by electrons with energies 90-120 keV, generated by using Penelope and Kawrakow cross sections. We can see that characteristic line intensities generated by Penelope cross section are in better agreement with experiment than those using the cross section by Kawrakow.

Figure 5.11: Comparison between experimental and simulated x-ray spectra from W target irradiated by electrons with energies of 90 keV using Kawrakow and Penelope cross sections. Experimental data are from PTB⁴ (section 3.2). Measurements are done in air.

Figure 5.12: Same as figure 5.11 except for impinging electrons with energies of 100 keV.

Figure 5.13: Same as figures 5.11 and figure 5.12 except for impinging electrons with energies of 120 keV.

Figure 5.14: Same as figures 5.8, 5.9 and 5.10 except W target irradiated by electrons with 90-120 keV energies(experimental spectra from PTB).

Figures 5.15 and 5.16 show comparisons of experimental spectra from W and Mo targets measured by Fewell and Shuping⁹ between two sets of the x-ray spectra simulated using Penelope and Kawrakow cross sections. To account for the resolution of the detector, Monte Carlo spectra are convoluted with a Gaussian distribution. The experimental spectra are multiplied by a scaling factor so as to match the simulated results at a given electron energy.

As can be seen from figure 5.15 the spectral shapes of the three spectra are similar. A notable difference is that the experimental spectrum has fewer photons/keV than the other two simulated spectra at energies between 12-18 keV and more photons/keV at energies more than 20 keV.

Figure 5.16 shows a comparison between the experimental and simulated spectra produced from a Mo target for 40 keV electron impact. The spectral shapes of experimental and two sets of simulated spectra using Kawrakow and Penelope cross sections are similar, but the experimental spectrum has relatively more photons/keV than simulated spectra at energies more than 10 keV. No matter how the measured values are normalized, the shapes of the bremsstrahlung component do not match the calculated shapes.

The discrepancies between the experimental and simulated spectra from W and Mo targets are because of not having detailed enough information about the experimental set-up. We use a 2.0 mm Be window as the x-ray tube's inherent filtration, which gave the closest fit as we varied it from 0.5 mm to 2.5 mm. The discrepancy may be from the anode material that was not properly polished or from other inherent filtration materials.

Figure 5.15: Comparison of experimental and simulated x-ray spectra from W target irradiated by electrons with energies of 40 keV using Kawrakow and Penelope cross sections. Measured spectra are from Fewell and Shuping⁹ (section 3.3).

Figure 5.16: Same as figure 5.15 except Mo target.

5.2 Kerma

Kerma, K , is the kinetic energy release per unit mass, and it is defined in the following equation:

$$K = \int_0^{h\nu_{max}} \frac{d\phi}{dh\nu} \left(\frac{\mu_{tr}}{\rho} \right) dh\nu \quad (5.1)$$

where, ϕ is the photon fluence, $h\nu$ is the photon energy, $h\nu_{max}$ is the maximum photon energy, and $(\frac{\mu_{en}}{\rho})$ is the mass energy transfer coefficient of the medium. An in-house program, kermadp, is capable of accepting a photon spectrum file and numerically integrating to obtain the kerma, using air as the medium.

In order to estimate for the contribution from characteristic lines to the air kerma from a tungsten target irradiated by 100 keV electrons, we have calculated kerma from simulated x-ray spectra using the kermadp code. Also, the comparison between the air kermas calculated with EII cross sections by Kawrakow and Penelope vs EII off showed that 47% of air kerma comes only from characteristic x-ray photons produced with EII cross sections by Kawrakow and 55% from characteristic x-ray photons produced by Penelope cross sections.

In order to compare the kerma calculated from the x-ray spectra obtained from the Penelope and Kawrakow cross-sections, we need to normalize the resulting kerma. To do this, the peaks in the x-ray spectra have been eliminated by linearly interpolating the fluence at the peripheries of each of the peaks. In essence, this patches over the segment with the peak. This allows the contribution of the peak to the entire kerma to be extracted by comparing the calculated kerma for the spectra with or without the peaks.

