Simulation of one-dimensionally polarized X-ray semiconductor detectors

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ABSTRACT

A pixelated X-ray semiconductor detector (=“direct converter”) is studied which contains an inhomogeneous electric field parallel to the depth axis caused by different concentrations of ionized dopants. X-ray energy depositions and charge movements within the detector are modeled in Monte-Carlo simulations giving access to a statistical analysis of electron drift times and current pulse widths for various degrees of static polarization. Charges induced on the pixel electrodes and pulse heights are evaluated and put to histograms of spectral detector responses and pulse height spectra, respectively, considering energy measurements before and after electronic pulse shaping. For n-doped semiconductors, the detector performance degrades due to pulse broadening. In contrast, a moderate p-doping can improve the detector performance in terms of shorter electron pulses, as long as the detector is not limited by dynamic polarization.

Keywords: x-ray photon counting detector, direct converter, polarization, polarized CZT, CdTe, Monte Carlo simulation, current pulse width, spectral response, pulse height spectrum

1. INTRODUCTION

Energy resolving direct conversion detectors promise several advances in X-ray medical imaging. The possibility to estimate the energy of transmitted photons enables additional features like material separation, higher spatial resolution, beam hardening correction and ideally a higher signal-to-noise ratio. Direct conversion X-ray and gamma ray detectors typically consist of a layer of semiconducting material with metal electrodes on the surface between which a voltage is supplied. Incident X-ray photons produce a large number of electron-hole pairs almost proportional to the absorbed photon energy. Due to the electric field, the holes and electrons drift in opposite directions until they are collected by the metal electrodes. Typically, the metal electrodes are segmented to spatially resolve the incident photons. A convenient segmentation is the use of a continuous metal electrode on the surface through which the photons are incident, and an array of pixel electrodes on the opposite surface. In this geometry, position and energy of an absorbed photon can be determined from the current pulse induced on the corresponding pixel electrode.

To understand the signal generation in more detail, one has to distinguish between three relevant mechanisms. Firstly, the X-ray transport within the detector needs to be modeled. Often, the photon energy is not deposited at a single position but can be spread to several positions within the detector if the photon undergoes Compton scattering or photoelectric absorption followed by an emission of a fluorescence photon. Secondly, the movement of a charge induces a current on all pixel electrodes, thus the physics of the movement of charge clouds has to be studied. Thirdly, it has to be analyzed how the electronics generates a digital signal from a specific pulse received from a pixel electrode.

In this work, we study pixelated CdTe or CZT detectors. These materials provide a high X-ray absorption with acceptable electron mobilities, which makes them suitable for spectral X-ray imaging of photon energies up to 150 keV typical for computed tomography (CT). Due to intra-pixel X-ray transport, multiple detections of a single incident photon are possible as its energy can be partly transferred to neighbor pixels and trigger simultaneous counts in all involved pixels. Energy transfer is mainly caused from K-fluorescence photons from Cd and Te atoms, but also from Compton scattering of high-energy photons. The K-fluorescence photons can easily propagate for a few hundred µm through the crystal, which results in the reduction of the original photon energy in case that the K-fluorescence photons escape a pixel, or in the measurement of K-fluorescence energies in case that a K-fluorescence photon is incident from a neighbor pixel.

In photoelectric absorptions as well as in Compton scatter events, energy is transferred to primary electrons, which dissipate their kinetic energy by creation of a large number of electron-hole pairs within a range of several µm. As a result, two charge clouds drift in the electric field into opposite directions. During the drift, an electric current is

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capacitively induced on the pixel electrodes. The current pulse shape strongly depends on the size of the pixels, and the location and velocity of the drifting charges, respectively. According to the Shockley-Ramo theorem, the charge $Q$ induced on an electrode by a charge $q$ at location $\vec{r}$ can be calculated with help of its weighting potential $\phi_w(\vec{r})$,

$$ Q = -q \cdot \phi_w(\vec{r}). \tag{1} $$

The weighting potential of a particular pixel is unitless with $0 \leq \phi_w(\vec{r}) \leq 1$, where $\phi_w(\vec{r})$ is unity in the considered pixel electrode and zero in all other electrodes. $\phi_w(\vec{r})$ can be calculated analytically for special geometric setups. The corresponding current $I(t)$ induced on the pixel electrode (i.e. with flow direction from the pixel to the amplifier) is

