A Fast General Spectrum Model for Quantitative Radiography Simulation

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Abstract. One essential step on the way towards accurate quantitative simulation of radiographic testing is an accurate description of the utilized energy spectrum of X-ray photons. For use in general purpose simulation tools, the spectra of X-ray tubes have to be described by a model covering at least the intended range of applications. This range includes transmission tubes as well as direct beam tubes with varying angles of incidence and emission, for a number of typical target materials. In radiographic testing acceleration voltages frequently reach up to 450 kV for direct beam targets and up to 225 kV for transmission targets, with even higher voltages available or being developed. Currently used models are unable to cover the whole range of configurations.

Here a model is presented that employs a unified approach for simulating the photon energy spectra for transmission and direct beam targets composed of arbitrary homogeneous materials. In order to achieve this, a detailed model of electron transport within the target is employed. The validity of the developed model is shown through comparisons with Monte Carlo simulations as well as measurements for a number of different configurations.

1 Introduction

Within the field of non-destructive evaluation simulation is more and more becoming an important tool for a variety of purposes. It is gainfully employed e.g. for assisting analysis of physical measurements, evaluating and optimizing techniques, and to generate exactly known input data for the development of processing or reconstruction algorithms. With increasing sophistication of available physical models the goal of fully quantitative simulation of complete techniques is within reach. In the case of industrial radiography there are three key component models: for the X-ray photon source, the interaction of photons with matter, and the detection of the photons. In general the latter two depend strongly on the distribution of photon energies. A sufficiently general and accurate model of the source spectrum is therefore required for any quantitative radiography simulation.

One important aspect of reliable quantitative simulation is the restriction of model parameters. In particular, quantitative models should not have any free parameters. That is, all model inputs should directly relate to physical quantities that can be determined by either the user of the model or the manufacturer of the modeled components. In order to be useful for a variety of applications, model runtimes should also be on the order of seconds or at most a few minutes.
2 Existing Spectrum Models

2.1 Model Classes

There are two main groups of models commonly employed for simulation of X-ray spectra. Monte Carlo models of coupled electron-photon transport are in principle capable of fully describing the relevant physics. Their use typically requires extensive knowledge about the particular software as well as significant computational resources. For these reasons semi-analytical models are much more frequently used. These are domain-specific algorithms, therefore taking a small number of parameters which are normally familiar to the user. In addition they achieve much faster execution times than Monte Carlo models. On the other hand, they lack the generality of a Monte Carlo model and can only be used within limited parameter ranges.

1.2 Range of Validity

Depending on the field a given model was developed in, target geometry and materials are typically restricted. Almost all common models are limited to either normal incidence or a 90° angle between electron beam and direction of photon emission. The latter configuration covers central emission of typical direct beam tubes, but cannot model variation of the spectrum over the emission cone. None of the commonly used models are applicable to transmission targets. In addition, models intended for use in diagnostic medicine or electron microprobe analysis (EPMA) do not cover the full kilovoltage range used in NDE. A comparison of several commonly used semi-analytical X-ray spectrum models is shown in Tab. 1, with the model presented here given in the last row. The first model was developed in the field of EPMA and is described by Ebel [1]. TASMIP [2] is based on polynomial fits to measured spectra and is therefore quite limited in its parameters. Consequently several variants for different types of X-ray tube exist. Two models by Tucker et al. are included, only differing in target material: tungsten [3] and molybdenum [4]. Despite being clearly aimed at use in diagnostic medicine, these find some use in NDE. Based on the works of Birch and Marshal [5] the Institute for Physics and Engineering in Medicine (IPEM) published a simulation software with their Report No. 78 [6], which is frequently used as reference for other models. The only listed model to support significantly higher acceleration potentials, 300 kV officially supported and 500 kV in an experimental version, is SpekCalc [7]. With the exception of the model presented here and one variant of TASMIP, these models are only applicable to direct beam targets.

2. Model Development

2.1 General Characteristics

This section will give an overview of the design principles for the developed model and the resulting characteristics. A more thorough discussion of the developed model can be found in [8]. One major goal for the developed model was to achieve generality in a fast, semi-analytical model without sacrificing accuracy of quantitative results. Direct beam and transmission targets (Fig. 1) are therefore supported by the developed model. The target is in both cases described by a plate of arbitrary thickness, consisting of an arbitrary homogeneous material. The incidence angle of the electrons as well as the take-off angle of the photons can be freely varied in the model. This allows describing variation over the emission cone as well as uncommon target geometries. For sufficient generality the angular de-
dependence of bremsstrahlung emission must be taken into account, which is not done in previous models. Since the model is intended mainly for use in the field of NDE, acceleration potentials from ca. 10 kV up to about 500 kV are targeted. Higher values can be used, but are out of scope for this work. In order to achieve these characteristics within a single model, a detailed distribution of energetic electrons has to be taken into account.

