Boundary Condition for the Modeling of Open-circuited Devices in Non-equilibrium

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A boundary condition specifically designed to model open-circuited devices in a macroscopic device simulator is introduced. Other simulation techniques have relied on an external circuit model to regulate the current flow out of a contact thus allowing the potential to remain the controlled variable at the boundary. The limitations of these methods become apparent when modeling open-circuited devices with an exceptionally small or zero output current. In this case, using a standard ohmic-type Dirichlet boundary condition would not yield satisfactory results and attaching the device to an arbitrarily large load resistance is physically and numerically unacceptable. This proposed condition is a true current controlled boundary where the external current is the specified parameter rather than the potential. Using this model, the external current is disseminated into electron and hole components relative to their respective concentration densities at the contact. This model also allows for the inclusion of trapped interface charge and a finite surface recombination velocity at the contact.

An example of the use of this boundary condition is performed by modeling a silicon avalanche photodiode operating in the flux integrating mode for use in an imaging system. In this example, the device is biased in steady-state to just below the breakdown voltage and then open-circuited. The recovery of the isolated photodiode back to its equilibrium condition is then determined by the generation lifetime of the material, the quantity of signal and background radiation incident upon the device, and the impact ionization rates.

Keywords: Current boundary condition, macroscopic simulation, charge storage, avalanche photodiodes

1. INTRODUCTION

Many macroscopic device simulators provide for a connection to an external circuit primarily through either ohmic or Schottky contacts. In these cases, the system variables are constructed such that the electrostatic potential is the independent parameter describing the boundary condition, and

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other values such as the current flowing through the contact are calculated in a post-processing step [1, 2]. These boundary conditions are adequate for situations where the device can be approximated as a voltage controlled current source; however, instances exist where this may not be the case. Most notably this occurs when the energy stored within the internal capacitance of a device becomes the dominant controlling factor for the prediction of the potential across the device. In these cases, the use of a current controlled boundary is more applicable.

A situation requiring a current controlled contact exists when simulating the recovery to equilibrium of an open circuited device. Such a condition occurs when examining the performance of an avalanche photodiode configured in the charge storage mode for imaging applications [3, 4]. In this configuration, the sensor is periodically reset by applying a large reverse bias to the device. Following the reset, the device is open-circuited and begins to equilibrate through carrier generation. If the device is used as a photodetector, light shining upon the structure generates excess charge which is then stored within the depletion region of the device. At the end of the integration cycle, the quantity of stored charge within the device is used as an indication of the total illumination upon the pixel [5].

The present work introduces a current controlled boundary condition which is capable of simulating an electrically isolated photodiode. With this model, a steady-state voltage is applied between the ohmic contacts using the traditional Dirichlet boundary condition. The device is then isolated from the external circuit. The voltage across the device is no longer fixed invalidating the use of a voltage controlled boundary condition. Alternatively, a current controlled boundary condition must be employed to describe the device which includes effects such as surface recombination, trapped surface charge, and leakage current from the read-out electronics. Application of this model to a generic APD is also presented.

2. BOUNDARY CONDITION

A current controlled boundary condition is required to accurately model the reverse recovery within a photodiode. When the diode is disconnected from the external circuit or driving bias, the voltage at the cathode floats. The metal contact can no longer be treated in its usual manner as an infinite source of carriers and the assumption that the electron and hole concentrations are dictated by their equilibrium values may not be valid. Moreover, the voltage across the device is determined solely by the distribution of charge and the internal capacitance of the diode and not by the external circuit. Simulation techniques which operate by allowing the potential to remain the independent variable, while acceptable for modeling switching characteristics, are inappropriate for cases with either very low or zero external current. Attempting to model the open-circuited device with the standard ohmic condition and a very large shunt load resistance is unacceptable on physical as well as numerical grounds.

The primary concern with developing the current controlled model lies in the apportioning of the electron and hole fluxes from the external current at the contact. It is assumed here that the total current is divided into the electron and hole currents relative to their respective densities at the contact. Thus, the relation between the currents is given by,

\[
\frac{n}{n+p} \cdot J_n - \frac{p}{n+p} \cdot J_p = qR_{surf} \quad (1)
\]

where \(J_n\) and \(J_p\) are the electron and hole currents leaving the contact as indicated in the illustration of the discretized control volume as shown in Figure 1 [6]. The carrier concentrations are taken to be those of the neighboring control volume within the device. \(R_{surf}\) is the recombinaiton rate owing to surface states at the contact [7] using the standard relation:

\[
R_{surf} = \frac{S_nS_p(n-p^2)}{S_n(n+n_1) + S_p(p+p_1)} \cdot \delta(x). \quad (2)
\]
where \( S_n \) and \( S_p \) are electron and hole recombination velocities. Additionally, Eqs. (3) and (4) below require that the carrier currents sum to the external current and that the band bending at the contact is proportional to the trapped interface charge.

\[
J_n + J_p = J_{\text{ext}} \quad (3)
\]

\[
\varepsilon \frac{\partial \psi}{\partial n} = Q_{\text{int}} \quad (4)
\]

Combining Eqs. (1) and (3) yields expressions setting the values of the current into a contact.

\[
J_p = qR_{\text{surf}} + \frac{p}{n + p} \cdot J_{\text{ext}} \quad (5)
\]

\[
J_p = -qR_{\text{surf}} + \frac{n}{n + p} \cdot J_{\text{ext}} \quad (6)
\]

These currents are used directly within the control volume formulation of the discretized continuity equations [8]. Furthermore, partial derivatives of the current expressions with respect to the system variables are analytically obtained thus leading to increased convergence of the non-linear system.