$$ I = q \cdot \nabla \phi_w(\vec{r}) \cdot \vec{r}. \tag{2} $$

with $\nabla \phi_w(\vec{r})$ representing the gradient of the weighting potential (known as weighting field), and $\vec{r}$ representing the velocity vector of the charge. The total current induced in a pixel is calculated as the sum of the currents of all moving charges according to Eq. (2). To calculate the trajectory of each charge, mainly three effects have to be taken into account. Firstly, the charges drift within an externally supplied electric field. Assuming a homogeneous electric field $E$ like that of an ideal plate capacitor to which a bias voltage $U_{bias}$ is supplied, a detector layer thickness $L$, and a charge mobility $\mu$, the drift velocity $v_d$ is

$$ v_d = \mu E = \mu \frac{U_{bias}}{L}. \tag{3} $$

Secondly, charges diffuse according to a diffusion coefficient $D$. Following the Einstein relation, $D$ is related to the mobility $\mu$ and the temperature $T$,

$$ D = \mu \frac{k_B T}{e}, \tag{4} $$

where $k_B$ is the Boltzmann constant and $e$ is the elementary charge. With time $t$, the charge cloud expansion in space can be approximately described by a Gaussian distribution having a standard deviation

$$ \sigma_r = \sqrt{Dt}. \tag{5} $$

for each direction. Thirdly, Coulomb repulsion occurs for all charges within a cloud, as well as for other charges existing within the detector or on the surface of the metallic conducting electrodes.

Due to the charge cloud extension, charge sharing can occur between neighbor pixels especially for photon energy depositions near pixel borders. This is a strongly unwanted effect, as it triggers multiple counts in the neighbor pixels destroying the original energy information.

A relevant factor for the current integration is the pulse detection electronics for each pixel, which usually has a limited time window for pulse integration. In the practical case of CZT or CdTe detectors as examined in this work, it has to be noted that the mobility of holes, $\mu_h \approx 120 \text{ cm}^2/\text{Vs}$, is by a factor of almost four smaller than the mobility of electrons, $\mu_e \approx 1000 \text{ cm}^2/\text{Vs}$. In consequence, a superposition of two current pulses is detected, one “fast” pulse generated by the electrons, and a “slow” pulse generated by the holes. For reasons of counting performance, it is preferred to detect only the “fast” electron signal, meaning that the available pulse integration time is adapted to the electron pulse. The holes’ signal can be strongly reduced by the “small-pixel effect”, which takes advantage of the weighting potential geometry for the case that the continuous electrode is the cathode (through which the photons are incident), and the electrodes of the pixel array are the anodes. For an appropriate large detector aspect ratio (i.e. the ratio between thickness $L$ and pixel size $w$, typically $L/w > 3$), the volume for which a relevant charge is induced on a particular anode is narrowed down to the immediate vicinity of the anode (see Figure 1 left). As for sufficiently thick material most electron-hole pairs are generated within a cathode-near volume, the holes drifting to the cathode generate a low-weighted signal which is in practice negligible compared to the high-weighted signal of the electrons which is created just shortly before the electrons enter the anode.

Another effect accounting for a charge loss during the integration time is charge trapping at dopants, impurities, dislocations and other crystal defects. In CdTe and CZT pixelated detectors, this could become relevant for electron trapping as long as the electron mean free path $\lambda_e$ is smaller than or comparable to the detector thickness $L$. 
The total charge $Q_e$ collected by a pixel can be approximated analytically under the assumption that within the integration time all non-trapped electrons are collected, all holes are almost stationary, gaps between pixels are negligible small, the electric field inside the detector is homogeneous, Coulomb repulsion is negligible, the drift velocity is much larger than the diffusion velocity, and the electron mean free path is much larger than the detector thickness, $\lambda_e > L$. The corresponding formula for electron and holes generated at a position $\vec{r}_e = (x_e, y_e, z_e)$ is reported to be:

$$Q_e = eN_e \left[ \frac{1}{4} \left[ \text{erf} \left( \frac{x_e + w/2}{\sqrt{2} \alpha z_e L} \right) - \text{erf} \left( \frac{x_e - w/2}{\sqrt{2} \alpha z_e L} \right) \right] \left[ \text{erf} \left( \frac{y_e + w/2}{\sqrt{2} \alpha z_e L} \right) - \text{erf} \left( \frac{y_e - w/2}{\sqrt{2} \alpha z_e L} \right) \right] \cdot \exp \left( -\frac{z_e}{\lambda_e} \right) - \Phi_e(\vec{r}_e) \right]. \tag{6}$$

