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TRANSIENT REGIMES OF HOT CARRIERS IN P-TYPE SILICON

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Résumé : On compare les régimes transitoires obtenus, sur Si-p à 300 K, par simulation de Monte Carlo et résolution itérative de l'équation de Boltzmann : l'accord est excellent. Le régime transitoire : a) dépend assez peu des formes de bandes d'énergie. b) dépend beaucoup de l'énergie initiale, une augmentation de celle-ci peut faire disparaître la survitesse. c) dépend peu de la forme de la distribution initiale. Dans tous les cas, le régime transitoire déterminé en utilisant les équations dynamiques donne un accord très satisfaisant avec les précédentes simulations.

Abstract : A comparison is made between transient regimes obtained, on p-Si at 300 K, by a Monte Carlo simulation and by an iterative solution of the Boltzmann equation : the agreement is excellent. The transient regime : a) depends relatively few on the energy bandshapes; b) Is strongly dependent on the initial energy, the increase of which may lead to a disappearance of the velocity overshoot; c) Slowly depends on the shape of the initial distribution function. In every cases, the transient regime computed using the balance equations is in very satisfactory agreement with the previous simulations.

1. INTRODUCTION

For studying transient regimes in homogeneous semiconductors, three methods can be used. i) iterative technique, ii) Monte Carlo simulation, iii) balance equations. Within the frame of the classical Boltzmann equation, the first two methods are exact numerical solutions ([1 - 6]). However, no direct comparison of the transient regime obtained by both methods have been performed till now. In this paper, various transient regimes are compared for the case of holes in Si using both methods with the same band structure and the same scattering mechanisms in order to check their reliability on a practical case of interest. Transient regimes corresponding to various initial conditions are studied. The influence of valence band particularities (such as nonparabolicity and warping) are investigated. Furthermore, comparison of these methods with the balance equations is carried out with the aim to provide a reference for estimating differences between realistic and simplified models used in practical calculations.

After a brief recall of the methods used (section 2), we shall compare (section 3) the various models, then study the influences of the dispersion relation $\varepsilon(\vec{k})$ (section 4), of the initial energy distribution (section 5), and of the initial distribution function (section 6), before giving an example showing an undershoot velocity (section 8).

2. METHODS USED

The values of the transport quantities of interest for a transport dynamic response can be obtained from a Monte Carlo procedure by simulating the behaviour of a number of independent particles and taking ensemble averages over the whole gas, at given values of time t [7]. For our case, 8192 particles have been considered and the space distribution has been assumed to be of a Dirac type; different initial energy distributions with different mean values have been considered, as will be discussed in the following. As in the stationary case, the self scattering mechanism has been included in the simulation. Of course, the results have been found to be independent from the choice of the self-scattering parameter Γ , contrary to what stated in refs. [8][9], provided that Γ is large enough.

The iterative method used for solving the Boltzmann equation was described in ref. [10], and has been extended here to the case of a two bands semiconductor.

The method of balanced equations was recently shown [11] to be a good approximation deduced from the Boltzmann equation. Its application proved to be successful [11][12] in n-Si, p-Ge and n-GaAs.

3. COMPARISON BETWEEN THE MODELS

In order to compare the Monte Carlo and iterative solutions on the same microscopic model, and to avoid too much time consuming computations, we used a simplified band structure model consisting in a single spherical band with an effective mass which, to account for nonparabolic effects, has been taken to be dependent upon the electric field strength through the stationary value of the hole mean energy. Acoustic scattering, which accounts for overlap effects, and non-polar optical scattering, have been considered. The values used in calculations are reported in Table 1, and Fig. 1 shows the dependence of the effective mass with the electric field strength. The reliability of the microscopic model, which differs from that of Ref. [13] only for warping effects, is checked with the comparison of theoretical and experimental results of the stationary values of the drift velocity and longitudinal diffusion coefficient [14], as shown in Fig. 2. The overlap was taken into account by setting $G(\vec{k}, \vec{k}') = 1/2$, thus having the effect of dividing by 2 the value of E_1^0 given in table 1.

The initial distribution function was assumed to be the thermal equilibrium Maxwell Boltzmann distribution at 300 K.