A two-dimensional analysis of the photodiode is necessary to study the full carrier transport of effects such as premature edge breakdown and pixel crosstalk; however, this study is concerned solely with the examination of the charge storage capabilities of the APD. Therefore, a one-dimensional analysis is satisfactory. This greatly simplifies the model by allowing the external current density, \( J_{\text{ext}} \), to be directly proportional to the cross sectional area of the device contact and the total current. Multi-dimensional extensions of this boundary can be produced by either imposing an additional constraint upon how the output currents sum over the range of the contact such as equipartitioning or by solving Gauss’ law describing the current flow through the metal comprising the contact [9].

To study the charge storage of the photodiodes, the current boundary condition is incorporated into a drift-diffusion simulator which self-consistently solves Poisson’s equation and the current continuity equations [10]. Since the smallest dimensions of the device structures are on the order of microns, it is believed that hot carrier transport can be neglected in these devices and that a full hydrodynamic simulation is unnecessary. Within this model, the generation-recombination rates include terms for SRH, Auger, and radiative recombination, impact ionization, and wavelength dependent photoillumination. Additionally, the standard field dependent mobility and impact ionization models for silicon are incorporated into the simulator [11]. By using a completely numerical model, many of the non-linear attributes of the carrier transport of a photodiode in charge storage mode can be included without the use of many of the simplifying approximations typically employed [3, 4].

3. EXAMINATION OF CHARGE STORAGE IN PHOTODIODES

To demonstrate the utility of the current controlled boundary condition, the reverse recovery of an avalanche photodiode designed for night-sky imaging is examined. Here the device, shown in Figure 2, is a reach-through avalanche photodiode 50 \( \mu m \) in length. During the initial reset period, a
large electric field is established in the $p$-type multiplication region and a modest drift field exists in the intrinsic region. The illumination spectrum used in this study is that of a cloudless, moonless, night sky with a total illumination of $5.4 \times 10^{16}$ photons per cm$^2$ over a range of wavelengths from 0.3 to 1.1 microns [12]. The total internal quantum efficiency for this spectrum is approximately 55%.

If the photodetector was continuously biased, the photo-generated carriers would be swept across the depletion region, collected at the device contacts, and interact directly with the external circuit. In the charge storage mode of operation, the connection to the external circuit is removed. In this case, the internally stored electric field still causes the carriers to be swept across the depletion region where they may impact ionize. However, the charge is stored near the edges of the depletion region as opposed to interacting with the external circuit. This accumulated charge counteracts the depleted charge from the reset and tends to drive the reverse recovery. Additional factors which promote the recovery of the diode include the leakage current inherent in the readout electronics, $J_{\text{ext}}$, the dark current due primarily to thermal generation of carriers from SRH centers, and surface recombination.

Figure 3 shows the dynamics of the charge storage within the APD for various photoillumination intensities. For this case, intensities ranging from 0.05 to 500 times the nominal night sky spectrum are considered ($2.7 \times 10^{15} - 2.7 \times 10^{19}$ photons per cm$^2$ per second). The initial bias on the device is established to produce an initial steady-state gain of fifteen. The first part of the voltage recovery is dominated by the influence of holes filling the intrinsic region resulting in a linear decay of internal bias with only a very small degradation in gain. Once the drift region has been filled, the charge is stored at the edge of the high field multiplication region giving rise to the expected parabolic voltage recovery. A non-linear decrease in the internal gain is observed as the high field region recovers. Under extreme illumination conditions, the diode completely recovers to its equilibrium level and begins to become forward biased. Recombination processes prevent the diode from continued storage of charge once the diode becomes sufficiently forward biased.
Typically, the actual stored charge rather than the device bias is quantified at the end of the integration period to determine the level of photoillumination [5]. Figure 4 illustrates the total electron charge stored within the diode as a function of the integration time. As expected, the first part of the integration gives rise to a linear collection of charge with a constant gain. As the amount of charge increases, the gain begins to saturate with a square root dependence [10, 13]. Once the device has recovered to the point where internal gain becomes negligible, the linear recovery is again observed. As the diode becomes significantly forward biased, as in an opencircuited solar cell, the charge saturates.

4. CONCLUSIONS

A current controlled boundary condition applicable to macroscopic device simulators is presented. This boundary type establishes the systems variables such that the external current becomes the independent quantity at the contact, thus allowing the contact potential to be self-consistently set within the simulation. As an example of this model, a reach-through avalanche photodiode, operating in the charge storage mode, is examined. Here it is observed that the model allows one to capture the full transient recovery of the device from the initial reset point all the way through the forward bias condition in the case of extreme photoillumination.

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