Full-Band Monte Carlo Study of Hot Carriers for Advection-Diffusion Monte Carlo Simulations

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***Abstract*—Diffusion of carriers under high electric field is studied using full-band Monte Carlo simulations. The diffusion of hot carriers is found to be strongly anisotropic with respect to the electric field direction and to be times higher than the one predicted by the Einstein's law. A new calibration of analytical models is proposed to account for the anisotropy of the diffusion coefficient as well of the impact of the electric field. The effect of the new model is illustrated by studying its impact on the lateral and longitudinal spread of the electronic avalanches that occur in single-photon avalanche diodes, using advection-diffusion Monte Carlo.**

***Index Terms*—electronic transport, full-band Monte Carlo, SPAD, diffusion, avalanche, photodiode**

I. INTRODUCTION

The diffusion of carriers is a fundamental transport process in semiconductors and is often treated by the Einstein's law in standard TCAD modeling. While the validity of the Einstein's law is well established at low electric fields, its validity at high electric fields is questionable.

In this work, we focus on the diffusion resulting from thermal excitation of carriers in silicon resulting from the mixing of the interaction with the lattice and the increase of the kinetic energy by an external electric field.

The electronic diffusion has been studied by several authors using measurements and Monte Carlo simulation [1]–[3] with electric fields up to around 50 kV/cm. In Single-Photon Avalanche Diodes (SPADs), the maximum electric field can be as high as 1 MV/cm, and there is no available data nor model for diffusion in this regime.

This paper aims to fill this gap by studying the lateral and longitudinal diffusion of carriers in silicon under high electric fields, using a Full Band Monte Carlo (FBMC) approach [4].

Finally, we used these FBMC results to calibrate the newly proposed Advection-Diffusion Monte Carlo (ADMC) model [5]. This approach reduces the computational burden, but requires a fine calibration of the transport parameters, among which the diffusion coefficient. We explore the impact of the new calibration of the diffusion coefficient on the avalanche spread SPAD devices.

II. METHODOLOGY

An FBMC code solving the Boltzmann transport equation is used to simulate the transport

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of electrons in silicon. The solver includes realistic band structure from tight-binding calculations and a full description of the scattering through phonon-assisted scattering and impact ionization with a Keldysh model. Implementation details can be found in [4]. The simulations are performed in pure silicon at 300K.

The diffusion coefficient is extracted from the variance of the position of the carriers as a function of the time.

$$D_{ij} = \frac{1}{2}\frac{d}{dt}\left\langle \left(x_i - \langle x_i \rangle\right)\left(x_j - \langle x_j \rangle\right)\right\rangle . \qquad (1)$$

With i and j the chosen spatial coordinate in (x, y, z), and x_α the trajectory of the particle in the real space, for the coordinate α.

Transverse and longitudinal diffusion coefficients are then calculated using adequate formulas including the dependence on the electric field orientation [6].

III. RESULTS AND DISCUSSION

To be meaningful as an intrinsic transport parameter (used for instance in TCAD or ADMC simulations), the diffusion coefficient must be independent of the time. This is indeed the case as illustrated in Fig. 1 where the variance of the position of the carriers as a function of time under three different electric fields is shown. The variance remains remarkably linear with time, even for very high electric fields. Because the carriers are initially injected according to the ambient thermal energy, a delay is required to reach equilibrium with the electric field, after which the diffusion coefficient is constant.

In Fig. 2, the total energy of carriers is shown as a function of the electric field. The carriers heating starts to be visible at 10^3 V/cm, and becomes dominant at 10^4 V/cm. We extracted an equivalent electronic temperature from the thermal velocity in order to test a modified Einstein's law, where the lattice temperature is replaced by the electronic temperature.

Interestingly, Fig. 3 shows that, even at 10^6 V/cm, the distribution of carriers is well described by a Gaussian distribution, both in the longitudinal and transverse directions. This fact accredits the Gaussian-based model, used in the ADMC solver, even for transport at very high fields, providing that overshoot phenomena have a negligeable impact on the diffusion coefficient. It is therefore critical to use an accurate field-dependent diffusion coefficient.

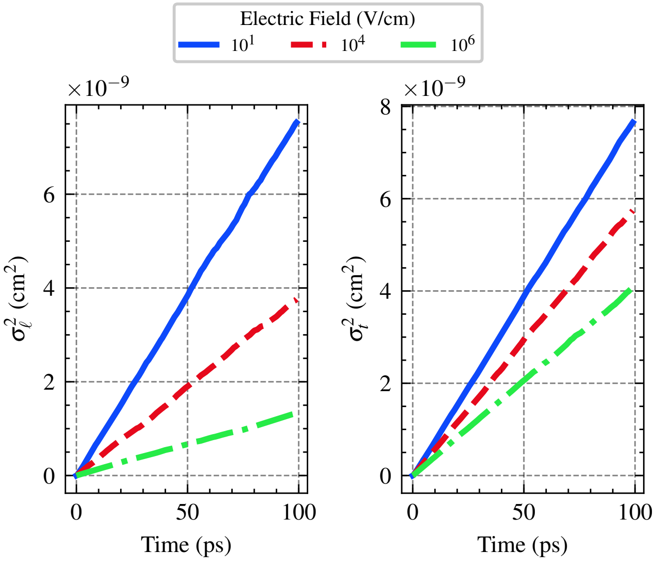

Fig. 1. Variance of the position of the carriers as a function of the time under three different electric fields. For both longitudinal (left) and transverse (right) directions, the variance is exactly linear with the time, which is in agreement with the Gaussian model. The diffusion coefficients are extracted from the slope of the linear fit.