Quantity	Unit	Value		
		One spherical parabolic band	Two spherical parabolic bands	Two spherical bands: one parabolic and one non parabolic
ρ [15]	gr/cm ³	2.33	2.33	2.33
θ_{op} [15]	K	735	735	735
s_e [15]	cm/s	9.04×10^5	9.04×10^5	9.04×10^5
s_t [15]	cm/s	5.34×10^5	5.34×10^5	5.34×10^5
m_{10}/m_0 [15]	-	-	-	0.50 [16]
m_{11}/m_0 [15]	-	-	-	1.16 [16]
m_h/m_0	-	$m(E)/m_0$ [see Fig. 1]	1.16 (see Fig. 3	-
m_e/m_0	-	-	0.30) of [16])	0.3 [16]
E_1 [13]	eV	5.0	5.0	5.0
d_0 [13]	eV	26.6	26.6	26.6

Table 1. Constants used in the calculations for the various band models used in the present paper. The notations are the usual ones and the quantities are defined or given in the references listed. The non parabolic band consists in two parabolic portions of masses m_{10} and m_{11} , linked by a linear portion [15].

Fig. 1 : Equivalent effective mass as a function of the electric field for the one band model, see Ref. [15].

Fig. 2 : Comparison between the experimental results, of drift velocity and diffusion, and the theory using the one band model (taken from [14]).

Figures 3a and 3b show the transient drift velocity and the transient energy for a set of electric fields suddenly applied at $t = 0$ ($E = 10, 20$ and 50 kV cm^{-1}). The values obtained with the Monte Carlo (circles, triangles and stars) and the iterative method (dotted curves) are found to coincide within the statistical uncertainty. This evidence proves the complete reliability of both methods to solve the Boltzmann equation under transient conditions. In particular, drift velocity is found to exhibit overshoot for field strengths above about 20 kV/cm . No overshoot was found for the energy.

On figure 3 are also plotted the transient regimes computed using the balance equations : these results are in agreement within 10 % with the "exact" ones, which is much satisfactory if one takes into account the great simplicity and rapidity of this method. These results are similar to those previously obtained [11] [12] on p-Ge, n-Si and n-GaAs.

Fig. 3 : Transient drift velocities (a) and energies (b) in p-Si at 300 K, for various values of suddenly applied electric fields at $t = 0$. Comparison between : iterative solution of the Boltzmann equation (dotted curves), Monte Carlo simulation (circles, triangles and stars), and balance equations (full curves).

4. INFLUENCE OF THE BANDSHAPES ON THE TRANSIENT REGIMES :

During the transient regimes, the "average position" of the carriers in the $|\vec{k}|$ space vary, so as their "average mass". Therefore, one could expect that for various bandshapes the transient motion is not the same. This is shown on Fig. 4 where the transient drift velocity is plotted for an electric field step of $E = 50 \text{ kV cm}^{-1}$, applied at $t = 0$, and for various dispersion laws $\epsilon(k)$. The following models have been used, their parameters are listed table 1 :

- (i) One spherical parabolic band described in the previous section
- (ii) Two spherical parabolic bands with effective masses m_h and m_e
- (iii) Two spherical bands, a light hole band parabolic and the heavy hole band non

parabolic consisting in two parabolic portions, of effective masses m_{10} and m_{11} , linked by a linear portion [15] .

(iv) One warped sphere band described in [13] .

Of course only the warped sphere model is able to exhibit anisotropy. As is shown on Fig. 4, the drift velocity (and so is the mean energy) is higher along a $\langle 100 \rangle$ direction than along a $\langle 111 \rangle$ direction. This reflects the lower value of the heavy hole effective mass along this direction. In particular, it has to be noted that the anisotropy exhibited by the drift velocity reaches its maximum value around the peak of the overshoot where, for the field strength considered, variations of about 30 % have been found.

Fig. 4 clearly shows that different bandshapes give different transient drift velocities, even when the steady state velocities are equal.

Figure 4 : Transient velocities for different bandshapes : warped spheres, $E//\langle 100 \rangle$ (Δ) and $E//\langle 111 \rangle$ ($\square$); two spherical bands, one parabolic and one non parabolic ($\bullet$); two spherical parabolic bands ($- -$); one spherical parabolic band ($-$).

5. EFFECT OF THE INITIAL ENERGY

In order to investigate the effect of the initial energy on the transient behaviour, an electric field step of 50 kV/cm was applied at $t = 0$ to p-Si at 300 K with the one spherical parabolic band model discussed above, corresponding to three different initial conditions described by the following distribution functions $f_0(\vec{k})$ (δ is the Dirac function) :

conditions 1 : $f_0(\vec{k}) \propto \delta(\vec{k})$: all the carriers are initially located at $\vec{k} = 0$, thus $\bar{v}(0) = 0$ and $\bar{\epsilon}(0) = 0$.

conditions 2 : $f_0(\vec{k}) \propto \delta(k_0)$ where $\epsilon(k_0) = 0.75$ eV : all the carriers have the initial energy 0.75 eV, but their velocities are randomly distributed : $\bar{v}(0) = 0$ and $\bar{\epsilon}(0) = 0.75$ eV. [17]

conditions 3 : $f_0(\vec{k})$ = thermal equilibrium distribution at 300 K : $\vec{v}(0) = 0$ and $\bar{\epsilon}(0) = 0.039$ eV.

