Simulating X-ray Spectra: From Tube Parameters to Detector Output

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Abstract
A model is discussed which describes the generation of X-rays in conventional tubes using tabulated bremsstrahlung energy spectra depending on three variables: the target atomic number, the incident electron kinetic energy, and the fraction of energy radiated. Additionally a parameter-free description of the characteristic radiation is included. The constructed model includes technical tube parameters like kilovoltage, target material, and angles of electron incidence and photon emission to also account for self-absorption in the target, as well as radiographic parameters like filtering. In order to verify model results, detector response is also considered. The validity of the proposed model is shown by measurements. Future work includes the extension of the model to transmission targets. This research was supported by the German Federal Ministry of Economics and Technology under contract MNPQ transfer II D 5-30/06.

Keywords
X-Ray, Spectrum, Simulation

1. Introduction

Frequently the output spectrum of x-ray tubes is estimated using analytical approximations, usually based on Kramers’ law, for the spectral shape and fit parameters to scale the intensity. Each incarnation of such a model is generally only valid within a limited range of electron energies and target geometries. A more general and potentially more accurate approach is the use of either specialized or off the shelf Monte-Carlo codes. This on other hand tends to require more computing time, so is oftentimes only viable for calculations not needing to be frequently rerun with different parameters. In order to overcome these limitations we have developed a fairly general model based on fundamental interaction cross sections, which still yields results significantly faster than typical Monte-Carlo calculations.

In order to verify the source model, simulated spectra have to be compared to actual measurements. This requires an understanding of the effects of the utilized detector, as well as filtering. We have therefore implemented a detector model focused on semiconductor spectrometers [1] as well. This is preferentially used to estimate the detected spectrum from a modeled input, though an attempt has been made to also implement the inverse operation, i.e. estimating an incoming spectrum from the detected one.

In order to fully utilize the model, ENDF [2] databases with photo-atomic and electro-atomic interaction and atomic relaxation data are needed. With some limitations MCNP and Elam style databases can also be used. All currently used material properties can also be calculated for compounds, except for the density and the mean excitation potential.
2. X-ray source model

2.1 Model description

A plane target is assumed. The target geometry is given by the angle between the target surface and the incident electron beam, and the angle between surface and emitted photon beam (i.e. only pencil beams are modeled with the intensity normalized per sterad). The implementation allows for transmission targets (i.e. emission from the surface opposite the incident beam), but only absorption targets have been experimentally verified so far. Improvement and verification of the model for transmission targets is planned for the near future.

The developed model is based on numerical integration of photon contributions from a number of processes. The primary contribution comes from interaction of the electrons accelerated by the high voltage potential with the target material. In order to calculate the absorption of the produced photons within the target, the depth of production has to be known. Additionally we require the direction of the electron at the time of interaction in order to consider the angular dependence of bremsstrahlung production [3-4].

Bremsstrahlung is produced through the deceleration of free electrons when interacting with bound atomic electrons. The modeling of bremsstrahlung production is based on tabulated cross sections depending on electron energy, photon energy and angle between incident electron and produced photon taken from [2-6]. The energy losses of the electrons are calculated according to [7].

The photons thus produced are partially absorbed within the target material and can thereby produce photons with characteristic energies for the element in question. Depending on tube acceleration potential and target material this can be an important contribution. We do not consider other processes leading to secondary photons.

In addition to generating bremsstrahlung the electrons can ionize the atoms of the target material, which leads to the production of the corresponding characteristic radiation. Originally a fit based model, taken from [8], was used to describe the production of characteristic radiation. This approach has its limitations, in that the above model is based on measurements within an energy range at the very bottom of or even below the one aimed for with this model. Being fit-based it is also not quite in line with our goals. Therefore a new model was developed, which describes the production of characteristic radiation based on fundamental cross sections. It is coupled to the bremsstrahlung code for two reasons. First of all both depend on the used distribution of electrons regarding depth and remaining energy. Secondly bremsstrahlung photons can also lead to ionization and those of high enough energy can in fact produce a significant portion of the characteristic radiation. For both, electrons and photons of all energies, the probability of ionizing a certain subshell is calculated and then multiplied by the transition probability for each radiative transition. Non-radiative transitions are not considered. The contributions from this process are then summed up over all depths within the target.

