Effect of random potential fluctuations on electron transport in *n*-type InSb

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(Received 22 January 1985)

A number of previous investigators have concluded that the low-temperature transport properties of *n*-type InSb can only be understood by assuming the existence of an impurity band which is separated from the conduction band by a finite binding energy. However, we show that the experimental results are fully consistent with a one-band interpretation as long as the effects of potential fluctuations due to random inhomogeneities in the impurity concentration are considered. Single-site electron mobilities are compared with a large body of experimental data from the literature covering the temperature range 1.3 to 80 K. Experiment and theory are found to agree well as long as the magnitude of the fluctuations γ is small compared to the thermal energy of the electrons E_0. However, when $\gamma \gg E_0$ in compensated samples at low temperatures, the experimental mobilities fall far below the results of the single-site theory (which ignores the fluctuations). This behavior is consistent with that observed for one-band conduction in other semiconductors. Also considered are effects of the potential fluctuations in the alternative case where an impurity band is assumed to be present.

I. INTRODUCTION

For close to 20 years, there has been an ongoing controversy concerning whether the impurity band in *n*-type InSb is separate from the conduction band or whether the two bands have merged. The argument used most often to support the existence of a separate impurity band has been that the low-temperature conductivity and Hall data can only be understood within a two-band context. The main purpose of the present paper is to show that, on the contrary, this data can be explained at least as well by a one-band treatment if one accounts for the effects of potential fluctuations due to random inhomogeneities in the impurity density. Korotin *et al.*[1] and Yaremenko *et al.*[2] have invoked this phenomenon previously in interpreting specific InSb transport data, and subsequent investigators[3,4] have noted that the fluctuations may be important in some regions. However, there has been no comprehensive study of the overall implications of the potential fluctuations in InSb. As part of the present analysis, we compare one-band theoretical results to a large body of experimental mobilities from the literature. We further examine whether the general behavior of the InSb data is consistent with that obtained for other semiconductors in regions where potential fluctuations are important but impurity-band conduction is negligible.

Section II below surveys the main arguments used to support the existence of a separate impurity band in InSb. In Sec. III, we discuss phenomenologically the effects of potential fluctuations on conduction-band transport. Section IV presents a broad comparison of the one-band theoretical and experimental mobility results for the temperature range 1.3—80 K. In Sec. V, incorporation of the potential fluctuations into the two-band model is considered, and some important consequences are discussed. Finally, in Sec. VI we assess the evidence provided by low-temperature transport measurements for or against the existence of a separate impurity band. We emphasize that our goal is to show the InSb experimental results to be consistent with a one-band interpretation rather than to conclusively refute the two-band model.

II. ARGUMENTS FOR THE TWO-BAND MODEL

In this section we review some of the low-magnetic-field transport data used by previous investigators in arguing for the existence of an impurity band distinct from the conduction band in *n*-type InSb. Most of the discussion in the literature has centered upon three phenomena: (a) "activated" low-temperature conductivity, (b) peaks in the temperature-dependent Hall coefficient, and (c) conductivity activation with electric field. Although the observation of negative transverse magnetoresistance[3,5,6] and peaks in the microwave photoconductivity[4,7] and absorption[8,9] spectra have also occasionally been cited as evidence for the two-band model,[10,11] those phenomena are outside the scope of the present work.

A number of investigators have noted that the low-temperature electrical conductivity of compensated InSb decreases much more rapidly with decreasing T than is predicted by conventional one-band transport calculations. This is illustrated in Fig. 1(a), which shows an InSb sample[1] for which the experimental conductivity (open circles) at 6 K falls to nearly an order of magnitude below the Brooks-Herring result[12] for ionized impurity scattering. While a few authors[1,2,13] have attempted to explain this phenomenon in terms of conduction-band electrons alone, most[5,8,14–17] have taken the low conductivities to be evidence for freeze-out into an impurity band. The latter usually assume that the conductivity may be written in the form[18]

$$\sigma_I \approx \sigma_1 e^{-\epsilon_1/k_B T} + \sigma_2 e^{-\epsilon_2/k_B T} + \sigma_3 e^{-\epsilon_3/k_B T} . \quad (2.1)$$

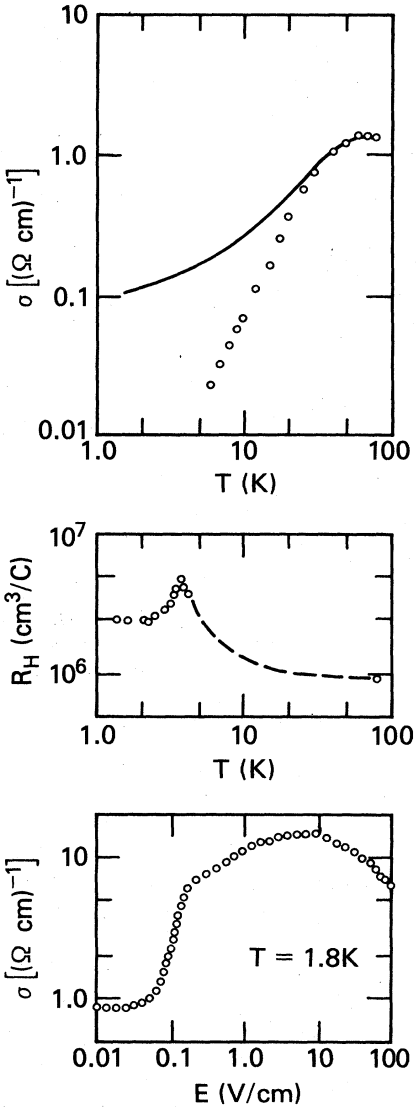

FIG. 1. Experimental transport data for InSb at low magnetic fields. (a) Conductivity vs temperature for sample 1 of Korotin *et al.* (Ref. 1) ($N_D - N_A = 4.3 \times 10^{13}$ cm^{-3}). Solid curve calculated from Brooks-Herring theory. (b) Hall coefficient vs temperature for sample 713-11a of Ishida and Otsuka (Ref. 3) ($N_D - N_A = 1.0 \times 10^{13}$ cm^{-3}). (c) Conductivity vs electric field for sample 57-S1 of Miyazawa and Ikoma (Ref. 6) ($N_D - N_A = 8.8 \times 10^{13}$ cm^{-3}).

Here the various activation energies ϵ_i correspond to (1) transitions from the impurity band to the conduction band (i.e., σ_1 is the conduction-band conductivity and $\epsilon_1 \rightarrow E_D$ is the donor binding energy), (2) transitions between "localized" states at the bottom of the impurity band to "metallic" extended states higher in the band, and (3) activation for hopping conduction. Since the corresponding conductivities are usually taken to satisfy the relation $\sigma_1 > \sigma_2 > \sigma_3$ while $\epsilon_1 > \epsilon_2 > \epsilon_3$, several investigators have claimed to observe more than one of these processes at different temperature ranges in the same sample.[3,15,17] It is widely acknowledged that an impurity band is present in n-type InSb whenever high magnetic fields are applied,[19–22] and that activation involving impurity-band conduction should then be observable. However, even in the high-field case there is sometimes disagreement concerning which of the three types of activation are actually observed.

