OPTIMIZATION OF X-RAY SOURCES BY MODELING

Andreas DERESCH[1], Gerd-Ruediger JAENISCH[1], Carsten BELLON[1],
Alexander WARRIKHOFF[2]
[1]FEDERAL INSTITUTE FOR MATERIALS RESEARCH AND TESTING, Berlin, Germany
[2]rtw RÖNTGENTECHNIK DR. WARRIKHOFF, Neuenhagen, Germany

INTRODUCTION

In order to reduce the amount of trial and error during optimization of x-ray tubes, one needs to have a good understanding of radiation production as well as electron behavior (e.g. backscattering). Using simulation software optimization of tubes can to a large extent take place during early development, without the need to fabricate many prototypes. In addition it becomes possible to separately study the influence of tube parameters (e.g. geometry).

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 the 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 attempt to develop 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 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, which will have to be provided.

X-RAY SOURCE MODEL

Bremsstrahlung Production

Bremsstrahlung is produced through the deceleration of free electrons when interacting with bound atomic electrons. Within this model a thick target approximation is currently used, i.e. no electrons are transmitted through the target – they are either absorbed or backscattered. Some work has been expended towards transmission targets, but this is neither fully implemented nor verified yet. Self-absorption in the target is considered by taking into account the depth of radiation production and applying the linear attenuation law accordingly. 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 [2-4].

In the past the distribution of electron counts, positions and directions were empirically estimated based on previous works [5-6]. Since the electron distributions obviously have a large impact on the energy and intensity of the radiation that will actually be emitted from the target in the direction of the observer (tube window, detector), our current focus is the improvement of this particular area. Using a separate Monte-Carlo model [7] to determine electron characteristics, much more realistic electron distributions can now be used. Figure 1 shows an example of one of the electron characteristics distributions calculated with this code. As a further example Figure 2 presents another view onto the same data: backscatter correction factors, i.e. relative number of electrons not yet backscattered at a certain energy – the asymptotically approached value for full energy loss represents the fraction of electrons completely depositing their initial energy. Within the radiation production code, the full angular distribution is used instead of this reduced dataset. Deriving a semi-analytical description of these distributions calculated for a set of typical tube parameters is envisioned as future development.

Characteristic Radiation

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 [5], 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. This contribution is especially important, if the highest electron energy is not significantly above the absorption edge in question (e.g. ~100 keV electrons in tungsten). 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. In order to accurately describe the production of characteristic radiation due to the bremsstrahlung photons, the depth of ionization due to those photons has to be estimated separately, as this can significantly differ from the depth of radiation production due to electrons.

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. The previous model remains as fallback, if insufficient data is supplied.

X-RAY DETECTOR MODEL

In order to compare the modeled spectra with measurements and therefore determine the quality of the model, it is necessary to take into account the effects of the acquisition process, e.g. the characteristics of the spectrometer and its associated electronics.

Photon Interaction with Detector Material

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 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 Ba-133 and Se-75 γ-spectra used for detector

calibration. These effects are modeled analogous to the recommendations from the manufacturer of our primary detector.

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 detected 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.

Results

Two examples of the application of the source and detector models for common x-ray tube geometry and parameters are shown in Figure 3 and Figure 4 together with the corresponding measurement. Apart from the line intensities the agreement is quite good. In addition several measurements with aluminum and steel objects of realistic thicknesses (depending on X-ray tube voltage), where absorption shifts importance to the high energy part of the spectrum, show no deterioration in agreement.

