SIMULATIONS OF HOLE INJECTION IN DIAMOND DETECTORS*

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Abstract

We present simulations of a semiconductor beam detector using the code VSim. The 3D simulations involve the movement and scattering of electrons and holes in the semiconductor, voltages which may be applied to external contacts, and self-consistent electrostatic fields inside the device. Electrons may experience a Schottky barrier when attempting to move from the semiconductor into a metal contact. The strong field near the contact, due to trapped electrons, can result in hole injection into the semiconductor due to transmission of electrons from the valence band of the semiconductor into the metal contact. Injected holes are transported in the applied field leading to current through the detector. We compare our simulation results with experimental results from a prototype diamond X-ray detector.

INTRODUCTION

Diamond is a promising material for use in X-ray and particle detectors [1–4]. The experimental setup for an X-ray detector is shown in Figure 1, it consists of a thin diamond sheet 90 μm thick which is placed in an X-ray beam line. On either side of the diamond sheet are metal contacts which can be held at different voltages, resulting in a voltage bias across the sheet. The bias is considered positive when the voltage is higher on the metal contact to the side of the beam (right).
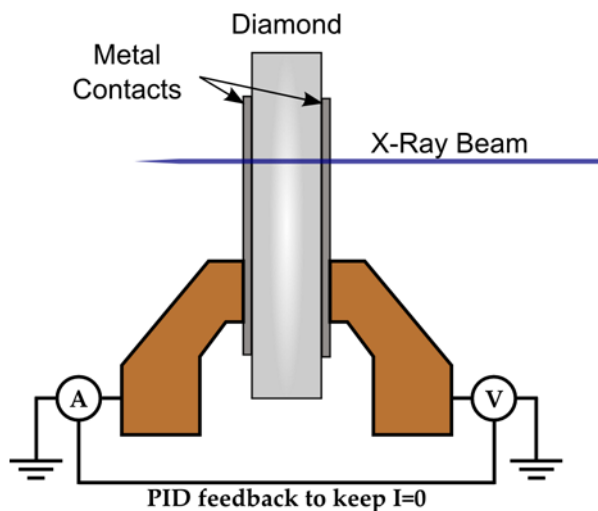

Figure 1: Schematic of an experimental X-ray detector.

When an X-ray photon passes through the thin diamond sheet, it may be absorbed, creating an electron-hole pair.

The electron and hole scatter inelastically in diamond, creating many more secondary electrons and holes. Further relaxation of low energy charge carriers is dominated by scattering with phonons. Under positive bias, electrons will tend to drift to the right and holes to the left, leading to separation of these charge carriers.

In these experiments an X-ray beam generates holes and electrons continuously inside the diamond detector. The experimental data of electron and hole responsivity versus bias shows a marked difference between electrons and holes. As holes are generated, they diffuse to the right under the negative bias, and are able to pass without difficulty into the right metal contact. The responsivity of holes increases when a negative bias is applied, but eventually saturates at a maximum value [3]. The maximum current is the rate at which holes are generated by the X-ray beam.

The resistivity of electrons under positive bias also shows an increase with the applied bias. The rate of increase is lower than that of holes, this was attributed to trapping of electrons inside the diamond, and to a lesser extend the different diffusion characteristics of holes versus electrons. As the bias is increased further, no saturation occurs; the current continues to increase with the bias.

The current eventually exceeds that generated by the beam. This is possible if electrons become trapped in the diamond, making it negatively charged. This could lead to holes being injected into the diamond from the right contact, where they drift across the diamond plate and pass into the left contact. Since these holes are not created by the beam, the current is not limited by the rate of hole production by the beam.

The hole current does not appear uniformly across the plate, but is isolated to small regions [5] with scale on the order of 50 μm. This supports the theory that the current is due to electron trapping localized in these small regions, perhaps due to surface defects. When electrons become trapped in these isolated regions near the right contact, they result in an increase in the electrostatic field in these regions, which can lead to hole injection. When holes are injected near the defect, they pass all the way through the diamond to the opposite contact in a well-defined current spike.

