Computational Toolset for X-ray Spectral Analysis

Cheol-Soon Shon\textsuperscript{1}, Ho Kyung Kim\textsuperscript{1,a}, Min Kook Cho\textsuperscript{1}, Min Ho Cheong\textsuperscript{1}, Chang Hwy Lim\textsuperscript{1} and Jung-Min Kim\textsuperscript{2}

\textsuperscript{1}School of Mech. Eng., Pusan National University, Jangjeon, Geumjeong, Busan 609-735, Korea
\textsuperscript{2}College of Health Sciences, Korea University, Jeongreung, Seongbuk, Seoul 136-703, Korea
\textsuperscript{a}Correspondence to hokyung@pusan.ac.kr

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Abstract. We have designed a computational tool for generating X-ray photon spectra for a range of applications both in diagnostic radiology and mammography. As a library, we have adapted the spectral data based on the interpolating polynomials methods by Boone et al\cite{5,6} as well as the computer data files given by Cranley et al\cite{8}. The attenuated spectra for element or compound materials can be calculated based on the mass-attenuation coefficients from NIST (National Institute of Science and Technology), which were also incorporated as a database. Furthermore, a function that a user can generate any filter material by editing the NIST data has been implemented. Parameters related to the beam quality, such as mean photon energy, fluence, exposure, half-value layer (HVL), etc., are considered as important outputs. All of functions and database are integrated in a form of graphical user interface (GUI) by using Microsoft Visual C++\textsuperscript{TM}. This self-developed spectrum-generating code can be usefully served to design X-ray sensors. In this study, we have applied the code to estimate quantum efficiency and charge collection efficiency in various detector materials.

Introduction

It is essential to know the detailed X-ray spectra for modeling, design, and optimization of imaging detectors or systems\cite{1,2}. The direct measurement of the spectra is desirable but difficult to be realized because of high rate of X rays, expensive experimental setups, and tremendous efforts on the analysis\cite{3,4}. Moreover, a wide range of energy and various combinations of X-ray tube settings in diagnostic radiology and mammography make the measurements time-consuming. When modeling or designing an imaging system, instead, many studies have been based on simple approximations, for example, a monoenergetic X-ray beam with mean or effective energy.

Prediction of the X-ray spectra can be alternative. There are several approaches of the prediction of the spectra such as empirical\cite{5,6}, semi-empirical calculations\cite{7,8} and Monte Carlo simulations\cite{1,3}. We have developed a user-friendly computational toolset for X-ray spectral analysis (we call it \textit{Xtailor}). Similar approach based on the empirical model, or TASMIP algorithm\cite{5} was previously reported\cite{9}, which was written by a high-level language, Matlab\textsuperscript{TM}. In addition to that empirical model, we incorporated semi-empirical model\cite{7,8} as an additional library for the complementary and comparative utility. The \textit{Xtailor} calculates various beam-quality characteristics of the spectra such as mean X-ray energy, fluence, exposure, and half-value layer (HVL). In this paper, we present a detailed algorithm of \textit{Xtailor} and demonstrate its usefulness related to the detectors design.

Methods and Validation

Using Microsoft Visual C++\textsuperscript{TM}, we have designed the \textit{Xtailor} in a form of graphical user interface (GUI) to allow convenient calculation and generation of the X-ray spectra. As shown in Fig. 1, the main window of the \textit{Xtailor} consists of four functional panels. Panel \textbullet\ provides a selection of library for the unattenuated X-ray spectra and a setup for X-ray tube operation such as the target material, the tube voltage, the voltage ripple, and the target (or anode) angle. The \textit{Xtailor} directly incorporates two
libraries for the unattenuated X-ray spectra; the empirical model based on the interpolating polynomials method of the measured spectra [5,6] and the semiempirical model [7,8]. Operation parameters and characteristics of the models are given in Table 1.

