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SEMICONDUCTOR RADIATION DETECTORS**

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**METHOD FOR MAPPING CHARGE PULSES IN SEMICONDUCTOR
RADIATION DETECTORS**

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METHOD FOR MAPPING CHARGE PULSES IN SEMICONDUCTOR RADIATION DETECTORS

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ABSTRACT

An efficient method for determining the distribution of charge pulses produced by semiconductor detectors is presented. The method is based on a quasi-steady-state model for semiconductor detector operation. A complete description of the model and underlying assumptions is given. Mapping of charge pulses is accomplished by solving an adjoint carrier continuity equation. The solution of the adjoint equation yields Green's function, a time- and position-dependent map that contains all possible charge pulses that can be produced by the detector for charge generated at discrete locations (e.g., by gamma-ray interactions). Because the map is generated by solving a single, time-dependent problem, the potential for reduction in computational effort over direct mapping methods is significant, particularly for detectors with complex electrode structures. In this paper, the adjoint equation is derived and the mapping method is illustrated for a simple case.

INTRODUCTION

Numerical modeling has been used routinely in the design and analysis of semiconductor devices, often resulting in significant savings in development effort and cost. At Los Alamos, we are investigating methods to model semiconductor radiation detectors with emphasis on room-temperature semiconductors such as CdZnTe. Our intent is to develop a comprehensive modeling tool that can be used for detector design and analysis.

In order to calculate the response of semiconductor detectors, the following physical processes must be treated: 1) production and transport of radiation; 2) ionization of the semiconductor; 3) separation and acceleration of electrons and holes by the electric field; 4) transport of charge carriers within the semiconductor and induction of charge on the electrodes (formation of the charge pulse); and 5) amplification and processing of the charge pulse. Each of these processes can be treated independently. For some applications, radiation transport processes are dominant and semiconductor effects can be ignored (e.g., estimating pulse-height spectra for medium-volume coaxial HPGe detectors). However, for many applications, semiconductor processes must be considered: for compound semiconductors, such as CdTe, CdZnTe, and HgI₂, carrier transport processes must be treated in order to model pulse-height spectra; For HPGe, the shape of the charge pulse must be known in order to evaluate pulse processing methods, such as digital signal processing.

In general, the dependence of the shape and magnitude of the charge pulse on the position of the interaction can significantly influence the performance of semiconductor detectors, particularly for spectroscopy, where ballistic deficit and incomplete charge

collection can degrade peak shape and resolution. For compound semiconductor detectors, elaborate electrode structures are often used to compensate for hole trapping for gamma-ray spectroscopy and to determine the location of interactions for imaging applications.

Because of the complexity of these devices, direct mapping pulse shapes using existing semiconductor models is impractical. A time-dependent, partial differential equation (the carrier continuity equation, described in the next section) must be solved for each point of interest within the volume of the semiconductor. For devices with complex electrode structures, such as coplanar-grid CdZnTe detectors, many points may be required to form an accurate map. Consequently, the time required to adequately characterize a detector using this approach is often prohibitive.

In this paper, a new method for mapping charge pulses produced by radiation interactions is presented that overcomes the limitations of direct mapping methods. Mapping charge pulses can be accomplished by solving an adjoint carrier continuity equation. The solution of the adjoint equation yields a time- and position-dependent map that contains all possible charge pulses that can be produced by the detector for charge generated at discrete locations (e.g., by gamma-ray interactions). Because the map is generated by solving a single, time-dependent problem, the potential for reduction in computational effort compared with direct mapping methods is significant, particularly for detectors with complex electrode structures. This method is being applied to investigate charge collection in CdZnTe detectors with complex electrode structures, to engineer improved electrode structures, and to devise analytical methods for gamma-ray

spectroscopy and imaging. The underlying physical assumptions of the mapping method are developed, the adjoint model is described, and a simple example is provided.

EXCESS CARRIER MODEL

Rigorous calculation of pulse shape involves the solution of a coupled, nonlinear system of equations. The most widely used semiconductor model consists of the following equations:

$$\text{Electron Continuity, } \frac{\partial n}{\partial t} = \nabla \cdot \mathbf{K}_n + G_n - R_n \quad ; \quad (1)$$

$$\text{Hole Continuity, } \frac{\partial p}{\partial t} = \nabla \cdot \mathbf{K}_p + G_p - R_p \quad ; \text{ and} \quad (2)$$

$$\text{Poisson's Equation, } \nabla \cdot (\epsilon \nabla \phi) = \rho(n, p) \quad ; \quad (3)$$

where $\mathbf{K}_n = -\mu_n n \nabla \phi + D_n \nabla n$ and $\mathbf{K}_p = \mu_p p \nabla \phi + D_p \nabla p$. The notation used in Eqs. 1-3 is standard and the reader is referred to a standard text on semiconductor physics for the definition of the parameters.¹ The local electron and hole current densities are $\mathbf{J}_n = \mathbf{K}_n$ and $\mathbf{J}_p = -\mathbf{K}_p$, respectively. The terms G and R in the continuity equations describe the generation and recombination of free carriers. An additional balance equation is used to describe the occupancy of traps. Equations 1-3 can be used to determine the steady-state conditions within a detector and to model transients caused by radiation interactions. With the appropriate boundary conditions and physical models, a variety of features common to semiconductor devices for radiation detection can be treated.

