AN ALTERNATIVE SOLUTION OF THE BOLTZMANN EQUATION: THE "SCATTERED PACKET METHOD"

J.P. NOUGIER, L. HLOU, P. HOULET, J.C. VAISSIERE, L. VARANI
Centre d'Electronique de Montpellier, Université Montpellier II
34095 Montpellier Cédex 5, France

Abstract

We present an original technique for the solution of the Boltzmann equation in bulk semiconductors: the *Scattered Packet Method*. This method intends to combine advantages and to overcome shortcomings of the direct solutions of the Boltzmann equation and of the Monte Carlo methods. The detailed procedure of the *Scattered Packet Method* is described and applied to the case of p-type silicon. The results obtained for first and second order transport parameters are found to be in excellent agreement with classical methods.

I. INTRODUCTION

Classical methods of solution of transport equations in semiconductors, such as the Monte Carlo (MC) method and the direct solution of the Boltzmann equation (BE), have shown their efficiency to provide transport coefficients. Anyway both methods have some inherent shortcomings. Direct solutions of the BE calculate distribution functions with high accuracy but don't take into account fluctuations. MC methods, due to the stochastic nature of the procedure and the limited number of carriers involved, meets with difficulties in calculating with high accuracy quantities on a hydrodynamic time scale such as the transient response of drift velocity and energy, small signal coefficients, etc. In order to combine the advantages of the above two methods, we have developed a new technique called the *Scattered Packet* (SP) *Method*. In this communication, the SP procedure is discussed in detail. Then, the theory is applied to the case of the p-type silicon and the results are compared with those obtained through classical methods.

II. THEORY

We consider a volume of the **k**-space large enough so that the number of carriers outside it is negligible. This volume is a sphere of radius k_{max} which, in spherical coordinates with the polar axis along the applied electric field E, is described by: $0 \le k \le k_{max}$, $0 \le \theta \le \pi$, $0 \le \varphi \le 2\pi$. The bandshapes are taken spherical, so that the variable φ can be omitted due to the symmetry around the electric field.

We discretize this volume in meshes $D_L = D_{ij}$ centered in $\mathbf{k}_L = \mathbf{k}(k_i, \theta_j)$ and limited as follows:

$$k_i - \Delta k/2 \le k' \le k_i + \Delta k/2 \quad and \quad \theta_j - \Delta\theta/2 \le \theta' \le \theta_j + \Delta\theta/2 \tag{1}$$

The volume of the mesh D_L is:

$$V_L = \int_{\varphi=0}^{\varphi=2\pi} d\varphi \int_{\theta_j-\Delta\theta/2}^{\theta_j+\Delta\theta/2} \sin\theta d\theta \int_{k_i-\Delta k/2}^{k_i+\Delta k/2} k^2 dk \tag{2}$$

Relations (1) and (2) are of course modified at the boundary of the domain.

The ensemble of carriers located in the volume V_L are defined as the *packet* P_L. $n_L(t) = n(k_i, \theta_j, t)$ is the number of carriers contained in V_L at time t. The distribution function is simply given by $f_L(t) = n_L(t)/V_L$.

The purpose of the method is now to determine a time-independent evolution matrix B that gives $n(t+\Delta t)$ when applied to $n(t)$, i.e. in matrix form:

$$[n(t+\Delta t)] = [B][n(t)] \tag{3}$$

The matrix element B_{ML} of [B] is the transition probability from the cell number L to the cell number M during the time interval Δt. In order to increase the accuracy in the calculations of [B] we divide each mesh in

submeshes of volume V_h so that $V_L = \sum_h V_h$. The number of carriers contained in the subcell h is given by $n_h = n_L V_h / V_L$. Now, we want to determine the repartition of this sub-packet on the different meshes of the domain after a time-step Δt sufficiently short so that the probability of having more than one collision during Δt is negligible. In order to calculate this repartition, we use some kind of Monte Carlo procedure with constant time-step. Under the application of an electric field, the carriers of the subcell h make a free-flight of duration Δt which transfer them into another subcell j of centered vector $\mathbf{k_j}=\mathbf{k_h}+e\mathbf{E}\Delta t/\hbar$. Let p_0 be the probability to have no collision during Δt, p_1 the probability for an optical phonon absorption, etc. Therefore the number of carriers having no collisions is $n_j = p_0 n_h$ and these carriers are located in the cell N which contains the subcell j. The element B_{NL} of [B] is incremented by n_j. The number of carriers undergoing an optical phonon absorption is $n_{circlek} = p_1 n_h$. These carriers are scattered along a sphere of constant energy according to the angular repartition probability. In a mesh M of this sphere, the number of carriers is (for an isotropic interaction):

