Field-dependent conductivity of lightly doped *p*-Si at 77 K

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A theoretical investigation and new experiments on the conductivity of lightly doped *p*-Si (boron) at 77 K are presented. The conductivity is studied as a function of the electric field in the range $10 < E < 10^4$ V/cm. The experimental results are interpreted within an original Monto Carlo simulation which includes the mechanism of generation and recombination from impurity centers, thus allowing a simultaneous calculation of the mobility and the fraction of ionized impurities. The good agreement between the theory and the experiments supports the reliability of the physical model suggested.

I. INTRODUCTION

The recent interest in the miniaturization of semiconductor devices requires a detailed knowledge of the transport parameters at increasing electric fields where deviations from ohm's law (hot-electron regime) are expected.[1] Despite the availability of low-field conductivity data,[2] to our knowledge no results exist at high fields for *p*-type Si at 77 K. Indeed, at this temperature the fact that the partial freeze-out of the ionized impurities is field dependent does not allow the conductivity to be evaluated from an independent knowledge of mobility[3] and doping. Therefore, more data and an appropriate theoretical calculation are needed to fill this lack of knowledge.

It is the aim of this paper to report an investigation on the conductivity of lightly doped *p*-Si at 77 K in a wide range of electric field ($10 < E < 10^4$ V/cm). We consider samples of highly controlled crystal perfection and doping concentration (boron) in the range $1.4\times10^{14} \leqslant N_A \leqslant 5.5\times10^{15}$ cm^{-3}. The conductivity is thus measured as a function of an applied electric field E where deviations from the ohmic behavior are clearly exhibited. The experiments are microscopically interpreted on the basis of an original Monte Carlo simulation which accounts for the carrier concentration by including the mechanism of generation and recombination (GR) from impurity centers. The GR mechanism is modeled on the cascade capture theory[4,5] according to which carriers become trapped through absorption and emission of long wavelength acoustic phonons. In this way, we are in the position to evaluate the current flowing in the device and therefore to obtain the conductivity at the given field. The theory does not contain arbitrary parameters, thus allowing us to check the reliability of the physical model suggested from the comparison with experiments. In particular, the field-dependent carrier concentration and mobility will be naturally provided by the simulation.

The paper is organized as follows: Section II presents the theoretical model. Section III reports the experimental details. The results are discussed in Sec. IV. Some conclusions are drawn in Sec. V.

II. THEORETICAL MODEL

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 flowing in the sample can be expressed by the two equivalent expressions:

$$I = eAN_A v_d' = eAN_A u v_d \,, \tag{1}$$

where e is the absolute value of the electron charge, N_A is the total concentration of acceptors, v_d' the total carrier mean drift velocity (reduced drift velocity) which accounts for the time spent by the carriers on the impurities, the so-called trapping time, u is the fraction of ionized carriers, and v_d is 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:

$$\sigma = eN_A v_d'/E = eN_A u v_d/E \,. \tag{2}$$

By introducing into a standard Monte Carlo procedure the GR processes as an additional scattering mechanism[6] we have calculated the reduced drift velocity at the given electric field. Therefore, through the knowledge of the acceptor concentration, the conductivity has been determined. The microscopic model follows from Ref. 7. In short, it uses a single valence band (the heavy one) warped with nonparabolic effects accounted for. Acoustic, nonpolar optical and ionized impurity scattering mechanisms are considered. A nonradiative GR mechanism assisted by acoustic phonons (cascade capture model) is introduced as reported in Ref. 6. The modeling of this last mechanism requires the knowledge of four parameters, namely: the acceptor concentration N_A, the recombination coefficient at equilibrium ρ_{eq}, the equilib-

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rium generation rate γ_{eq}, and the fraction of ionized impurities at equilibrium u_{eq}. Indeed, since the balance equation at equilibrium implies the following standard relationship:

$$N_A \rho_{eq} u_{eq}^2 = \gamma_{eq}(1 - u_{eq}) \tag{3}$$

for a given acceptor concentration only two parameters are needed and we choose ρ_{eq} and u_{eq}.