<table>
<thead>
<tr>
<th>Model</th>
<th>Diagnostic radiology</th>
<th>Mammography</th>
<th>Diagnostic radiology</th>
<th>Mammography</th>
</tr>
</thead>
<tbody>
<tr>
<td>Target material</td>
<td>W</td>
<td>W, Mo, Rh</td>
<td>W</td>
<td>Mo, Rh</td>
</tr>
<tr>
<td>Tube voltage [kV]</td>
<td>30 – 140</td>
<td>20 – 40</td>
<td>30 – 150</td>
<td>25 – 32</td>
</tr>
<tr>
<td>Voltage interval [kV]</td>
<td>1</td>
<td>5</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Energy bin [keV]</td>
<td>1</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>Ripple [%]</td>
<td>0 – 100</td>
<td>NA</td>
<td>0 – 30(^a)</td>
<td>NA</td>
</tr>
<tr>
<td>Ripple interval [%]</td>
<td>Arbitrary</td>
<td>NA</td>
<td>5</td>
<td>NA</td>
</tr>
<tr>
<td>Anode angle [°]</td>
<td>NA</td>
<td>NA</td>
<td>6 – 22</td>
<td>9 – 23</td>
</tr>
<tr>
<td>Angle interval [°]</td>
<td>NA</td>
<td>NA</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

\(^a\)For tube voltage from 55 [kVp] to 90 [kVp] with an interval of 5 [kV].

In order to meet various imaging conditions in diagnostic radiology and mammography, it is necessary to tailor the unattenuated X-ray beam profile. The Xtailor uses the Lambert-Beers law of exponential attenuation for the specified materials and thicknesses. Elemental filter materials and their mass-attenuation coefficients \(\mu/\rho(E)\), in which \(\mu\) is the linear-attenuation coefficient and \(\rho\) is the physical density of the material, are based on the database of NIST (National Institute of Standard and Technology, USA). Specification of elemental materials and thicknesses is given by the panel \(\oplus\). For a flexible design of the compound materials and the corresponding \(\mu/\rho(E)\), the panel \(\otimes\) provides an additional function in the form of separate window as shown in Fig. 2. A compound material can be defined by stoichiometric number of constituents or weight fraction (see the panel \(\oslash\) of Fig. 2). The resultant \(\mu/\rho(E)\) can be displayed (see the panel \(\odot\) of Fig. 2) and transferred to the main window for the further analysis.

After manipulation of beam tailoring, the resultant X-ray spectrum is displayed in the panel \(\ominus\) of the main window. Quantitative beam-quality characteristics are simultaneously shown in the panel \(\ominus\) such as mean photon energy, fluence per unit exposure and exposure, and HVL, which are estimated as follows.

The mean photon energy is calculated by

\[
\bar{E} = \frac{\int_0^{kVp} \Phi(E)dE}{\int_0^{kVp} \Phi(E)dE}
\]  

where \(\Phi(E)\) is the X-ray spectrum and kVp is the applied tube peak voltage. The fluence per unit exposure can be estimated for a given spectrum as

\[
\phi_X = \frac{\int_0^{kVp} \Phi(E)[\Phi_X(E)]dE}{\int_0^{kVp} \Phi(E)dE}
\]  

where \(X\) is the exposure in Roentgen or [R]. In this equation, the fluence per unit exposure for monoenergetic beam with energy \(E\) is calculated by

\[
\phi_X(E) = \frac{Q_{air}W_{air}}{qE\left(\frac{\mu_{en}(E)}{\rho}\right)_{air}}
\]
where $Q_{air}$ is the charge generated in air by one Roentgen ($= 2.58 \times 10^{-4} \text{ C/kg-R}$) and $W_{air}$ is the average ionization energy of air ($= 34 \text{ eV}$), $q$ is the electronic charge ($= 1.6 \times 10^{-19} \text{ C}$), and $(\mu_{en}(E)/\rho)_{air}$ is the mass-energy-absorption coefficient [cm$^2$/g] as a function of energy for air. The exposure can therefore be calculated by

$$X = \int_0^{kVp} \frac{\Phi(E)}{\Phi/X(E)} dE.$$  \hspace{1cm} (4)

The HVL is the thickness of aluminum required to reduce the calculated exposure by 50% and computed in this study by the numerical bisection method. All the beam-quality characteristics as well as the X-ray spectrum are evaluated at a distance of 1 m. After the spectrum is specified and the beam-quality characteristics are evaluated for the input parameters, any change of distance can be applied and the Xtailor instantly recalculates the change.

