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Theoretical characterization of imaging performance of screen-printed mercuric iodide photoconductors for mammography

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ABSTRACT: We theoretically characterize the imaging performance of a hypothetical mercuric iodide (HgI₂) photoconductor prepared by a screen printing method in terms of the spatial-frequency-dependent detective quantum efficiency (DQE) using the cascaded-systems analysis. In the DQE model, we use the “photon-interaction process” in order to represent both the selection of interacting photons and subsequent conversion gain as a single process because both processes are not statistically independent but their probabilities are determined by the photon energy. We further include the thermal generation process of leakage current charges and the incomplete charge-collection process in the DQE model. Theoretical imaging performances of the hypothetical HgI₂ photoconductor sample are compared with those of a 0.2-mm thick amorphous selenium (a-Se) under mammographic imaging conditions. It is shown that the hypothetical HgI₂ with a smaller value of the average ionization energy than a-Se gives a better DQE performance at lower exposure levels, which suggests that a HgI₂-based photoconductor may have the potential to reduce the

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patient dose in mammography applications. We believe that our theoretical assessment of imaging performances will be useful for determining the feasibility of novel photoconductor materials for x-ray imaging applications.

KEYWORDS: Detector modelling and simulations II (electric fields, charge transport, multiplication and induction, pulse formation, electron emission, etc); Detector modelling and simulations I (interaction of radiation with matter, interaction of photons with matter, interaction of hadrons with matter, etc); X-ray radiography and digital radiography (DR); X-ray detectors
1 Introduction

The imaging performance of a radiography detector is limited by the statistical properties and spatial correlation of the number of secondary quanta (e.g., optical photons in a scintillator or electron-hole pairs in a photoconductor) liberated in an x-ray convertor material [1]. Signal and noise properties of the detected secondary quanta are determined by complicated combinations of x-ray interaction physics, secondary quanta transport, and material/device properties. The cascaded linear-systems theory describing signal and noise propagation through image-forming processes is a powerful tool for the analysis of imaging performance of digital radiography detectors, and has been practically and successfully used for the evaluation of various radiography detectors [2–7]. The cascaded-systems analysis (CSA) approach enables an understanding of detector performance limitations as governed by the statistical characteristics of image-forming processes, making CSA analyses a critical step in the design and optimization of new digital radiography detectors [8].

While only amorphous selenium (a-Se) has been successfully commercialized as a photoconductor for direct-conversion digital mammography detectors because of its own advantages, such as large-area fabrication and reproducibility, other candidate photoconductor materials are being investigated by several researchers [9] to advance the performance of photoconductor-based x-ray imaging detectors. We are developing polycrystalline photoconductors consisting of high atomic number materials, such as mercuric iodide (HgI$_2$) and cadmium telluride (CdTe), using screen printing and vacuum deposition methods respectively, for low-dose imaging applications.

To study the feasibility of screen-printed HgI$_2$ for low-dose mammography, in this study we theoretically characterize its imaging performance in terms of the spatial-frequency-dependent detective quantum efficiency (DQE) using the CSA approach, and compare its performance with that of 0.2-mm thick a-Se under mammographic imaging conditions (W/Rh spectrum). To reflect its electrical properties, we have extended previous work on the DQE model described by the photon-interaction process [10] to include the influence of thermally generated leakage current.
Figure 1. Schematic block diagram describing the signal and noise propagations in photoconductor-based x-ray detectors. The overhead tilde designates a random variable.

charges [11] and incomplete charge collection [12] and use this to develop an analytic expression to describe the DQE of photoconductor-based x-ray imaging detectors. We believe the analytic approach described in this study provides important insight in designs and development directions of new radiographic detectors.

2 Theoretical background

Since CSA is only successful for linear and shift-invariant imaging systems [13], we have made the same assumption on the development of a theoretical DQE model of photoconductor-based x-ray imaging detectors.

