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DIRECT MONTE CARLO SIMULATION OF HOT-CARRIER CONDUCTIVITY

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ABSTRACT

We present a Monte Carlo procedure which, by including the mechanism of generation and recombination from impurity centers, enables us to calculate directly from the simulation the field dependent conductivity for the first time. The reliability of the theoretical model has been checked by comparing numerical results with experiments provided by the Montpellier group and performed on p-Si at different acceptor concentrations and temperatures.

KEYWORDS

Electronic transport, semiconductors, impurity centers, scattering mechanisms, Monte Carlo method.

INTRODUCTION

One of the main limitation in using Monte Carlo (MC) simulations is to treat the case of a field independent carrier concentration. Thus, once the drift velocity versus field is obtained, the calculation of conductivity is straightforward inferred from the knowledge of the sample geometry and of the equilibrium carrier concentration. However, at lowering temperature and/or increasing doping concentration partial freeze-out of the ionized impurities occurs and the well-known phenomenon of field-assisted ionization is observed under hot-carrier regime. As a consequence, the calculation of the conductivity requires the knowledge of the free carrier concentration at the given field. Within a single impurity approach (Hydrogenic-model) two effects concur in determining the free carrier concentration. Firstly, the field dependence of the recombination rate induced by carrier heating. Then, the modification of the impurity potential (the so called Poole-Frenkel effect) which implies a field dependent generation rate.

In this communication we present a MC procedure which, by including the mechanism of Generation and Recombination (GR) from impurity centers, enables us to calculate directly from the simulation the field dependent conductivity for the first time.

THEORY AND RESULTS

We consider a uniform semiconductor sample of cross-sectional area A in which charge transport occurs through a two level system: the valence band and the impurity centers which supply the carriers. Under stationary conditions, the current I flowing in the sample can be expressed by the two equivalent expressions:

$$I = eAN_A v_d^r = eAN_A u v_d \tag{1}$$

where e is the absolute value of the electron charge, N_A is the acceptor concentration, v_d^r is the total carrier mean-drift velocity (reduced drift velocity) which accounts for the time spent by the carriers on the impurities, u is the average-fraction of ionized carriers and v_d the mean-drift velocity associated with the carrier motion in the conducting band. By definition, from Eq. (1) the conductivity σ is given by the two equivalent expressions:

$$\sigma = eN_A v_d^r / E = eN_A u v_d / E \tag{2}$$

We introduce into a standard MC procedure the GR processes as an additional scattering mechanism (Reggiani and others, 1987) parametrized by a volume recombination rate B_T^{eq} and a generation rate $A_{T,ac}^{eq}$. The physical model is naturally extended at increasing temperatures by scaling appropriately the GR coefficient rates, on the basis of a non-parabolic band model and of the temperature dependent capture cross-section given by Abakumov and others (1978), as reported in Table 1. Then, by using the standard stationary algorithm (Jacoboni and Reggiani, 1983), the reduced drift velocity at the given field is calculated and, through the knowledge of the acceptor concentration, the conductivity is determined from Eq. (2). We apply the above scheme to the case of boron doped p-type Si, where a direct comparison with the experiments performed by the Montpellier group (Vaissiere, 1987) can be carried out. Here impact ionization of impurities is found of negligible importance for the doping concentration considered and therefore is disregarded.

TABLE 1 - GR coefficients at different temperatures

T (K)	B_T^{eq} $cm^3 s^{-1}$	$A_{T,ac}^{eq}$ s^{-1}
77	4.20×10^{-6}	2.90×10^{9}
110	1.66×10^{-6}	1.49×10^{10}
160	6.22×10^{-7}	5.04×10^{10}

The field dependent conductivity is reported in Fig. 1 for the case of samples oriented along the < 100 > crystallographic direction. A satisfactory agreement is found between theory and experiments. The systematic decreases of the conductivity with the field reflects the prevailence of the decrease in mobility, v_d/E, over the increase in free carrier concentration, N_Au . These are well known effects associated with a hot-carrier regime (Reggiani, 1985). Indeed, from the MC simulation one can evaluate separately the dependence with field of the free carrier concentration and of their mobility (Reggiani and others, 1989).

