Hot-electron galvanomagnetic conduction in n-InSb at 77 K

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The Monte Carlo (MC) method is used to analyze high-field Hall-effect measurements on n-InSb at 77 K in a magnetic field of 5 mT. The Hall factor, the Hall mobility, and the drift mobility are calculated as a function of the electric field. A nonparabolic conduction band is used and polar LO-phonon, acoustical-phonon, and ionized impurity scattering are incorporated in the MC calculations. The acoustical deformation potential is determined from the high-electric-field ($E > 150$ V/cm) mobility. Good agreement with experiment is found for an acoustical deformation potential between 18 and 30 eV. The impurity concentration is then determined from the low-field mobility results.

I. INTRODUCTION

Much work has been done on hot-electron galvanomagnetic properties in n-type InSb, governed by various scattering mechanisms, but some points remain unclear. The value of the acoustic deformation potential ε_D as found in the literature[1-7] ranges from 4 to 30 eV. Moreover, the impurity content N_i of samples of n-InSb is not known precisely. Usually it is estimated by comparing the experimental low-electric-field Hall mobility to a theoretical calculation.[8] In order to realize this, one needs to know the deformation potential ε_D. Given ε_D, the concentration of impurities N_i will be fixed. In this way the problem of determining ε_D and N_i are coupled: a higher value of ε_D results in a lower value of N_i. At low electric fields both the acoustical deformation-potential scattering and ionized impurity scattering have roughly the same effect, they are both elastic processes. They have a slightly different temperature dependence, a fact which was used by several authors[4,7] to estimate ε_D. In this paper we present a method which will make it possible to determine ε_D independently from N_i. Only one experiment at a given temperature is needed.

The purpose of this paper is to study theoretically the transport properties of InSb in the presence of an electric as well as a nonquantizing magnetic field. The Monte Carlo (MC) method has been adopted for this purpose. An analysis is made of the experimental results of Alberga *et al.*[9,10] on InSb at 77 K.

II. MONTE CARLO METHOD USED IN THE CALCULATION

The MC procedure follows the same lines as discussed by Fawcett *et al.*[11] and Boardman *et al.*[12] (for a recent review see Ref. 13). Scattering of electrons by ionized impurities, acoustical and polar optical phonons is included and described essentially in the same way as was done by Ruch and Fawcett[14] but using different parameter values. The electron concentration is sufficiently low that electron-electron scattering is unimportant.

The conduction band of InSb is strongly nonparabolic and is described within the Kane model.[15] The effect of nonparabolicity was taken into account both in the electron equations of motion and in the different scattering rates. The trajectory of an electron in crossed electric $\mathbf{E}=(E,0,0)$ and magnetic $\mathbf{B}=(0,0,B)$ fields and within a Kane band, differs appreciably from a circular orbit.[16] The magnitude and type of deviation depends on the ratio E/B. The nonparabolicity limits the velocity of high-energy electrons, thereby preventing the "runaway" effect. It also affects scattering probabilities and in this way the heating of the electrons.

The equations of motion for an electron in crossed fields and within a Kane band are

$$\frac{d\mathbf{p}}{dt} = e(\mathbf{E} + \mathbf{v}_d \times \mathbf{B}) , \tag{1}$$

where

$$\mathbf{v}_d = \nabla_p \epsilon(\mathbf{p}) \tag{2}$$

is the electron velocity and

$$\epsilon(\mathbf{p}) = \frac{1}{2\gamma}\left[-1+\left[1+4\gamma\frac{p^2}{2m^*}\right]^{1/2}\right] \tag{3}$$

is the nonparabolic electron energy-momentum relation with

$$\gamma = \frac{1}{\varepsilon_g}\left[1-\frac{m^*}{m_e}\right] [=0.1046(\hbar\omega_{\mathrm{LO}})^{-1} \text{ in InSb}] ;$$

γ is the nonparabolicity coefficient and m^* the effective electron mass at the bottom of the conduction band.