In most applications, semiconductor detectors operate in a quasi-steady-state mode. The excess charge produced by radiation interactions does not significantly perturb the field within the detector. Consequently, the continuity equations can be

decoupled from Poisson's equation. We will further assume that the electron and hole continuity equations can be decoupled and that the generation-recombination terms can be linearized. These assumptions have been used routinely in the analysis of semiconductor detectors.²⁻⁵ Linearization of the recombination-generation terms, for example, is valid when the excess carrier concentration is small compared to the number of available trapping and recombination centers and when the detrapping time is small compared to the transit time. In this case, the rate of removal of carriers is proportional to the carrier concentration. Detrapping can also be included in the model and will be discussed in a later section.

These assumptions lead to the following equation for the concentration of excess carriers (x) within the semiconductor:

$$\frac{\partial x}{\partial t} = \nabla \cdot \mathbf{K}_x - x/\tau_x + G, \quad (4)$$

where $x = p$ for holes or $x = n$ for electrons. The parameters of the excess carrier equation, including the mobility, diffusion coefficient, and free-carrier lifetime can vary with position and electric field. The initial condition for the problem is $n(\mathbf{r}, 0) = 0$ for $\mathbf{r} \in \Omega$ where Ω is the set of points within the semiconductor. For mapping charge pulses, the generation term is selected to be an impulse of unit charge: $G = \delta(\mathbf{r} - \mathbf{r}') \delta(t)$.

Equation 4 is valid for all points within the semiconductor ($\mathbf{r} \in \Omega$). Boundary conditions can be specified by dividing the surface of the semiconductor into three parts: $S = S_O \cup S_B \cup S_I$ (Fig. 1). The set of points on the surface underneath ohmic contacts is S_O . The set of points on general metal-semiconductor interfaces is S_B (e.g., rectifying contacts). The set of points on semiconductor-insulator interfaces is S_I . The boundary

conditions for Eq. 4 are $x(\mathbf{r},t)=0$ for $\mathbf{r} \in S_O$; $\hat{n} \cdot \mathbf{J}_x = vx$ for $\mathbf{r} \in S_B$, where v is the surface recombination velocity and $\hat{n}$ is the unit outward surface normal vector; and $\hat{n} \cdot \nabla x = 0$ for $\mathbf{r} \in S_I$.⁶

The current induced in electrodes by the motion of charge can be estimated using the weighting potential method.^{7,8} Using this method, the charge induced on individual electrodes or groups of electrodes connected to a common circuit can be determined. In this paper, the analysis is confined to cases in which the electrode potential is not influenced by charge motion, which is consistent with the assumptions used to decouple the semiconductor equations. Note that the analysis method is not restricted to contacts: the current induced in conductors outside the semiconductor volume can also be modeled.

The charge induced in an arbitrary set of electrodes connected to a common circuit (denoted k) is given by

$$Q_{xk}(t) = -q \int_0^t dt' \int_{\Omega} d^3\vec{r} \ x \ \mathbf{v}_x \cdot \nabla \phi_k \quad , \quad (5)$$

where $\mathbf{v}_x$ is the drift velocity, q is the charge on a single carrier, and ϕ_k is the weighting potential given by the solution of Poisson's equation when the electrodes connected to circuit k are set to unit potential and all other electrodes are grounded. In determining the weighting potential, the space charge is set to zero. The charge measurement efficiency for circuit k is defined as $\eta_{xk}(\mathbf{r},t) = Q_{xk}(t)/q$, when x is the solution of Eq. 4 for an impulse of unit charge at $\mathbf{r}$. Note that the charge measurement efficiency is Green's function for the electron continuity equation and gives the shape of charge pulses for charge generated at discrete locations.

