# An Efficient Impact Ionization Model for Silicon Monte Carlo Simulation

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In the field of Monte Carlo ($MC$) simulations of silicon devices the capabilities of isotropic band models in reproducing the essential features of the anisotropic silicon band structure ($ASBS$) has been demonstrated [1][2][3] and justify further work in the development of microscopic models consistent with the isotropic bands.

In this paper, we present an *electron* impact ionization ($II$) model for $MC$ simulation which is directly derived from the accurate calculations of Bude et al. [4] carried out for the $ASBS$ and including collisional broadening and intra-collisional field effects.

Compared to simplified $II$ models [5], the present one features the same average behavior of the different $II$ processes of the $ASBS$ calculated in [4], is consistent with the isotropic band structure [2][7] based on, and allows a correct generation of the secondary carriers.

To develop the $II$ model we followed the same methodology of [2] by attributing to each of the three isotropic bands of [2] (corresponding to the regions $\mathcal{P}_i$ of the Brillouin zone around the 0.85X, L, $\Gamma$ symmetry points) an $II$ rate as a function of energy. These $II$ rates $P_i^{iso}(E)$ were computed by integrating, over the equi-energy surfaces of each region of the $ASBS$, the wave vector dependent $II$ rate of [4]. This implies the following equation to be satisfied for each isotropic band $i$:

$$P_i^{iso}(E)DOS_i^{iso}(E) = \int_{\mathcal{P}_i} P(\vec{k})\delta(E - E(\vec{k}))d^3\vec{k} \tag{1}$$

where $DOS_i^{iso}(E)$ is the density of states ($DOS$) of the isotropic band $i$ and $P(\vec{k})$ is the $II$ rate of $ASBS$ at $\vec{k}$. The integration over each $\mathcal{P}_i$ is obtained following the method reported in [8]. Thus, the new $II$ model features, at each energy, the same *average* $II$ scattering rate as the $ASBS$ if the electrons were uniformly distributed over the equi-energy surface of the $ASBS$. The three $P_i^{iso}(E)$ are only calculated once (Fig. 1) and stored in files for routine simulation.

As for the final states of particles, the energies of the primary and secondary electrons are chosen according to the energy distributions of the scattered particles computed by [13]. In addition, the three final particles fulfill both energy and momentum conservation.

Several simulations of homogeneous silicon bars were performed to validate the model against available experimental data. Since no free parameters are present in our $II$ model, the electron-phonon coupling constants have been adjusted in order to reproduce electron drift velocity [9], ionization coefficients $\alpha$'s [10], and quantum yield data [11][14] (defined as the number of $II$ events experienced by an electron relaxing from a certain energy $E$).

The optimized parameters used in this work are listed in Table 1: a single value, well within the range found in the literature, has been used for the optical phonon deformation potential for all bands.

The results, illustrated in Figs. 2-4, show a good agreement with the experimental data. Since the quantum yield experiment gives information about the ratio between the $II$ and the electron-phonon scattering rate as a function of energy, and since the $II$ rate of the present model relies on a sound theoretical calculation, the results of Fig. 3 give confidence on the choice of the electron-phonon scattering strength. In Fig. 4 we also show the electron mean energy for different electric fields. The discrepancy between our results and the ones of Ref.[12] can be explained in the following way: our model is based on a higher $II$ rate (see Fig. 1) and consequently a higher electron-phonon scattering rate is obtained, which is responsible for a weaker energy vs. field dependence.

In conclusion, the $II$ model of this work allows to use the results of accurate calculations based on the $ASBS$ in the frame of a more simplified silicon isotropic band structure. It has been shown that the model is able to well reproduce available data on ionization coefficients and quantum yield experiments, and being free of fitting parameters it is very useful for determining the correct strength of the electron-phonon deformation potential for the isotropic band model which corresponds most closely with full band results.

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| optical deformation potential($D_tK$) | $eV/cm$ | $5.85 \times 10^8$ |
| optical phonon temperature($T_{op}$) | $°K$ | 600 |
| acoustic deformation potential | $eV$ | $5.8(E < 0.18eV); 4.0(E > 0.4eV)$ |

Table 1: Parameters used in calculations

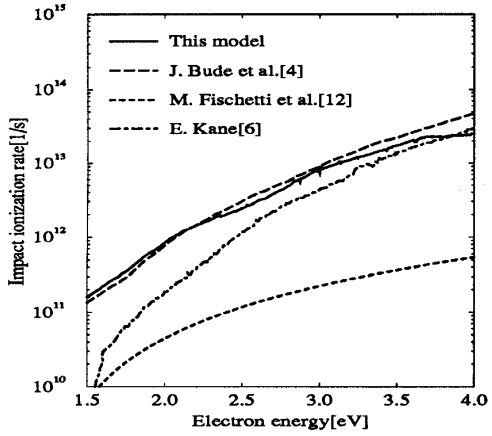


Fig. 1: $II$ rate of different models[4][6][12].

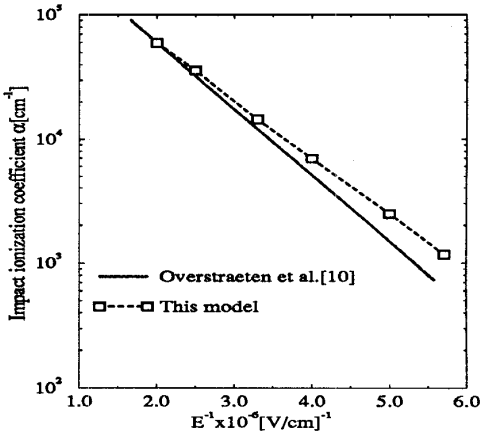


Fig. 2: $II$ coefficient in Si[10].

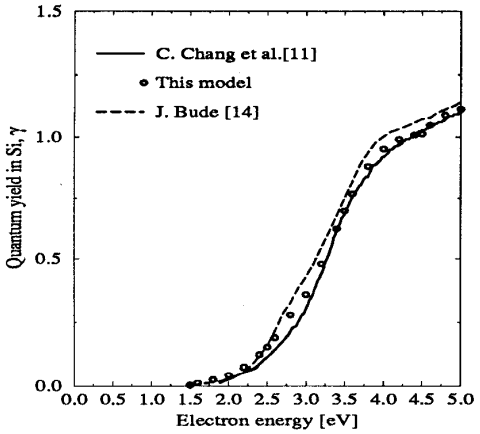


Fig. 3: Simulated and experimental quantum yield results [11][14].

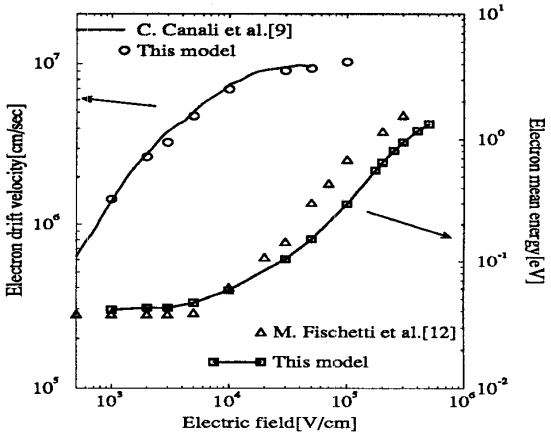


Fig. 4: Electron drift velocity (left axis) and mean energy (right axis) from this model and Ref.[9][12].