Signal and noise transfer in photoconductor-based x-ray detectors can be described by a cascade of serial stages representing elementary image-forming processes, as shown in figure 1. The model starts with a “coupled interaction” stage [14] to simultaneously describe an interaction of incident x-ray photons with the photoconductor and its conversion to secondary quanta (i.e., electron-hole pairs), which was firstly introduced by our group [10]. This process was devised based on the fact that, when an x-ray photon is incident on a detector, both the probability of interaction and the energy deposited are functions of the energy of the incident photon, and those are not statistically independent. To reflect the respective electrical properties in different photoconductors, unlike the previous model [10], we considered two more processes: (1) the thermal generation of leakage current charges which are spatially uncorrelated and statistically independent with signal charges generated by incident photons [11]; and (2) the incomplete collection of generated charges due to the charge trapping and insufficient integration time [12]. Both of these processes are mainly determined by the electrical properties of photoconductors such as the dark current density $J$, which is dependent upon the electric field intensity $F$ applied to photoconductors, and the mobility-lifetime product $\mu_j \tau_j$, where $\mu_j$ and $\tau_j$ denote mobility and lifetime for the charge carrier of $j$. In addition to material properties, the integration time $\tau_{\text{int}}$ of the imaging detector, which is the detector operation parameter, was also considered.

Based on the previous works [10, 11], the analytic expression of spatial-frequency-dependent DQE describing the model under investigation in this study can be given by

$$DQE(u,v) = \frac{\tilde{q}_0 (a^2 \eta M_1 / w)^2}{\tilde{q}_0 a^2 \eta^2 M_1 w \sum_{n=0}^{\infty} \left\{ \left[ \frac{M_1}{w \tau_{\text{int}}} - 1 \right] T_x^2 \left( u \pm \frac{n \pi}{p}, v \pm \frac{n \pi}{p} \right) + \frac{w \delta_{\text{gen}}}{M_1 \tau_{\text{int}} + \frac{1}{\eta}} \right\} T_d^2 \left( u \pm \frac{n \pi}{p}, v \pm \frac{n \pi}{p} \right) + p^2 \sigma_{\text{add}}^2},$$

(2.1)
where \((u, v)\) is the Fourier conjugate of the two-dimensional (2D) spatial variables, \(\overline{q}_0\) is the average number of incident photons \([\text{mm}^{-2}]\), \(w\) is the average energy (in eV) to liberate an electron-hole pair, and \(\eta\) is the collection efficiency of generated charges. Assuming square pixel geometry, \(a\) and \(p\) denote active aperture width and pixel pitch, respectively. \(T_x\) and \(T_a\) denote the modulation-transfer functions describing the scattering of x-ray photons and the blurring due to the pixel aperture, respectively. We note that \(T_a\) is described by the “sinc” function. \(M_i\) is the \(i\)-th moment of the absorbed energy distribution (AED) which describes the average distribution of deposited energies in photoconductors for incident photons \([10, 15]\). Uncorrelated noise terms due to additive readout electronic noise \(\sigma_{\text{add}}\) and thermal noise \(\delta_{\text{gen}}\) were also considered. Thermal noise \(\delta_{\text{gen}}\) can be defined as \([5]\)

\[
\delta_{\text{gen}} = \sqrt{\frac{J_{\text{int}}}{e}},
\]

where \(e\) is the electronic charge \((1.6 \times 10^{-19} \text{ C})\). When \((u, v) = (0, 0)\), we have the zero-spatial-frequency DQE such that

\[
\text{DQE}(0) = \left[ \frac{M_2}{M_1^2} + \frac{w}{M_1} \left( \frac{1}{\eta} - 1 \right) + \frac{1}{\overline{q}_0} \left( \frac{w}{M_1} \right)^2 \left( \delta_{\text{gen}}^2 + \frac{p^2 \sigma_{\text{add}}^2}{a^2 \eta^2} \right) \right]^{-1}.
\]

### 3 Methods

#### 3.1 Material parameters for calculations

Table 1 summarizes material parameters for \(\text{HgI}_2\) and \(a\)-Se required for the CSA analysis in this study. The \(a\)-Se detector with a thickness of 0.2 mm was selected as a reference because it is widely used for the current generation of digital mammography detectors. In order to emphasize the effects of secondary quanta transport on the DQE performance, we selected \(\text{HgI}_2\) with a thickness of 0.185 mm, which provides a quantum efficiency similar to the reference \(a\)-Se system. In addition, we performed the CSA assuming that \(\sigma_{\text{add}} = 0\) to exclude the effects of electronics; hence investigating the performances due only to photoconductors themselves. It is noted that the material parameters describing \(\text{HgI}_2\) in table 1 are the values taken from reference \([16]\) and the measured values from the fabricated screen-printed \(\text{HgI}_2\) layers in this study. We call these the ideal and measurement parameters, respectively, hereafter.