Although for most model components the tabulated cross sections and other data can currently be taken from databases in Elam, MCNP or ENDF format, the new model for characteristic radiation depends on data not present in either Elam or MCNP style databases.
2.2 Electron distributions

As the basis of the developed model we require the probability density distribution of electrons regarding electron energy, position, and direction. In order to reduce the dimensionality, we only consider depth within the material. This distribution depends on target material, angle of incidence, and initial electron energy. In the case of transmission targets it additionally depends on the target thickness. It is possible to precalculate such distributions using a Monte Carlo model for coupled electron-photon transport and configure our model to use these. An example is shown in figure 1, where the angular dependency has been integrated over. If this is not done, as will usually be the case, the implementation estimates electron distributions based on previous works [8-11] and our own Monte Carlo computations. This estimate works very well for typical x-ray tubes, but becomes increasingly incorrect for small angles of incidence and large deviations from a 90° angle between incidence and emission.

In order to estimate the electron distribution, we follow an electron from its initial energy down to some cutoff energy in a reasonable number of steps. By default the lower threshold as well as the number of steps are directly determined from the energy resolution of the x-ray spectrum to be calculated. The fraction of electrons lost to backscattering at the current energy is estimated using the results of Storm [10], and Hunger [11] in combination with an empirical dependence on the incidence angle (figure 2). Electrons are assumed to be uniformly distributed between the surface and a maximum depth determined from their path length in continuous slowdown approximation and the energy diffusion depth [9]. The angular distribution is approximated as the superposition of two components: a narrow beam in the direction of incidence, and a broad component uniformly distributed within a varying opening angle. The relative weights of these components as well as the width of the broad component depend on the fraction of path length in continuous slowdown approximation, i.e. roughly on the number of previous interactions.

A noticeable improvement of the results can be expected, when the approximate electron distributions become more realistic. It is our goal to replace this approximation with a functional description fitted to results obtained from Monte Carlo simulations.

![Figure 1](image-url) Normalized electron density distribution plotted over energy and depth for normal incidence on a tungsten target with 100 keV initial energy
3. **X-ray detector model**

3.1 **Photon interaction with detector material**

In order to reduce calculation complexity over full Monte Carlo simulations, we again consider a pencil beam. The angular distribution of photons scattered within the sensitive volume is neglected. Considered effects include photo absorption, i.e. the detector quantum efficiency, Compton scattering, Fano broadening, photon escape (detector material fluorescence) and charge transfer losses as well as pile-up and system noise (broadening). Since there are a number of effects depending on the position within the detector, namely transfer losses, all effects are calculated for a configurable number of slices along the incident beam. For each slice the events are registered and the photon spectrum is updated with scattered photons, photon escapes or characteristic radiation of the detector material.

Photo absorption is simply modeled by taking the tabulated cross section from the database and calculating the absorption probability within the current slice. Photon escape can play an important role if there is a high chance of characteristic X-ray emission upon absorption as well as a low chance of immediate re-absorption (comparably high energy of characteristic radiation). For segmented detectors there is the additional possibility of recapturing in a different segment.

For the energy range of current industrial NDT applications Compton scattering in the detector has little influence on the continuous spectrum. Fano broadening takes into account the statistical uncertainty due to the electron cascade initiated in the detector material. Especially for compound semiconductors, like the CdTe detector primarily used for our measurements, charge transfer losses can significantly influence the detected spectral shape. In our case this is most visible for high characteristic energies, as encountered in the $^{133}$Ba and $^{75}$Se $\gamma$-spectra used for detector calibration. These effects are modeled in accordance with the recommendations from the manufacturer of our primary detector.
3.2 *Pile-up*