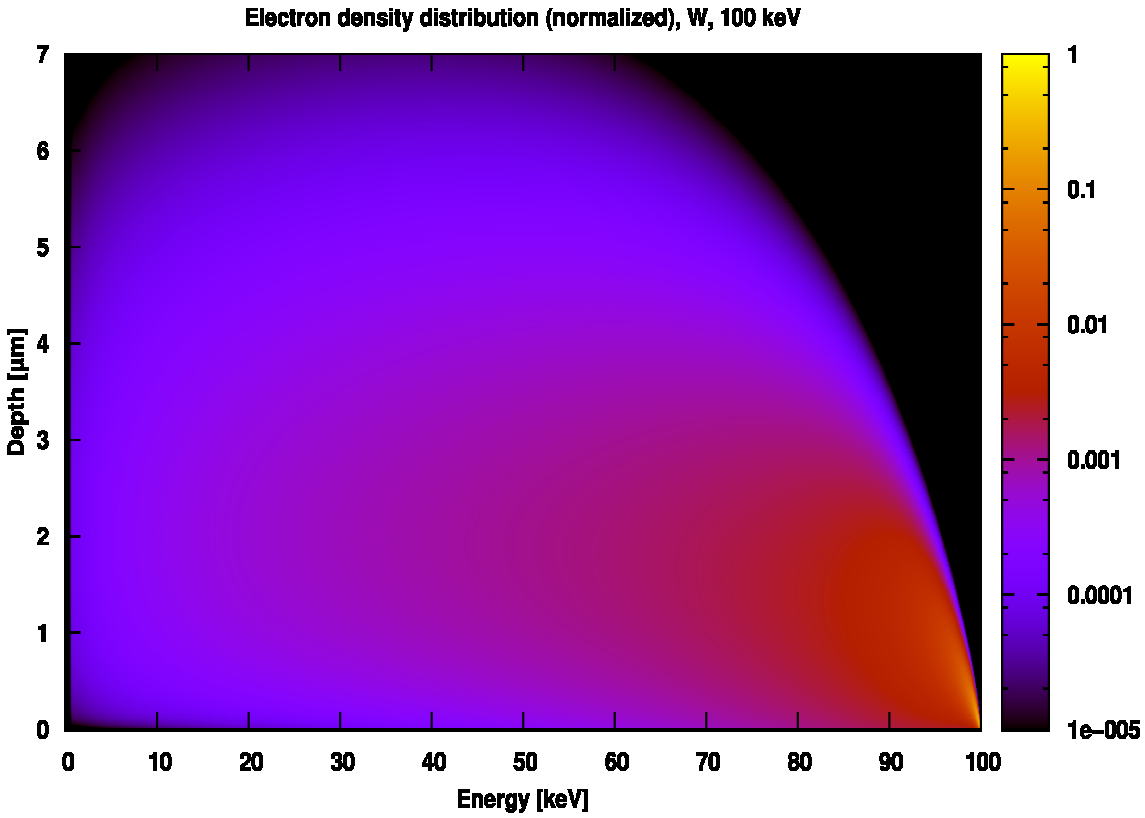

Figure 1. Probability density distribution of an electron in energy and depth.