The equation of motion (1) with the conduction band (3) is impossible to solve analytically. A numerical solution of Eq. (1) increases the MC simulation time dramatically. Therefore we linearized Eq. (1) at *each* MC free flight by expanding the Kane dispersion law (3) around the initial electron momentum $\mathbf{p}_0$ of the free flight up to second order in the difference $(\mathbf{p}-\mathbf{p}_0)$:

$$\epsilon(\mathbf{p}) = \epsilon(\mathbf{p}_0) + \left[1+4\gamma\frac{p_0^2}{2m^*}\right]^{-1/2}\left[\frac{\mathbf{p}_0}{m^*}(\mathbf{p}-\mathbf{p}_0)+\frac{(\mathbf{p}-\mathbf{p}_0)^2}{2m^*}\left[1-4\gamma\frac{p_0^2}{m^*}\frac{1}{1+4\gamma(p_0^2/2m^*)}\right]\right] . \tag{4}$$

The replacement of (3) by (4) at each free flight makes the differential equation (1) linear in $\mathbf{p}$ and then Eq. (1) can be solved analytically. Equation (4) corresponds to a local parabolic approximation of Eq. (3) which, in view of the short times of the electron free flight, is reasonable. We checked that this approximation induces an error of less than 1% in the results of the MC simulation for the Hall and the drift mobility as compared to the corresponding results from a numerical solution of Eq. (1). Recently, Brazis *et al.*[16] used a different approach and solved Eq. (1) iteratively. An independent check of our MC results was obtained by comparing the electron drift mobility as obtained from the present MC simulation with the results of Kranzer *et al.*[17] who solved the Boltzmann equation numerically. In the case of the absence of acoustical-phonon scattering and for an ionized impurity concentration of $N_i = 4\times10^{14}$ cm^{-3} we could reproduce their results within 1%.

Values of the parameters of InSb, which were used in the MC simulation, are listed in Table I. Consistent polaron constants were used.[18,19]

III. RESULTS

The electric-field dependence of the Hall mobility μ_H (Fig. 1), the drift mobility μ_D (Fig. 2), and the Hall factor $r_H = \mu_H/\mu_D$ (Fig. 3) were calculated for sample H286 of Ref. 9. The electron density of this sample is $n_e = 1.8\times10^{14}$ cm^{-3}, the lattice temperature was taken to be 77 K, and a magnetic induction $B = 5$ mT is applied perpendicular to the electric field. The MC results are given by the different symbols in Figs. 1–3 with their corresponding error bars. The solid curves in Figs. 1–3 represent the experimental results of Ref. 9, *uncorrected* for the geometry of the side contacts.

Usually, the impurity concentration in a sample is determined from the low-field mobility. This is a reliable method if all the other scattering mechanisms, which limit the electron mobility, are fully known. In the case of InSb, the parameters for all scattering mechanisms are fairly well known except for the acoustical-phonon scattering mechanism. The importance of the latter in InSb is not yet fully understood. In the literature there exists a large discrepancy between the numbers quoted for the deformation potential; they range roughly between 7.2 and 30 eV. Note that the transition rate for acoustical-phonon scattering depends quadratically on the deformation potential ε_D and thus the acoustical-phonon scattering rates, for the range $\varepsilon_D = 7.2$–30 eV, can lead to a difference of a factor of almost 20. Depending on the value of ε_D other values for the impurity concentration will be obtained. It would be very important to determine ε_D independently from the low-field mobility result. This will be done in the present analysis. Once we know ε_D we can determine N_i from the low-field mobility results.

In this paper we performed our MC calculation for three different values of the deformation potential which are most often quoted in the literature, namely, $\varepsilon_D = 7.2$, 18, 30 eV. The impurity concentration is then determined such that the low-field Hall mobility fits the experimental low-field Hall mobility. We opt for fixing the N_i from the Hall mobility because μ_H was determined experimen-

TABLE I. Parameters of InSb used in the MC calculations.

Electron-phonon coupling constant	α	0.0197
Effective-mass ratio	m^*/m_e	0.0138
LO-phonon energy	$\hbar\omega_{\mathrm{LO}}$	24.2 meV
Static relative dielectric constant	ε_s	17.64
Band gap	ε_g	225 meV
Mass density	ρ	5.8 g/cm^3
Acoustic velocity	u	3.75×10^5 cm/sec