The coordinate axes $x$, $y$ and $z$ point parallel to the directions of pixel rows, pixel columns, and drift direction of charges, respectively; note that other than in reference [9] we define $z = 0$ as the anode pixel plane, $z = L$ as the cathode plane, set the coordinate origin to the pixel center, and do not normalize geometrical quantities to the detector thickness. $N_e$ is the number of electron-hole pairs created at $\vec{r}_e$. The subtracted weighting potential term $\Phi_e(\vec{r}_e)$ takes into account the remaining charge induction caused by holes which are considered to be stationary relative to the electrons. The parameter $\alpha$ is defined as the ratio between the diffusion and the drift contribution:

$$\alpha = \frac{2D}{v_e L} = \frac{2k_e T}{eU_{bias}}. \tag{7}$$

The error function terms in Eq. (6) are the result of an integral of the charge density over the pixel area after diffusion, with the charge density modeled as a Gaussian distribution $\exp \left( -r^2 / (2\sigma_{xy}^2) \right) / (\sigma_{xy} \sqrt{2\pi})$, where $r_{xy}$ represents the lateral distance to the cloud center, and $\sigma_{xy}$ represents the lateral cloud extension with

$$\sigma_{xy} = \sqrt{\alpha z_e L}. \tag{8}$$

The charge mobility $\mu$ does not contribute to $\sigma_{xy}$, therefore the findings of Eq. (6) to (8) are material independent.

In technical practice, it is not possible to integrate all charges of the electron pulse, as the pulse shape strongly depends on the trajectory of the charge cloud. As an additional challenge, “crosstalk” pulses caused by charge cloud trajectories ending on neighbor pixels have to be correctly identified; these pulses at first generate a positive pulse component which is followed by a compensating negative pulse component, such that the integral current for these pulse types is zero. For trajectories ending near pixel borders, a positive pulse component is followed by a partially compensating negative pulse component, generating typical charge-shared counts in both neighbor pixels, with each count representing only a part of the original total charge. One possibility to deal with such a variety of pulses is to use electronics with an integrating stage followed by a pulse shaper stage. The integrator stage integrates the current pulse and converts it to a step-like voltage function with a long exponential decay time. The pulse shaper stage is essentially a band pass filter which
transforms the integrator signal into a pulse with a pulse height ideally proportional to the integral current. The pulse height is electronically compared to the pre-defined values of a set of discriminator stages representing the energy thresholds. If the pulse height exceeds a threshold of any discriminator, the associated counter is incremented. The described method can be approximated by a convolution of the current pulse $I(t)$ with a pulse shape function $f(t')$,

$$p(t) = \int_{-\infty}^{\infty} I(t') f(t-t') \, dt'.$$

(9)

where $f(t')$ has a width corresponding to the integration time. The detailed form of $f(t')$ is determined by the electronic circuit used; ideally, $f(t') = 1$ corresponds to an exact current integral. As an advantage, the pulse shaping method allows a fast pulse integration at high counting rates with reduced pileup effects. As a disadvantage, the integration is not ideal for non-rectangular pulse shape functions; especially pulse components away from the pulse maximum are not considered adequately.

So far, the electric field $E$ within the detector layer has been considered to be homogeneous. This is however not any more the case if the conversion material is doped by an acceptor concentration $n_A$ or a donor concentration $n_D$. It is known that commercially available CdTe and CZT crystals for imaging purposes have certain doping of both types which are partially compensating each other.\textsuperscript{4} We consider here the case that at the surface of one electrode a “rectifying” contact is made by heavily doping of a thin layer with atoms of the opposite doping type, which creates a pn-junction.\textsuperscript{11} Typically, almost all dopants near the band edges are ionized at room temperature, i.e. donors are positively charged and acceptors are negatively charged. By applying a reverse voltage across the junction, the bulk region gets depleted as free charges are removed by a $z$-directed electric field.\textsuperscript{11} Usually, detectors are operated in a fully depleted mode, i.e. the absolute value of the bias voltage $U_{bias}$ is larger than the absolute value of a characteristic depletion voltage $U_{dep}$. For this case, all free charges are removed and collected by the external electrodes, such that a spatially fixed charge density $\rho_0$ of the ionized dopants remains,

$$\rho_0 = e (n_D - n_A).$$

(10)

The depletion voltage built up by this charge is given by

$$U_{dep} = -\frac{L^2 \rho_0}{2 \varepsilon_0 \varepsilon_r},$$

(11)

with $\varepsilon_0 \varepsilon_r$ being the absolute permittivity of the material.\textsuperscript{11} In the case of full depletion with constant space charge, the electric field depends linearly on $z$ as shown in Figure 1 right,

$$E(z) = \frac{U_{bias}}{L} - \frac{U_{dep}}{L} \left( \frac{2z}{L} - 1 \right),$$

(12)

where the pixel anodes at $z = 0$ are on ground potential, and the cathode at $z = L$ is set to a negative potential corresponding to the bias voltage $U_{bias} < 0$. In consequence, an n-doping weakens the electric field near the anode pixels, and strengthens it near the cathode. Vice versa, a p-doping weakens it near the cathode and strengthens it near the anode pixels.