In all cases we consider, a photon eventually produces an electron cloud, which is accumulated at a readout electrode in order to determine the total charge. Neglecting losses this charge is proportional to the deposited energy. This accumulation takes a certain amount of time, the integration time, during which more than one photon might strike. In this case the detected energy is increased by whatever amount of charge the second photon contributed during the integration time of the first – frequently this means the sum of both energies. In part this can be recognized by the electronics and such events discarded, but this is never fully possible. Within our model the probability of such a coincidence is estimated by assuming Poisson statistics. This is not quite correct, as given inelastic scattering one photon can produce several events that are not completely independent. It is immediately clear, that the higher the rate of photons of a certain energy, the higher the probability for coincidence. Therefore in the presence of characteristic radiation one can usually discern a doubling of at least the more prominent characteristic energies. For spectral measurements it is good practice, though, to choose filtering, measurement times, and target currents as to minimize this effect. Accordingly it can frequently be neglected.

4. **Validation**

In order to validate our approach and judge its merits, we have compared the calculated spectra to measurements as well as Monte Carlo simulations. As an example, comparisons for tungsten targets at 100 kV and 200 kV acceleration potential are shown in figure 3 through figure 6. The plots comparing with measurements are shown in linear scaling, while the plots for Monte Carlo results are scaled logarithmically to show the bremsstrahlung continuum as well as the sharp features at the characteristic energies.

Measurements have been taken with an AmpTek CdTe-Stack spectrometer, positioned with a 16 m evacuated tube with inbuilt collimators between it and the source. This setup together with additional collimation supplied with the spectrometer reduces the x-ray photon flux sufficiently to allow spectral measurement at normal tube operating parameters. For the purpose of comparison the detector characteristics have been modeled in accordance with the manufacturer’s specification and our own calibration measurements carried out with $^{133}$Ba and $^{75}$Se $\gamma$-emitters. Our model was configured to return results for the exact setup including tube current, measurement time, and opening angle of the illuminated spectrometer surface. No additional scaling was applied.

For the Monte Carlo calculations our in-house code McRay [12] was used, and the model described here was configured to return results for the same opening angle and number of electrons. Again, no additional scaling was applied.

In general we find good to excellent agreement with measured spectra as well as Monte Carlo results. For an acceleration potential significantly below 100 kV we find deviations from measurements in the absolute intensity, reaching approximately 20% at 30 kV. As the agreement with our Monte Carlo model is excellent in this case, this cannot be attributed to the simplicity of the model. The exact cause will have to be investigated. Additionally, for initial electron energies close to the highest absorption edge of the target material, i.e. below about 100 keV, the intensity of characteristic radiation shows some deviation from the measured spectra. This limitation will be difficult to overcome within the scope of this simplified model.
Figure 3  Comparison of the described model to Monte Carlo calculation for a tungsten target and 100 keV initial energy

Figure 4  Comparison of the described model to measurement for a tungsten target and 100 keV initial energy
Figure 5  Comparison of the described model to Monte Carlo calculation for a tungsten target and 200 keV initial energy

Figure 6  Comparison of the described model to measurement for a tungsten target and 200 keV initial energy
5. Conclusion

The source model includes bremsstrahlung production due to the interaction of free electrons with atomic matter as well as the production of characteristic radiation by the same electrons and the bremsstrahlung photons. Given sufficient data the model is completely based on interaction cross sections. This physics-based model allows improvement over simple fit-based models, as it is capable of producing the spectral shape instead of imposing it. Additionally, the model is more general in that it makes fewer assumptions about the geometry.

Calculation times vary with configuration, but on current office hardware typically amount to a few seconds. The agreement with Monte Carlo computations, which take many hours on the same hardware, is very good for all tested configurations up to several hundred keV, and still quite good at 2 MeV.

For acceleration potentials from 100 kV to 300 kV we found good to excellent agreement with our measurements. Comparison to available spectra between 450 kV and 800 kV also showed good agreement, but the setup was less rigorously defined for these, as they were not specifically taken with this goal.

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References