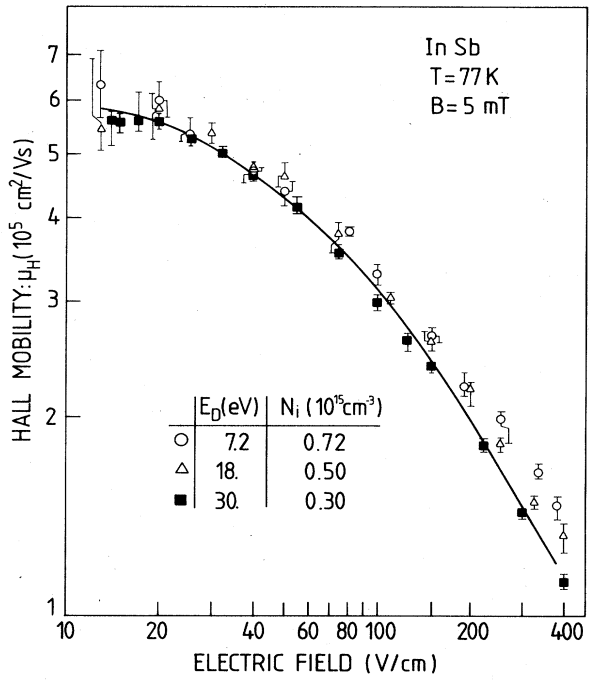

FIG. 1. Hall mobility as a function of the electric field at a fixed magnetic field strength of 5 mT. The different symbols correspond to the present MC results for three different sets of values for the deformation potential (ε_D) and the ionized impurity content (N_i). The solid line represents the experimental values of Ref. 9.

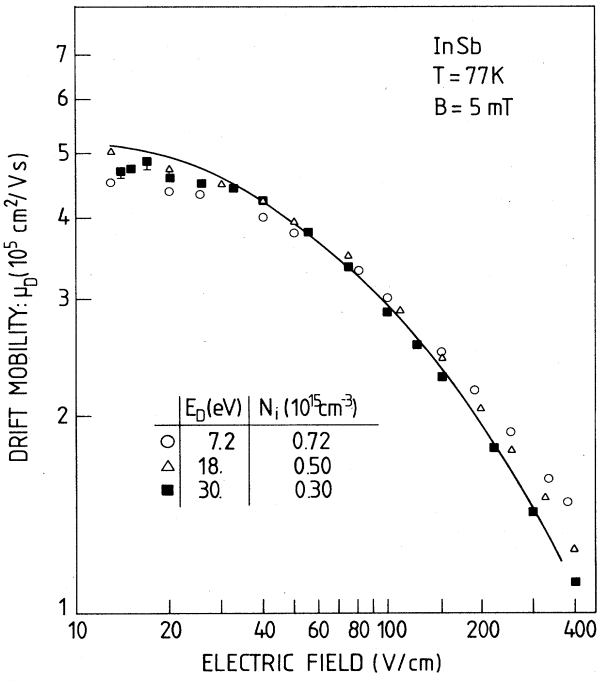

FIG. 2. Same as Fig. 1, but now for the drift mobility.

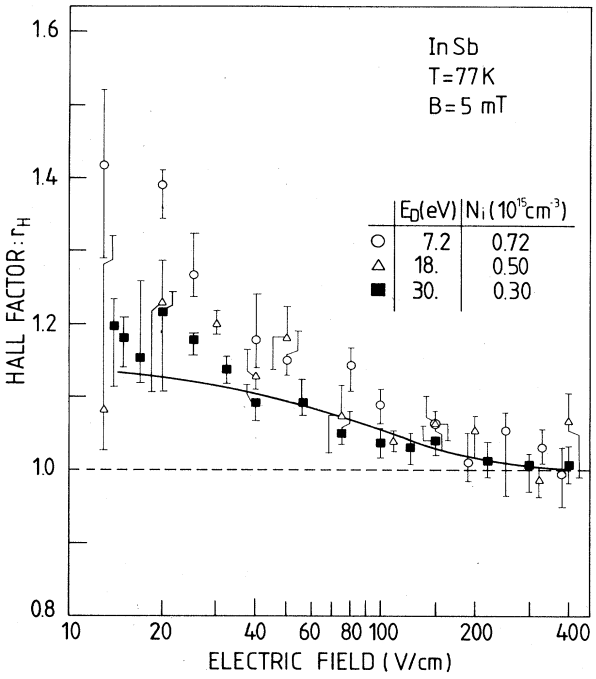

FIG. 3. Hall factor as a function of the electric field. The same notations are used as in Fig. 1. The solid line does *not* represent the experimental data of Ref. 9, but is the quotient of the two experimental lines in Figs. 1 and 2.

tally in a direct way. The experimental drift mobility is obtained indirectly: In Ref. 9 μ_D was a derived quantity.