The aim of this work is to study the impact of the static polarization caused by the dopants to relevant detector performance parameters. “Dynamic” polarization,\textsuperscript{12} i.e. the build-up of a space charge due to trapped electrons or holes is not considered here. With the help of simulations we analyze pulse widths, spectral responses and pulse height spectra in dependence on the dopant concentration.

2. METHODS

All simulations are performed on an $L = 3$ mm thick CZT layer with a 3x3 pixel matrix at room temperature ($k_B T = 0.02526 \text{ eV}$). Each pixel square has a size of $w = 300 \text{ µm}$ without a gap between the pixels. The pixel anodes are held on ground potential, while the cathode is biased with $U_{bias} = -900 \text{ V}$. For CZT, we assume a relative permittivity $\varepsilon_r = 10$, an electron mobility of $\mu_e = 1000 \text{ cm}^2/(\text{Vs})$, and a hole mobility of $\mu_h = 120 \text{ cm}^2/(\text{Vs})$. Assuming an ideal material which is almost free of dislocations or traps, we set $\lambda_e$ to infinity. According to Eq. (11), the limiting doping
concentration \( n_{\text{max}} = |\rho_0| / e \) still allowing full depletion corresponds to \( n_{\text{max}} = 2 |e| \epsilon |U_{\text{bias}}| / (\epsilon L^2) = 1.1053 \cdot 10^{15} \text{ cm}^{-3} \) with the parameters reported above. For the parameterization of the doping concentration we varied the ratios \( n / n_{\text{max}} = |U_{\text{dep}}| / |U_{\text{bias}}| = 0\%, 50\%, 75\%, 90\%, 95\% \) or 99\% for pure n-doping \( (n = n_p) \) and p-doping \( (n = n_h) \), respectively.

For each doping concentration, \( 1 \cdot 10^6 \) X-ray photons with energy 100 keV were simulated, except for the n-doped case \( n_p = 0.99 \cdot n_{\text{max}} \), for which due to increased computational efforts only \( 4 \cdot 10^5 \) Photons were simulated. The photons are incident through the cathode at \( z = L \) within a random position of the center pixel area. In a first step, the energy deposition of X-ray photons is tracked in a Monte Carlo simulation including photoelectric absorption (potentially followed by K-fluorescence), Compton scattering, and coherent scattering.\(^{14} \) At each location of energy deposition, an electron cloud with zero initial diameter is generated according to a conversion constant of 4.6 eV per \( e/ h \) pair,\(^{13} \) and the drift/diffusion motion of each charge is Monte-Carlo simulated according to Eq. (3) to (5) in time steps of \( \Delta t = 0.2 \text{ ns} \). To speed up simulation time, however, 271 electrons (corresponding to a deposited energy of 1 keV) were bundled, respectively, and tracked in a single simulated trajectory. The electric field for a particular doping concentration is calculated according to Eq. (12). Coulomb interaction between charges in a cloud and their image charges is neglected. Optionally, also a hole cloud can be generated and tracked. The current induced in each pixel is calculated with help of Eq. (1) and (2), wherein \( \phi_i(r) \) is calculated with the method of infinite image charges.\(^{15} \) Current pulses created from energy depositions at different locations but originating from the same photon are superposed. For the center pixel, each electron current pulse is analyzed for its width by extracting the time which passed between the detection of 10\% and 90\% of the integral current, respectively.

For each pixel, the total integral current induced by electrons is calculated and related to the charge of electrons which would be generated by the deposition of the original photon energy. This quantity is interpreted as that part of the original photon energy which can be measured with ideal electronics performing a complete integration of the electron current pulse. The corresponding measured photon energy is registered in a histogram plot we refer to as spectral response (SR) in the following.