#### 3.2 Monte Carlo simulations

To simulate x-ray photon transport in each photoconductor material, we used the latest version of Monte Carlo N-Particle transport code (MCNP Version 5, the Radiation Safety Information Computational Center or RSICC, Oak Ridge, TN). The particle tracking (pTrac) tally was used to track the interaction locations and deposited energy for each incident photon. It was assumed that the pencil-like photon beam was incident perpendicular to the center position of the semi-infinite thin slab geometry. We considered the photon beam as the W/Rh spectrum, which was obtained from the IEC standard radiation quality \([17]\), for the simulation of mammography. From the Monte Carlo simulation results, we obtained 2D spatial distributions of energy absorption, and then calculated AED, \(M_i\), and \(T_x\) for the CSA simulations \([10]\).
Table 1. Material parameters used for the cascaded-systems analysis.

<table>
<thead>
<tr>
<th>Material</th>
<th>( a\text{-Se} )</th>
<th>( \text{HgI}_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Preparation</td>
<td>Vacuum deposition</td>
<td>Screen printing</td>
</tr>
<tr>
<td>State</td>
<td>Amorphous</td>
<td>Polycrystalline</td>
</tr>
<tr>
<td>Parameters</td>
<td>Taken from reference [16]</td>
<td>Measurements</td>
</tr>
<tr>
<td>Density, ( \rho ) (g/cm(^3))</td>
<td>4.3</td>
<td>6.3</td>
</tr>
<tr>
<td>( w ) (eV)</td>
<td>45</td>
<td>5</td>
</tr>
<tr>
<td>( \mu_c \tau_c ) (cm(^2)/V)</td>
<td>( \sim 5.15 \times 10^{-6} )</td>
<td>( \sim 5.5 \times 10^{-6} )</td>
</tr>
<tr>
<td>( \mu_h \tau_h ) (cm(^2)/V)</td>
<td>( \sim 3.05 \times 10^{-5} )</td>
<td>( \sim 10^{-7} )</td>
</tr>
<tr>
<td>( F ) (V/( \mu )m)</td>
<td>( \sim 10 )</td>
<td>( \sim 1 )</td>
</tr>
<tr>
<td>( J ) (pA/mm(^2))</td>
<td>(&lt; 10 ) up to ( F = 20 ) V/( \mu )m</td>
<td>( \sim 8 ) at ( F = 1 ) V/( \mu )m</td>
</tr>
</tbody>
</table>

Figure 2. 3D representations of the calculated DQE\((u)\) performances: (a) \( a\text{-Se} \), (b) \( \text{HgI}_2 \) with the measured parameters, and (c) \( \text{HgI}_2 \) with the ideal parameters with respect to spatial frequency and exposure.

4 Results and discussion

Figure 2 shows the calculated DQE performance as a function of spatial frequency and x-ray exposure in three-dimensional (3D) representations. For the given exposure range \( (10^{-4}-1 \) mR or equivalently \( 8.71 \times 10^{-4}-8.71 \mu \text{Gy} \) or \( 2.58 \times 10^{-11}-2.58 \times 10^{-7} \) C/kg), the DQE\((u)\) of \( \text{HgI}_2 \) calculated with the measured parameters is slightly better than that of \( a\text{-Se} \), as shown in figures 2(a) and (b). We note that the DQE\((u)\) performance of both materials gradually degrades with decreasing x-ray exposure and the speed of these degradations is accelerated for exposure levels less than \( \sim 10^{-3} \) mR \( (8.71 \times 10^{-3} \mu \text{Gy} \) or \( 2.58 \times 10^{-10} \) C/kg). These degradations are due to non-negligible thermal noise at lower exposures. Since the thermal noise was modeled as an additive white noise in the Fourier domain, which is true for uniform photoconductors over area in this study, it can significantly reduce DQE\((u)\) especially at higher spatial frequencies where the number of secondary quanta lessens. On the other hand, this observation is negligible in the DQE\((u)\) of \( \text{HgI}_2 \) calculated with the ideal parameters, as shown in figure 2(c). As noted in table 1, we can speculate that the \( w \) value plays a primary role in these observations. In other words, the lowest \( w \) value implies the largest number of secondary quanta, thereby making DQE\((u)\) insensitive to the addition of thermal noise at lower exposure levels.
Figure 3. 3D representations of the calculated DQE(u) performances: (a) α-Se, (b) HgI₂ with the measured parameters, and (c) HgI₂ with the ideal parameters with respect to spatial frequency and integration time.