Figure 5.17 shows comparison between the ratio of the air ketma with the characteristic peaks included to that with the peaks excluded for two sets of spectra gen-

erated using Penelope and Kawrakow cross sections from W (see figure 5.1), Mo (see figure 5.2) and Ti (see figure 5.3) targets irradiated by electrons with energies 10-25 keV. Air kerma due to X-ray spectra generated using Penelope cross sections is higher compared to Kawrakow cross sections. The significant impact of the peaks is due to the very low energy peaks below 3 keV, where the mass energy transfer coefficient has become very large.

Figure 5.18 shows the contribution to the air kerma from L and K lines together and from only L lines for 90, 100 and 120 keV energy spectra from a W target. It is clearly dominated by the contribution from the L lines around 10 keV.

Figure 5.19 shows the contribution to the air kerma from only K characteristic lines of a W spectra. The K x-ray contribution to the air kerma is determined by removing the characteristic L lines from the calculated W spectra and then calculating the air kerma either with the K lines included in the spectrum or not. As expected high energy K lines do not contribute to the air kerma, since their fluence is small compared to the bremsstrahlung fluence. That said, one must recall that the calculated K lines significantly underestimate the magnitude of the experimentally measured lines (see figure 5.14). The L lines have much more impact because the mass energy absorption coefficients are much larger at low energies. However these lines are usually filtered out in clinical x-ray tubes.

Figure 5.17: Normalized kerma for W, Mo and Ti targets. Air kerma calculated from spectra including all the characteristic peaks is divided by air kerma calculated using bremsstrahlung x-ray background.

Figure 5.18: Same as figure 5.17, except spectra are from a W target and for higher energy incident electrons.

Figure 5.19: Normalized kerma for W target. Air kerma calculated from spectra including only K characteristic peaks is divided by air kerma calculated using bremsstrahlung x-ray background.

5.3 Characteristic peak ratios by different authors

In the diagnostic radiology and mammography energy range, Ay. et al.²⁰ have assessed the x-ray spectra parametrized by empirical, semi-empirical and Monte Carlo modelling by comparison with measured spectra. The spectra were simulated with the same parameters as in the experimental measurements.

The measured spectra in diagnostic radiology energy range from the Eimac x-ray tube with 12.5 degree tungsten target angle and 1.2 mm Al inherent filtration were taken from the Handbook of Computed Tomography X-ray Spectra²⁵.

Mammography energy range spectra measured from a Dynamax M64 molybdenum and a Dynamax M64 tungsten target x-ray tubes with 12 degree target angle and 0.6 mm Al filtration were taken from the Handbook of Mammography X-ray Spectra⁹. Both radiology energy range and mammography energy range spectra were measured with a high purity germanium detector^{9,25}.

K x-ray yields - the contribution from the K x-rays to the total spectra were determined by subtracting the bremsstrahlung part of the spectra from total counts in the desired region and dividing them by the sum of bremsstrahlung and K x-rays.

The MCNP4C Monte Carlo model of total K characteristic peak's intensities is 67%, 20%, 11% and 8% greater than the measured values reported in IPEM Report 78 for respectively 80, 100, 120 and 140 keV electrons on a tungsten target. The differences decrease as the tube voltage increase.

The EGSnrc Monte Carlo model of the total K x-ray intensities are 76%, 72%, and 66% lower for EII by Kawrakow and 71%, 71% and 69% lower for EII by Penelope compared to the PTB experimental values for respectively 90, 100 and 120 keV electrons on a tungsten target.

The EGS4 Monte Carlo model of the K x-ray intensities for tungsten target is 10% lower than the measured values for 100 keV electrons on a tungsten target. The low characteristic x-ray intensity in the EGS4 spectra is because Electron Impact Ionization was not included in the EGS4 code system during the simulation.