Furthermore, the processing of a current pulse by the electronics is simulated according to Eq. (9) with a Gaussian pulse shape function \( f(t') = \exp \left( -t'^2 / (2 \sigma_p^2) \right) \) with a two-sigma width of \( 2 \sigma_p = 20 \text{ ns} \). The maximum of the convolution result \( p(t) \) is taken as pulse height and related to an ideal pulse height which would be measured if the complete electron charge generated by the original photon energy is injected as a delta-peak to the electronic circuit. The measured pulse height is correspondingly converted into a measured photon energy and registered in a histogram distribution which we refer to as pulse height spectrum (PHS) in the following. Thus, in contrast to the SR, the PHS contains also the non-idealities of the pulse processing by the electronics.

The SR and PHS can be calculated for two illumination modes, i.e. an illumination of the center pixel only, or a homogeneous illumination of the complete 3×3 pixel matrix, respectively. In the latter case, SR and PHS can be composed from the data which was simulated for the center pixel illumination. For symmetry reasons, the SR or PHS of a border pixel under center pixel illumination is identical to the SR or PHS of a center pixel under solely illumination of the corresponding border pixel. Thus, a SR or PHS for a homogeneous 3×3 pixel illumination is identical to the superposition of the SR or PHS of all 9 pixels obtained for a center pixel illumination.

Finally, we perform an analytical calculation of the SR, for which we slightly modify the model reported by Kozorezov et al.\(^{7} \) to take into account an inhomogeneous electric field. For that, we calculate the mean drift time of an electron using the differential \( dt = dz \nu_E(z) = dz [\mu E(z)] \) where \( \nu_E \) and \( \mu \) are the drift velocity and the mobility of electrons, respectively. Using \( E(z) \) as expressed in Eq. (12), the total drift time for the case \( 0 < |U_{\text{dep}}| < |U_{\text{bias}}| \) is calculated by

\[
 t = \int_0^L \frac{dz}{\mu E(z)} = - \frac{1}{\mu} \frac{L^2}{2 |U_{\text{dep}}|} \ln \left( 1 + \frac{2 z_{\text{max}}}{L \left( \frac{U_{\text{bias}}}{|U_{\text{dep}}|} - 1 \right)} \right) . \tag{13}
\]

Using furthermore Eq. (4) and (5), one can calculate the lateral sigma-extension \( \sigma_y \) of the electrons cloud at the anode plane (in two dimensions) by
\[ \sigma_{xy} = \sqrt{2Dt} = \sqrt{-\frac{k_B T}{e} \frac{L^2}{U_{dep}} \ln \left( 1 + \frac{2z_a}{L} \left( \frac{U_{bias}}{U_{dep}} - 1 \right) \right)} \]  

(14)

With Eq. (8), the term \( \sqrt{2z_a L} \) in Eq. (6) can be replaced by \( \sqrt{2} \cdot \sigma_{xy} \) with \( \sigma_{xy} \) as defined in Eq. (14).

\[ Q_e = \frac{e}{\Delta V} \left[ \frac{1}{4} \left( \text{erf} \left( \frac{x + w/2}{\sqrt{2} \cdot \sigma_{xy}} \right) - \text{erf} \left( \frac{x - w/2}{\sqrt{2} \cdot \sigma_{xy}} \right) \right) \right] \left( \frac{y + w/2}{\sqrt{2} \cdot \sigma_{xy}} - \text{erf} \left( \frac{y - w/2}{\sqrt{2} \cdot \sigma_{xy}} \right) \right) \exp \left( \frac{-z_a}{\lambda_a} - \Phi(x) \right). \]  

(15)

To calculate an analytical SR, Eq. (15) is used to determine the total collected charge for each energy deposition of a particular photon. The total collected charge can be converted into a corresponding measured photon energy for registration in the SR histogram.

### 3. RESULTS AND DISCUSSION

In Figure 2, a spectral response is shown which was determined by three different methods of charge tracking and charge collection, i.e. by an analytical calculation according to Eq. (15), by a Monte Carlo simulation involving only electron transport, and by a Monte Carlo simulation involving electron as well as hole transport (the first two methods base on 4 \( \times \) 10^3 photons, the latter method on 4 \( \times \) 10^5 photons).

![Figure 2](image-url)

Figure 2. Spectral response for a strongly n-doped CZT detector (\( U_{dep} \)/\( U_{bias} = 0.99 \)) at center pixel illumination, plotted with linear scaling (left) and logarithmic scaling (right). The plots represent different ways of current integration, i.e. an analytical calculation, a Monte Carlo simulation involving only electron movement, and a Monte Carlo simulation involving both electron and hole movement, respectively.