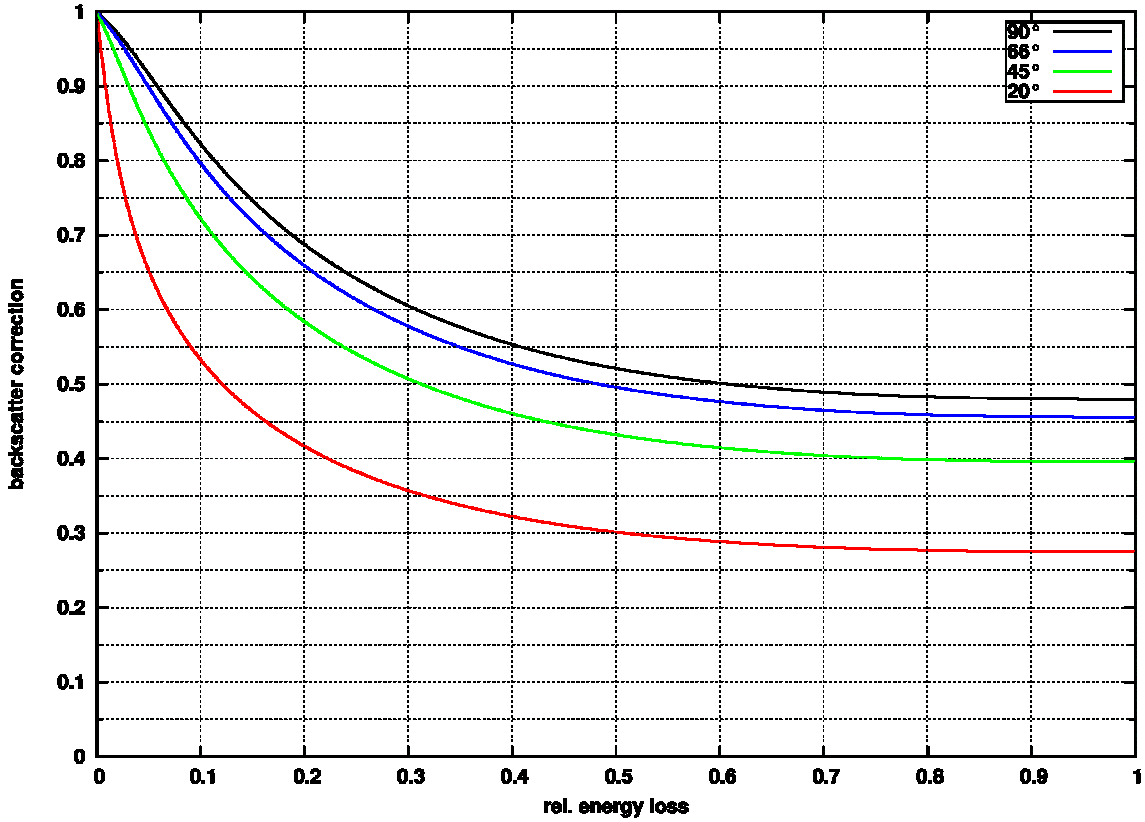

Figure 2. Backscatter correction curves for tungsten, 100 keV, several incidence angles.