For $\varepsilon_D=7.2$ eV an impurity content $N_i=0.72\times10^{15}$ cm^{-3} was taken as estimated in Ref. 9. From Fig. 1 we observe that the MC results are in reasonably good agreement with the uncorrected experimental results for electric field $E<60$ V/cm. At higher electric fields ($E>100$ V/cm) a systematic difference is found in μ_H which is higher than the maximal experimental error of 10%. The drift mobility (Fig. 2) for $E<60$ V/cm lies well below the experimental result. For $E>60$ V/cm the MC results for μ_D are systematically larger than the experimental results. For $\varepsilon_D=18$ eV we took $N_i=0.50\times10^{15}$ cm^{-3} to fit the experiment for μ_H at low fields. The agreement with experiment is reasonable and the systematic difference in μ_H and μ_D at high fields is smaller than for $\varepsilon_D=7.2$ eV. The MC results for $\varepsilon_D=18$ eV are just at the border of the experimental 10% error region. For $\varepsilon_D=30$ eV we took $N_i=0.30\times10^{15}$ cm^{-3} to fit the low-field Hall mobility. These results show an overall agreement with the experimental results. Note that in the 100 V/cm $<E<400$ V/cm region μ_H and μ_D have the same inclination as the experimental results.

The MC results indicate that (1) at high electric fields impurity scattering has little effect, (2) the relative contribution of acoustic-phonon scattering is significant as opposed to the conclusion of Ref. 9. This is not surprising since the acoustic-phonon scattering rate increases monotonically with electron momentum. It is clear from Figs. 1 and 2 that the best agreement with experiment is obtained for $\varepsilon_D=30$ eV rather than 18 eV. The value

$\varepsilon_D = 7.2$ eV can be ruled out. This is consistent with the conclusion of Asauskas *et al.*[3] for the case of electric field only. Asauskas *et al.* compared their MC calculations with (1) direct measurements[3(a)] of the high-field drift velocity and (2) weak field mobility measurements[3(b)] as a function of temperature, doping level, and hydrostatic pressure and also obtained $\varepsilon_D = 30$ eV for the deformation potential.

IV. DISCUSSION AND CONCLUSION

Alberga *et al.*[9] corrected their measured Hall voltages for the geometry of the side contacts. Since the contact dimensions in the experiment are of the same order of magnitude as the thickness of the sample one should in principle expect some influence of the geometry on the Hall mobility result. Based on a calculation by Haeusler,[20] the geometrical correction was estimated to be of the order of 40% (the correction was slightly electric-field dependent). The drift velocity is not influenced by the geometry of the side contacts. But note that μ_D was not a directly measured quantity in Ref. 9. r_H has the same geometry correction as μ_H.

Comparing the MC results for μ_H (Fig. 1) with the uncorrected experimental results it is hard to believe that such a large geometrical correction of about 40% is necessary. All the MC results give evidence that this correction is unnecessary or at least very small at high electric fields and at most 10% in the low-electric-field region. The problem is to understand the reason why in Ref. 9 only a small geometrical correction is necessary in contrast to the estimated correction of around 40%.

Three remarks are in order here: (i) It is not established experimentally whether the physical size of the side contacts equal the optical size. The current carrying part of the contact (i.e., the physical size), which is the physically relevant size here, could be much smaller than experimentally measured (i.e., the optical size, which was measured optically in Ref. 9). This would lead to a much smaller geometrical correction than estimated by Alberga *et al.*, as was already mentioned in Ref. 10, (ii) the experimental value of the equilibrium carrier concentration n_e is subject to uncertainty: sample H268 from the same ingot as sample H283 has $n_e = 1.59 \times 10^{14}$ cm^{-3} in Ref. 9 as compared to $n_e = 1.81 \times 10^{14}$ cm^{-3} for H283. This would lead to lower values for the corrected experimental Hall factor. In order to get agreement in this way with the high-field MC result of $r_H \approx 1.0$ one has to take $n_e = 1.3 \times 10^{14}$ cm^{-3}, which is a highly improbable value, however, (iii) the expression (2) of Ref. 9 for the geometrical correction factor g_H is derived by Haeusler[20] starting from a fairly simple force equation for an infinite sample [Eq. (2.1) of Ref. 20(b)]:

$$\mu(\mathbf{E} + \mathbf{v}_d B) = \mathbf{v}_d$$

with

$$\mu = \frac{e\tau}{m^*}$$

in which the electron scattering is described by an energy-independent relaxation time τ. In this model the Hall factor equals 1 exactly, independent of E, B, and before correcting for side contact geometry. Without a geometrical correction factor the MC results show that r_H differs already appreciably from 1 (20 to 30%) at low electric fields. Thus, Haeusler's starting point is already wrong. This led us to believe that the formula for the geometrical correction factor is much more complicated than derived in Ref. 20. Apparently, r_{Hc}, as given in Ref. 9, is not the scattering factor but $g_H r_H$. When the data of Fig. 10 in Ref. 9 are divided by g_H, they compare very well with Fig. 3.

