Three-Dimensional Simulation of Signal Generation in Wide-Bandgap Semiconductor Radiation Detectors

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Abstract: We demonstrate the use of Comsol Multiphysics with Matlab to model signal generation in wide-bandgap semiconductor radiation detectors. A quasi-hemispherical detector design is compared with a simple, planar detector. Results show that the quasi-hemispherical design can simply and effectively compensate for the poor hole transport of most compound semiconductor materials.

Keywords: radiation detector, compound semiconductor, cadmium zinc telluride

1. Introduction

Semiconductor detectors are widely used for gamma-ray imaging and spectroscopy in a variety of applications, including nuclear medicine, national security, astrophysics and environmental science. However, one dominant detector technology, high-purity germanium, suffers from the need for cooling to liquid-nitrogen temperature, while the leading alternative, scintillator crystals, has inadequate energy resolution for many applications.

Much research has been devoted to the use of compound semiconductors, such as cadmium telluride, cadmium zinc telluride, gallium arsenide and mercuric iodide, for hard x-ray and gamma-ray detection. These materials have good stopping power due to their high atomic numbers, can operate at room temperature due to their wide band gaps, and ideally can provide better energy resolution than scintillators. Their primary drawback is the poor transport properties of holes relative to electrons, which creates a non-uniformity in charge collection characteristics that is detrimental to energy resolution.

Several schemes have been devised to implement "electron-only" device structures to compensate for the poor hole transport in these materials, including coplanar-grid[1], longitudinal Frisch grid[2], segmented detectors[3], and similar structures. Accurate prediction of performance of these devices requires good computational methods for calculating electric field profiles and integrating the induced currents.

In this paper, we demonstrate the use of Comsol Multiphysics with Matlab to model signal generation characteristics in planar and quasi-hemispherical detectors and show that the quasi-hemispherical geometry provides a substantially more uniform charge collection profile.

2. Model Construction

2.1 Theory

The simplest type of semiconductor detector is essentially a slab of high-resistivity material with metal electrodes deposited on its surfaces. In operation, one or more of the electrodes is held at a non-zero bias voltage, while others are grounded. When an x-ray or gamma-ray photon interacts with a semiconductor, either by photoelectric absorption or Compton scattering, it generates a number of electron-hole pairs that is proportional to its energy. As an approximation, this bundle of charge can be regarded as originating at a point. As the electrons and holes drift to opposite electrodes under the applied potential difference, they induce signal currents on the electrodes. The crux of the problem is to compute the total signal - the induced current integrated over time - as a function of the location within the detector where the interaction occurs. The uniformity of this charge collection efficiency function determines the energy resolution that can be achieved with the detector design.

The basis for computing signal generation in a semiconductor radiation detector is Ramo's theorem[4]:

$$i = q\, \boldsymbol{v} . \boldsymbol{E_1} \qquad (1)$$

This equation states that the induced current (i) on a given electrode due to the motion of a charge (q) is equal to the velocity (**v**) of that charge dotted with the weighting field, $\mathbf{E_1}$. $\mathbf{E_1}$ is not necessarily the actual electric field, but a computational construct equal to the field that would exist with the signal electrode held at unit potential and all other electrodes grounded. For the simplest class of detectors, consisting of two electrodes, one of which is grounded, $\mathbf{E_1}$ differs from the physical field only by a factor of the applied bias potential.

The drift velocity of an electron (hole) in a semiconductor under the influence of an electric field E is

$$\boldsymbol{v} = \mu_{e(h)}\boldsymbol{E} \tag{2}$$

where $\mu_{e(h)}$ is the electron(hole) mobility, which is assumed to be independent of the field for our purposes.

When integrating the current over time, it is necessary to take into account the fact that the number of free carriers (and therefore the charge) decreases due to trapping according to:

$$N(t)=N_0\, e^{-t/\tau_{e(h)}} \tag{3}$$

where $\tau_{e(h)}$ is the trapping lifetime of electrons(holes). This equation assumes that both de-trapping and space charge effects due to trapped charge are negligible. Since electrons and holes will in general have different mobilities and lifetimes and follow different trajectories, it is necessary to calculate the electron and hole contributions to the signal separately.

The process of calculating the charge collection in a detector consists of computing the physical and weighting fields for use in equations (1) and (2), then integrating the electron and hole currents over time, taking equation (3) into account. The latter step is repeated for a number of different origination points to determine the charge collection profile. In this work we compute the electric fields by finite element analysis with Comsol and export the solution to Matlab, where the integration is performed.

