Optimization of physical parameters for high energy transport simulation in Si based on efficient electron energy distribution calculations

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In this paper the iteration technique (IT) for the solution of Boltzmann transport equation (BTE) [1] has been applied to determine a consistent set of physical parameters important for electron transport at high energies in silicon.

IT directly solves BTE in 1-D **k** space in the field direction. Given the electric field (F), IT provides noiseless and efficient calculation of the electron energy distribution (EED) in sub-micron devices, correctly accounting for non-local effects [1]. Compared to Monte Carlo (MC), the main drawbacks, arising from the 1-D approximation [1], are: i) the approach is limited to the high field case ($F > 10^4 V/cm$); ii) it makes use of isotropic semiconductor models; iii) F is given as input and is not computed self-consistently. The Si model used in this work [2] features four isotropic bands for electrons and accounts for electron-phonon interaction and impact ionization (II) (modeled by Keldish formula). Fig.1 reports the comparison between EED's calculated with IT and MC [4] for homogeneous Si (in the following EED=$f(E)g(E)$, where $f(E)$ is the occupation probability and $g(E)$ the density of states).

Simulation of modern sub-micron MOSFETs requires accurate transport models for high energy electrons. The basic set of transport parameters includes: acoustic phonon deformation potentials ($\mathcal{E}_1$), optical phonon deformation potentials ($D_t K$) for both intra- and inter-band transitions and the II parameters which in the simple Keldish formulation are the II energy threshold E_{th} and the II rate at $E = 2 \cdot E_{th}$, $P/\tau_{op}(E_{th})$ [3]. In previous works [2,5,6] the values of these parameters were obtained by fitting only experimental data of drift velocity at relatively low fields ($F \leq 5 \cdot 10^4 V/cm$).

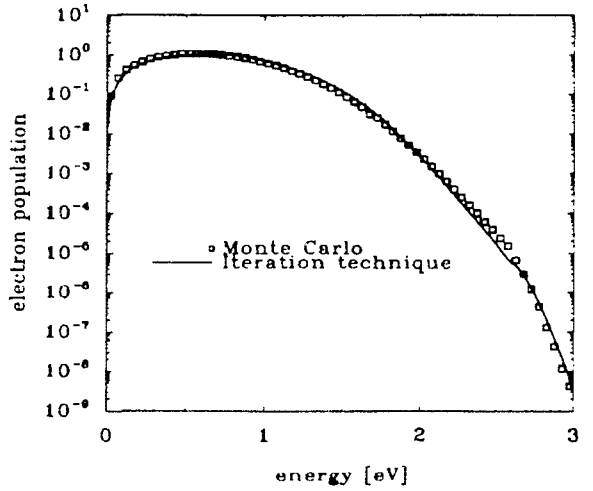

Fig.1 EED in homogeneous Si calculated by MC (squares) and IT (line): F=200kV/cm

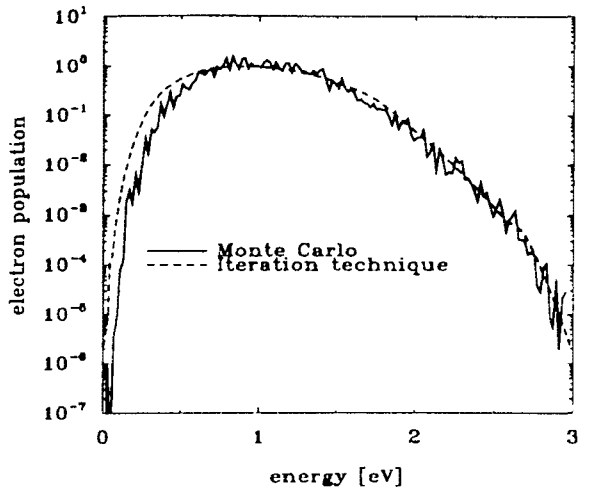

Fig.2 EED at the interface of the MOSFET 15-2-9 [8] V_{bulk}= -18V

In this work, in addition to low field mobility and drift velocity, we exploit II rates (α) [7] and the electron injection probability into the SiO_2 of MOSFETs structures (as measured by Ning [8]), that provide a set of informations related to high energy transport. In particular the transport parameters are determined by comparing the above quantities with IT calculations. A similar procedure was already used in [3] where MC calculations were used instead of IT. However, the MC simulation of Ning's experiments suffers from relevant statistical noise because: i) the very high energy tail of the electron population must be computed; ii) the simulated region (the MOSFET depletion region which is $\approx 2\mu m$) is approximately one order of magnitude larger than the typical MC MOSFET application [4,6]. Conversely, IT is well suited for this application due to the 1-D nature of the problem and to the absence of statistical noise.

