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A general spectrum model for X-ray generators

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ABSTRACT

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1. Introduction

Motivation: The goal of this work was to develop a model for the energy spectra of photons emitted by X-ray tubes that, due to its very general design, is applicable to a wide range of configurations. In particular, the same model shall apply to thin targets employed in transmission configuration and thick targets employed in direct beam configuration, with no limits placed on the target material. With a focus on sources used in radiographic imaging, acceleration potentials of up to approximately 500 kV, as commonly used in non-destructive evaluation, must be supported. In addition, arbitrary combinations of incidence and take-off angles shall be supported to enable use in optimization of target geometries. While available Monte Carlo models can achieve all this, the required computational resources are oftentimes prohibitively large. Consequently a semi-analytical approach was chosen to allow simulation times on the order of seconds for a typical personal computer. One use of the developed model is in simulation of the complete radiographic process, e.g. in *aRT*ist [1].

Existing models: Most dedicated X-ray spectrum models found in the literature have been developed in fields such as diagnostic medicine (e.g. [2–4]) or electron microprobe analysis (e.g. [5,6]). They are typically limited to the range of target materials, geometries, and acceleration potentials commonly used in their respective fields. These limitations allow employing relatively simple estimates of the electron distributions in depth and energy.

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http://dx.doi.org/10.1016/j.ndteint.2015.12.007 0963-8695/© 2015 Elsevier Ltd. All rights reserved. The angle dependence of bremsstrahlung emission is usually neglected. This is justified by the assumption that the electron scattering quickly reduces anisotropy of electron movement. This last approximation does not hold for target geometries that significantly deviate from the classic geometry with 90° between electron beam and central photon beam, i.e. transmission targets as well as some modern direct beam configurations. In some models, empirically determined scaling factors are employed to adjust the resulting photon flux. The model developed here places fewer restrictions on the range of allowable configurations.

2. Model description

A fast quantitative model for the energy spectra of radiation emitted by X-ray tubes is described,

handling thin as well as thick plane targets of arbitrary materials. The developed model is based on

fundamental interaction cross sections, describing electron and photon transport via numerical inte-

gration of discretized distributions. While the focus lies on bremsstrahlung production, modeling of

characteristic radiation is fully integrated. The model does not include any free parameters. The validity

of the model is shown through comparison with measurements and Monte Carlo simulations for several

combinations of target material and acceleration potential between 30 kV and 450 kV.

Technical X-ray sources are composed of an electron source, normally a hot or cold cathode, a means of applying a potential difference to accelerate the electrons, and a metal target in which the electrons are slowed down and produce radiation. The basic target geometry considered in this model is a single semi-infinite plate of arbitrary thickness, i.e. lateral plate borders are considered unreachable by transported particles. The plate must consist of a single homogeneous material, the elemental composition and density of which are input parameters. Interaction cross sections for compounds are calculated internally from element data, which is normally taken from ENDF databases [7]. A pencil beam of electrons with a fixed kinetic energy corresponding to the configured acceleration potential is assumed. The output of the model is the spectrum of X-rays emitted within an infinitesimally small solid angle, i.e. a single direction is considered for determining angles of emission. This output is scaled according to a configurable solid angle, the measurement time, and the target current.









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This allows calculation of an absolute photon flux. Both the incidence angle and the take-off angle can be freely chosen. The incidence angle θ_{e^-} is defined here as the angle between target surface and electron beam within a plane spanned by electron beam and surface normal. The take-off angle θ_{γ} in turn is defined as the angle between target surface and direction of photon emission, opposite the incidence angle (Fig. 1). We use the notation $\langle \theta_{e^-} \rangle / \langle \theta_{\gamma} \rangle$ to describe target geometries, e.g. 78°/12° denotes a target with 78° incidence angle and 12° take-off angle.

In order to take into account the angle of emission for the produced bremsstrahlung photons, the distribution of electron directions is required. The depth of emission is needed to calculate attenuation of the produced photons, i.e. self-absorption within the target. Consequently, the first step of the model is to prepare a discretized distribution of electron travel paths, differential in electron energy, depth within target, and direction of electron movement. This distribution is used to calculate the bremsstrahlung emission as well as the atomic excitation due to electrons and the subsequent emission of characteristic radiation. The photons emitted along the configured take-off direction can be immediately added to the resulting spectrum. In addition, the full emission for each depth is stored for use in calculating secondary contributions of characteristic radiation. Self-absorption is considered for all contributions by attenuating them according to the distance traveled inside the target depending on depth of emission and the take-off angle. During this step scattering inside the target is not considered, as it has been found to be of negligible impact. At low photon energies absorption is the dominant process, while at higher energies the overall interaction probability is very low. This latter fact is due to the mean free path for a photon of such an energy being much larger than the penetration depth of the electrons. See Fig. 2 for an overview of the calculation scheme.

2.1. Electron transport

Preparing the distribution of electron travel distances is done by evaluating the probability density distribution of electron depths and directions after each scatter interaction, i.e. a singlescattering approach is used. Initially the electrons are assumed to be located at the target surface and have kinetic energy corresponding to the acceleration potential. Their direction of movement is given by the angle of incidence, although there is an inherent uncertainty in representation due to the angle discretization of the distribution. A typical discretization choice is 40 bins uniformly distributed in -1 to 1 for $\cos(\theta)$, where θ is the polar angle of the electron's direction relative to the surface normal, 18 bins uniformly distributed in 0 to π for the azimuth angle ϕ , and 50 uniformly distributed bins for the depth. The considered depths range from the target surface to the minimum of the target thickness and twice the electron diffusion depth as defined in [8]. A finer discretization choice, in particular for the angles, can improve results, but will also increase calculation times. A coarser discretization can be used for fast estimates.

The mean free path between electron scatter interactions for the current electron energy is determined from the input material data. The current probability density distribution and this path are used to update the result distribution, i.e. the electron travel distances and the depth distribution of electrons. The updated distribution of directions for each depth is determined by approximating the convolution of the current electron directions with the probability density distribution of scatter angles for the current electron energy. Finally, the average energy loss between scatter interactions is calculated according to [9,10]. This procedure is repeated until the minimum electron energy is reached. Secondary electrons are not currently taken into account. A more detailed description of the electron transport model is given in [11].

2.2. Bremsstrahlung

Bremsstrahlung is directly produced by the energetic electrons inside the target. Modeling this contribution is therefore relatively straightforward. Bremsstrahlung production cross sections can be taken either from the input material data or from [12,13]. The total bremsstrahlung emission at different depths can be calculated from the production cross sections and the distribution of electron travel distances (see Section 2.1). Since all produced photons can interact before leaving the target and in doing so create characteristic radiation, this full emission is stored for later use (see Section 2.3). For directional emission according to the chosen take-off angle, the angular dependence of bremsstrahlung emissions is taken into account using shape functions from [14] below 500 keV and from [15] for higher electron energies.

2.3. Characteristic radiation

Characteristic radiation results from atomic excitation due to either electrons or photons. Subsequent relaxation of excited atoms leads to emission of photons with energies characteristic for the material. The direct contribution due to electrons is calculated at the same time as the bremsstrahlung contribution. This step uses excitation and relaxation probabilities from the loaded material data in addition to the previously calculated electron



Fig. 1. Definition of incidence angle θ_{e^-} and take-off angle θ_{γ} .

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