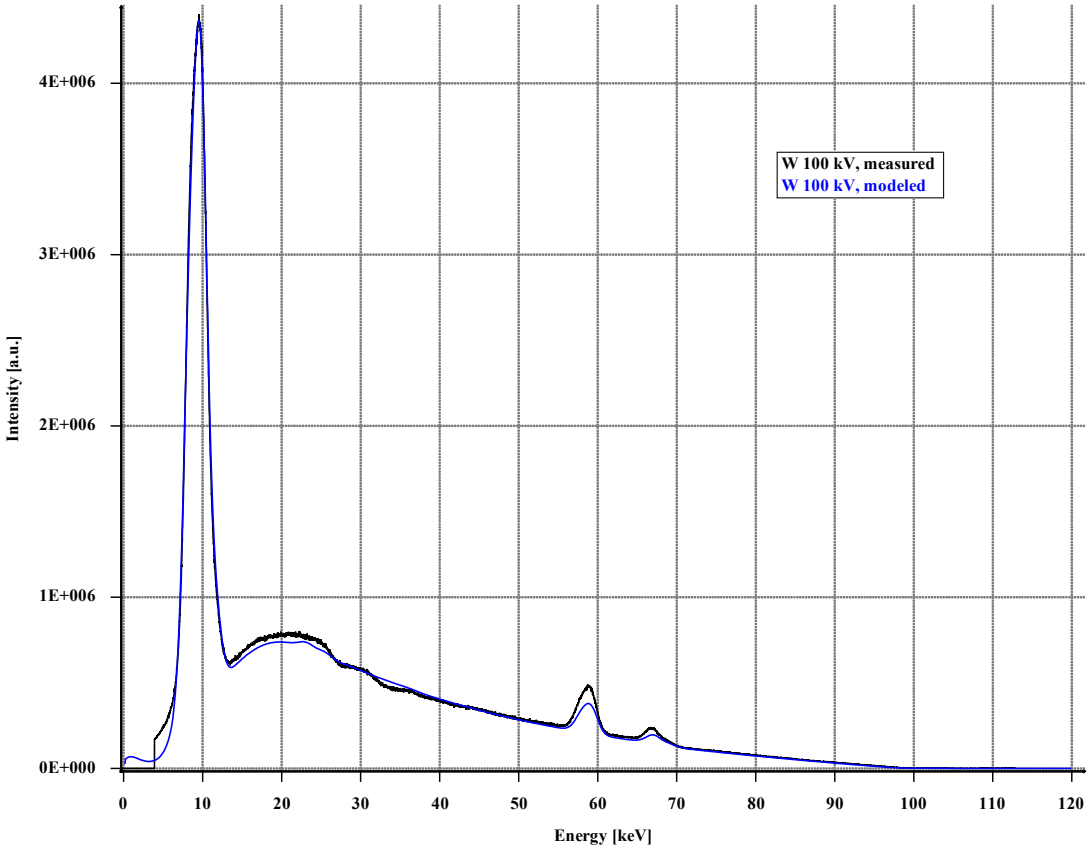

Figure 3. Comparison of a modeled spectrum to the corresponding measurement

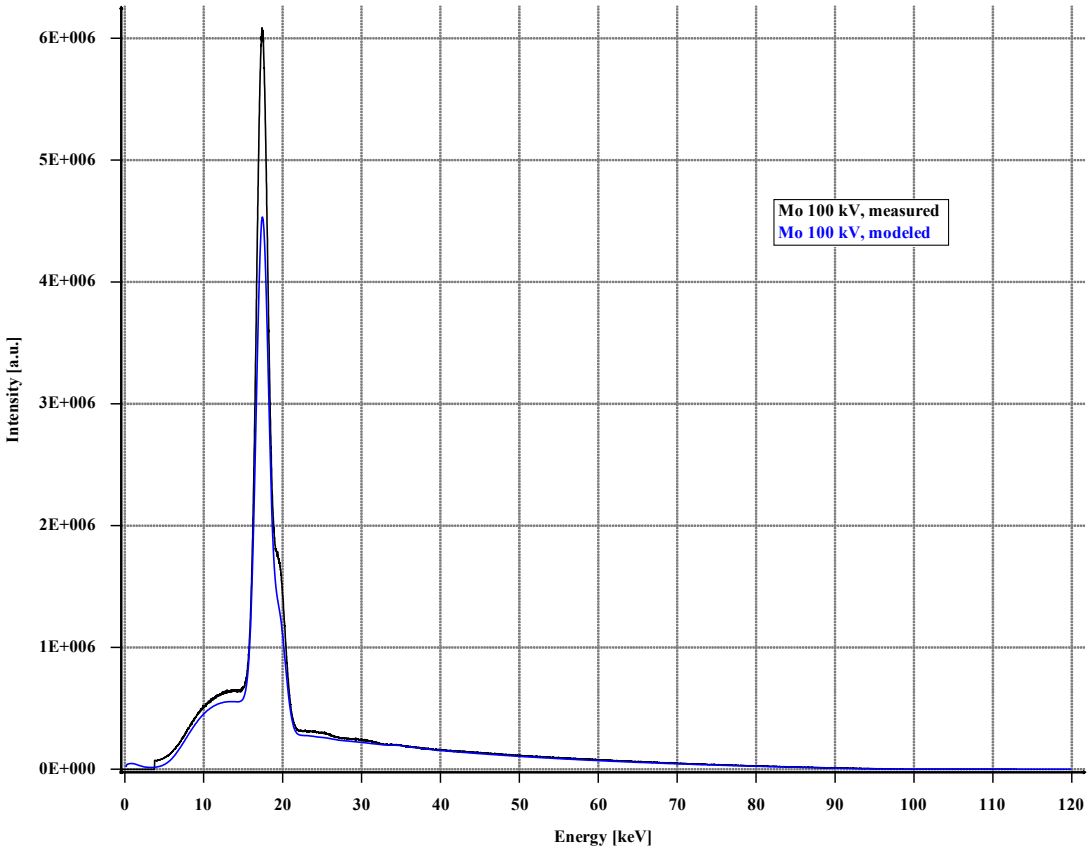

Figure 4. Comparison of a modeled spectrum to the corresponding measurement

INVERSION OF DETECTOR MODEL

The inversion is completely based on the same functions used for estimating the detector effects in the first place. In this way the model is kept self-consistent at all times and any changes or improvements of the detector model are immediately present here.

Pile-Up

As a first step pile-up effects are estimated and removed. This is done by simply using the input spectrum as a starting guess and iteratively setting it to the difference between the input spectrum and the current pile-up estimate. This process usually converges very quickly.

Iterative Deconvolution

The general idea of deconvolution, given some output data and a convolution kernel, is to estimate the input data that would yield this output after having this kernel applied. For iterative deconvolution this is achieved by repeatedly applying the given kernel, comparing the result to the output data and somehow redistributing the differences to the current estimate. Depending on the circumstances there are of course many possible ways of actually implementing this scheme. Frequently one has fairly simple, symmetrical kernels, e.g. a Gaussian distribution, and some expected properties of the result to impose on the estimates, greatly facilitating convergence. Unfortunately, without over-simplification, neither is the case here. Strictly speaking not the whole spectrum is being (de)convolved, but there rather is one distinct convolution kernel for each energy bin. Those for close energies are fairly similar, so interpolation can be used to some extent, but there is no way to describe the detector effects for all bins in the same way. In addition, when all effects are considered, the kernels are noticeably asymmetrical.

