AN EFFICIENT METHOD FOR EVALUATING THE ENERGY DISTRIBUTION OF ELECTRONS IN SEMICONDUCTORS BASED ON SPHERICAL HARMONIC EXPANSION [1]

D. Ventura, A. Gnudi, G. Baccarani

Dipartimento di Elettronica, Informatica e Sistemistica
Università di Bologna, viale Risorgimento 2
40136 Bologna, Italy

Modeling hot electron effects in silicon has gained considerable attention in recent years, with the aim of predicting substrate currents and aging due to hot carrier injection into the gate oxide in MOSFET's, and impact ionization at the base-collector junction in BJT's. Two main approaches are found in the literature: the *hydrodynamic* (HD) or *energy balance* approach, and the Monte Carlo (MC) simulation. Criticism has been moved to both methods for different reasons: the former can with relatively little CPU time provide reasonable average quantities, such as mean velocity and energy, but it does not provide any direct information on the high-energy distribution of electrons, while the latter lends itself to a thorough physical investigation, at the expense of very large computational resources. Some proposals have been made to overcome the above limitations [1,2]. The basic idea of these papers is to derive from the Boltzmann Transport Equation (BTE) a simpler equation in the space-energy domain, which can include also non-local effects. An approximate analytical solution is then found under simplifying assumptions, such as high energy and constant effective mass [2].

In this work, we also reduce the BTE to the space-energy variables, but we do not introduce any further assumption by numerically solving the resulting equations. We validate the approach by comparing our results with those of MC calculations in homogeneous silicon with uniform electric field.

We begin with expanding the distribution function in series of spherical harmonics [3]:

$$f(\mathbf{r},\mathbf{k}) = f_0(\mathbf{r},k) + f_1(\mathbf{r},k)\cos\theta + f_2(\mathbf{r},k)\frac{1}{2}(3\cos^2\theta - 1) + \ldots \tag{1}$$

where θ is the angle between $\mathbf{k}$ and the current density $\mathbf{J}$. Only the first three terms of the series are considered in our calculations. A system of equations for the unknown functions f_i is obtained by substituting the expression (1) for f into the BTE and by balancing the coefficients of the harmonics of the same order. The procedure is quite general. Considering acoustic and optical phonon interactions, as well as ionized impurity scattering, and a spherically symmetric band structure, the equations for f_0 and f_1 in the spatially uniform case are

$$q^2F^2\lambda^2\left[f_0'' + \left(\frac{\lambda'}{\lambda} + \frac{\gamma'}{\gamma}\right)f_0'\right] + \tag{2,a}$$

$$+3c_{op}\,\tau\left[g(E+\hbar\omega_{op})\left(N_{op}^{+}\,f_0(E+\hbar\omega_{op}) - N_{op}\,f_0(E)\right) - g(E-\hbar\omega_{op})\left(N_{op}^{+}\,f_0(E) - N_{op}\,f_0(E+\hbar\omega_{op})\right)\right] = 0$$

$$f_1 = -q\,F\,\lambda\,f_0' \tag{2,b}$$

where $\lambda(E)$ is the mean free path, $\tau(E)$ the inverse scattering rate, $\gamma(E)$ the band-shape function, $g(E)$ the density of states, N_{op} the optical phonon occupation number, $N_{op}^{+} = N_{op} + 1$, $\hbar\omega_{op}$ and c_{op} the optical phonon energy and coupling constant respectively, and, finally, F the electric field. A similar set of equations has been derived including the next term of the expansion f_2.

The phonon coupling constants and the band structure are taken from [4]. More precisely, we have so far taken into account the two lowest bands of the model given in [4], thus fitting the density of states in silicon up to 2.6 eV, much beyond the parabolic band approximation. Ionized impurity scattering is included in the Brooks-Herring formulation. The screening length is adjusted so as to match the empirical mobility model [5].

From the numerical point of view we have faced the problems stemming from *i)* singularities in the coefficients near the energy extrema, *ii)* definition of suitable boundary conditions, *iii)* efficiency of the discretization scheme in view of the extension of the code to the non-uniform case.

In Figs. 1 and 2 the electron distributions (normalized such that $\int f\,g\,\mathrm{d}E = 1$) as a function of energy obtained with our method both including and neglecting f_2 are compared with MC data from [4] for two different electric fields. The agreement is excellent when f_2 is taken into account, even in the high-energy tail, which is beyond the modeling capabilities of the HD model, and creates noise problems in a MC approach. As emphasized by several authors, the distribution departs from the Maxwellian shape. It is also seen that a reasonable approximation is obtained with f_0 and f_1 only. The spike at energy around $\hbar\omega_{op}$ in the curve relative to the solution with f_2 is due to the aforementioned singularities in the coefficients.

The mean energy and velocity vs. electric field curves are shown in Fig. 3. The small velocity decrease at high fields is due to the particular band shape, and is observed also in the MC data reported in the same figure. It is worth noticing that the evaluation of these average quantities involves only f_0 and f_1, whereas f_2 slightly affects the results because of the weak coupling with the other terms. Finally, Fig. 4 shows the calculated mobility as a function of doping concentration, compared with the empirical model [5].