$$n_M = n_{circlek} \left[\int_{\theta_M - \Delta\theta/2}^{\theta_M + \Delta\theta/2} \sin\theta' d\theta' \right] \left[\int_0^{\pi} \sin\theta' d\theta' \right]^{-1} \tag{4}$$

The element B_{ML} of [B] is then incremented by n_M. For anisotropic interactions Eq. (4) is slightly modified. The column L of [B] is filled when all the sub-packets of P_L have been scattered in **k**-space. By repeating the same procedure for all the initial packets we finally evaluate the evolution matrix [B] which satisfies Eq. (3). We notice that [B] depends only on the material, the carrier concentration, the lattice temperature, the electric field, the time-step and the number of meshes used for the discretization of the **k**-space.

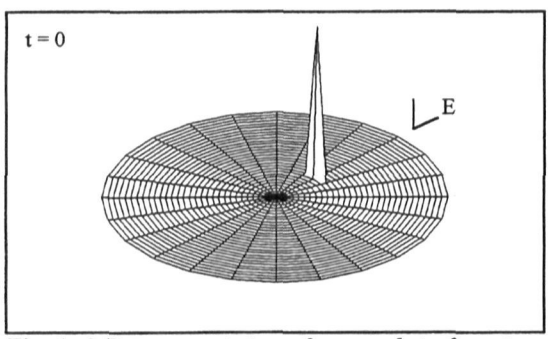

Fig. 1: *3-D representation of one packet of carriers centered in* $k = 10^9 m^{-1}, \theta = 0$. *Calculations are performed for the case of p-Si with Na=0, T=300 K and E=20 kV/cm.*

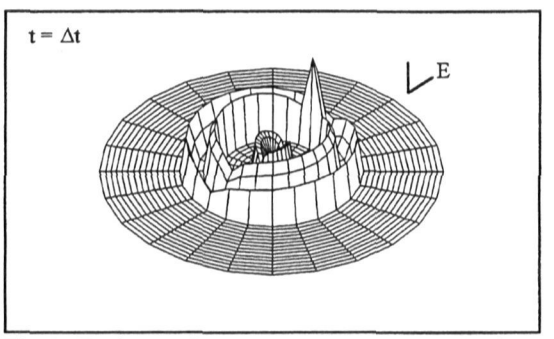

Fig. 2: *Evolution during one time-step* Δt*=1fs of one packet initialy centered in* $k = 10^9 m^{-1}, \theta = 0$. *Calculations are performed for the case of p-Si with Na=0, T=300 K and E=20 kV/cm. The vertical scale is not linear in order to enhance small values of n(k,*Δt*).*

To better clarify for the reader the repartition of a packet in **k**-space, let us consider one packet P_L centered in $k = 10^9 m^{-1}$ and $\theta = 0$ at time t=0 as shown in Fig. 1. By construction, the column L of the matrix [B] represents the packet repartition at time Δt when the initial number is equal to unity and located in $\mathbf{k}_L$. We have drawn on Fig. 2 n(t=Δt) which is proportional to the column L. The peak corresponds to the carriers that have been only displaced by the electric field without being scattered, and the circle at the same $|\mathbf{k}|$ refers to carriers which have undergone an elastic scattering. The inner and outer circle correspond to carriers having emitted or absorbed an optical phonon, respectively.

To study the transient regime, at time t=0 the number of carriers in the state k_L is n_L chosen equal to the thermodynamic value of the number of carriers of this state. Then, using Eq. (3) n(k,Δt) is computed and so on untill the stationary regime is obtained.The resulting algorithm (similar to the lattice-gas cellular-automaton method [1]) is physically equivalent to an ensemble MC method, using a considerable amount of carriers and without any use of random number.