Consequently the detector model is applied to build one convolution kernel for each energy bin. These are then used for all convolution steps as well as for the error redistribution. In order to reduce oscillations to an acceptable level, the program attempts to estimate two spectral components: one smooth, mostly equivalent to the continuum, and one containing narrow spectral features, mostly equivalent to the discrete spectrum. The critical part here is to separate the two as cleanly as possible. This is attempted by imposing a continuity as well as smoothness constraint onto one component, while minimizing the other. Both are separately subjected to a non-negativity constraint.

Redistributing the error onto the current estimate is a critical part of the whole process, as this step strongly influences not only the final result, but also the convergence rate. Good results were only achieved by a fairly complicated scheme. The error of each bin is distributed across all other bins, according to how large a contribution those bins might have made to this particular one. In other

words in each iteration the current estimate is used as weighting factors to the corresponding convolution kernels during redistribution.

Results

This somewhat generic approach is fairly slow, but has the important advantage of fully utilizing any work expended on the detector model itself. This makes it seem the most flexible solution for arbitrary detector configurations and reduces the workload for implementing any future improvements. Figure 5 shows a comparison of the simulated tube spectrum used for Figure 3 and the corresponding detector model inversion. As can be seen, the inversion process is very good at removing the forward application of the detector model, including finding the original line positions and preserving integral quantities (photon count, total and average energies). Oscillations from deconvolving sharp features are not fully suppressed yet.