Comparison of the X-ray spectra calculated from the Xtailor and the original empirical and (Right) semiempirical models for a tungsten target. The relative error between them is also given.

Comparison of the X-ray spectra calculated from the Xtailor and the original empirical model for a tungsten target is shown in Fig. 3 (Left). Filtration by a 2.5-mm-thick aluminum was considered.
Relative error between them was calculated, and the maximum error was about 3.5% at the lower energy region. This is due to the slight difference of the interpolated \( \mu/\rho(E) \) values. Figure 3 (Right) also shows comparison between the Xtailor and the original semiempirical model for the same conditions. The relative error in the worst case is about 1%.

### Table 2 Various detectors and their mean ratio of atomic number-to-mass.

<table>
<thead>
<tr>
<th>Detector</th>
<th>Si</th>
<th>GaAs</th>
<th>Se</th>
<th>CdZnTe(^a)</th>
<th>Gd(_2)O(_2)S</th>
<th>CdTe</th>
<th>CsI</th>
<th>HgI(_2)</th>
<th>PbI(_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Z/A</td>
<td>0.49848</td>
<td>0.44246</td>
<td>0.43060</td>
<td>0.42391</td>
<td>0.42265</td>
<td>0.41665</td>
<td>0.41569</td>
<td>0.40933</td>
<td>0.40781</td>
</tr>
</tbody>
</table>

\(^a\)Cd\(_{0.1}\)Zn\(_{0.9}\)Te.

Applications

**Detector Quantum Efficiency.** One of the most important performances of detectors is quantum efficiency. We have calculated the quantum efficiency of the various detector materials by simple exponential attenuation accounting for the X-ray spectrum. The X-ray spectrum was obtained from the Xtailor for a tungsten target operated at 120 kVp and beam filtration by a 40-mm-thick aluminum, which corresponds to the radiation quality number 9 or RQA9 of IEC (International Electrotechnical Commission). The considered detector materials are described in Table 2 in which \( Z/A \) is the mean ratio of atomic number-to-mass. The thickness of detector was assumed to 500 \( \mu \)m. For comparison, the quantum efficiency was also calculated for the monoenergy approximation with the mean photon energy of the X-ray spectrum. Figure 4 compares the results. Overall the monoenergy approximation underestimates. In order to validate the result, Monte Carlo simulation was performed, which gives a good agreement with the results of the X-ray spectrum except Cd\(_{0.1}\)Zn\(_{0.9}\)Te.

**Charge Collection Efficiency.** Compound semiconductor such as CdZnTe, HgI\(_2\) and PbI\(_2\) is recently paid attention as a new detector material for large-area digital radiography because of high quantum efficiency as shown in Fig. 4 [10]. Nevertheless, the compound semiconductor suffers from incomplete charge collection with a large fluctuation due to trapping-detrapping of charge carriers, and which may restrict the operation in real-time imaging. For the reliable use of the compound detector in an imaging system, the optimal design of the operation parameters, for example, charge integration time and applied bias voltage, should be made. In this study, we have theoretically investigated the charge collection property in compound detectors with an X-ray spectrum and monoenergy approximation.