Ishida and Otsuka[3] claim that their low-field data shows evidence for a "Mott transition"[23] if the conductivity at 1.3 K is plotted as a function of compensation for nearly constant donor concentrations. Mott proposed that the impurity-band conduction should become "metallic" if the donors are close enough together that[23,24]

$$N_D \gtrsim \left[\frac{0.25}{a_0}\right]^3 \tag{2.2}$$

since the wave functions of electrons bound to neighboring donors then overlap significantly. Here N_D is the donor density and $a_0 = \hbar^2\kappa_0/m_e e^2$ is the effective Bohr radius. However, rather than criterion (2.2), Ishida and Otsuka used the misleading criterion

$$n = N_D - N_A \gtrsim (0.25/a_0)^3, \tag{2.3}$$

where n is the total electron density in both conduction and impurity bands. Following an argument by Mott,[25] they assert that as $T \rightarrow 0$, the mobility of electrons at the Fermi level in highly compensated material should be low because the degenerate electrons populate localized states at the bottom of the impurity band even though metallic states exist higher in the band. While it is reasonable to expect this effect to be observable (assuming that impurity-band conduction dominates), criterion (2.3) should not be relied upon as a valid indicator of the critical density n_c. Using criterion (2.3), Ishida and Otsuka obtained $n_c \approx 6 \times 10^{13}$ cm^{-3}, which appears to be in good agreement with their data. However, we show in Sec. IV that when one accounts for the potential fluctuations, the one-band model predicts a similar transition at nearly the same electron density.

As discussed in the Appendix, the two-band model also predicts that there should be a peak in the Hall coefficient as a function of temperature. The observation[3,6,14,26] of such a peak in $R_H(T)$ at temperatures T_P on the order of 4 K has therefore been interpreted as evidence for two-band conduction. This is illustrated in Fig. 1(b), which shows Hall-coefficient data for a highly compensated ($K \equiv N_A/N_D \approx 0.98$) InSb sample[3] for which $R_H(T_P)/R_H(77\text{ K}) \approx 5$. Comparison of the curves for different compensations shows that the magnitude of $R_H(T_P)/R_H(77\text{ K})$ increases with increasing K while the peak temperature T_P decreases. Both of these effects are predicted by the two-band model (see the Appendix) as long as the impurity-band mobility μ_I is assumed to decrease strongly with increasing compensation. At the lowest temperatures the Hall coefficient usually levels off at a constant value $R_H(0\text{ K})$, which approaches $R_H(77\text{ K})$ in relatively uncompensated samples. However, it can be seen from Fig. 1(b) that $R_H(0)/R_H(77\text{ K})$ sometimes exceeds a factor of 2 when K approaches unity.[3,14] This latter finding has not been explained within

the two-band model, which predicts

$$R_H(0\ \mathrm{K})/R_H(77\ \mathrm{K}) < 1$$

since the Hall factor r_H exceeds unity at $T = 77$ K and $r_H \to 1$ as $T \to 0$ K (see the Appendix). For some of their more compensated samples Bannaya *et al.*[14] observe a second increase in the Hall coefficient when $T \lesssim 1$ K, although this is not observed by Ishida and Otsuka[3] for samples with comparable doping.

In arguing against the existence of a separate impurity band in n-type InSb, Sandercock[27] and Crandall[28] suggested that the behavior of R_H may be due to the dependence of the conduction-band Hall factor r_H^e on T (see the Appendix). While the particular scattering processes suggested by those authors apparently do not explain the data, we show in Sec. IV that scattering by random fluctuations of the impurity potential may produce the required $R_H(T)$.

For highly compensated samples in which the low-field conductivity is quite small, a number of investigators[2,6,14,16,29] have observed that σ increases sharply with electric field for E in the range $0.1 < E < 1.0$ V/cm [see Fig. 1(c)]. Most[6,14,16,29] have attributed this phenomenon to two-band processes in which either carrier heating or impact ionization of the bound electrons leads to the increased conductivity.[6,29] A one-band interpretation of these data will be discussed in Sec. IV.

III. RANDOM POTENTIAL FLUCTUATIONS

In this section, some qualitative effects of the random potential fluctuations on electron transport will be considered for the case in which no impurity band is present. A comparison of the one-band theory with experiment is made in Sec. IV, and the effect of fluctuations on the two-band problem will be treated in Sec. V.

We consider the regime in which one has considerable overlap of neighboring impurity potentials, i.e.,

$$d \equiv (\lambda_s/D)^3 \gg 1. \tag{3.1}$$

Here λ_s is the screening length, $D\ (= 4\pi N_I/3)^{1/3}$ is half the average distance between impurities, and $N_I = N_D + N_A$ is the total impurity density. We assume that the net impurity potential may be represented by a superposition of screened Coulomb potentials.[30–32] Keldysh and Proshko[33] and Kane[34] independently pointed out that when $d \gg 1$, the net potential fluctuates with position due to random inhomogeneities in the donor and acceptor densities. Consider for simplicity an uncompensated n-type sample, i.e., $N_I \to N_D$. Because the impurities are very close together, a test electron interacts with an average of $N = 4\pi N_I \lambda_s^3/3 = d$ donors at a time. One result of these overlapping negative potentials is to lower the effective bottom of the conduction band by an average amount of $V_0 = -3Ne^2/\kappa_0\lambda_s$. However, when N is large the local donor density displays random fluctuations about the average, leading to fluctuations in the local potential, $V(\mathbf{r})$. For Gaussian statistics the fluctuations in N are of magnitude $N^{1/2}$, implying that the offset potential should display fluctuations of order $3N^{1/2}e^2/\kappa_0\lambda_s \to (12\pi N_I\lambda_s)^{1/2}e^2/\kappa_0$. A more rigorous calculation[33,34] including compensation shows that the rms potential due to the random fluctuations is $\gamma/2^{1/2}$, where

$$\gamma^2 = \frac{4\pi N_I \lambda_s e^4}{\kappa_0^2}. \tag{3.2}$$

The correlation length for the fluctuations is simply λ_s, and with compensation the average potential offset is $V_0 = -4\pi(N_D - N_A)\lambda_s^2 e^2/\kappa_0$.

We recently showed[31] that in the large-d limit, i.e., when

$$d \gtrsim b^{3/2}/(8g)^{3/4}, \tag{3.3}$$

where $b \equiv 4k^2\lambda_s^2$ and $g \equiv \ln(b+1) - b/(b+1)$, the potential fluctuations represent the dominant electron scattering mechanism. Only ions closer than the average impurity separation D contribute significantly to short-range scattering by individual ions, and this scattering becomes negligible as $D \to 0$. For small γ, the random-potential-scattering theory of Yussouff and Zittartz[35] may be used to calculate the transition rates due to the fluctuations. Their lowest-order formalism yields the same net relaxation time[36] as that predicted by Brooks-Herring theory[12] under the assumption of single-site scattering by screened Coulomb potentials. This is a striking result considering the significant phenomenological differences between the two regions. At small d the potential overlap is unimportant, whereas at large d the overlap is severe and potential fluctuations dominate the scattering. The intermediate d region is difficult to treat rigorously, since both long-range scattering by the potential fluctuations and short-range scattering by the individual impurities are important. However, because the single-site theory yields accurate scattering rates per ion at both large and small d, it seems reasonable to interpolate by employing the same form at intermediate d.[31] The accuracy of this procedure for "weak" scattering [see criterion (3.3) above] appears to be verified by the good agreement with experiment which is obtained, for example, in the case of compensated n-type GaAs.[37]

Thus far we have considered only the weak-scattering limit, where electron mobilities calculated with the single-site scattering theory usually agree well with experimental values.[38] This limit may be delineated by the following simple criterion:[31]

$$\frac{4d}{by^2} \gtrsim 1, \tag{3.4}$$

where $y \equiv \frac{1}{2}ka_0$. For small d criterion (3.4) is related to the breakdown of the free-electron quasiparticle picture, which occurs when [38,39] $\langle \tau_D/\tau_R \rangle \gtrsim 1$. Here τ_D is the duration of the collisions, τ_R is the momentum relaxation time, and the angular brackets denote a weighted average over scattering events. As long as b and y are not too small ($b \gtrsim 1$ and $y \gtrsim 0.05$), $\langle \tau_D/\tau_R \rangle \approx 4d/by^2$ to within about 25%.