III. CALCULATION OF THE VELOCITY AUTOCORRELATION FUNCTION

By neglecting cross correlation terms between velocities of different carriers, the autocorrelation function of the fluctuations of the drift velocity can be written as follows:

$$C(t) = \overline{\sum_{i=1}^{N} (v_i(t) - \overline{v_d})(v_i(0) - \overline{v_d})} \qquad (5)$$

where N is the total carrier number, $v_i(t)$ the velocity of the carrier i at time t, $\overline{v_d}$ the drift velocity.

Let us define by $F_{LM}(t)$ the ensemble of carriers leaving the state $\mathbf{k}_L$ at an initial time and reaching the state $\mathbf{k}_M$ at time t. By construction, these ensembles verify the two following properties:

(i) they constitute a partition of the whole system,

(ii) the carriers belonging to a given ensemble have the same initial and final velocity: $v(0)=v_L$ and $v(t)=v_M$, where v_L and v_M are the projections along the electric field of the carrier velocities in state L and M.

Therefore, the correlation given by Eq. (5) can be obtained by summing elementary contributions from each family $F_{LM}(t)$:

$$C(t) = \sum_L \sum_M C_{LM}(t) \qquad (6)$$

with

$$C_{LM}(t) = n_{LM}(t)(v_L - \overline{v_d})(v_M - \overline{v_d}) \qquad (7)$$

where $n_{LM}(t)$ is the carrier number of the family $F_{LM}(t)$. At time t=0 the number of carriers in the state $\mathbf{k}_L$ is n_L chosen equal to its steady state value in the applied electric field E and $n_{L'\neq L}$ is taken equal to zero. Using the SP method $n_{LM}(t)$ and $C_{LM}(t)$ are computed. The number of simulations is equal to the number of meshes in k space (about 500). An acceleration technique described in Ref. [2] is used in order to reduce the CPU time. The diffusion coefficient can then be obtained taking the Fourier transform of Eq. (6).

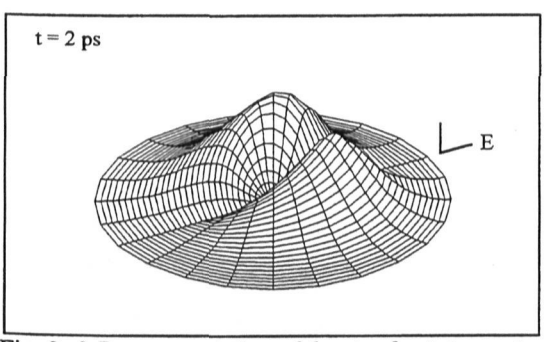

Fig. 3: *3-D representation of the steady-state carrier population. Calculations are performed for the case of p-Si with Na=0, T=300 K and E=50 kV/cm.*

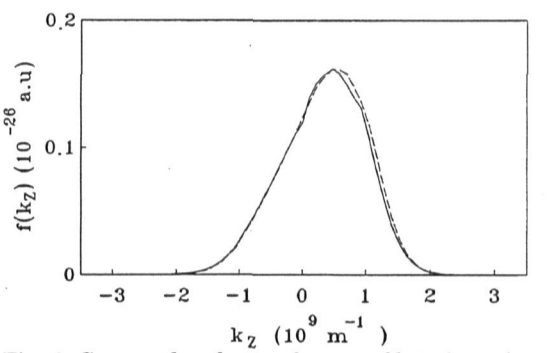

Fig. 4: *Carrier distribution function $f(k_z)$ along the electric field in p-Si with Na=0, T=300 K and E=20 kV/cm. The dashed line refers to the direct solution of the BE and the solid line to the SP method.*

IV. RESULTS

We present the results obtained for the first and the second order transport coefficients in the case of a p type silicon at T=300 K. The microscopic model is based on a single spherical nonparabolic-band and considers scattering with acoustic, impurity and non-polar optical phonon mechanisms as described in Ref. [3].

Figure 3 shows the steady-state number of carriers given by the SP method. The number of carriers in the cells located near k=0 (centre of the plot) and along the direction of the field is small, due to $k \sin\theta \cong 0$ (cf Eq. (2)).