In this work Ning's experiments have been simulated applying the IT to the field profile given by a drift-diffusion simulator, and calculating the EED at the $Si - SiO_2$ interface. Fig.2 reports the EED of carriers hitting the interface calculated by both MC and IT: a substantial agreement is obtained between the two methods, but the MC simulation is more noisy and required a longer CPU time ($\approx$ 40 times) than IT (IT requires 20 minutes on an IBM RISC6000 320 per bias point).

The injection probability is calculated as the ratio between the number of electrons with $E > E_B$ and the total number of carriers reaching the interface (E_B is the $Si - SiO_2$ energy barrier lowered by the oxide field effects [8]).

α's have been calculated performing homogeneous IT simulations and applying the following expression:

$$\alpha = \frac{q}{J} \int_{E_{th}}^{\infty} f(E) g(E) R_{II}(E) dE, \tag{1}$$

where J is the current density and $R_{II}(E)$ the II scattering rate.

The low field mobility μ_0 is calculated as a function of total scattering rate as:

$$\mu_0 = \frac{q < \tau >}{m^*}, \tag{2}$$

where $< \tau >$ is the mean scattering rate averaged over $\mathbf{k}$ and m^* is the effective mass.

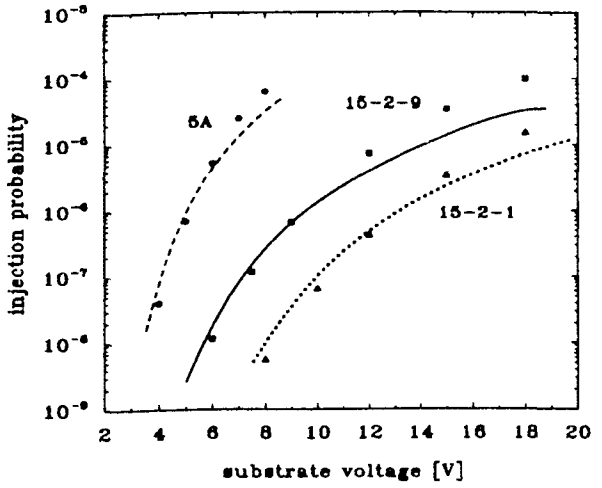

Fig.3 Injection probability for three MOSFETs [8]; lines: Fig.8 of [8], points: IT

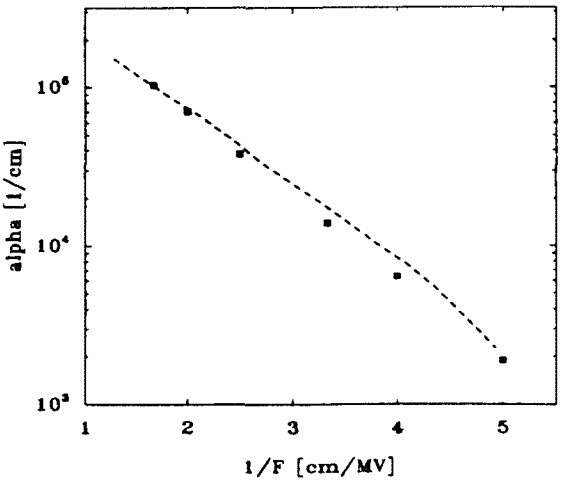

Fig.4 II rates for electrons in Si; lines: [7], points: IT

Our fitting procedure was aimed at obtaining the values for $D_t K$, $P/\tau_{op}(E_{th})$ and E_{th}, in order to reproduce Ning's injection probabilities and $\alpha(F)$; then $\mathcal{E}_1$ has been calculated in order to obtain $\mu_0 = 1420 cm^2/Vs$ from equation (2). Fig.3 reports a comparison between the measured and calculated injection probabilities for three different devices and for several bias conditions: the agreement is quite good over five orders of magnitude. With the same set of parameters an excellent agreement is obtained for the II rates (Fig.4).

The final set of parameters is reported in the following table.

optical deformation potential ($D_t K$)	eV/cm	6×10^8
optical phonon temperature (T_{op})	$^\circ K$	600
impact ionization threshold (E_{th})	eV	1.2
impact ionization rate @ $2E_{th}$ (P/τ_{op})	$1/s$	5×10^{12}
acoustic deformation potential ($\mathcal{E}_1$)	eV	6.4
sound velocity (v_s)	cm/s	9×10^5

Notice that a single value of $D_t K$ has been used for both inter- and intra-band transitions for all bands (the reference values given in [2] account for band multiplicity z, therefore for the sake of comparison, they must be divided by $\sqrt{z}$), and that the II parameters are similar to those obtained in [3]. The results of this work represent an important quantitative ingredient for MC device simulations which are still mandatory in full 2-D problems as self-consistent MOSFET calculations [4,6].

References

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