When $d \gg 1$, potential fluctuations are important and one has $4d/by^2 = \frac{1}{3}(\gamma/E_0)^2$, where the electron thermal energy E_0 is given by $\frac{3}{2}k_BT\mathcal{F}_{1/2}(\eta)/\mathcal{F}_{-1/2}(\eta)$, $\eta \equiv E_F/k_BT$ is the reduced Fermi energy, and $\mathcal{F}_p$ is the Fermi integral of order p. In this region, criterion (3.4)

indicates that the lowest-order calculation of Yussouff and Zittartz[35] breaks down whenever the magnitude of the fluctuations becomes large compared to the electron energy. In particular, Shklovskii and Éfros[40] pointed out that for a distorted conduction band with spatial fluctuations, the electrons preferentially populate those locations with the lowest potential energy.[41] This causes a general lowering of the Fermi level and a decrease in the mobility due to the smaller electron energies. Furthermore, the resulting inhomogeneities in the electron density lead to an electrical conductivity $\sigma(\mathbf{r})$ which varies with position.[40] The net conductivity σ_s will then always be lower than the spatial average $\langle\sigma(\mathbf{r})\rangle$.[42] In the limit of extremely large fluctuations one can in principle obtain σ_s orders of magnitude below $\langle\sigma\rangle$, since virtually all of the electrons will be localized in isolated "droplets" at positions where the potential energy is lowest.[40] These considerations suggest that when the potential fluctuations are large, i.e., $4d/by^2 \gg 1$, the conductivity may fall far below the value predicted by the single-site scattering theory.[43]

Comparison of the single-site theory to experimental results for Si (Ref. 44), GaAs (Ref. 45), ZnSe (Ref. 46), and CdTe (Ref. 47) verify this conclusion. As long as criterion (3.4) is satisfied, the agreement between theory and experiment is good. However, when $4d/by^2 > 1$ at lower temperatures, the experimental mobility usually falls below the theoretical result, often by over a factor of 2. Since the samples studied in Refs. 44—47 were at most only moderately compensated ($K \lesssim 0.8$), the region $4d/by^2 \gg 1$ was not reached (e.g., see Table 1 of Ref. 38). However, at the lowest temperatures $4d/by^2 \gtrsim 10$ for some of the more compensated InSb samples discussed in the next section, so much larger changes in μ are expected. Unfortunately, there is presently no reliable, comprehensive theory[48] for correcting the single-site mobilities in the region $4d/by^2 \gtrsim 1$.

While it was verified in Refs. 31, 38, and 44—47 that potential-fluctuation (and multi-ion scattering) effects account for the low-temperature breakdown of the single-site scattering picture in those semiconductors cited above, no such broad analysis has been performed previously for InSb. In the next section, we therefore compare the one-band, single-site theory with a large body of n-type mobility data from the literature. We seek to determine whether the rapid conductivity decrease with decreasing temperature discussed in Sec. II may be attributable to the influence of the potential fluctuations, or whether the two-band model must be invoked.

IV. ONE-BAND TRANSPORT WITH FLUCTUATIONS

In this section we compare temperature-dependent electron mobilities calculated in the one-band picture with experimental results for n-type InSb. Although the potential fluctuations are not explicitly included in the calculation, deviations of the data from single-site theory will be correlated with the magnitude of $4d/by^2$.

The mobility formalism uses Kohler's variational principle[49] to solve the Boltzmann equation, where the method has been generalized to fully account for the nonparabolic band-structure and wave-function admixture. Since similar calculations have been performed previously by several investigators,[50—52] we do not reproduce the rather lengthy expressions here. Details on incorporating the Kane band model are discussed elsewhere.[53]

The most important difference between our approach and that of previous studies for InSb (Refs. 13, 54, and 55) is that rather than relying on the Born approximation to treat ionized impurity scattering, cross sections have been calculated by a nonparabolic generalization of the partial-wave phase-shift method.[53] Electron-electron scattering[56] and scattering by optical, deformation-potential acoustic, and piezoelectric acoustic modes[57] have also been taken into account. At temperatures above about 50 K, the high inelasticity of the optical phonon transitions requires that the variational calculation be carried to sixth order.

InSb material parameters employed in the calculations are listed in Table I. The largest uncertainty is in the acoustic deformation potential, E_1. Although a number of investigators[58—61] have employed band-structure considerations to estimate E_1, the values obtained differ by nearly a factor of 3 (most fall between 7 and 19 eV). Other workers have treated E_1 as a parameter to be adjusted in fitting mobilities[54,55,62—69] and other transport properties[50,70—75] to experiment. These results are even less consistent with one another, giving deformation potentials in the range $7 \lesssim E_1 \lesssim 41$ eV. In the present broad comparison of calculated and experimental mobilities, we find that the overall fit is poor for $E_1 \gtrsim 25$ eV. However, since the calculated results are relatively insensitive to the deformation potential when $E_1 \gtrsim 16$ eV, we conclude that the comparison of theoretical and experimental mobilities does not represent a reliable method for accurately determining E_1. For definiteness, we follow Rode[57] and employ $E_1 = 7.2$ eV, for which one obtains approximately equal numbers of cases with $\mu_{\text{theor}} > \mu_{\text{expt}}$ as opposed to $\mu_{\text{theor}} < \mu_{\text{expt}}$ in the temperature range $40 \lesssim T \lesssim 70$ K where acoustic mode scattering has its greatest effect.

Whenever possible, we follow Kinch[13] by comparing theoretical mobilities with the experimental quantity $\mu(T) = \sigma(T)/ne$, where σ is the temperature-dependent conductivity, $n = -(r_H/R_H e)$, and R_H is the Hall coefficient at a suitable intermediate temperature such as 77 K where mixed conduction effects are unimportant and the Hall factor r_H can be straightforwardly calculated. Were the Hall mobility employed, the low-temperature peak which is sometimes observed in $R_H(T)$ would be folded into the data. In the presence of an impurity band, the total electron density obtained above,

TABLE I. InSb material properties (taken from Ref. 57).

Effective mass at $k = 0$	$0.013 m_0$
Low-frequency dielectric constant	17.5
High-frequency dielectric constant	15.8
Deformation potential	7.2 eV
Longitudinal elastic constant	7.89×10^{10} N/m^2
Piezoelectric coefficient	0.027
Polar-phonon Debye temperature	278 K

$n = n_e(T) + n_I(T)$, should remain constant at temperatures below the intrinsic region. Thus $\mu(T)$ as defined above represents the composite drift mobility for electrons in both bands:

$$\mu(T) = \frac{n_e(T)\mu_e(T) + n_I(T)\mu_I(T)}{n}. \quad (4.1)$$

However, in some cases comparison must be made with the Hall mobility at some given magnetic field below the high-field limit. In these instances the field-dependent Hall factor r_H has been calculated as discussed in Ref. 44. The drift mobility is then the Hall mobility divided by r_H. In the mobility plots discussed below, each figure caption indicates whether the quantity shown is a drift or Hall mobility.

The calculated mobilities have been compared with a broad range of experiments[1,2,13,17,63,66,67,76] from the literature. In each case, the Hall measurements at intermediate temperatures have been employed to obtain $N_D - N_A$. Unfortunately, $N_D + N_A$ cannot be straightforwardly determined by the usual methods employed in wide-gap semiconductors due to the weakness of the low-temperature electron freeze-out (if it occurs at all). The total impurity density was therefore estimated by fitting calculated mobilities near $T \approx 20$ K to the experimental values. This temperature is sufficiently low that phonon scattering is unimportant, yet sufficiently high that the potential fluctuations are expected to be small compared to $k_B T$ [see criterion (3.4)]. The resulting $N_D - N_A$ and $N_D + N_A$ are given in Table II. Since these values were obtained assuming that no impurity band is present, $N_D + N_A$ must be altered if the experimental mobilities are compared to a two-band theoretical fit (see the next section).