2.2 Comsol Electrostatic Model

The 3D, Electrostatics with Conductive Media application mode was used to compute the physical and weighting fields within the detector crystal. The geometry was defined as a simple cube, 1 cm on each side. The conductivity of the material was set to 10^{-8} S/m, consistent with the properties of $Cd_{0.9}Zn_{0.1}Te$ radiation detector material.

The electrode surfaces were defined with either a fixed potential or ground boundary condition. The free surfaces of the semiconductor crystal were assumed to be perfectly insulating.

2.3 Matlab Post-processing

Having used Comsol to compute the physical and weighting fields (which, in the examples treated in this paper are identical except for a factor of the applied bias voltage), the charge collection efficiency for a given interaction location is calculated in Matlab by integrating equation (1) in conjunction with equations (2) and (3):

$$\frac{Q_{e(h)}}{eN_0} = \int_0^{t_{c,e(h)}} \mu_{e(h)} e^{-t/\tau_{e(h)}}\, \vec{E}\cdot\vec{E}_1 dt \tag{4}$$

Here $t_{c,e(h)}$ is the collection time for electrons(holes) – the time at which the charge carriers reach the electrode.

Equation (4) is discretized, but rather than a uniform time step, we use a uniform distance step (Δr), so that in weaker-field regions larger time steps can be taken to improve computational efficiency. The computation sequence is therefore:

1. Given the starting coordinates, obtain the electric field at that point from the FEM structure.
2. Calculate the electron or hole velocity using equation (2).
3. Calculate the time step as $\Delta t=\Delta r/|\mathbf{v}|$.
4. Add to the charge collection as $\Delta Q=i\Delta t$, with i given by equation (1).

5. Calculate the next coordinates as $\mathbf{r}_1=\mathbf{r}_0+\mathbf{v}\Delta t$
6. Adjust the number of free charge carriers at the end of the time step according to equation (3).
7. Repeat until the charge carriers reach a boundary of the detector.

The signals due to electrons and holes are calculated separately and added. As a by-product, the electron and hole current vs. time waveforms can also be obtained. The entire process is repeated for numerous starting points to generate a charge collection profile.

3. Results

3.1 Planar Detector

To verify the model, we first consider the simplest case, for which an analytical solution is available. In an ideal, planar detector, the charge collection efficiency as a function of interaction depth is given by the Hecht relation[5]:

$$\frac{Q}{eN}=\frac{\mu_h\tau_h E}{W}\left(1-e^{-z_0/\mu_h\tau_h E}\right)+\frac{\mu_e\tau_e E}{W}\left(1-e^{-(W-z_0)/\mu_e\tau_e E}\right) \quad (5)$$

where z_0 is the distance from the cathode at which the interaction occurs and W is the thickness of the detector. Because of the unequal values of the drift lengths, $\mu\tau E$, for electrons and holes, the charge collection depends strongly on z_0. This phenomenon, commonly called "hole tailing", produces a grossly asymmetrical line shape in the spectrum.

Figure 1 shows the calculated charge collection profile as a function of z_0 using the Comsol-Matlab model along with the expected result from equation (5). In this case, due to the uniformity of the electric field, the transverse coordinates (x,y) do not affect the result. The close agreement confirms that the model is functioning properly.

To compute a simulated pulse-height spectrum would involve Monte Carlo methods and the use of radiation transport codes that are beyond the scope of this paper. However, a qualitative picture of the photopeak line shape for high energies can be obtained by plotting a histogram of the values from Figure 1. Figure 2 shows the result for the ideal, planar detector. The severe asymmetry due to hole tailing is apparent.

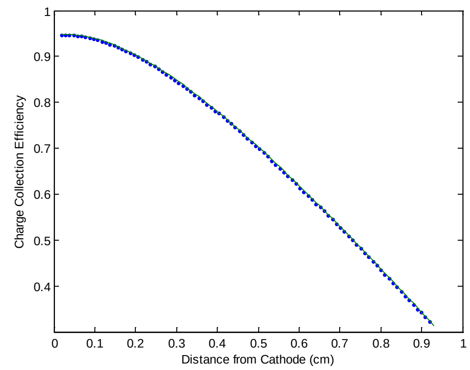

Figure 1. Computed charge collection profile for ideal, 1.0x1.0x1.0 cm^3 planar detector with $(\mu\tau E)_e$ = 9.1 cm, $(\mu\tau E)_h$ = 0.25 cm. Comsol-Matlab model (dots) vs. equation (4) (line).