Of course the condition number 1 is unrealistic (the case number 2 could describe carriers injected using an electron gun), but these three cases are interesting for testing the reliability of the methods since they represent very extreme conditions.

Figure 5a and 5b show the results obtained on the transient velocity and energy using the three techniques of simulation (Monte Carlo, iterative, balance equations). As can be seen on Fig. 5a, the overshoot is maximum with the condition 1, while it disappears for the condition 2. In fact, in the former case the carriers start to accelerate before to dissipate energy and, provided that the field strength is high enough, as it is in this case, due to the streaming effect of the field they have the possibility to reach velocity values higher than the stationary one. In the case number 2 the carriers simultaneously start to accelerate and dissipate energy through phonon emission; this process is quite randomizing in momentum and leads to a smooth increase with time of the drift velocity, so that overshoot effects disappear. Thus the influence of the initial energy and distribution is quite important on the transient velocity. The slight discrepancy appearing between the Monte Carlo and iterative simulations comes to the fact that, with our iterative technique, discontinuities are forbidden, so that we are unable to simulate delta functions : these were then replaced by narrow Gaussian distributions, which tends to lower the overshoot in the case number 1. As concerning the transient energies (see Fig. 5b), no overshoot is observed. Finally it can be remarked, on Fig. 5a, that the slopes of $v(t)$ at the origin are identical : this is quite normal, and eq. (16) of reference [11] shows that, without any approximation: when $v(t=0)=0$: $(dv/dt)_{t=0} = eE/m$ and thus does not depend on the initial distribution provided that $v(t=0)=0$. However, as can be seen from eq. (24) of ref. [11], $(d\epsilon/dt)_{t=0}$ depends on $\epsilon(t=0)$ even when $v(t=0)=0$, as is obviously confirmed by Fig. 5b.

Finally one should note that the balance equations give transient curves in quite good agreement with the exact methods.

Fig. 5 : Transient velocities (a) and energies (b) computed using the three techniques of simulation: (Monte Carlo (★)), iterative (.....), and balance eqs. (—)), for various initial conditions : ① : $f_0(k) \propto \delta(0)$; ② : $f_0(k) \propto \delta(k_0)$ where $\epsilon(k_0) = 0.75 \text{ eV}$; ③ : $f_0(k) = \text{thermal equilibrium distribution at } 300 \text{ K}$.

6. INFLUENCE OF THE INITIAL DISTRIBUTION FUNCTION

The balance equations do not take into account the distribution function, they describe only the notion of the average velocity and of the average energy. In order to get an idea of the error performed by neglecting the shape of the distribution function, we study the transient velocities (Fig. 6a) and energies (Fig. 6b) for a step of electric field $E = 50 \text{ kV/cm}$ applied at $t = 0$, the carriers being, at $t=0$, distributed according to the two following laws giving both $\bar{v}(0) = 0$ and $\bar{\epsilon}(0) = 0.5 \text{ eV}$: 1) $f_0(\vec{k}) \propto \exp(-\hbar^2 k^2 / 2m k_B T_0)$ with $3 k_B T_0 / 2 = 0.5 \text{ eV}$ (thermal equilibrium at $T_0 = 3870 \text{ K}$). This condition is of course unrealistic, but corresponds to a limiting case where all the energies in the $\{\vec{k}\}$ space are occupied. 2) $f_0(\vec{k}) \propto \exp[-\hbar^2 (k-k_1)^2 / 2m k_B T_1]$ with k_1 such that $\hbar^2 k_1^2 / 2m = 0.5 \text{ eV}$ and $T_1 = 40 \text{ K}$. This corresponds to carriers located in a narrow region of $\pm 5.2 \text{ meV}$ around the energy 0.5 eV .

The transient responses were computed using the iterative method, for the single spherical parabolic band model. Fig. 6a and 6b show that the discrepancy between the two transient responses is not very large. As a consequence, the description given by the balance equations is, in this case two, quite satisfactory as shown in Fig. 6.

Figure 6 : Transient drift velocities (a) and energies (b) for p-Si, 300 K, in a step of $E = 50 \text{ kV/cm}$, for two initial distributions $v(0) = 0$ and $\epsilon(0) = 0.5 \text{ eV}$; (.....)all the carriers have an energy equal to $500 \pm 5.2 \text{ meV}$, and the directions of the $\mathbf{k}$ vector are randomly distributed, iterative method; (---)maxwillian distribution centered at $k = 0$, with average energy 0.5 eV , iterative method; (—)balance equations.