The electric field may influence the ionization process by changing the shape of the impurity potential (Poole-Frenkel effect). In an attempt to estimate the importance of this effect, a phenomenological approach is used (Hartke, 1968) so that the ionization rate in the presence of the electric field is given by:

$$A_{T,ac}(E) = A_{T,ac}^{eq} \, exp(a\beta E^{1/2}/KT) \tag{3}$$

where for the present case of Si $\beta = 3.55 \cdot 10^{-24} J/(V/m)^{1/2}$ and a is a numerical parameter comprised between 0.5 and 1. The reason for introducing this variability is due to the fact that the lowering of the potential barrier occurs only in the direction of the electric field and therefore by taking $a = 1$ the effect is strongly overestimated. Figure 2 reports an investigation of this effect on the relative conductivity for an acceptor concentration $N_A = 5.5 \cdot 10^{15} cm^3$. The higher values for the ionization rate given by Eq. (3) lead to a further increase in the fraction of ionized impurities with the field, while the change in the mobility is found negligible. Because of that, we find higher values for the conductivity at intermediate electric field strengths. At the highest fields, as well as at lower doping, practically all the impurities are ionized and the values for the conductivity no longer depend from the Poole-Frenkel effect. By comparing these results with the experiments of Fig. 1 we find that the fitting gets worse by including this effect. We conclude that no evidence of Poole-Frenkel effect in experiments may be proved from the present analysis.

The field dependent conductivity at increasing temperatures is reported in Fig 3. As a general feature, in all cases the conductivity decreases systematically from its Ohmic value at increasing field strengths. However, the threshold field for such a decrease increases with temperature. This reflects the lowering of the Ohmic mobility with increasing temperature which displaces at higher fields the onset for the hot-carrier regime. Again, the satisfactory agreement found with the experiments of the Montpellier group confirms the physical reliability of the theoretical model suggested.

CONCLUSIONS

A direct Monte Carlo simulation of hot-carrier conductivity in the presence of field assisted ionization from shallow impurity levels is here presented. The satisfactory agreement found with experiments for the case of boron doped p-type Si supports the physical reliability of the theoretical model. It further confirms the importance of the cascade capture mechanisms assisted by acoustic phonons in the determination of the free carrier concentration.

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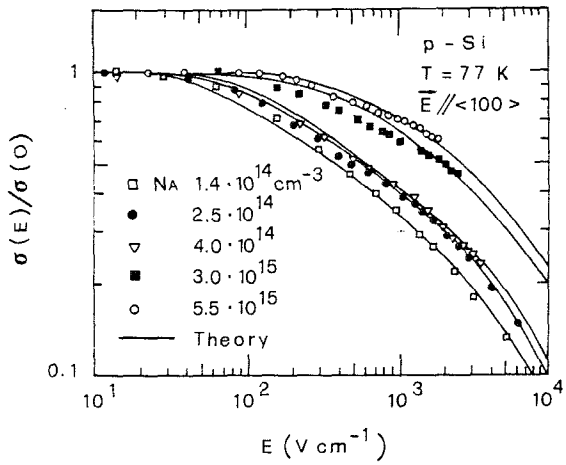

Fig. 1 - Conductivity normalized to its Ohmic value as a function of the electric field for the different acceptor concentrations reported in p-Si at 77 K. Symbols refer to experiments (Vaissiere, 1986), the lines to MC simulation.

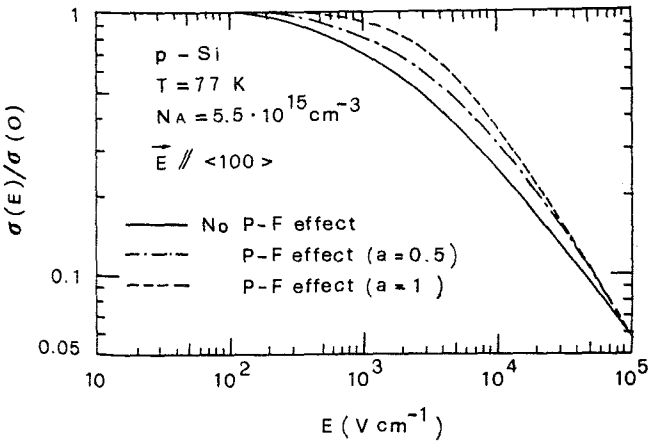

Fig. 2 - Conductivity normalized to its Ohmic value as a function of the electric field for the acceptor concentration reported as obtained from the Monte Carlo simulation with and without Poole-Frenkel effect in p-Si at 77 K.

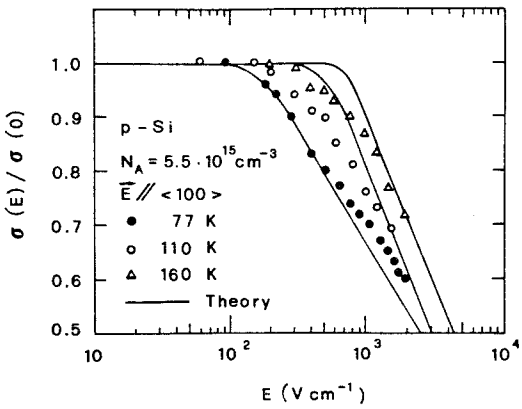

Fig. 3 - Conductivity normalized to its Ohmic value as a function of the electric field for the different temperatures reported in p-Si with $N_A = 5.5 \times 10^{15}\ cm^{-3}$. Symbols refer to experiments (Vaissiere, 1986), the lines to MC simulation.