Figure 4. 3D representations of the calculated DQE(0) performances: (a) α-Se, (b) HgI₂ with the measured parameters, and (c) HgI₂ with the ideal parameters with respect to exposure and integration time.

The effects of integration time on the DQE(u) performance calculated for three photoconductors are summarized in figure 3. Even when decreasing the integration time down to $10^{-3}$ seconds, degradation in DQE(u) performance is not noticeable. While it is obvious that the insufficient integration time limits the charge collection efficiency [12], the thicknesses of photoconductors and/or $\mu_j \tau_j$ characteristics considered in this study are thin and/or large enough for the full charge collection even for the small integration time of $10^{-3}$ seconds.

Figure 4 shows the DQE(u) performance as a function of exposure and integration time, and the trends are similar to figure 2: slightly better performance of HgI₂ with the measured parameters than that of α-Se, and excellent performance of HgI₂ with the ideal parameters. These observations can be more clearly illustrated by one-dimensional (1D) representations with respect to each parameter.

For the low exposure level (0.1 mR or $8.71 \times 10^{-1} \mu\text{Gy}$ or $2.58 \times 10^{-8} \text{C/kg}$) and integration time ($10^{-1}$ seconds), as shown in figure 5(a), HgI₂ provides a DQE(u) performance comparable to that of α-Se, with the DQE(u) of HgI₂ slightly better than that of α-Se at spatial frequencies less than 3 mm$^{-1}$. The gain in dose reduction when we use the HgI₂ for mammography is well illustrated in figure 5(b), and this gain comes from the lower $w$ value as explained earlier. If we can lower the $w$ value down to the ideal value of 5 eV, we can achieve $\sim 90\%$ of DQE at the zero frequency due to the HgI₂ itself even for the extremely low exposure level of $10^{-4}$ mR.
The collection noise factor [18], which describes statistical noise due to incomplete charge collection accounting for the random depth positions at which charges are generated, was also calculated. For the given electrical properties, the effect of collection noise on DQE($u$) performance of HgI$_2$ was negligible. Although it is known that a poor charge collection results in a secondary quantum sink [3], and which can cause a degradation in DQE performance, this problem may be partly mitigated by a smaller $w$ value which can provide higher secondary quantum conversion gain.

Although we analyzed the DQE performance of HgI$_2$ with the assumption that $\sigma_{\text{add}} = 0$, the effect of non-zero $\sigma_{\text{add}}$ values on the DQE performance was more significant than that of $\delta_{\text{gen}}$. As shown in eqs. (2.1) and (2.3), $\sigma_{\text{add}}$ appears in the spatial-frequency domain as white noise. Therefore, $\sigma_{\text{add}}$ can significantly reduce DQE($u$) at higher spatial frequencies where the number of secondary quanta lessens, similar to the effect of $\delta_{\text{gen}}$. The last parenthesis term, $\delta_{\text{gen}}^2 + p^2 \sigma_{\text{add}}^2 / a^4 \eta^2$ in eq. (2.3), clearly shows the competition between the two additive noise terms. Since $a \approx p$ with a width less than 0.1 mm in most photoconductor-based detectors for mammography, the last parenthesis term can be approximated to $\delta_{\text{gen}}^2 + 10^2 \sigma_{\text{add}}^2$ with negligible incomplete charge collection. Therefore, the effect of the electronic noise on the DQE performance is larger than that of the photoconductor thermal noise by at least a factor of $10^2$.

5 Conclusion

We have developed the DQE formula for assessing the impact of x-ray and secondary quanta interactions in photoconductor detectors, and applied it to hypothetical HgI$_2$ photoconductors for investigating their use in mammography. Compared to a conventional $\alpha$-Se photoconductor, the effect of signal loss and additional noise from incomplete charge collection had negligible impact on the DQE performance, whereas the larger secondary quantum gain due to the lower $w$ value made HgI$_2$ photoconductors immune to the addition of thermal noise; hence providing the potential for the low-dose mammography. Consequently, finding or developing a photoconductor having a $w$ value as low as possible will be key for the realization of low-dose mammography.
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