For all three methods, the same result is obtained within statistical fluctuations. A photo peak between 95 and 100 keV represents energy depositions which occurred almost completely in the considered pixel volume. Some characteristic peaks are present at about 72 keV and 76 keV, which is caused by escape of K-fluorescence photons emitted after photoelectric absorption of the original photon, such that the registered energy is the original photon energy reduced by the corresponding K-fluorescence energy. Furthermore, a so-called low-energy tailing is seen mainly in the range between 30 keV and 90 keV, which indicates charge loss mainly due to charge sharing with neighbor pixels. Here, however, we are most interested in the similar results of the spectral response for each of the three methods applied. The identical histograms give confidence in a correct implementation of the charge tracking Monte Carlo code, and also in a correct theoretical treatment of the charge collection in an inhomogeneous electric field (correct with respect to the proposed model described above). Furthermore, there is evidence that the holes transport is negligible for the chosen detector geometry. In more detail, we intentionally chose an n-doping concentration close to the limit which still allows...
Figure 3. Current pulses obtained for the Monte-Carlo simulation of an electron cloud generated by a 100 keV energy deposition at the cathode above the pixel center, for different concentrations of n-doping (left) and p-doping (right).

Figure 4. Mean drift time (left) and lateral sigma-extension (right) of an electron cloud created at a location $z_a$ within the detector, for p-doping and n-doping, in different concentrations: a) no doping; b)-f) n-doping with ratios $U_{dep}/U_{bias}$ of b) 0.5, c) 0.75, d) 0.9, e) 0.95, f) 0.99; g)-k) p-doping with ratios $U_{dep}/U_{bias}$ of g) -0.5, h) -0.75, i) -0.9, j) -0.95, k) -0.99.

Figure 5. Histograms of obtained pulse widths (i.e. times which passed between the detection of 10% and 90% of the integral current) for n-doping (left) and p-doping (right) in different concentrations.

full depletion, $n_f = 0.99\ n_{max}$, which from all studied doping concentrations creates the strongest electric field near the cathode, and the weakest electric field near the anode pixels. For this configuration, we expect the largest contribution of holes drifting to the cathode, and the weakest contribution of electrons drifting to the anodes. However, even for this extreme case the holes contribution is negligible, which is explained according to Eq. (2) by a relatively low gradient of
the weighting potential in almost the whole detector volume except in the immediate vicinity of a detector pixel. In addition, holes drift by a factor of almost 8 more slowly than electrons due to their reduced mobility. We performed similar tests for other doping concentrations (not shown here), and found for each case again that hole movement is negligible. Therefore, we skipped hole tracking in all following simulations, and performed instead electron tracking with a larger number of photons allowing better statistics of the results.

The hypothesis, that only the weighting potential in the vicinity of a pixel is relevant for the current induction, is supported by Figure 3, in which simulated electron current pulses for different concentrations of p-doping and n-doping are shown. If the CZT is undoped, electrons drift constantly for a time of about 100 ns (see black plots in Figure 3). The relevant part of the current pulse is generated for the last 15 ns of the drifting time interval, i.e. the last 450 µm before the electrons are collected by the anode. According to this, in the following, the “bubble”-like volume around a pixel within a relevant part of the current pulse is generated for the last 15 ns of the drifting time interval, i.e. the last 450 µm before the electrons are collected by the anode. According to this, in the following, the “bubble”-like volume around a pixel within which the “relevant” part of a current pulse is induced is denoted as “relevant region of the weighting potential”. The current curves for doped CZT can be understood well in combination with Figure 4 left, which shows the mean drift times of electrons in dependency on the position $z_a$ of creation according to Eq. (13), and with Figure 5, which shows a histogram of pulse widths obtained in the Monte Carlo simulations. For the case of n-doping, the electric field is weakened in the relevant region of the weighting potential, accompanied with a slower drift of electrons near the pixel anodes, and a longer total drift time. For this reason, the current pulses get increasingly broadened (from 11 ns without doping up to 130-190 ns for $n_p = 0.99 \cdot n_{\text{max}}$ as seen in Figure 5 left) and delayed for increasing donor concentrations (from 100 ns without doping up to 270 ns for $n_p = 0.99 \cdot n_{\text{max}}$ as seen in Figure 4 left). A different characteristic is found for the case of p-doping. The electric field is weakened near the cathode, but strengthened in the relevant region of the weighting potential. In consequence, the pulse shape depends strongly on the start position $z_a$ of the cloud. According to Figure 4 left, the drift time through the relevant region of the weighting potential is shorter than that for the undoped CZT.