According to the literature[5] and previous findings[6] we take $\rho_{eq} = 4.2 \times 10^{-6}$ cm^3/s. The fraction of ionized impurities at equilibrium is calculated as follows. From statistics, under the hypothesis of neglecting compensation, we obtain[8]

$$u_{eq} = \frac{2}{1 + [1 + (4g_A/N_N m^{*3/2}) T^{-3/2} N_A \exp(\epsilon_A/KT)]^{1/2}} \tag{4}$$

with $g_A = 4$ the degeneracy factor, $N_N = 4.83 \times 10^{21}$ m^{-3} K$^{-3/2}$ a universal constant factor, $m^* = 0.75$ the density of states effective mass in units of the free-electron mass at 77 K, $\epsilon_A = 45$ meV, the ionization energy of the acceptor level.

If u_{eq} given by Eq. (4) is substituted into Eq. (3), we obtain the well-known relationship $\gamma_{eq}/\rho_{eq} = N_N (m^* T)^{3/2}/[g_A \exp(\epsilon_A/KT)]$, which shows that γ_{eq}/ρ_{eq} does not depend on the acceptor concentration, while it strongly depends on temperature. The values given by Eq. (4) well agrees with available data provided by Hall-effect measurements in a wide range of temperatures and acceptor concentrations.[9–11] We notice that the Monte Carlo method enables a self-consistent calculation of u_{eq} to be carried out from the knowledge of γ_{eq}, ρ_{eq}, and N_A (therefore in a microscopic way from the scattering mechanisms). As a matter of fact, by using an iterative procedure the initial value $u_{eq}^{(0)} = 1$ can be introduced in the simulation. Then, the output $u_{eq}^{(1)}$, obtained as the ratio between the total time of free flight and the total time of simulation, is used as the new input for a second simulation, and so on until convergence is reached.

Figure 1 shows the values for u_{eq} as function of N_A calculated by using the above technique and compares them with the results given by Eq. (4) and the available data in the literature.[9–11] The agreement between Monte Carlo calculations and statistics is at worst within 20% and thus considered satisfactory. It represents a formidable check for the theory here presented. We also remark that, taking into account the spread of the experimental data found in the literature, probably due to a significant compensation of different samples, theory well agrees with experiments.

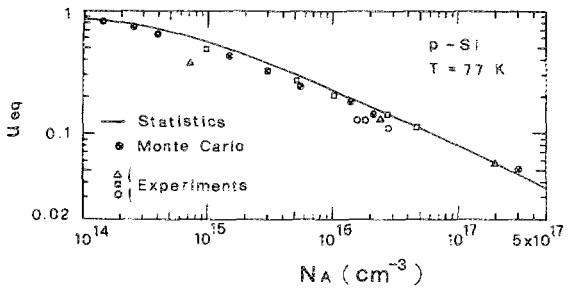

FIG. 1. Fraction of ionized impurities at equilibrium as a function of the acceptor concentration in p-Si at 77 K. The line is obtained from statistics. Full circles refer to to the Monte Carlo simulation, other symbols to experiments (Refs. 9–11).

So far the Poole–Frenkel effect has been neglected in the evaluation of the generation rate; we shall comment on this point later. Furthermore, impact ionization of impurities has been found of negligible importance for the doping concentration here considered and therefore has been disregarded.

III. EXPERIMENTS

All the samples investigated belong to slices of ingots of p-type silicon doped with boron and nominally uncompensated. Ohmic contacts have been performed through a p^+ diffusion of boron on both slice surfaces. Finally, a metallization has been made by depositing a thick film of aluminum covered by silver and then performing an annealing process. Different slices have been prepared at LAAS (Laboratoire d'Automatique et d'Analyse des Systemes, Toulouse, France) and at the Modena University (Italy); then they have been cut either by scribing or by using an ultrasonic machine to obtain the samples for the measurements. The acceptor concentration has been derived from the room-temperature ohmic resistivity by using the Irvin curves.[12] The main characteristics of the samples used in present experiments are summarized in Table I.

To determine the conductivity we have performed measurement of the current-voltage characterics. To avoid Joule heating of the samples, which at the highest electric field can be over 10^6 K/s, we have used a measurement technique of short time pulses within 0.3 and 3 μs. Furthermore, to avoid

TABLE I. Summary of the main characteristics of the samples used in the field-dependent measurements.