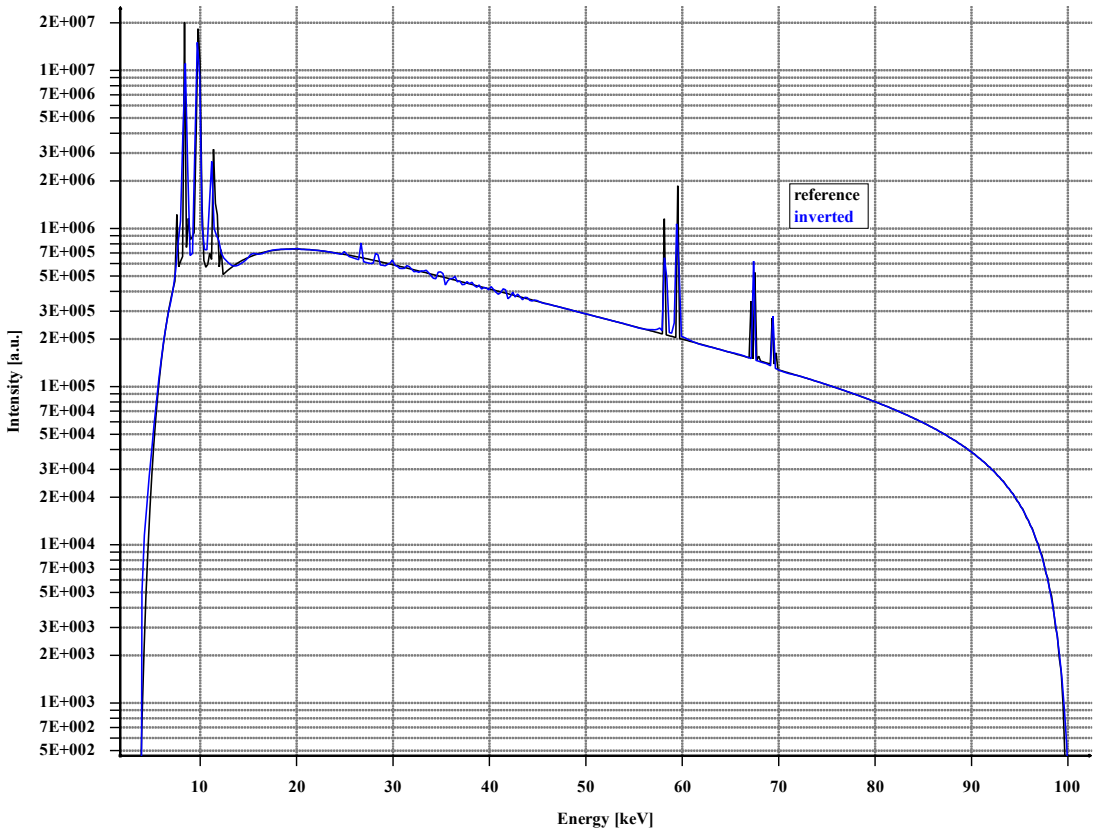

Figure 5. Comparison of detector model inversion to theoretical tube spectrum (tungsten, 100 kV, 24° target angle)

SUMMARY AND OUTLOOK

X-Ray Source Model

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. 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. The model has been extended to utilize externally supplied electron distributions (energy, depth, direction of motion), which has improved the results significantly. Implementing a semi-analytical description of these distributions would immensely improve usability, as the companion code [7] would not be needed.

Depending on configuration (e.g. requested number of energy bins in spectrum, chosen characteristic radiation model, size/resolution of provided electron distributions) execution times on a single 3.2 GHz Pentium4 core range between a few seconds and a few minutes, typically noticeably below one minute. On newer, multi-core processors or multi-processor machines execution times will be significantly reduced, as the model scales quite well with the number of threads. This makes it possible to quickly calculate spectra for parameter variations, which is potentially useful for optimization during tube development.

Detector Model

The detector model includes all major effects, yet it is rather difficult to fully model all of them. In general simplifications have to be made, the applicability of which has to be judged against the work needed to improve upon them. In particular refinement seems needed regarding the contribution of Compton scattering events. Among the included effects are losses due to charge trapping, which is especially important for compound semi-conductors.

Inversion of Detector Model

As can be seen from Figure 5, the detector model inversion tends to produce false peaks. For measured spectra, which will not be perfectly described by the model and also contain noise, this is frequently even more pronounced. This has to be taken into account when interpreting spectra and will be subject of further work.

ACKNOWLEDGEMENTS

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