![Figure 6](image_url)

**Figure 6.** Spectral responses of the center pixel for different concentrations of n-doping, linearly scaled (left) and logarithmically scaled (right), with illumination of the center pixel area only. The inset shows a strong enlargement of the photo peak.

![Figure 7](image_url)

**Figure 7.** As Figure 6, but for a 3x3 pixel illumination, containing crosstalk counts from neighbor pixels.
case, which results in most cases in even shorter pulses down to 5-6 ns as seen in Figure 5 right. For $z_a < 0.8$, also the total drift time is shorter than that for the undoped case. In contrast, for $z_a > 0.9$, the total drift time increases. In Figure 3 right, pulse examples are shown for the case that the electron cloud is generated directly at the cathode at $z_a = 1$. We consider this as an “extreme” case, as the electrons have to traverse completely the region of the weakest electric field near the cathode. As to be expected, the total drift times increase with the doping concentration $n_A$. Agreeing to Figure 5 right, the pulse widths for moderate doping concentrations ($n_D \leq 0.75 \cdot n_{max}$) are reduced or at least similar to the undoped case. For strong p-doping concentrations, however, broader pulses are seen than those expected from Figure 5 right. We explain this finding by a diffusive charge cloud extension in $z$-direction especially within the low-field region near the cathode. For p-doping, the case $z_a/L = 1$ seems to represent the worst-case scenario with respect to pulse width. Therefore, we can interpret the histogram distribution presented in Figure 5 right as a composition of a large number of energy depositions well below the cathode generating short pulses, and a relatively small number of energy depositions very close to the cathode generating quite broad pulse widths as those shown in Figure 3 right.

Figure 6 and Figure 7 show Monte-Carlo simulated spectral responses for the case of n-doping. By definition of the spectral response, the influence of the pulse width is eliminated; nevertheless, it is clearly seen that the low energy tail becomes more dominant with increasing doping concentrations. We interpret this as a result of lateral charge cloud extension by diffusion due to a longer drift time, which results in stronger charge sharing between neighbor pixels. The analytically calculated width of a Gaussian distribution according to Eq. (14) is shown in Figure 4 right. The thesis of charge sharing is supported by Figure 7 representing 3×3 pixel illumination, which shows a strong increase of low energy counts (< 20 keV) with increasing donor concentration. We assume that these counts originate from energy depositions in neighbor pixels close to the border to the center pixel. At 22 keV and 25 keV, peaks are seen originating from K-fluorescence photons originating from neighbor pixels.

Figure 8. Spectral responses as in Figure 6 (center pixel illumination), but for the case of p-doping. Note the strongly enlarged scaling of the inset in Figure 8 left compared to that of Figure 6 left.

Figure 9. As Figure 8, but for a 3×3 pixel illumination, containing crosstalk counts from neighbor pixels.
Figure 8 and Figure 9 show accordingly the simulated spectral responses for the case of p-doping. The results show only a very weak dependency on the acceptor concentration, with a slightly reduced low-energy tailing (i.e. charge sharing) for moderate acceptor concentrations \( n_A \leq 0.75 \times n_{\text{max}} \), and a slightly strengthened low-energy tailing for larger acceptor concentrations, which indicates a faster mean total drift time and therefore weaker lateral diffusion of electrons for moderate acceptor concentrations. The best result in terms of reduced low-energy tailing and photo peak height are found for an acceptor concentration of \( n_A = 0.5 \times n_{\text{max}} \).

Figure 10. Pulse height spectra for different n-doping concentrations, for a center pixel illumination (left), and a 3×3 pixel illumination (right).

Figure 11. Pulse height spectra for different concentrations of p-doping at center pixel illumination, linearly scaled (left) and logarithmically scaled (right).

Figure 12. Pulse height spectra as in Figure 11 (p-doping) but for a 3×3 pixel illumination.
Figure 10 shows pulse height spectra for different n-doping concentrations, as resulting for a Gaussian pulse shaper function with $2\sigma_p = 20$ ns as described in the methods section. For an ideal delta-function pulse, a pulse height corresponding to 100 keV is expected. In realistic cases, like for a mean pulse width of 11 ns for the undoped case (see Figure 5), almost 9% of the total charge gets lost during the pulse shaping, which results in an energy-scaling of the pulse height spectrum such that the photo peak is found at 91 keV. Clearly seen is, that with increasing donor concentrations the photo peak shifts lower energy (down to 18 keV for $n_D = 0.99\cdot n_{\text{max}}$), which is explained by the broader pulse widths as seen in Figure 5 left.