ρ at 300 K ($\Omega \times$cm)	N_A (10^{15} cm^{-3})	Direction	Length (10^{-2} cm)	Surface (10^{-2} cm^2)	Origin
2.9	5.5	⟨100⟩	3.50	0.42	LAAS
4.8	3.0	⟨100⟩	1.50	0.36	LAAS
32	0.40	⟨100⟩	3.55	0.70	LAAS
50	0.25	⟨100⟩	2.35	0.70	Modena
64	0.18	⟨111⟩	3.00	0.70	Modena
90	0.14	⟨100⟩	3.00	1.0	Modena

cumulative heating effects, we have made the measurements at a low repetion rate of 0.1–10 Hz. Then, an average of the current-voltage measurement has been performed by using a current and voltage probe from Tektronix coupled with a numerical oscilloscope. Thus, the conductivity has been finally obtained from the knowledge of the sample geometry.

The accuracy of the results obtained at the different electric fields is estimated to be within $\pm 5\%$. (This by taking into account the indetermination in the dimensions, in the contact resistance and in the doping level of different samples.[13]) The same accuracy can be attributed to the Monte Carlo calculations.

IV. RESULTS AND DISCUSSION

The ohmic conductivity as a function of the acceptor concentration is shown in Fig. 2 where for completeness available data from literature[2] have been also reported. The agreement between theory and experiments is found to be at worst within 20% and thus considered satisfactory, in view of the lack of any arbitrary parameter entering the theory. The sublinear behavior exhibited by the conductivity is mainly attributed to a decrease in the fraction of ionized impurities at increasing acceptor concentrations. Moreover, this effect is enhanced by the decrease in the mobility associated with the increased efficiency of the ionized impurity scattering.

The field-dependent conductivity is reported in Fig. 3 for the case of the samples oriented along the ⟨100⟩ crystallographic direction. Again, a satisfactory agreement is found between theory and experiments. The systematic decreases of the conductivity with the field reflects the prevalence of the decrease in mobility over the increase in free-carrier concentration caused by the increase in free-carrier lifetime as discussed below. These are well-known effects associated with a hot-carrier regime.[1] Indeed, from the Monte Carlo simulation we have evaluated separately the dependence with field of the free-carrier concentration and of their mobility.

The increase in the fraction of ionized carriers reported in Fig. 4 is due to the rise in the carrier mean energy. Because of that, the low-energy population in the carrier distribution function, which is responsible for capture processes, decreases, thus lowering the average recombination rate at the

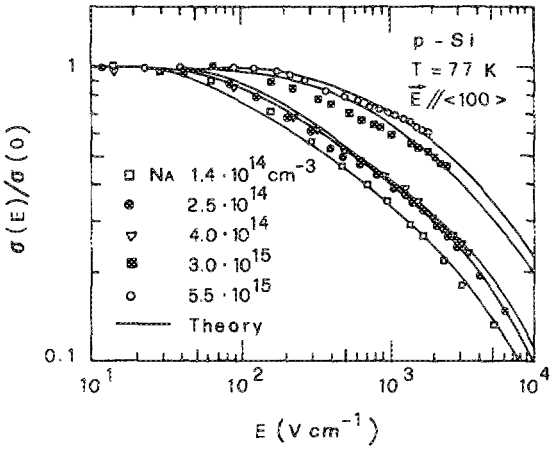

FIG. 3. Conductivity normalized to its ohmic value as a function of the electric field for the different acceptor concentrations reported in p-Si at 77 K. Symbols refer to present experiments, the lines to the Monte Carlo simulation.

given field with respect to its equilibrium value. As a consequence, we have found an enhancement of the free-carrier lifetime, which in turn leads to a net increase in their concentration.

Concerning the mobility, we see from Fig. 5 a systematic decrease from its ohmic value due to an increase of the scattering efficiency with increasing fields. At higher doping levels the effect is smoothed because of the lowering of the ohmic value which displaces to higher fields the onset for hot-electron regime. At the highest fields the mobility becomes practically independent of the acceptor concentration because of the Coulomb nature of the ionized impurity scattering which implies a vanishing efficiency of this mechanism at increasing carrier energies.