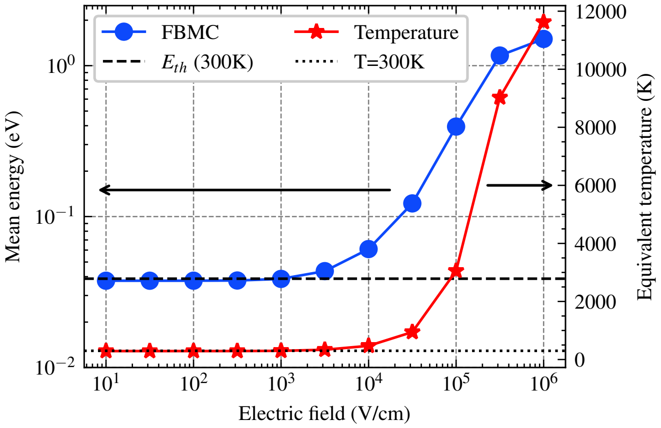

Fig. 2. Mean carrier energy extracted from the Full-Band Monte Carlo simulation as a function of the electric field in the (100) direction. By assuming a Boltzmann distribution, and using the formula: $\langle E \rangle = \frac{3}{2}k_B T/q$, we extracted the electron equivalent temperature. We show in Fig. 4 that injecting this temperature into the Einstein's law ($D = \mu_e k_B T_e/q$) improves the agreement with the FBMC results.

The extracted diffusion coefficients are shown in Fig. 4 as a function of the electric field in a range

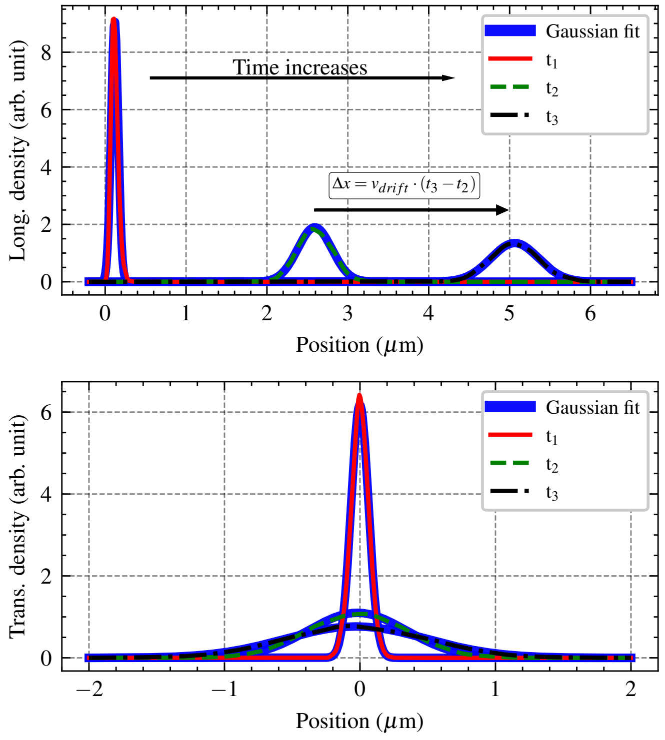

Fig. 3. Longitudinal (upper) and transverse (lower) density of carriers at three different times under a 1e5 V/cm electric field at 300K. In thick blue, the Gaussian fit of each density profile. Even at very high field, the diffusion is remarkably well described by a Gaussian model. For short times, non-linear effects are visible.

from 10^3 to 10^7 V/cm, for the <100> and <111> directions. The diffusion coefficient is found to be strongly anisotropic with respect to the electric field direction and to be times higher than the one predicted by the Einstein's law for very high electric fields. The lateral diffusion coefficient is found to be completely uncorrelated with the original Einstein law for field higher than 10^4 V/cm. Yet, the Einstein law can be greatly improved by replacing the lattice temperature by the electronic temperature extracted from the Full-Band Monte Carlo simulation (Fig. 2), in particular for the transverse diffusion coefficient.

Using a field-dependent diffusion coefficient, we also studied the spread of the electronic avalanches that occur in SPAD. In a SPAD, an initial photo-generated electrons drifts towards the diode junction, where the very high electric field accelerates it up to giving rise to an impact ionization process, yielding a new electron-hole pair. The newly generated carrier suffer the same mechanism, which eventually give rise to a self sustained electronic avalanche. We used the Advection-Diffusion Monte Carlo (ADMC) model [5] to simulate the avalanche with up to 10^7 active particles in the junction in a realistic SPAD geometry (see Fig. 5). This figure shows the importance of a well-calibrated diffusion coefficient to accurately capture the so-called space charge effects. The charge dipole created by the generated electrons and holes have an impact on the SPAD timing characteristics, through the induced electric field that counterbalances the external electric field [7].