![Schematic view of the considered target geometries.](image)

**Fig. 1.** Schematic view of the considered target geometries.

**Table 1.** Validity ranges of several semi-analytical spectrum models

<table>
<thead>
<tr>
<th>Model</th>
<th>Materials</th>
<th>Kilovoltage</th>
<th>Incidence angle</th>
<th>Emission angle</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>min  max</td>
<td>min  max</td>
<td>min  max</td>
</tr>
<tr>
<td>Ebel</td>
<td>Al, Cu, Mo, Au, ...</td>
<td>10  50</td>
<td>30   90</td>
<td>15   90</td>
</tr>
<tr>
<td>TASMIP</td>
<td>W</td>
<td>30  140</td>
<td>—    —</td>
<td>—    —</td>
</tr>
<tr>
<td>Tucker</td>
<td>W</td>
<td>70  140</td>
<td>—    —</td>
<td>&lt;12  &gt;20</td>
</tr>
<tr>
<td>Tucker</td>
<td>Mo</td>
<td>20  55</td>
<td>—    —</td>
<td>&lt;12  &gt;22</td>
</tr>
<tr>
<td>IPEM78</td>
<td>W</td>
<td>30  150</td>
<td>—    —</td>
<td>6    22</td>
</tr>
<tr>
<td>IPEM78</td>
<td>Mo, Rh</td>
<td>25  32</td>
<td>—    —</td>
<td>9    23</td>
</tr>
<tr>
<td>SpekCalc</td>
<td>W</td>
<td>40  300</td>
<td>—    —</td>
<td>6    30</td>
</tr>
<tr>
<td>XRayTools</td>
<td>Al, Ti, Cu, Mo, W, ...</td>
<td>10  500</td>
<td>10   90</td>
<td>1    179</td>
</tr>
</tbody>
</table>

2.2 Electron Transport

As a first step electron transport within the target geometry is carried out. The algorithm employs a single-scattering approach, where a discretized distribution of electron characteristics is developed after each elastic electron scatter event. The tracked characteristics are the remaining electron energy, the depth within the target, and the direction of movement. These quantities are required for accurate modeling of photon emission and attenuation. During this step backscattering of electrons as well as transmission through a thin target are naturally taken into account. No separate model for these aspects is therefore needed.

2.3 Photon Emission

Modeling of photon emission in turn is split into two components. The first step uses the previously described electron distribution to model the direct emission of bremsstrahlung and characteristic radiation due to these electrons. The availability of electron directions allows for taking into account the angular dependence of bremsstrahlung emission in this step. The attenuation of all photons is modeled taking into account the emission angle as well as the depth of emission within the target.
For some source configurations a significant fraction of the emitted characteristic radiation is not directly excited by the electrons. Instead, the primary photons, bremsstrahlung as well as characteristic radiation, lead to the production of secondary photons. This contribution is described by applying a simple photon transport model to primary photons, tracing their interaction depths within the target. From this, the emission of secondary photons can be modeled, taking into account the attenuation for this depth.

3. Results

The comparison of simulated spectra is carried out mainly with Monte Carlo codes and measurements where available. Other semi-analytical models are too limited in scope for a broad comparison. The main Monte Carlo code used is BEAMnrc [9], as it has been independently validated and is particularly well suited to this type of simulation. While originally targeted at high-energy applications, e.g. linear accelerators, it can model all physical processes relevant for the description of X-ray spectra in the kilovolt range. One capability setting it apart is the possibility to configure directional bremsstrahlung splitting, which allows significantly faster spectrum calculations compared to other Monte Carlo models. McRay [10], developed at the German Federal Institute for Materials Research is also included, since it considers the same physical effects and utilizes the same material data as the presented model.

Three different configurations for the same kilovoltage, 100 kV, were chosen for comparison. These are: a molybdenum target with 66° incidence and 24° emission angle (Fig. 2), a tungsten target with 70° incidence and 20° emission angle (Fig. 3), and a tungsten transmission target of 5 µm thickness with normal incidence and emission (Fig. 4). Excellent agreement is seen in both shape of the spectrum and absolute photon intensity. While this is typical for direct beam targets, absolute intensities show larger deviations at some acceleration potentials for transmission targets. Photon count for the L-characteristic radiation of tungsten is not correctly predicted by any of the models.

In addition a comparison was carried out for the highest kilovoltage in common use, i.e. 450 kV. A typical tungsten target with 70° incidence and 20° emission angle was used for this comparison (Fig. 5). Unfortunately the corresponding measurement has so far not been taken, so the comparison includes only several simulation results. The model presented here is again in excellent agreement with McRay, while both show decreased flux when compared to BEAMnrc. This is attributed to secondary electrons not being taken into account in McRay and the presented model. The only other semi-analytical model available in this energy range, an experimental version of SpekCalc, shows a very similar result.

In order to demonstrate applicability of the developed model to more unusual configurations a 20° copper target at 30 kV is shown as well (Fig. 6). While no measurement was taken for this configuration, agreement to BEAMnrc as well as McRay is excellent.

4. Summary

A fast general model for the energy spectra of photons emitted by industrial X-ray tubes was presented. The model is applicable to direct beam and transmission targets with varying angles of incidence and emission. Arbitrary homogeneous target materials are supported. The model is capable of producing equivalent results to common Monte Carlo models, while requiring significantly fewer computational resources. The model requires only geometrical and physical parameters describing the actual measurement; there are no free parameters such as scaling factors for the user to change. This is an important aspect for the creation of a tool chain for fully quantitative simulation of radiographic inspections.
Fig. 2. Comparison of models for 24° molybdenum target at 100 kV.

Fig. 3. Comparison of models for 12° tungsten target at 100 kV.

Fig. 4. Comparison of models for tungsten transmission target at 100 kV.
Fig. 5. Comparison of models for 20° tungsten target at 450 kV.

Fig. 6. Comparison of models for 20° copper target at 30 kV.

References