SIMULATION SETUP

The models for charge transport in diamond are described in Ref. [6]. To model electrons transmission across the potential barrier of a diamond interface (e.g., with a metal or vacuum) we use the transfer matrix method [7, 8], which has been implemented in VSim [9].

Our 3D simulations of the diamond detector use a domain of size $30 \times 500 \times 500$ μm. The thickness of the plate is $d = 30$ μm. We use periodic boundaries in y and z. The

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electrostatic field is calculated at each time step by doing a Poisson solve based on the current charge density, with boundary conditions in x using the applied voltage difference (4.13 V). The electrostatic field in the diamond is constant (without particles) at around -0.1 MV/m. This field strength gives a hole drift speed of $v \approx 2 \times 10^4$ m/s, so free holes should drift across the domain in around 1.3 ns. In this field strength, the drift speed for free electrons in diamond is less than for holes, around 1×10^4 m/s.

There is a 1/2 µm gap at the right edge of the domain between the diamond and metal contact. This gap effectively represents the metallic contact region, and allows electrons with sufficiently high energy to transition into the metal contact.

In order to simulate electron trapping, we initialize the simulation with $Q_e = 1.6 \times 10^{-11}$ C (1×10^6) thermal electrons in a small region $2 \times 50 \times 50$ µm to correspond with the scaling of the trapped electron features. We place these electrons first at the right edge of the diamond, and second in the center of the diamond. We run the simulation for 30 picoseconds, during this time the electrons diffuse and drift to the right. In the first case they encounter the metal contact region, and their energy is too small to cross the potential barrier (Figure 2). In the second case the electrons become effectively trapped in the middle of the diamond.
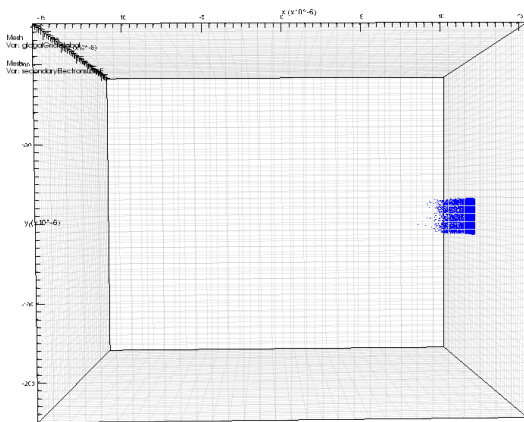

Figure 2: Electrons initialized near the right wall and allows to drift into it for 30 ps.

At 30 ps, we freeze the electron density to simulate trapped electrons which do not move. If we did not do this the electrons would continue to diffuse inside the diamond. At this time, Figure 3 shows the energy bands inside the diamond for the conduction and valence bands. Conditions are favorable for an electron on the right edge to pass from the valence band of diamond into the metal contact, or in other words a hole to pass from the right contact into diamond.

Figure 4 shows the electrostatic field inside the device at 30 ps. The red curve shows the field when the electrons are initialized near the right boundary, while the blue curve shows the field when the electrons are initialized in the center of the diamond.
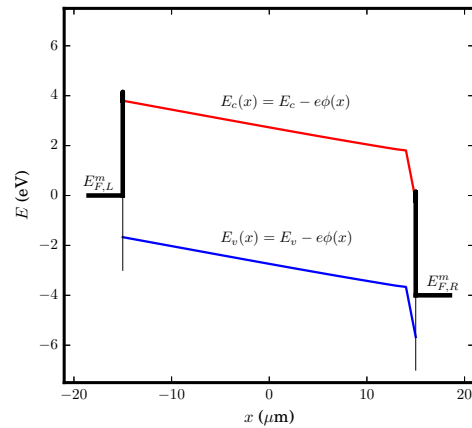
Figure 3: Energy bands for the conduction (upper) and valence (lower) bands across the diamond detector, including the electrostatic field due to trapped electrons near the right boundary.
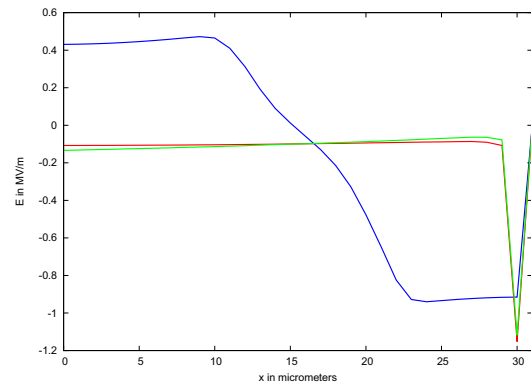