TABLE II. Doping levels estimated from mobility

Reference	Sample designation	$N_D - N_A$ (cm^{-3})	$N_D + N_A$ (cm^{-3})
13	9	5.4×10^{13}	6.7×10^{14}
67	1	1.9×10^{13}	1.25×10^{14}
	4	6.2×10^{13}	2.9×10^{14}
	5	5.0×10^{13}	2.9×10^{14}
66	4	7.9×10^{13}	4.8×10^{14}
	2	4.3×10^{13}	5.6×10^{14}
	1	1.35×10^{13}	8.7×10^{14}
2	1	1.2×10^{14}	5.1×10^{14}
	2	1.9×10^{14}	1.11×10^{15}
	3	9.8×10^{13}	1.47×10^{15}
63		1.0×10^{14}	5.2×10^{14}
76	2	9.8×10^{14}	2.5×10^{15}
1	1	4.3×10^{13}	2.2×10^{15}
17	3	1.95×10^{15}	6.5×10^{15}
	4	6.9×10^{13}	3.9×10^{14}

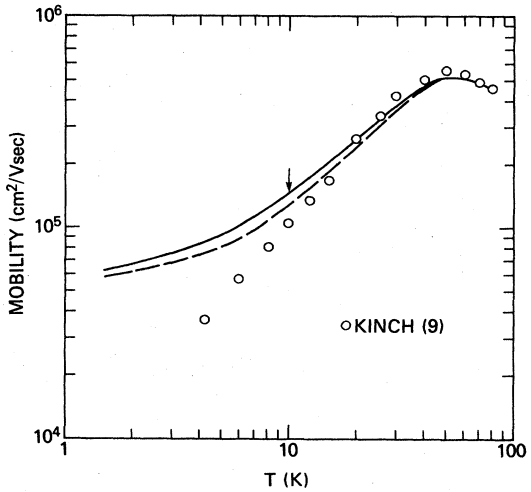

FIG. 2. Experimental drift mobilities (open circles) for InSb, along with theoretical values obtained using Brooks-Herring theory (dashed curve) and the partial-wave phase-shift method (solid curve). At temperatures below the arrow on the solid curve, $4d/by^2 \gtrsim 1$ and the single-site scattering theory is inappropriate.

Figure 2 shows a typical comparison between theoretical (solid and dashed curves) and experimental[13] (open circles) results for the electron mobility in a moderately compensated sample as a function of temperature. The dashed curve was obtained using the Born approximation to treat ionized impurity scattering, whereas the solid curve was obtained using the more general partial-wave phase-shift method. In contrast to the sizable errors introduced by the Born approximation in semiconductors with larger effective masses,[44–47] the phase-shift correction for electrons in InSb is typically no more than

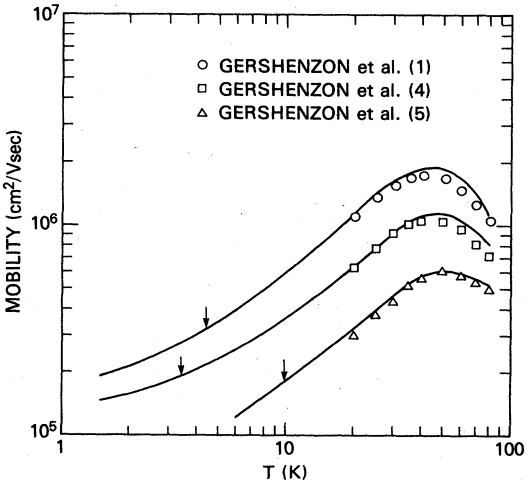

FIG. 3. Comparison of theoretical and experimental Hall mobilities (1 kG) for InSb. Arrows indicate the temperature at which $4d/by^2 \approx 1$.

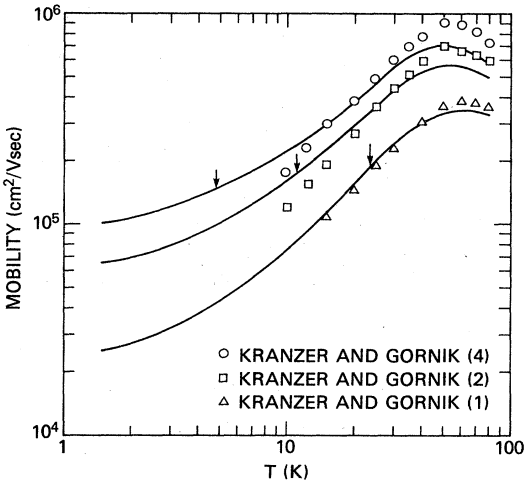

FIG. 4. Comparison of theoretical and experimental Hall mobilities (low field) for InSb. Arrows indicate the temperature at which $4d/by^2 \approx 1$.

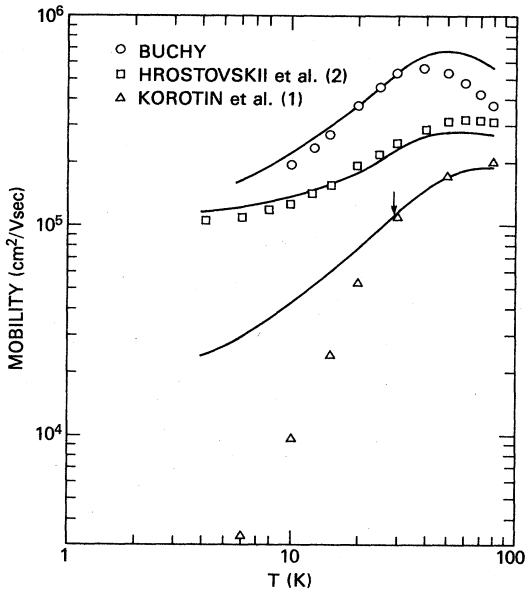

FIG. 6. Comparison of theoretical and experimental drift mobilities for InSb. For the upper two curves, $4d/by^2 < 1$ at all temperatures shown. The arrow on the lower curve indicates the temperature at which $4d/by^2 \approx 1$.

$\sim 10\%$. However, it can exceed 20% when the comparison is made for the most compensated samples.

The arrow at $T \approx 10$ K on the solid curve in Fig. 2 indicates the temperature at which $4d/by^2 \approx 1$. Below this temperature, criterion (3.4) predicts that the single-site scattering model should become inaccurate due to large fluctuations in the random potential. It is evident from the figure that the theoretical and experimental mobilities do begin to diverge in the region near the arrow.

Figures 3–7 show results for 14 additional samples studied by 7 different groups, and the pattern is similar in each. The figures indicate that no divergence between theory and experiment is observed whenever the compensation is low enough that $4d/by^2 \lesssim 1$ at all temperatures investigated. However, μ_{theor} can exceed μ_{expt} by factors of between 2 and 10 when $4d/by^2 \gg 1$ at the lowest temperatures.

Unfortunately, mobilities were not given over a broad enough temperature range to allow the same comparison with the extensive low-temperature data of Ishida and Otsuka.[3] It is, however, useful to examine the dependence of their results at $T = 1.3$ K on compensation. Shown in

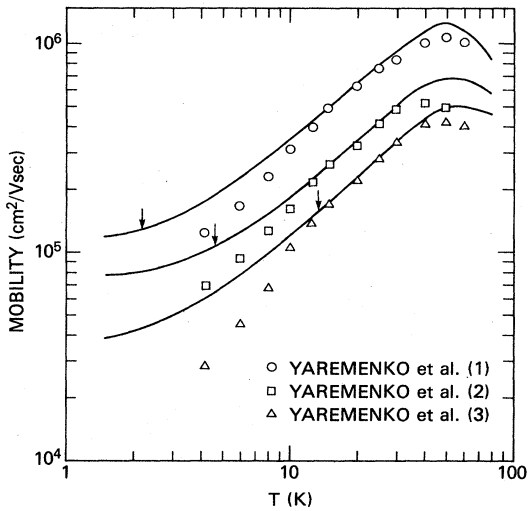

FIG. 5. Comparison of theoretical and experimental Hall mobilities (low field) for InSb. The arrow on each curve indicates the temperature at which $4d/by^2 \approx 1$.