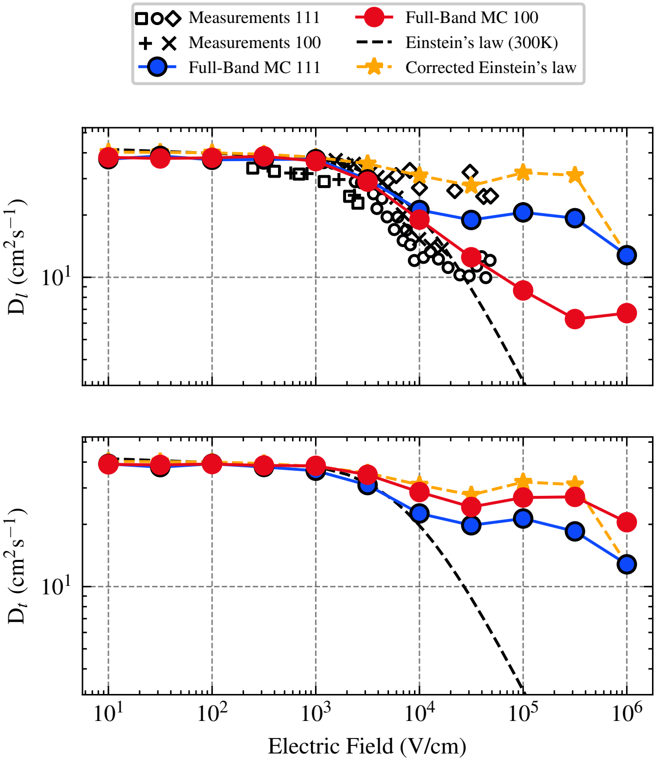

Fig. 4. Longitudinal diffusion coefficient in <100> and <111> directions as a function of the electric field. The result of the Full-Band Monte Carlo simulation is compared to data reported in [1]. In the <100> direction, we find a very good agreement with the available data. In the <111> direction, there is an important discrepancy among the measurements. Our results are in a reasonable range whatsoever. As expected, the Einstein law is not valid for very high electric fields.

IV. CONCLUSION

The diffusion of electron in Silicon under very high electric field has been studied. A new calibration of an Advection-Diffusion Monte Carlo enables to accurately predict the spatial extension of the avalanche that occurs in SPAD devices. In

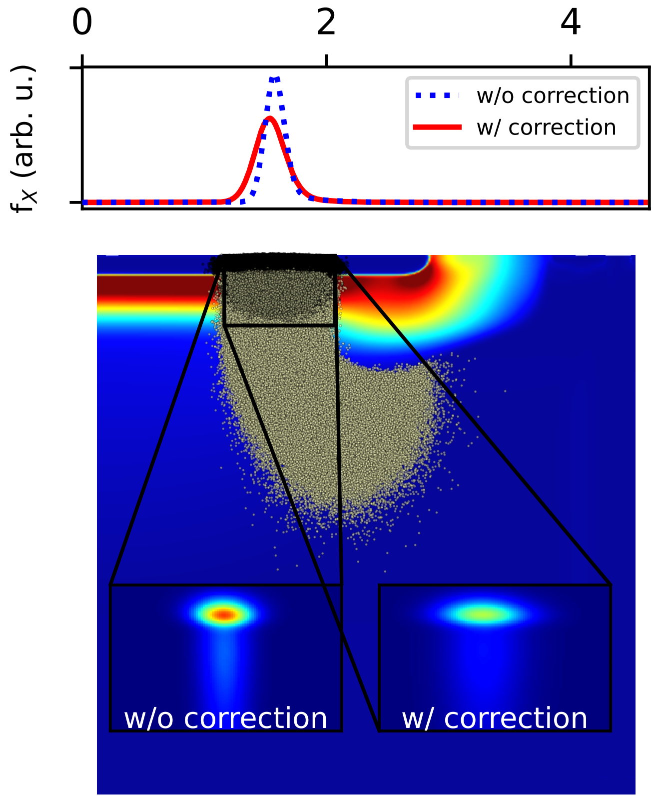

Fig. 5. Avalanche in a realistic SPAD architecture is shown. The dots represent the position of electrons and holes at the end of the simulation for the corrected diffusion coefficient. The avalanche is simulated with up to 10^7 active particles in the junction under a frozen electric field. We compare the resulting density of carriers created by the avalanche, using the usual Einstein's law and the diffusion coefficient extracted from the Full-Band Monte Carlo simulation. The insets show the density of carriers for both cases, with the same color scale. The marginal distributions of the density of carriers in the x direction (f_X) is shown. It is noticeable that the correct diffusion coefficient leads to a lower density of carriers in the junction.

future work, the new diffusion model could be used in a self-consistant Monte Carlo simulator of the transient SPAD operation, to accurately predict the space charge effect of the avalanche on the quenching process.

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