From the above three remarks and from the present MC analysis we conclude that the magnitude of the correction for side contact geometry must be calculated in an essentially different way than suggested by Haeusler[20] and that its magnitude appears to be much smaller than was estimated in Refs. 9 and 10. This implies that the experimental results in Refs. 9 and 10 are much closer to the results for bulk electrons in a sample of infinite dimensions than was anticipated.

In conclusion, MC simulation of the conduction of electrons in n-InSb in crossed electric and magnetic fields was performed at 77 K for $B = 5$ mT. The acoustical deformation potential ε_D is determined from the experimental high-electric-field Hall mobility result, in contrast to the usual approaches where ε_D is determined from the low-field electron mobility results, with the exception of Asauskas *et al.* (Ref. 3). We found ε_D to be close to 30 eV although the range 18—30 eV cannot be ruled out, due to (experimental) accuracy problems. The ionized impurity concentration is subsequently obtained from the low-

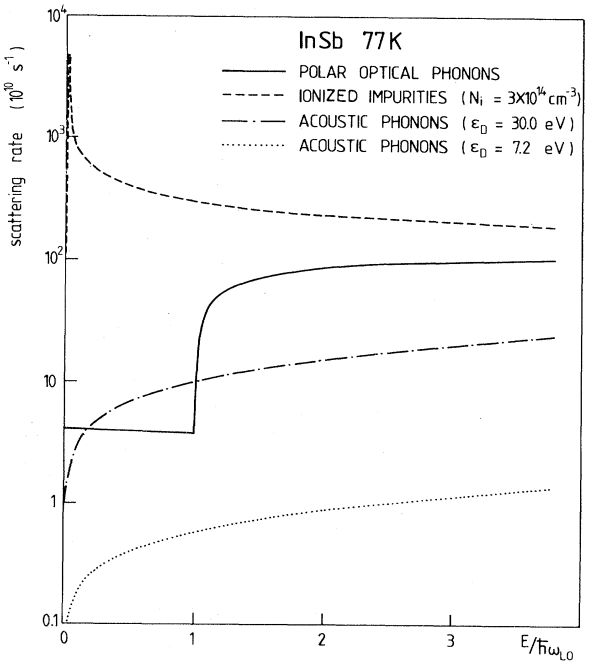

FIG. 4. Transition rate as a function of the electron energy for the different relevant scattering mechanisms in InSb at 77 K. $\hbar\omega_{LO}$ is the optical-phonon energy.

electric-field mobility. This new method for determining ε_D, allows one to determine ε_D and N_i with an experiment performed at one temperature, here $T=77$ K. Impact ionization plays no role in the experiment, since it was pulsed.[3(b),9] Although the ionized impurity scattering rate is large at high electron energies (Fig. 4), ionized impurity scattering has little effect in this electric-field range, because of the elastic nature of this scattering mechanism and because this scattering is predominantly in the forward direction.

At high electric fields ($E\sim 60$—300 V/cm) the relative importance of acoustical-phonon scattering increases because (1) the acoustical-phonon scattering rate at high electron energies increases faster than the polar LO-phonon scattering rate (see Fig. 4) and (2) acoustical-phonon scattering can reverse the electron momentum (backscattering) which is very efficient in reducing the mobility.

The reason for the discrepancy between the quoted numbers for ε_D is not fully understood. A possible reason may be that the Hamiltonian for deformation-potential scattering is in essence derived in the limit of long-wavelength phonons. These phonons are triggered by a pressure experiment which leads to $\varepsilon_D\sim 7$ eV. Optical measurements favor $\varepsilon_D\sim 15$ eV, while high-electric-field transport measurements seem to lead to $\varepsilon_D\sim 30$ eV. In the latter type of experiments short-wavelength phonons are also involved. From this we may conclude that the deformation-potential interaction is not fully understood; and that more theoretical work has to be done on the deformation-potential interaction in order to get a consistent description of the different types of experiments.

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