The anisotropy effect of the field-dependent conductivity has been theoretically investigated along the ⟨100⟩ and ⟨111⟩ orientations for the case of $N_A = 2.5\times10^{14}$ cm^{-3}. Figure 6 shows that above 50 V/cm the conductivity along the ⟨100⟩ becomes greater than along the ⟨111⟩ direction by about 20%. In analogy with previous findings[3] we ascribe this behavior to the warped shape of the heavy-hole band. As a matter of fact, the lower value for the local effective mass

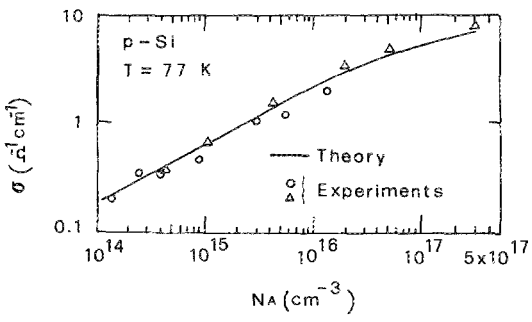

FIG. 2. Low field (ohmic) conductivity as a function of the acceptor concentration in p-Si at 77 K. Open circles refer to present experimental data, triangles to those Ref. 2, and the line to the Monte Carlo simulation.

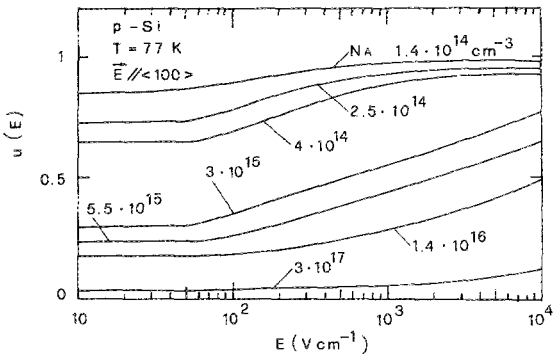

FIG. 4. Fraction of ionized carriers as a function of the electric field for the different acceptor concentrations reported as obtained from the Monte Carlo simulation in p-Si at 77 K.

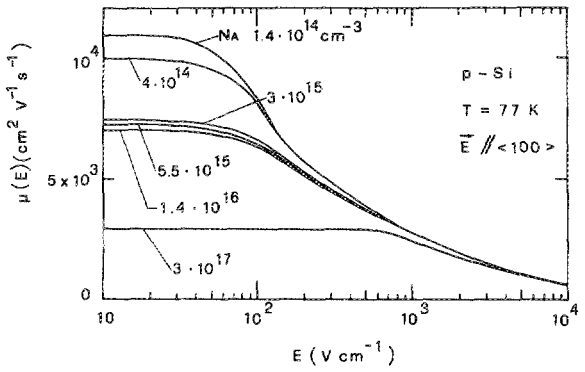

FIG. 5. Free-carrier mobility as a function of the electric field for the different acceptor concentrations reported as obtained from the Monte Carlo simulation in p-Si at 77 K. Notice that curves for $N_A = 2.5\times10^{14}$ and 4×10^{14} cm^{-3} are found to coincide within the numerical uncertainties.

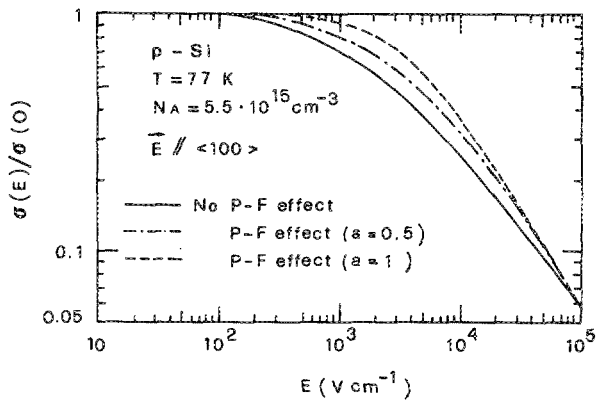

FIG. 7. Conductivity normalized to its ohmic value as a function of the electric field for the acceptor concentration reported as obtained from the Monte Carlo simulation with and without Poole–Frenkel effect in p-Si at 77 K.

along the ⟨100⟩ with respect to the ⟨111⟩ direction is responsible for a correspondent higher mobility, while the carrier concentration has been found to be practically insensitive to the orientation.