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The extension to the non-uniform case is currently in progress, as well as the inclusion of the full energy-band model of [4]. From the results obtained so far, and considered the computational advantages of this method over the MC approach, we believe an efficient tool for device simulation can be developed.

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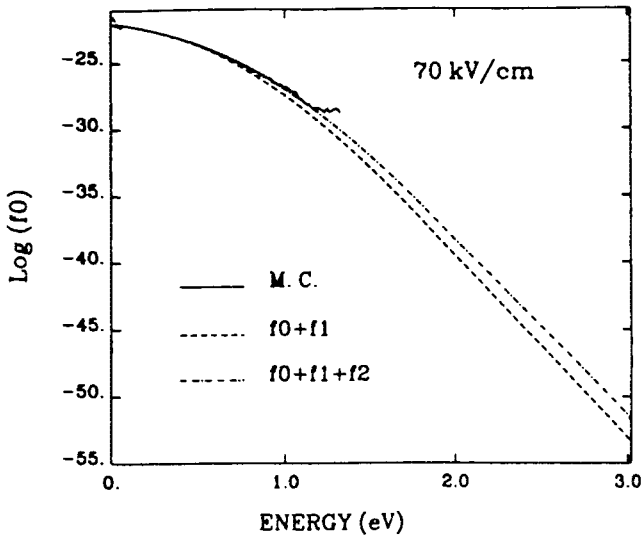

Fig. 1. Electron distribution vs. energy from the present model and from the MC procedure.

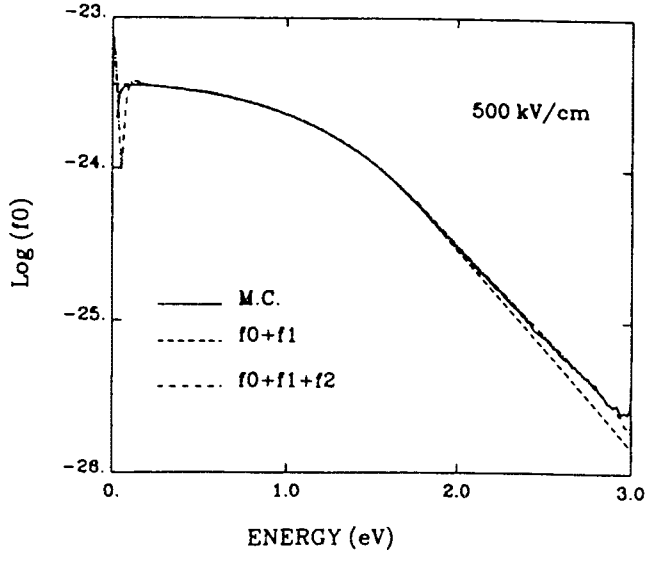

Fig. 2. Electron distribution vs. energy from the present model and from the MC procedure.

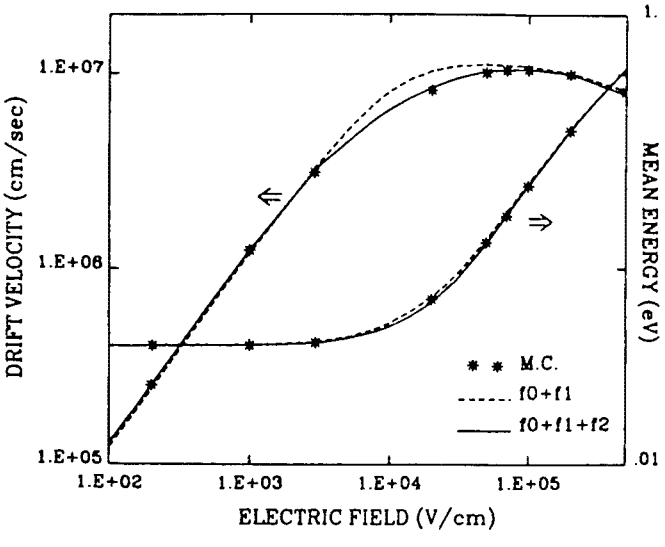

Fig. 3. Electron mean velocity and energy vs. field from the present model and from the MC procedure.

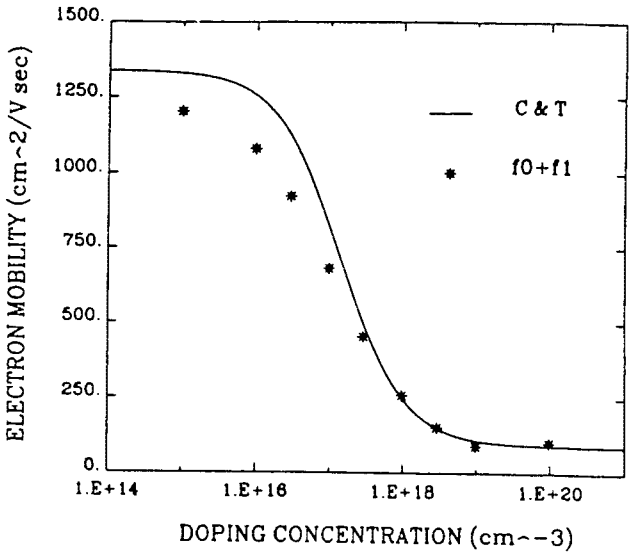

Fig. 4. Electron mobility vs. field from the present model and from the empirical model [5].