Equations 4 and 5 provide a complete description of charge transport and current induction for excess carriers produced by radiation interactions. The steady-state electric field, which appears in the excess carrier continuity equation, can be determined by solving the semiconductor equations (Eqs. 1-3). The boundary conditions for Eq. 4 are general enough to model a wide variety of semiconductor effects. Equation 5 can be used to approximate the output of a charge-sensitive preamplifier and is the starting point for more detailed calculations of the response of pulse-processing electronics. Ballistic deficit, for example, can be modeled by convolving the charge pulse given by Eq. 5 with the transfer function of the charge-sensitive preamplifier.

PULSE MAPPING METHOD

An efficient method can be derived for estimating all of the pulses that can be produced by a detector for a selected circuit and charge carrier. Since the excess carrier continuity equation involves linear operators, an adjoint continuity equation can be constructed. For example, the adjoint electron continuity equation is given by

$$\frac{\partial n^+}{\partial t} = -\mu_n \nabla \phi \cdot \nabla n^+ + \nabla \cdot (D_n \nabla n^+) - n^+ / \tau_n + G_n^+, \quad (6)$$

where n^+ is the adjoint electron concentration. If the adjoint generation term is selected to be $G_n^+ = \mu_n \nabla \phi \cdot \nabla \phi_k$, then the solution to Eq. 6 yields a spatial and temporal map of the charge measurement efficiency for circuit k . Namely, it can be shown that

$$n^+(\mathbf{r}, t) = \eta_{nk}(\mathbf{r}, t) \quad (7)$$

In other words, all of the charge pulses that can be produced by a detector for impulses of charge at discrete locations can be determined by solving a single, time-dependent problem.

The boundary conditions for Eq. 6 are given in Table 1. All of the assumptions that are stated for Eqs. 4 and 5 are valid for the adjoint model. An expression similar to Eq. 6 can be developed for excess holes with the same interpretation, $n^+(\mathbf{r}, t) = \eta_{pk}(\mathbf{r}, t)$. The generation term for the adjoint hole continuity equation is $G_p^+ = \mu_p \nabla \phi \cdot \nabla \phi_k$, and the sign is reversed on the drift term (see Table 1).

DETRAPPING

Detrapping of carriers causes additional dispersion of charge, delays charge collection, and enhances ballistic deficit. Detrapping can be included in the model by introducing an additional continuity equation describing the population of trapped carriers. For the model to be strictly valid, the number of unoccupied trapping centers must be large compared to the number of excess free carriers. The continuity equation is given by

$$\frac{\partial n_t}{\partial t} = n/\tau_n - n_t/\tau_n^* \quad , \quad (8)$$

where n_t is the concentration of trapped, excess carriers and τ_n^* is the lifetime of trapped carriers. By definition, there are no excess, trapped carriers in steady state, so

$n_t(\mathbf{r}, 0) = 0$. The adjoint equation for trapped carriers is

$$\frac{\partial n_t^+}{\partial t} = n^+/\tau_n - n_t^+/\tau_n^* \quad , \quad (9)$$

where the initial condition for the concentration of trapped adjoint carriers is $n_t^+(\mathbf{r}, 0) = 0$.

It is very easy to show that the solution of the coupled system of adjoint equations (Eqs. 6

and 9) has the same interpretation as before: $n^+(\mathbf{r}, t) = \eta_{nk}(\mathbf{r}, t)$. So, a map of charge pulses can be constructed that includes both trapping and detrapping.

SIMPLE DEMONSTRATION

To illustrate the mapping method, we calculated charge-pulses for points underneath a collecting electrode in a coplanar grid CdZnTe detector. Luke gives a detailed description of the coplanar grid method.^{11, 12} The device modeled was 1 cm x 1 cm x 0.5 cm and is described in detail elsewhere.¹³ The electrostatic potential and the weighting potential for both the collecting and noncollecting electrodes were determined using a two-dimensional finite elements code (Fig. 2). Space charge was neglected. The mobility of electrons was assumed to be 600 cm²/V-s. The electron lifetime was 5 μ s. Detrapping was not modeled. The adjoint electron continuity equation (Eq. 6) was solved in 25-ns time steps using finite differences in one dimension along the chord A-B shown in Fig. 1. Lateral charge motion was ignored. The electrostatic potential and weighting potential for the collecting and noncollecting circuit used in the calculation are shown in Fig. 3. The results of the simulation, including Green's function for charge induction by electrons, are displayed in Fig. 4. Note that the adjoint electrons flow in the same direction as the holes. In fact, if there is no space charge in the device, the adjoint continuity equation has exactly the same form as the continuity equation for holes (see Table 1). Consequently, production semiconductor codes can easily be modified to solve the adjoint continuity equation for Green's function, provided the adjoint source term can be modeled and the user is willing to ignore the effect of space charge on the adjoint drift term.