The signal generation or charge collection in a planar semiconductor detector is described by the well known Hecht equation [11], in which the incomplete charge collection is handled by the simple deep trapping approximation and the concept of mean lifetime. We applied the Hecht equation to the case of the distributed charge generation through the detector by the incident X-ray photons in a direction perpendicular to the electrodes. Total induced charge at the external circuit for a given detector thickness \( L \) and a charge integration time \( \tau_C \) is given by integrating the induced current due to...
\[ Q_{\text{ind}} = \int_0^L dx_0 \int_0^\tau_{x_0} I_{\text{ind}}(x_0, t) dt \]  
\[(5)\]

and

\[ I_{\text{ind}, j}(x_0, t) = \frac{\mu_j V_A}{L^2} \times n_0(x_0) e^{-t/\tau_j} \]  
\[(6)\]

where the subscript \( j \) implies the corresponding charge carrier, \( \text{viz.}, e \) and \( h \) for the electron and hole. \( \mu \) and \( \tau \) describe the mobility and the lifetime of the charge carrier, respectively. \( V_A \) is the applied bias voltage. It is noted that the number of charge carriers generated at a position \( x_0 \) or \( n_0(x_0) \) has a unit of \([\text{cm}^{-1}]\).

The transit time larger than the integration time causes a ballistic deficit and this can cause an image lag in imaging application. In such cases, some of the charges are regarded as fully collected charges whereas the others are not. However, it is important to note that the charges other than the fully collected still contribute to the induced charge (or signal) by drift motion during the charge integration time. This fractional signal contribution was also considered in this study by identifying the location of the non-fully collected charges. This approach was experimentally verified in the previous work \([11]\).

We have calculated the charge collection efficiency for two compound detectors; \( \text{Cd}_{0.1}\text{Zn}_{0.9}\text{Te} \) and \( \text{Hgl}_2 \). The thickness was assumed to 500 \( \mu \text{m} \). The applied bias voltage is based on \( 10^4 \) V/cm. \( \mu_e, \mu_h, \tau_e, \) and \( \tau_h \) of \( \text{Cd}_{0.1}\text{Zn}_{0.9}\text{T} \) were taken to 1000 \( \text{cm}^2/\text{V} \cdot \text{s} \), 50 \( \text{cm}^2/\text{V} \cdot \text{s} \), 5 \( \mu \text{s} \), and 1.5 \( \mu \text{s} \), respectively. Those of \( \text{Hgl}_2 \) were 80 \( \text{cm}^2/\text{V} \cdot \text{s} \), 5 \( \text{cm}^2/\text{V} \cdot \text{s} \), 50 \( \mu \text{s} \), and 4 \( \mu \text{s} \). For the incident X rays upon the electrode biased negatively, the X-ray spectrum was calculated from the \textit{Xtailor} for IEC’s RQA8 (100 kVp and filtration of 34-mm-thick aluminum), and the corresponding mean photon energy was 67.2 keV. Figure 5 shows the calculated charge collection efficiency as a function of integration time. For two detectors, the results show an opposite trend; monoenergetic approximation overestimates \( \text{Cd}_{0.1}\text{Zn}_{0.9}\text{Te} \) whereas underestimates \( \text{Hgl}_2 \). In addition, significant difference is found for \( \text{Hgl}_2 \). The same tendency is observed in the charge collection efficiency as a function of field intensity as shown in Fig. 6. Therefore, the elaborate design of a detector or an imaging system, the X-ray spectral analysis is necessary.

![Fig. 5 Calculated charge collection efficiency as a function of integration time.](image1)

![Fig. 6 Calculated charge collection efficiency as a function of field intensity.](image2)
Summary
A user-friendly computational toolset to allow convenient calculation of the X-ray spectrum, filtration, and spectral characteristics such as mean photon energy, fluence, exposure, and HVL has been developed in the form of GUI. The unattenuated X-ray spectra were straightforwardly integrated from the well-known empirical and semiempirical models. Based on the attenuation coefficients from NIST, any compound filter material can be designed. From the comparison with the original models, the calculated X-ray spectra showed a good agreement. Compared with the detector quantum and charge collection efficiencies calculated based on the monoenergy approximation, the importance and utility of the X-ray spectral analysis have been addressed. The developed toolset will be very useful for the X-ray spectral analysis of a detector or an imaging system.

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