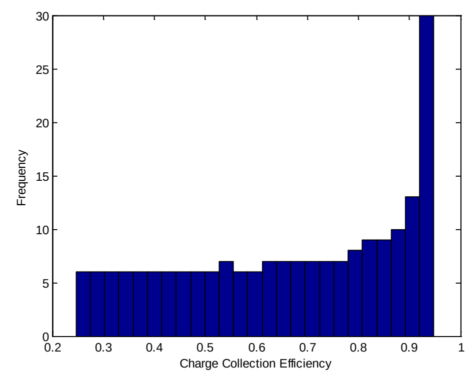

Figure 2. Histogram of charge collection efficiency for the ideal planar detector. This plot is a qualitative representation of the photopeak shape for high energies, where interaction is nearly uniform through the detector volume and the contribution of noise is relatively small.

3.2 Quasi-Hemispherical Detector

One solution to the hole-tailing problem is to use an electrode geometry that concentrates the electric field near the anode. In that way, most of the signal generation occurs in a small region near the anode so that holes, which move in the opposite direction, make only a minor contribution.

One approach is a “quasi-hemispherical” design, in which the anode, rather than covering the entire face of the crystal, has a circular shape. The cathode covers not only the opposite face, but all of the side faces as well. This electrode configuration concentrates the field lines near the circular anode, as shown in Figure 3. In the specific case used here, the crystal dimensions are 1.0x1.0x.10 cm^3, and the anode is a 0.5 cm-diameter circle, centered on the top face.

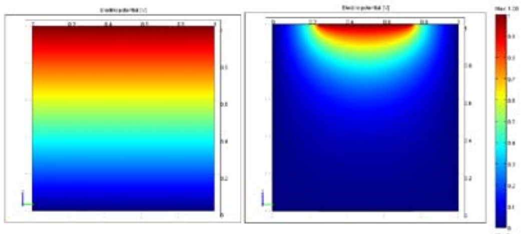

Figure 3. Cross-section of equipotential map for planar (left) and quasi-hemispherical detectors.

Because of the non-uniformity of the electric field, the charge collection efficiency now depends on the (x,y) coordinates as well as the interaction depth, z. The charge collection profile for this design along three lines parallel to the z-axis is shown in Figure 4. Whether the line is taken along the center of the crystal (blue), near the edge of the anode (green) or closer to the corner of the crystal (red), the uniformity of charge collection is substantially better than for the planar case.

Because of the field non-uniformity in the quasi-hemispherical case, it is necessary to sample the charge collection efficiency at a large number of points to produce a representative histogram. The plot of Figure 5 is based on 200 points sampled along ten lines parallel to the z-axis. This qualitative representation demonstrates the potential for improved spectral resolution and photopeak efficiency compared to the planar detector.

4. Conclusions

A three-dimensional model of charge collection efficiency in semiconductor radiation detectors with arbitrary electrode configurations has been implemented in Comsol Multiphysics with Matlab. Results show that a quasi-hemispherical detector design can provide enhanced energy resolution and photopeak efficiency compared to planar detectors, without the use of a guard ring, grid bias or multiple readout amplifiers. A further characteristic of this geometry is that crystals can be directly abutted, a significant advantage in nuclear imaging applications.

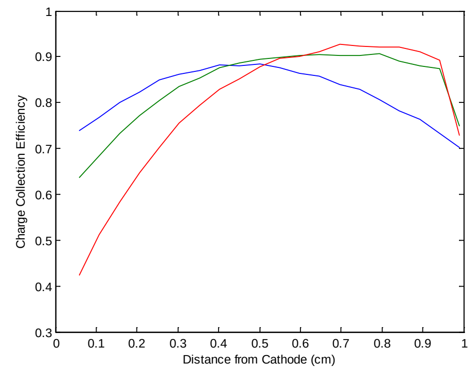

Figure 4. Charge collection profiles for quasi-hemispherical detector along the lines [0.5,0.5,z] (blue), [0.25,0.25,z] (green) and [0.125,0.125,z] (red).

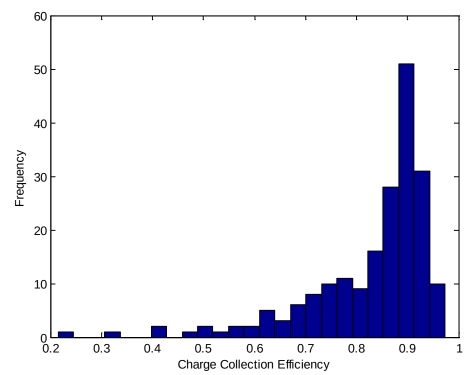

Figure 5. Histogram of charge collection efficiency for the quasi-hemispherical detector.

6. References

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