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 has been used[14–16] by introducing an exponential factor so that the ionization rate in the presence of the electric field is given by

$$\gamma(E) = \gamma_{eq} \exp(a\beta E^{1/2}/KT)\,, \qquad (5)$$

where for the present case of Si $\beta = 3.55\times10^{-24}$ 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 7 reports an investigation of this effect on the relative conductivity for an acceptor concentration $N_A = 5.5\times10^{15}$ cm^{-3}. The higher values for the ionization rate given by Eq. (5) lead to a further increase in the fraction of ionized impurities with the field, while the change in the mobility has been found negligible. Because of that, we find higher values for the conductivity at intermediate electric field strengths. At the highest fields, practically all the impurities are ionized and the values for the conductivity no longer depend upon the Poole–Frenkel effect. At lower doping levels the fraction of ionized impurities is closer to unity (see Fig. 1) and the Poole–Frenkel effect on the conductivity is expected to become weaker. By comparing these results with the experiments of Fig. 3 we have seen that the fitting gets worse by including Poole–Frenkel effect. We conclude that no evidence of this effect in experiments may be proved from the present analysis.

Finally, we wish to remark that the fitting of the present data is, to a large extent, sensitive only to the ratio γ_{eq}/ρ_{eq} and not to their absolute values; this because for the parameters used the carrier lifetime ($\gtrsim 10^{-10}$ s) is much longer than the scattering time ($\lesssim 10^{-12}$ s). In other words, the carrier distribution function is practically independent on GR mechanisms and once u_{eq} is given then the results will depend only on the ratio given above. To obtain separate information of γ_{eq} and ρ_{eq} the fitting of other transport parameters, such as the noise spectral density, is required.[17,18]

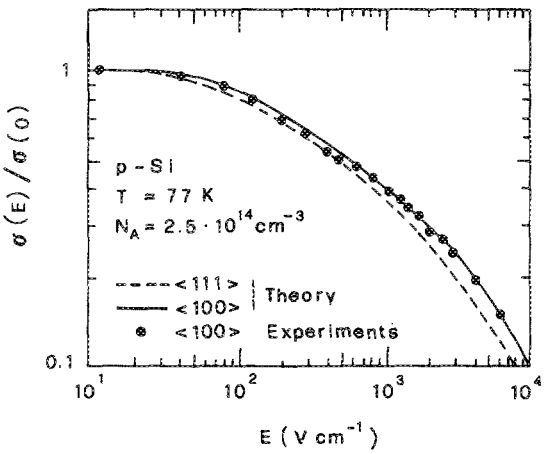

FIG. 6. Conductivity normalized to its ohmic value as a function of the electric field for the acceptor concentration and the crystallographic directions reported in p-Si at 77 K. Full circles refer to experiments already reported in Fig. 3; the lines refer to the Monte Carlo simulation.

V. CONCLUSIONS

We have reported a systematic analysis of the field-dependent conductivity in lightly doped p-Si at 77 K. To this end new measurements are provided and an original microscopic interpretation is given. This last is based on a Monte Carlo simulation which enables us to account simultaneously for the change in the mobility and concentration of free charge. The field-dependent conductivity has been described by the competitive effect of an increase in the free-carrier concentration and decrease in their mobility, both behaviors occurring within the hot-carrier regime. The satisfactory agreement found supports that the cascade capture assisted by acoustic phonons, which has been introduced in the simulation to model generation recombination processes, is the

basic mechanism responsible for the determination of the carrier concentration at any increasing electric field. The theoretical model predicts an effect of anisotropy with a greater conductivity along the ⟨100⟩ crystallographic direction. In the region of fields and acceptor concentrations investigated no evidence of Poole–Frenkel effect has been noticed.

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