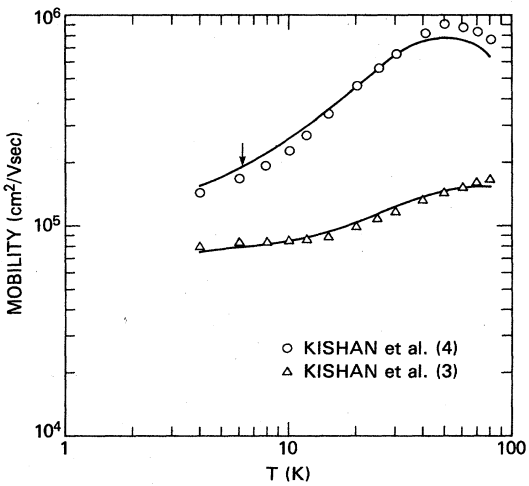

FIG. 7. Comparison of theoretical and experimental drift mobilities for InSb. The arrow on curve (3) indicates the temperature at which $4d/by^2 \approx 1$, while $4d/by^2 < 1$ at all temperatures on curve (4).

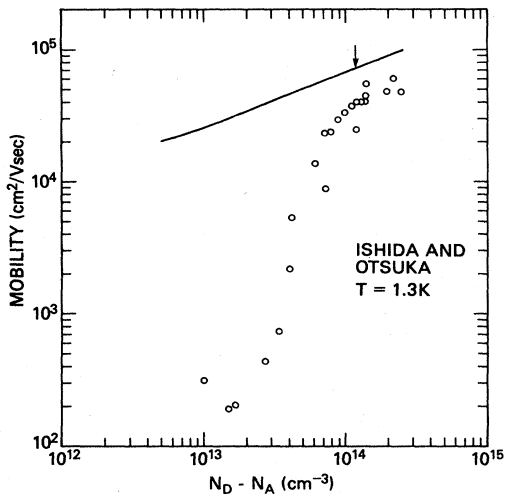

FIG. 8. Experimental mobility vs excess donor density for InSb at $T = 1.3$ K [Ishida and Otsuka (Ref. 3)]. Each point represents a different sample. The solid curve is the single-site theoretical result obtained when their reported doping levels as a function of $N_D - N_A$ are averaged.

Fig. 8 is μ versus $N_D - N_A$ for 23 different samples with donor concentrations varying between 2×10^{14} and 6×10^{14} cm^{-3}. Also shown as the solid curve is the single-site theoretical result which one obtains using averages of their reported doping levels as a function of $N_D - N_A$. As was mentioned in Sec. II, Ishida and Otsuka attributed the rapid decline of the mobility at low n to an impurity-band metal-insulator transition. They argued that below a critical electron density $n_c \approx 6 \times 10^{13}$ cm^{-3}, the Fermi level is lowered to the tail of the impurity band where the states are localized. However, their data are also fully consistent with a one-band interpretation if one accounts for the potential fluctuations. The arrow in the figure indicates that $4d/by^2 \gtrsim 1$ whenever $n < n_c \approx 1.2 \times 10^{14}$ cm^{-3}. Since the transition is rather broad, this value for n_c is in as good agreement with the data as the value 6×10^{13} cm^{-3} specified by Ishida and Otsuka. For the highest compensation shown in Fig. 8 ($n = 10^{13}$ cm^{-3}), one has $4d/by^2 \approx 13$ and the rms potential of the fluctuations is four times the electron Fermi energy. As was pointed out in Sec. III, one then expects the electrons to be effectively "localized" at those locations where the fluctuating potential is lowest. It is not surprising, therefore, that the measured mobility is two orders of magnitude below its value at higher n for which $4d/by^2 < 1$.

We may also compare with data for the more heavily doped sample ($N_D \approx 8.65 \times 10^{16}$ cm^{-3}, $N_A \approx 8.33 \times 10^{16}$ cm^{-3}) studied by Sethi *et al.*[5] Those authors point out (see their Fig. 3) that the experimental mobilities fall below the one-band theoretical results when $T \lesssim 160$ K. They attribute the divergence to the presence of an impurity band, whose mobility must exceed 10^5 cm^2/V sec when $T \gtrsim 110$ K. However, their results are precisely what one expects when the potential fluctuations are included in the one-band model, since $4d/by^2 \approx 1$ at $T \approx 130$ K.

Summarizing, we have demonstrated that the incorporation of potential-fluctuation effects into the one-band model qualitatively accounts for the large body of low-temperature mobility data from the literature. A number of previous investigators[3,5,8,14–17] have asserted that these data can only be explained if one assumes the existence presence of a separate impurity band in n-type InSb. Although present theories do not enable one to accurately calculate the electron mobility in regions where $4d/by^2 > 1$, criterion (3.4) is remarkably successful at predicting where experimental mobilities should diverge from the single-site theoretical results. It was previously shown that this criterion is equally successful when applied to the wider-band-gap semiconductors Si, GaAs, ZnSe, and CdTe.[38,44–47] We now briefly examine whether the inclusion of potential fluctuations in the one-band model might also account for the experimentally observed electric field dependence of the conductivity and the large peaks in the temperature-dependent Hall coefficient which were discussed in Sec. II.

Whenever the low-temperature conductivity is quite small, σ is usually observed[2,6,14,16,29] to increase markedly with electric field for E in the range $0.1 < E < 1.0$ V/cm. Chusov and Gulyaev[77] pointed out that if the electrons are effectively "localized" in potential wells caused by the random fluctuations, the application of an electric field has the effect of "tipping" the wells and "pouring out" the electrons.[2] Even if the fluctuations are not large enough to cause localization, one expects the preferential population of low-potential regions to be less pronounced in the presence of an electric field. A detailed quantitative theory for $\sigma(E)$ is not available at present.

Potential fluctuations may also account for the observation of sizable peaks in the temperature-dependent Hall coefficient (see Sec. II). When the fluctuations are large compared to the electron energy, the momentum relaxation time $\tau(E)$ is expected to decrease rapidly with decreasing E. It is pointed out in the Appendix that the Hall factor r_H for nondegenerate electrons can then increase considerably with decreasing temperature (the magnitude of r_H is related to $d\tau/dE$). However, as long as the conductivity remains finite as $T \to 0$ [i.e., states at the Fermi level are not strictly localized even though $\tau(E_F)$ is small], degeneracy causes r_H to return to a constant value near unity (see below) in the low-temperature limit. A large peak in $R_H(T)$ is thus expected when $4d/by^2 \gg 1$ at low temperatures. Also in accordance with experimental observation (see Sec. II) is the prediction that as the compensation is increased, T_P should become smaller (because degeneracy occurs at lower temperatures) while the magnitude of the peak $R_H(T_P)/R_H(77\text{ K})$ should become larger (because γ/E_0 and hence $d\tau/dE$ is larger). If the usual expressions for the onset of degeneracy in an undistorted conduction band are employed for the most compensated sample of Ishida and Otsuka[3] ($n \approx 10^{13}$ cm^{-3}), one obtains T_P about a factor of 2 smaller than the experimental value $T_P \approx 4$ K. However, this may be attributable to the induced spatial inhomogeneities of the electron distribution, i.e., the electrons occupy only those regions where the random potential is lowest.[40] Electrons in those

restricted locations should become degenerate at higher temperatures than in the unperturbed case since their density is larger than the average value, n.