Figure 4: Electric field in diamond. Red: electrons trapped at the right edge, blue: electrons trapped in the center, green: steady state with edge trapping after hole injection.

The main difference between the electrons trapped at the edge of the domain and the center is that in the first case the field is negative across the device. If a hole is injected from the right, this field allows it to drift across the entire domain. In the case of the electrons initialized in the center, the field goes positive to the left of these electrons, which prevents holes from drifting across the domain.

SIMULATION RESULTS

After 30 ps, the electron density is frozen and we begin to inject holes into the 50×50 µm patch at the right edge of the domain. Holes are injected at a constant rate (one every 10 timesteps or $I_h = 3.2$ µA). We have also started to investigate controlling hole injection using a Fowler-Nordheim approach, this will be used in future models.

After holes are injected they drift to the left in the (approximately) constant electrostatic field. As additional holes are injected, they begin to modify the electrostatic field, but for small currents the holes will drift across the entire plate and exit the left side. The total hole charge in the device at steady state will be $I_h d/v$, or 3×10^5 holes in this case. For this small current the electrostatic field across the center is only slightly modified (the green curve in Figure 4).

Figure 5 shows the steady-state density of holes. The gap on the right side is due to the 1/2 μm gap at the right edge of the domain.
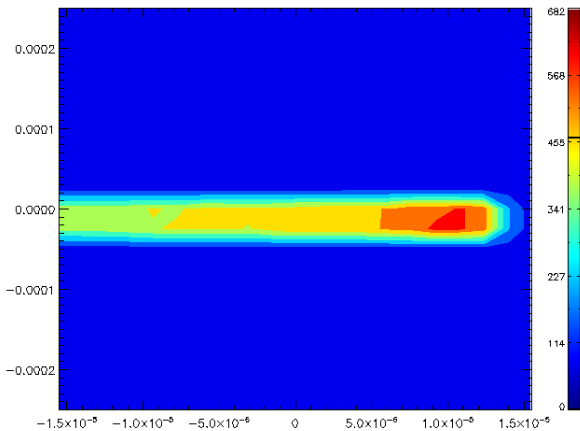

Figure 5: The density of holes when the simulation reaches steady state.

As the hole current is increased further, eventually the field inside the diamond goes to zero, which shuts off the hole current. This happens when the total number of holes is around the total number of trapped electrons, which will occur when the hole current reaches

$$I_{max} \approx \frac{Q_e v}{d}. \tag{1}$$

This current increases with the applied bias, because the hole drift speed v increases with the applied bias. One can think of the trapped electrons and holes as a dipole which oppose the applied field, eventually cancelling it out. In the simulation example the limiting hole current is 107 μA.

SUMMARY

We have demonstrated that electrons which become trapped in a small 50μm region at the right edge of the domain can lead to a situation favorable for hole injection. The trapped electrons lead to a localized increase in the electrostatic field, and it is possible that the overall electrostatic field has the right sign to allow holes to drift all the way across the diamond in a thin current spike. When electrons become trapped in the middle of the domain, conditions are not favorable for holes to drift across the entire domain, because the field reverses.

This hole drift is shut off when the number of holes in the device is the same order as the trapped electrons. However, as the bias is increased the hole drift rate increases, so there is no limit to the hole current with bias increase, in agreement with experimental results.

In reality, the rate of hole injection is limited by the maximum electric field at the right wall. If the perpendicular electric field is not large enough, no holes will be injected. These simulation results indicate that the hole injection current is probably due to electron trapping near the diamond-metal interface and not within the bulk of the diamond detector.

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