Figure 11 and Figure 12 show pulse height spectra for different p-doping concentrations. In contrast to the n-doping case, the photo peak shifts towards higher energies compared to the undoped case. This is explained by on average shorter pulse widths as shown in Figure 5 right, i.e. the current pulse gets closer to a delta-function, and correspondingly more electrons are collected per pulse. For any simulated acceptor concentration, less charge sharing is observed for low energies smaller than 20 keV. For moderate p-doping $n_A \leq 0.9\cdot n_{\text{max}}$, also less low energy tailing is seen for energies above 30 keV up to the photo peak.

In summary of all findings, n-doping in any concentration results in broader pulses and a degradation of the spectral response and pulse height spectrum. In contrast, a moderate p-doping $n_A \leq 0.9\cdot n_{\text{max}}$ provides on average shorter pulses with less charge cloud extension, which improves spectral response and pulse height spectrum.

An ideal crystal contains only acceptor atoms in concentrations as reported in the results above. The ionized acceptor states are negatively charged, i.e. they can act as trap for holes, but not as trap for electrons. Consequently, in an extreme case of dynamic polarization, one can assume that all acceptor states become electrically neutral by hole trapping, which would generate an electric field like that of an undoped semiconductor. In a case of partial dynamic polarization, a “mixed” electric field between that of an undoped semiconductor and that of a p-doped semiconductor without trapping occurs. The holes would be preferentially trapped near the cathode, with the result that the electric field gets strengthened in the region of trapped charges and weakened near the anode; however, the electric field near the anode would be still larger than in the undoped case, therefore providing the beneficial effects of shortened pulse width. In summary, for an idealized semiconductor containing no other traps than acceptor atoms, we expect also for high photon rates a preservation of the beneficial effects of a shorter pulse width, improved spectral response and improved pulse height spectrum, although the characteristics are approaching those of an undoped semiconductor as soon as dynamic polarization occurs.

In realistic semiconductors, however, a certain density of unwished traps exists, like substituting atoms, vacancies, dislocations and other crystal defects. Also, an effective p-doping might be a result of much larger concentrations of acceptors as well as donors which compensate each other. Especially the trapping of holes is reported, which might cause dynamic polarization near the cathode. In worst case, “catastrophic” dynamical polarization occurs, i.e. the electric field breaks completely down at a “pinch point” located near the cathode. Electrons created on the cathode site of this field-free “barrier” can neither traverse this region nor create a relevant current pulse. Unfortunately, the weakening of the electric field at this pinch point is accumulatively supported by the static polarization created by ionized acceptors. Thus, it happens that a p-doped semiconductor gets earlier (i.e. at lower photon rates) into the state of “catastrophic” polarization than an undoped semiconductor.

The benefits of a p-doped semiconductor reported in this work are therefore limited to detector applications with very pure semiconductor crystals (i.e. without potential traps or compensated doping), or to applications with photon rates low enough to not generate significant dynamic polarization.

4. CONCLUSIONS

We performed Monte-Carlo simulations of energy deposition and charge movement within pixelated photon counting direct conversion detectors made of doped semiconductors of different acceptor or donor concentrations. Induced currents were statistically evaluated with the help of histograms of pulse width and total integral currents (represented before consideration of pulse shaper electronics in spectral responses, and after consideration of pulse shaper electronics
in pulse height spectra, respectively). The electric field close to anode pixels was identified as the main quantity defining the pulse characteristics. For n-doped semiconductors, a weaker electric field near the pixel anodes and longer total electron drift times are seen, which results in broader pulse widths and a degradation of the spectral responses (by enhanced charge sharing) and pulse height spectra. In contrast, for p-doped semiconductors, a strengthened electric field near the anodes and an, on average, reduced total drift time is seen, which results in shorter pulse widths. For moderate p-doping concentrations $n_A \leq 0.9\cdot n_{\text{max}}$, an improvement of the spectral response (less charge sharing) and pulse height spectrum is seen. For p-doping concentrations close to the limit still allowing full depletion, $n_A > 0.9\cdot n_{\text{max}}$, the spectral response and pulse height spectrum degrade again due to charges which experience long drift times when created in a region with weakened electric field near the cathode. We conclude that using moderately p-doped semiconductor material, $n_A \approx 0.5\cdot n_{\text{max}}$, improves detector performance as long as the detector is not limited by dynamic polarization. In the latter case, it has to be noted that a p-doped semiconductor reduces the maximum count rate at which catastrophic dynamical polarization occurs.

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