7. EXAMPLE : UNDERSHOOT VELOCITY :

Let us apply at time $t = 0$, a constant electric field E_1 : after an overshoot (if $E_1 \geq 20 \text{ kV cm}^{-1}$), the velocity reaches its stationary value. If then, at time t_1 , the field is suddenly lowered and takes the constant value E_2 , the velocity may exhibit an undershoot value before stabilizing at the steady state corresponding to the field E_2 . This phenomenon is shown on figure 7a and 7b where E_2 was taken equal to 10 kV cm^{-1} , starting at time $t_1 = 1.5 \text{ ps}$. The simulation was performed using three values of E_1 ($20, 50$ and 100 kV cm^{-1}) with the balance equations (respectively dotted, dashed and full curves of figures 7a and 7b). It was checked at 50 kV cm^{-1} by comparing the result obtained, with the iterative solution of the Boltzmann equation for the one parabolic band model, the system being at $t < 0$ in thermal equilibrium : the agreement between the iterative method and the balance equation is excellent. The drift velocity, shown in Fig. 7a, exhibits an overshoot at the increase of electric field. An undershoot appears at the decrease of electric field, the more pronounced as the intermediate field E_1 is higher. Figure 7b shows that no overshoot nor undershoot are observed on the average energy. For both the energy and (even more) the velocity, the transient regime is almost twice longer for the decrease of the electric field than for the increase. The velocity undershoot had already been predicted on multivalley semiconductors (n-Si and n GaAs [12]). However it is shown here to be possible even with a single band structure.

When the electric field is suppressed instead of being lowered ($E_2 = 0$), the velocity remains positive, but the decay time decreases with increasing E_1 .

Figure 7 : Transient velocity (a) and energy (b) responses to an electric field E_1 applied at $t=0$ and E_2 applied at $t=t_1$. $t_1 = 1.5 \text{ ps}$, $E_2 = 10 \text{ kV cm}^{-1}$. The iterative method ($\square$) was applied for $E_1 = 50 \text{ kV cm}^{-1}$, and the balance equations were used for $E_1 = 20 \text{ kV cm}^{-1}$ (....), $E_1 = 50 \text{ kV cm}^{-1}$ (---) and $E_1 = 100 \text{ kV cm}^{-1}$ (—).

8. CONCLUSION

Transient regime of hot holes in Si has been studied using three different methods. Iterative technique and Monte Carlo simulation have been proved to produce the same results when the microscopic model is kept to be the same. Due to the lack of experimental data, the present investigation has been devoted to analyze systematically some physical situations in order to offer plausible expectations on transient regime effects. So, overshoot of the drift velocity has been found to be magnified by lowering the initial carrier energy and, by considering warping, when the field is oriented along $\langle 100 \rangle$ direction.

The transient regimes were found to depend strongly on the initial average velocities and energies : diminishing the initial energy enhances the velocity overshoot. However, the transient regime depends very few on various initial distributions corresponding to the same initial average velocity and energy.

In every case, in spite of the great variety of conditions studied, the balance equations gave results in quite satisfactory agreement with iterative or Monte Carlo methods. This strongly justifies the use of the balance equations, which is a very fast and cheap method.

Of course the steady state regime is completely independent from the initial conditions. On the basis of these new results and of our experience with the three methods discussed above, we have drawn a general synthetic overview on the advantages and limitations of each method, which is reported in tables 2 and 3.

Balance equations	Iterative technique	Monte Carlo simulation
Simple and fast method. A desk computer is sufficient.	An exact solution of the Boltzmann equation is obtained	
	The carrier distribution function is obtained with great detail and in a very direct way	The microscopic dynamics is quite transparent since each scattering process can be analyzed in full detail.
	Different initial conditions and initial distribution functions can be simulated in a rather simple way.	
Time dependent electric fields are easily included	Time dependent electric fields can be included	
	Realistic band structure models can be fully accounted	

Table 2 : Possibilities of the various methods

Balance equations	Iterative technique	Monte Carlo simulation
No rigorous justification of the validity of the equations can be given	The microscopic dynamics of the scattering process is somewhat hidden	Details of the distribution function are not easily obtained
The stationary values of the drift velocity, of the mean energy and of the effective mass should be known a priori	To fully exploit the potentiality of the method, very fast computers are needed	
Realistic band structure models cannot be included		

Table 3 : Limitations of the methods

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