The same comparison has been performed for molybdenum spectra predicted by different computational models with measured spectra published by Fewell et al⁹, for a Dynamax M64 x-ray tube at voltages of 25 and 30 kV. The MCNP4C Monte Carlo model of total K characteristic peak's intensities is 73% and 42% greater than the measured values for respectively 25 and 30 keV electrons on a molybdenum target. The MASMIP empirical model is 20% and 13% lower than the measured data for respectively 25 and 30 keV electrons on a molybdenum target. The numbers show that the MASMIP empirical model underestimates the characteristic line intensities whereas the difference decreases as the tube voltage increases.

The EGSnrc Monte Carlo model of the total K x-ray intensities are 44% lower for EII by Kawrakow and 1% lower for EII by Penelope compared to the Tian et al's. experimental values for 25 keV electrons on a molybdenum target.

A similar study has been done by Verhaegen et al²⁶. Their measurements of tungsten x-ray spectra were done using a Philips MCN421 tube for different radiation qualities and the results were compared to the Monte Carlo EGS4/BEAM spectra with an EII subroutine added by Namito et al²⁷. The ratios of measured to calculated K x-ray characteristic photons for a Philips MCN421 x-ray unit are 1.34, 1.09 and 1.20 for $K_{\alpha 2}$, $K_{\alpha 1}$ and K_{β} peaks for a radiation quality of 100 kV with 1.0 mm added Al filtration and 0.78, 0.75 and 0.77 for a radiation quality of 250 kV with 1.0 mm Al and 1.0 mm Cu added filtration. These results are similar to the present results: the ratios of measured to calculated area under the K x-ray peaks are 0.88, 0.94 and 1.06 for $K_{\alpha 2}$, $K_{\alpha 1}$ and K_{β} peaks from a tungsten target for radiation quality 100 kV in vacuum and no added

filtration calculated using EII by Kawrakow and 0.83, 0.91 and 1.01 calculated using the Penelope EII option.

Chapter 6

Conclusions

The electron impact ionization cross-sections present an interesting physical problem. Although the underlying theory of the interaction is known, a clear-cut method for determining the appropriate values of these cross-sections has yet to be determined. We elucidate this through a comparison of calculations of x-ray spectra via EGSnrc using two different sets of elemental cross-sections which account for electron impact ionization. These two data sets are available to users of EGSnrc, and it would be useful to conclude if one option is superior to the other. We have determined that the Penelope cross-sections is the better choice for users, but there is still considerable room for improvement in the results.

We calculated the x-ray spectra resulting from electrons of varying energy incident on titanium, tungsten, and molybdenum. This allowed exploration of any energy and material dependencies. From the x-ray spectra the intensity of the peaks relative to the bremsstrahlung continuum in comparison to the experimental results were studied. These comparisons reveal that the Penelope cross sections yielded a closer match to the experimental magnitudes of the peaks relative to bremsstrahlung for the L-lines of all of the materials, and comparable or slightly poorer matching for the K-lines of tungsten. Although the intensities of the peaks relative to bremsstrahlung appear to be in better agreement with experiment, their values can still deviate from the measured peaks

anywhere from an overestimate of about 27% to an underestimate of approximately 70%, depending on the material and incident electron energy. In regards to the K-lines, the deviations are of the same order. The fact that the Penelope cross section option is more accurate in most cases is expected in the sense that the Penelope option for the EII cross section combines the relativistic plane-wave Born approximation (PWBA) with a semi relativistic version of the distorted-wave Born approximation (DWBA), whereas the Kawrakow option for the EII cross section calculates them using a PWBA.

The contribution to the air kerma from K characteristic lines is not significant and as well few effects in dose calculation are expected, since the total fluence in the characteristic peaks is a small fraction of the total fluence, in practical situations where the very low energy photons are filtered out.

As a conclusion, in order to predict characteristic x-ray lines accurately, more theoretical research is required for Electron Impact Ionization cross sections.

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