Figure 4 shows the steady-state distribution function $f(k_z)$ along the electric field for an acceptor concentration Na=0. We observe an excellent agreement with results obtained from the direct solution of the BE [3]. The same agreement is found for the drift velocity as a function of time which is reported in Fig. 5, for three different electric fields.

Therefore we have shown that the SP method keeps the accuracy of the direct solution of the BE in calculating first order transport parameters.

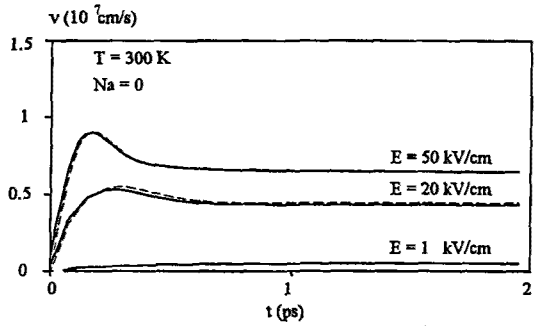

Fig. 5: *Average velocity as a function of time for the reported electric fields in p-Si with Na=0 and T=300 K. The dashed line refers to the direct solution of the BE and the solid line to the SP method.*

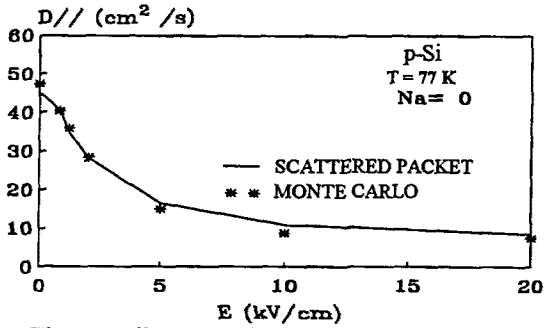

Fig. 6: *Diffusion coefficient as a function of the electric field in p-Si with Na=0 and T=77 K. The stars refer to the MC method and the solid line to the SP method*

As concerning second order transport parameters, Fig. 6 shows the low frequency diffusion coefficient as a function of the electric field. Also in this case the agreement between results obtained by the MC method [5] and the SP method is excellent.

Using about 500 cells, in order to compute precisely the 500*500 matrix elements B_{ML}, we compute (see Eq.(4)) how many particles from each of the 62500 subcells of each cell L are scattered in each of the 500 cells M. Due to the energy conservation, with about 16 steps in θ, this requires 62500*17*500 computations for each scattering mechanism. With optical absorption and emission, acoustical and impurity scatterings, the calculation of the matrix [B] takes about 30 minutes, the stationary regime of the distribution function is obtained after few seconds for a time-step of 1 fs and the correlation functions after few minutes on an IBM 3090.

V. CONCLUSIONS

We have presented a new technique to simulate carrier transport in bulk semiconductors based on an original numerical solution of the Boltzmann Equation. The results obtained for the distribution function, the first and second order transport coefficients have been found to be in excellent agreement with classical methods. The advantages of this method can be summarized as follows: a procedure closed to the corpuscular reality, a high accuracy calculation of distribution functions and fluctuations within a reasonable CPU time.

Developments of the *Scattered Packet Method* towards the device simulation and the study of electronic noise seems to be promising.

ACKNOWLEDGMENTS

This work have been performed within the *European Laboratory for Electronic Noise* (ELEN) and supported by the CEC through the contracts ERBCHRXCT920047 and ERBCHBICT620162. Partial support from the *Centre de Compétences en Calcul Numérique Intensif* (C3NI) and the italian *Consiglio Nazionale delle Ricerche* (CNR) is gratefully acknowledged.

REFERENCES

[1] K. Kometer, G. Zandler and P. Vogl, Phys. Rev. **B46**, 1382 (1992).

[2] L. Hlou, Thèse de Doctorat, Université Montpellier II (France), 1993 (available upon request).

[3] J.C. Vaissiere, Thèse de Doctorat ès Sciences, Université Montpellier II (France), 1986 (available upon request).

[4] J.P. Aubert, J.C. Vaissiere, J.P. Nougier, J. Appl. Phys. **56**, 1128 (1984)

[5] T. Kuhn, L. Reggiani, L. Varani, D. Gasquet, J.C. Vaissiere, J.P. Nougier, Phys. Rev. **B44**, 1074 (1991).