Another consequence of the spatially inhomogeneous electron density is that it can lead to a zero-temperature Hall coefficient $R_H(0\text{ K})$ which is larger than $R_H(77\text{ K}) \approx 1/ne$. Shik[78] and Karpov *et al.*[79] have calculated $R_H(T)$ for inhomogeneous semiconductors using percolation theory. Since their model gives a vanishing conductivity at zero temperature (due to localization in the valleys of the random potential), the Hall coefficient increases exponentially with T^{-1} even in the regime of extreme degeneracy. This type of behavior appears to be observed experimentally at the lowest temperatures (down to $T \approx 0.3$ K) for some of the more compensated samples of Bannaya *et al.*[14] (A similar dependence of R_H on temperature is predicted by the two-band model if one assumes freeze-out into localized states in the tail of the impurity band as $T \rightarrow 0$ K.)

In other cases,[3,6,14,26] $R_H(T)$ for $T \lesssim 2.5$ K appears to approach a constant value, which is sometimes as much as a factor of 2 larger than $R_H(77\text{ K}) \approx 1/ne$. This is what might be expected in an inhomogeneous system with degenerate electrons for which σ ($T = 0$ K) remains finite. Although an exact calculation of $R_H(0\text{ K})$ is quite difficult, Cohen and Jortner[80] used effective-medium theory to calculate R_H for a two-component system in which the electron density and mobility at a given location are either n_1 and μ_1 or n_2 and μ_2. The average carrier density is then $n = Cn_1 + (1 - C)n_2$, where C is the volume fraction occupied by component 1 and $1 - C$ is the fraction occupied by component 2. Their results give $R_H > 1/ne$, which should also hold for the more realistic case in which many components are present, i.e., n and μ are random functions of position. The observation of a constant $R_H(0\text{ K})/R_H(77\text{ K}) > 1$ has not been explained within the two-band model.

We have sought to demonstrate in this section that the main features of the low-temperature transport data for n-type InSb can be explained, at least qualitatively, without invoking the existence of a separate impurity band.[81] It is not a coincidence that many of the phenomena usually attributed to an impurity band are also expected to occur as a result of the random potential fluctuations. This is because both models are characterized by a freeze-out of the electrons into "low-mobility" states as the temperature is decreased. In one case these are impurity-band states, while in the other they are states near the bottom of the conduction band which have energies smaller than the magnitude of the random fluctuations.

V. TWO-BAND MODEL WITH POTENTIAL FLUCTUATIONS

It was shown in the last section that the transport properties of n-type InSb at low temperatures and low magnetic fields can be explained at least qualitatively by the one-band theory. In this section we illustrate how one could also account for the temperature dependence of the mobility using a standard two-band fit similar to those found in the literature. However, it will then be shown that such a fit is not very realistic, even if one accepts the existence of a separate impurity band, since it ignores important consequences of the random potential fluctuations.

Several authors have fit the low-temperature ($T \lesssim 10$ K) transport data by assuming two-band mixed conduction with a small, nearly constant mobility ratio:[6,14,26] $3 \lesssim b_\mu \lesssim 10$, where $b_\mu \equiv \mu_e/\mu_I$. It is often not recognized that an impurity band should also have an important effect on the measured mobilities at higher temperatures in the range $10 < T \lesssim 50$ K. This is because even at these temperatures where the donor binding energy is smaller than k_BT, n_I/n_e is sizable since N_D is comparable to the effective density of states in the conduction band, N_c [see Eq. (A3)]. For this reason it is necessary to adjust the compensation assumed if, as in the previous section, the intermediate-temperature mobility is employed in fitting $N_D + N_A$.

Figure 9 shows net mobilities [see Eq. (4.1)] for three of the same samples[13,17,64] discussed in Sec. IV. Following the practice of previous workers, b_μ has been assumed to increase with increasing compensation. Hall-coefficient data was not included in the fits, except to determine $N_D - N_A$. The agreement between experiment and the two-band theory is seen to be relatively good even with the simple assumption that b_μ is constant. However, in the cases of both the upper and lower curves, a better fit would have been obtained for b_μ close to unity and $N_D + N_A$ the same as in Table II [$\mu(T)$ then reverts to the one-band form shown in Figs. 4 and 7]. The indicated values of b_μ roughly correspond to those employed in the literature[6,14,26] for similar $N_D - N_A$. Comparison of the two-band-fit N_I values (given in the caption of Fig. 9) with those in Table II shows that the required impurity densities are 26% to 52% smaller than the values obtained from the one-band fit. In choosing between the

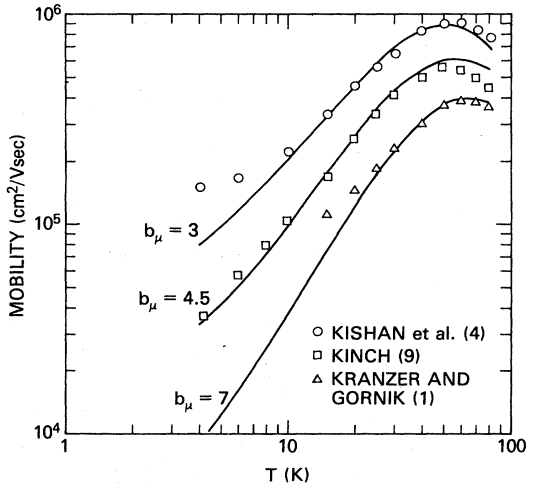

FIG. 9. Experimental mobilities for InSb compared with values calculated assuming two-band conduction with b_μ as shown on each curve. The fits shown are for $N_I = 3.1 \times 10^{14}$ cm^{-3} [Kishan *et al.* (Ref. 17)], $N_I = 4.4 \times 10^{14}$ cm^{-3} [Kinch (Ref. 13)], and $N_I = 6.1 \times 10^{14}$ cm^{-3} [Kranzer and Gornik (Ref. 66)].

two models, it would therefore be quite helpful to have an independent characterization of $N_D + N_A$. The photo-Hall technique discussed in Ref. 53 may provide a reliable means of performing such a calibration.

Actually, the assumption of constant b_μ may be unreasonable. The conduction-band mobility decreases by about an order of magnitude as the temperature is lowered from 50 to 4 K (and a factor of about 3 between 10 and 4 K), mostly due to the decrease of the average electron energy [$E_0 = \frac{3}{2}k_BT$ for nondegenerate statistics]. At the same time, it seems that μ_I should vary relatively little until k_BT becomes comparable to the "width" of the impurity band. Only at temperatures somewhat below 4 K should one expect the lower-mobility states in the tail of the impurity band to be populated preferentially over the higher-mobility states in the middle of the band. At higher temperatures, the main effect on μ_I is probably the change in the screening length with temperature, and this should cause μ_I to increase rather than decrease with decreasing temperature. One might therefore expect $b_\mu(T)$ to have a fairly strong dependence on temperature, a consideration which may alter somewhat the two-band fit one performs to the experimental data. However, if the middle curve[13] of Fig. 9 is recalculated assuming the same N_D and a temperature-independent impurity-band mobility of 2.8×10^4 cm^2/V sec, the agreement with experiment is at most only 25% worse than that shown in the figure.

We conclude that as long as potential-fluctuation effects are ignored, previous investigators[6,14,26] are correct in asserting that the two-band model can be made to yield reasonably good agreement with experiment. This is of course at the expense of introducing $b_\mu(T)$ as an adjustable parameter which is difficult to estimate *a priori*.