CONCLUSIONS

The adjoint mapping method enables the efficient calculation of charge-pulses produced by semiconductor radiation detectors: the solution of a single, time-dependent problem is required to compute Green's function for selected electrodes, provided the weighting potential for the electrodes and the steady-state electric field within the device are known. The underlying assumptions of the method are consistent with assumptions routinely used for semiconductor detector analysis. For example, for planar detectors, the model is consistent with Hecht's relation. Within the framework of the mapping algorithm, a wide range of carrier transport physics can be modeled, including trapping and detrapping, the diffusion and drift of charge carriers, arbitrary electric fields, and non-ideal contacts (e.g., Schottky effect). No assumptions are made about the geometry of the device or the electrodes. Consequently, the mapping method should prove effective in modeling complex structures envisioned for compound semiconductor detectors and imagers.

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APPENDIX: DERIVATION OF THE MAPPING METHOD

Adjoint operators were derived for the continuity equation using the identity $(n^+, Ln) = (n, L^+ n^+) + C$,* where L is the forward operator, L^+ is the adjoint operator, and C is the conjunct.^{9, 10} Boundary conditions for the adjoint problem (Table 1) were established by requiring the conjunct to vanish.

The forward equation for excess carrier concentration is given by $G = Ln$, where L can be determined by inspecting Eq. 4. The adjoint equation is given by $G^+ = L^+ n^+$. Multiplying the forward equation by n^+ and the adjoint equation by n , subtracting the result, and integrating over the volume of the detector and time, yields

$$(n^+, G) - (n, G^+) = (n^+, Ln) - (n, L^+ n^+) = 0. \text{ Consequently, } (n^+, G) = (n, G^+). \text{ If}$$

$$G = \delta(\mathbf{r} - \mathbf{r}')\delta(t), \text{ then } n^+(\mathbf{r}', t') = (n, G^+). \text{ If } G^+ = \mu_n \nabla \phi \cdot \nabla \phi_k, \text{ then}$$

$$n^+(\mathbf{r}', t') = (n, -v_n \cdot \nabla \phi_k), \text{ which is the charge measurement efficiency (see Eq. 5).}$$

*The inner product is given by $(x, y) = \int_0^t dt \int_V d^3\bar{r} \ x y$.

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Figure 1. Diagram of a coplanar-grid detector illustrating different types of boundaries.

Table 1. Summary of operators and boundary conditions for the electron continuity equation.

Forward	Adjoint	Associated initial and boundary conditions for the adjoint problem.
$\frac{\partial n}{\partial t}$	$\frac{\partial n^+}{\partial t}$	$n^+(\mathbf{r}, 0) = 0 \quad \forall \mathbf{r} \in \Omega$ $t \geq 0$ (Note 1)
$\nabla \cdot (\mu_n n \nabla \phi)$	$-\mu_n \nabla \phi \cdot \nabla n^+$ (Notes 2 and 3)	$n^+(\mathbf{r}, t) = 0 \quad \forall \mathbf{r} \in S_B \cup S_I$ (Note 4)
$\nabla \cdot (D_n \nabla n)$	$\nabla \cdot (D_n \nabla n^+)$	$\hat{n} \cdot \nabla n^+ = 0 \quad \forall \mathbf{r} \in S_B \cup S_I$ $n^+(\mathbf{r}, t) = 0 \quad \forall \mathbf{r} \in S_O$

Notes:

1. The adjoint model is derived as a final value problem and has been transformed into an initial value problem by a change of variables.
2. $-\mu_n \nabla \phi \cdot \nabla n^+ = -\nabla \cdot (n^+ \mu_n \nabla \phi)$ if $\nabla^2 \phi = 0$ and μ_n is spatially invariant, in which case the adjoint electron continuity equation has the same form as the hole continuity equation.
3. The adjoint term for the hole continuity equation is $\mu_p \nabla \phi \cdot \nabla p^+$.
4. This condition can be eliminated on surfaces for which $\hat{n} \cdot \nabla \phi = 0$.

Figure 2. Potential (a) and weighting potential for the collecting circuit (b) for a coplanar grid detector. The solution of the example is defined on the chord A-B. The weighting potential for the noncollecting circuit is the mirror image of the weighting potential for the collecting circuit.

Figure 3. Electric field and weighting fields for the collecting and noncollecting electrodes, where z is the distance from the anode.

Figure 4. The adjoint generation terms for the collecting and noncollecting electrodes are shown in 4a and 4b, respectively, where z is the distance from the anode. The adjoint electron concentrations (Green's function) for the collecting and noncollecting electrodes are shown in 4c and 4d, respectively. Adjoint electrons move towards the cathode (as do holes). Charge pulses determined from the adjoint solutions are shown as a function of depth in 4e and 4f for the collecting and noncollecting electrodes, respectively.