We now examine some important consequences of introducing the random potential into the two-band picture. We first note that for n-type InSb with impurity densities of mid-range 10^{14} cm^{-3}, the effective Bohr radius a_0 is very nearly equal to half the average distance between impurities, D. Depending on the value of $d \equiv (\lambda_s/D)^3$, one then has two phenomenologically different regimes: (1) $d > 1$, for which the random fluctuation analysis is valid [see criterion (3.1)] and (2) $d < 1$, which implies that $\lambda_s/a_0 < 1$. One does not expect to observe bound states in region (2) because electron-ion interactions at distances on the order of the Bohr radius are weakened too much by the screening.[82] We therefore focus our attention on region (1), which for $N_I \approx 7 \times 10^{14}$ cm^{-3} at 10 K is restricted to moderately compensated samples having $n \lesssim 1.7 \times 10^{14}$ cm^{-3}.

We next point out that in the region of interest, the potential fluctuations are virtually always larger than the donor binding energies $0.14 \lesssim E_D \lesssim 2.0$ meV claimed by most investigators.[3,6,14,15,26] Assuming the hydrogen-model value $E_D^0 = e^2/2\kappa_0 a_0 \approx 0.69$ meV and $N_I \approx 7 \times 10^{14}$ cm^{-3} at 4 K, one obtains $\gamma/E_D^0 \approx 3$ for $n = 1.7 \times 10^{14}$ cm^{-3} and 6 for $n = 10^{13}$ cm^{-3}. This relation is illustrated in Fig. 10, which shows the fluctuating bottom of the conduction band $V(\mathbf{r})$ along with the impurity levels at $V(\mathbf{r}) - E_D$ (Shklovskii and Éfros[40] gave a similar figure for the opposite limit, $\gamma \ll E_D$). As discussed in Sec. III, the rms magnitude of the fluctuations is $\gamma/2^{1/2}$, while the correlation length is the screening radius λ_s

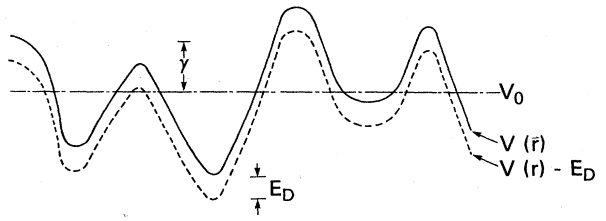

FIG. 10. Fluctuating bottom of the conduction band (solid line) and impurity band (dashed line) for $\gamma/E_0 \gg 1$.

One obvious consequence of the energy-band structure shown in Fig. 10 is that when $k_BT \lesssim \gamma$, the total electron density $n(\mathbf{r}) = n_e(\mathbf{r}) + n_I(\mathbf{r})$ is strongly inhomogeneous (see the discussion in Sec. III). At the same time, the ratio of average densities in the two bands, n_e/n_I, is also affected since conduction-band states in the valleys are energetically preferred over impurity-band states in the peak regions.[83] We are not aware of any detailed accounting for these phenomena in the two-band InSb literature.

The mobility of electrons in the impurity band should also be much different from that obtained in the absence of fluctuations. In semiconductors such as Ge and Si doped to "metallic" impurity densities just above the Mott transition,[24] $d \ll 1$ and the potential fluctuations may be ignored. One then has a picture in which electrons may travel within the impurity band in any spatial direction while remaining at a constant energy.[84] However, when $d > 1$ and fluctuations are present as in Fig. 10, electrons can remain at the same energy[85] only by traveling along certain restricted contours of the fluctuating band (it can be shown[40] that tunneling from one valley to the next is negligible). While the details of the effect on the impurity-band mobility are unclear at this time,[86] the fluctuations introduce significant phenomenological differences between the $d \ll 1$ (Ge and Si) and $d > 1$ (InSb) regimes.

In addition, the potential fluctuations produce static electric fields which may significantly reduce the ionization energy of the impurity states. A number of investigators have studied the effect of an external electric field on the binding energy of ionized impurities in a solid.[87–90] It can be shown that a uniform field of magnitude F lowers the barrier height for a Coulomb well by the amount[87]

$$\Delta E_L = e\left[\frac{eF}{\pi\kappa_0}\right]^{1/2}. \tag{5.1}$$

The typical electric fields produced by the random potential can be estimated from the magnitude of the fluctuations divided by the correlation length: $eF_0 \approx \gamma/\lambda_s$. Using the hydrogen-model value for the binding energy, substitution into Eq. (5.1) leads to the relation

$$\frac{\Delta E_L}{E_D^0} \rightarrow \left[\frac{8}{\pi\chi}\right]^{1/4}, \tag{5.2}$$

where

$$\chi \equiv \frac{b}{(192d)^{1/2}y^2} \tag{5.3}$$

and the dimensionless parameters b, d, and y are defined in Sec. III. Equation (5.2) predicts that for $N_I = 7 \times 10^{14}$ cm^{-3}, the donor states should be completely ionized at any electron density above 10^{13} cm^{-3} and any temperature below 10 K. On the other hand, in semiconductors such as Ge and Si with larger effective masses, $\Delta E_L/E_D \ll 1$ since E_D is much larger.

Even in cases where ionization has not occurred, one expects significant broadening of the levels due to tunneling. From the uncertainty principle the energy broadening is $\Delta E_T \approx \hbar/\tau_T$, where τ_T is the time an electron spends in the impurity band before tunneling to the conduction band. Using the tunneling emission rate calculated by Korol',[88] we obtain

$$\frac{\Delta E_T}{E_D^0} \approx \frac{1}{\chi} e^{-\chi/3}. \tag{5.4}$$

One finds that when $\chi \lesssim 3$, the broadening of the levels should be significant even if the electric field is not quite strong enough to cause ionization. Although the models employed in obtaining Eqs. (5.2) and (5.4) are somewhat crude, they yield ionization-energy reductions which agree well with experiment in such semiconductors as ZnTe (Ref. 89) and Si (Ref. 90). The calculations are based on the assumption of isolated impurity sites (i.e., N_D is below the metal-insulator transition point), but Pautrat has shown that a further reduction in the ionization energy is obtained if neighboring impurity potentials overlap.[89]

The preceding discussion has been based on an estimate of the "typical" electric field F_0 set up by the random potential. However, the actual field varies with position, so that the binding energy may be inhomogeneous in $\mathbf{r}$. The estimates for $\Delta E_L/E_D^0$ obtained above suggest the possibility that while most of the donors are ionized, bound states may exist in restricted regions where the electric field is smallest, i.e., at the peaks and valleys of the potential $V(\mathbf{r})$ in Fig. 10. As long as the average density of such states is relatively small, their presence would not necessarily have a significant effect on the low-temperature transport properties. The one-band description would then yield accurate mobilities even though a small density of bound states is present.

We conclude that the two-band treatments used in the InSb literature to fit experimental transport data are far too simple, since they fail to account for important consequences of the random potential fluctuations.

VI. CONCLUSIONS

In the preceding sections, we have considered the effects of random potential fluctuations on the low-temperature transport properties of n-type InSb. Although the central issue of whether a separate impurity band exists in this material has not been finally resolved, we feel that a number of important points have been clarified. We now summarize those conclusions which are possible at this time.

A priori, it is difficult to assess on theoretical grounds the extent to which the impurity band may be considered separate from the conduction band. Although the hydrogen model predicts a small but finite binding energy ($\approx$0.69 meV), there are several processes which may either remove the level or broaden it sufficiently that it merges with the conduction band. These include the following: (1) At low compensation ($n \gtrsim 1.7 \times 10^{14}$ cm^{-3} when $N_I \approx 7 \times 10^{14}$ cm^{-3}), the screening length λ_s is smaller than the Bohr radius a_0. One then expects the binding energy to vanish. (2) Spatial overlap of the bound-state wave functions when $a_0 \gtrsim D$ leads to a broadening of the levels. (3) Since $\gamma > E_D$ in most regions of interest, there is significant overlap between conduction-band and impurity-band states in energy space[83] (see Fig. 10). However, this does not preclude the two bands being discrete at any given spatial location $\mathbf{r}$. (4) Static electric fields produced by the fluctuations should lead to inhomogeneous reductions in the binding energy. A first-order estimate of ΔE suggests that this effect may lead to ionization of the bound states everywhere except in the peaks and valleys of the fluctuations where the electric field is weakest. (5) If ionization does not occur, the electric field can still lead to broadening of the levels due to tunneling transitions from the impurity band to the conduction band. Unfortunately, a reliable quantitative characterization of these effects would require more detailed theoretical treatments than are presently available, as well as a more accurate knowledge of such parameters as the unperturbed Bohr radius a_0 and binding energy E_D.

Since a direct calculation of the band structure is quite difficult, most attempts to determine whether the bands are separate or merged have focused on the interpretation of experimental evidence. In particular, it has been argued by a number of investigators[3,4,6,14,15,26] that the low-temperature transport data are best explained by the two-band model. The rapid mobility decrease with T at low temperatures in the more compensated samples is then attributed to electron freeze-out from the conduction band to the impurity band. The assumption of two-band mixed conduction also accounts for the sharp increase of the conductivity with electric field as well as large peaks in the Hall coefficient as a function of temperature.

Conventional one-band analyses employing Brooks-Herring theory to treat ionized impurity scattering do not provide for these effects. However, it has been noted[1-4] that the introduction of random potential fluctuations can significantly alter the low-temperature transport properties. When the magnitude of the fluctuations is large compared to the thermal energy of the electrons ($4d/by^2 \gtrsim 1$), the electron density becomes inhomogeneous and the Fermi level is lower than in the absence of fluctuations.[40] Large fluctuations therefore lead to a decrease in the electron mobility. This appears to be verified when single-site theoretical mobilities (ignoring fluctuations) are compared to a wide range of experimental results from the literature at temperatures between 80 and 1.3 K (see Figs. 2—8). There is found to be a strong corre-

lation between the magnitude of $4d/by^2$ and the degree to which theory and experiment agree. This behavior is fully consistent with results obtained previously[38,44–47] for wider-gap semiconductors such as Si, GaAs, ZnSe, and CdTe. We have discussed how the potential fluctuations also account qualitatively for the electric field dependence of the conductivity and the temperature dependence of the Hall coefficient.

We conclude that one may qualitatively account for the main features of the transport data in either a one-band or a two-band context. Unfortunately, present theories do not allow for a general, quantitative calculation of the electron mobility in either case. The one-band model is somewhat less arbitrary in that, *a priori*, one can obtain a reliable criterion ($4d/by^2 \gtrsim 1$) for the conditions under which the conventional single-site scattering theory becomes inadequate. On the other hand, the two-band fit is obtained by varying the mobility ratio b_μ arbitrarily since accurate impurity-band mobilities are extremely difficult to calculate. Several investigators[21,28] have argued that the μ_I required in these fits (often 10^4 to 10^5 cm^2/V sec) are orders of magnitude higher than is reasonable for impurity-band conduction. Although relatively large μ_I (100–1000 cm^2/V sec) have been claimed in Ge and Si,[24,91,92] the phenomenology of the impurity-band conduction is much different since $d \ll 1$ and potential fluctuations are unimportant in those materials at the relevant doping levels. Furthermore, the existence of an impurity band above the metal-insulator transition in Ge and Si has more recently been questioned.[93] For InSb with $4d/by^2 < 1$ over the entire temperature range, we find that the best fits to the mobility data are usually obtained by letting b_μ approach unity, which is equivalent to assuming one-band conduction.

It has often been asserted that only the two-band picture can account for the low-temperature transport data in n-type InSb. However, we feel that the present analysis considerably shifts the burden of proof. We contend first that the experimental data is fully consistent with the one-band interpretation as long as one accounts for the potential fluctuations caused by random inhomogeneities in the impurity concentration. At the same time, proper consideration of the fluctuations within the two-band model would require extensive modifications which have not received detailed treatment in the InSb literature. We cite in particular the following effects: (1) Spatial fluctuations of the bottom of the conduction band lead to overlap of the two bands in energy space (see Fig. 10). This affects the population statistics. (2) Impurity-band mobilities may be strongly affected by the fluctuations since electrons cannot travel in arbitrary direction at the same energy while remaining within the band. (3) Static electric fields produced by the fluctuations may lead to spatially inhomogeneous ionization or broadening of the impurity states.

We finally note that an accurate, independent determination of $N_D + N_A$ should be quite useful since the one-band and two-band fits tend to require values which differ by 25–50%. The photo-Hall technique discussed in Ref. 53 may provide a reliable means for accomplishing this.

APPENDIX: TWO-BAND MIXED CONDUCTION

In the two-band model, the net conductivity is given by

$$\sigma = n_e e\mu_e + n_I e\mu_I, \tag{A1}$$

where n_e and n_I are the densities for electrons in the conduction and impurity bands, respectively, and the mobilities μ_e and μ_I represent a weighted average over the various energy states in a given band:[94] $\mu_i \equiv \langle \mu(E) \rangle_i$. Similarly, the net Hall coefficient at zero magnetic field is given by the relation

$$R_H = -\frac{n_e \langle \mu^2 \rangle_e + n_I \mu_I^2}{e(n_e\mu_e + n_I\mu_I)^2}. \tag{A2}$$

For simplicity, we have made the usual approximation $\langle \mu^2 \rangle_I \rightarrow \mu_I^2$, which is valid as long as the impurity band is characterized by a single level with a single mobility: $\mu_I \approx \mu_I(-E_D)$, where E_D is the donor binding energy. The temperature-dependent densities n_e and n_I can be determined from the statistical relation

$$\frac{n_e}{n_I} \approx \frac{N_c e^{-E_D/k_B T}}{2N_D}, \tag{A3}$$

where $N_c = 2(m_e k_B T/2\pi\hbar^2)^{3/2}$ is the effective density of states in the conduction band. The total electron density $n = n_e + n_I = N_D - N_A$ must remain constant as a function of temperature.

In the limit $n_i \gg n_j$, Eq. (A2) reduces to

$$R_H \approx -\frac{r_H^i}{ne}. \tag{A4}$$

Here the Hall factor r_H^i is given by

$$r_H^i = \frac{\langle \mu^2 \rangle_i}{\mu_i^2} \tag{A5}$$

from which $r_H^I \rightarrow 1$. For the usual conduction-band relaxation processes, such as phonon and ionized impurity scattering in the Brooks-Herring approximation, one has $1 \lesssim r_H^e \lesssim 1.93$. Since $n_e \gg n_I$ at 77 K while $n_I \gg n_e$ as $T \rightarrow 0$ K, Eq. (A2) predicts that $(1.93)^{-1} < R_H(0\text{ K})/R_H(77\text{ K}) < 1$. However, at intermediate temperatures where $n_e\mu_e \approx n_I\mu_I$, $R_H(T)$ can exceed both $R_H(77\text{ K})$ and $R_H(0\text{ K})$ by an amount which increases with the mobility ratio $b_\mu \equiv \mu_e/\mu_I$. The two-band model therefore predicts a sizable peak in $R_H(T)$ for cases where $b_\mu \gg 1$.

While r_H^e is always less than 1.93 for the standard Brooks-Herring treatment of ionized impurity scattering, it can greatly exceed this value if the mobility (or relaxation time τ) decreases rapidly with decreasing energy near $E \approx k_B T$. For example, if $\tau(E) \sim E^s$ one has[95]

$$r_H^e = \frac{3\pi^{1/2}}{4} \frac{(2s + \frac{3}{2})!}{[(s + \frac{3}{2})!]^2} \tag{A6}$$

which is 1.93 for $s = \frac{3}{2}$, but increases rapidly with increasing s. It is pointed out in the text that large random potential fluctuations in highly compensated material can lead to a strong dependence of τ on E.

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