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Elastic Electron Scattering in InSb-Type Semiconductors

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Relaxation times for elastic electron scattering in III-V compounds of InSb type are calculated taking into account consistently the nonparabolic structure of the conduction band, both in the density of states and electron wave functions. The calculations are based on the Kane model of band structure, including explicitly mixing of p-like components into the total wave function of the conduction band. Electron scattering by charged impurities and heavy holes, optical phonons (polar interaction), acoustic phonons, and piezo-acoustic modes are considered. Screening by free electrons is included in the long-range interactions and shown to play an important role at higher electron concentrations. Both spin-conserving and spin-flip transitions are considered for all modes. It is demonstrated that transverse branches participate appreciably in acoustic scattering at high electron energies. In all cases, the presented calculations give much higher values of the theoretical mobilities for heavily doped samples than those obtained up to now taking into account only the proper density of states.

Die Relaxationszeiten für elastische Elektronenstreuung in III-V-Verbindungen vom InSb-Typ werden unter konsistenter Berücksichtigung der nichtparabolischen Struktur des Leitungsbandes sowohl in der Zustandsdichte als auch in der Wellenfunktion berechnet. Die Berechnungen beruhen auf dem Kanesischen Bandstrukturmodell, wobei explizit die Zumischung von p-artigen Komponenten in die Gesamtwellenfunktion des Leitungsbandes eingeschlossen wird. Elektronenstreuung durch geladene Defekte und schwere Löcher, optische Phononen (polare Wechselwirkung), akustische Phononen und piezo-akustische Moden werden berücksichtigt. In den langreichweitigen Wechselwirkungen wird Abschirmung durch freie Elektronen eingeschlossen und gezeigt, daß sie eine bedeutende Rolle bei höheren Elektronenkonzentrationen spielen. Es werden sowohl spin-erhaltende als auch spin-flip-Übergänge für alle Moden berücksichtigt. Es wird gezeigt, daß transversale Zweige einen beträchtlichen Anteil an der akustischen Streuung bei hohen Elektronenenergien haben. In allen Fällen ergeben die dargelegten Berechnungen viel höhere Werte der theoretischen Beweglichkeiten für stark dotierte Proben als die bisher erhaltenen, die nur die richtige Zustandsdichte berücksichtigen.

1. Introduction

Since the nonparabolic structure of the conduction band in InSb was derived by Kane [1], it has been realized that the non-parabolicity must strongly affect transport properties of small-gap materials. General formulas for various kinetic coefficients in terms of the relaxation time have been derived by various authors for a spherical nondegenerate energy band with arbitrary non-parabolicity [2]. It has been demonstrated among other things that the effective mass which enters the general transport theory is not the one given by the second derivative

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of energy *versus* momentum, which had been in common use for parabolic bands, but one deals with the energy-dependent mass defined as

$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{d\varepsilon}{dk}. \quad (1.1)$$

It was also realized that the scattering itself is affected by the non-parabolicity of the band. The relaxation time in case of elastic scattering is in general given by

$$\frac{1}{\tau(\varepsilon)} \sim \varrho(\varepsilon) W(\varepsilon), \quad (1.2)$$

where $\varrho(\varepsilon)$ is the density of states per unit energy and $W(\varepsilon)$ is the scattering probability. In early attempts to calculate the relaxation times for various scattering modes the nonparabolic character of the band was taken into account only via the appropriate change of the density of states, $\varrho(\varepsilon)$, which is determined by the dispersion relation $\varepsilon(k)$ of the band in question. And so, for polar optical phonons it was done by Howarth and Sondheimer [3], for acoustic scattering by Radcliffe [4], for charged impurities and nonpolar optical modes by Barrie [5]. It turned out that the final results of these theories can be obtained from the corresponding formulas for a parabolic band by replacing the usual effective mass by the mass defined in equation (1.1). This property becomes clear if one notices that the density of states per unit energy for a spherical band is

$$\varrho(\varepsilon) = \frac{1}{\pi^2} k^2 \frac{dk}{d\varepsilon}. \quad (1.3)$$

For a parabolic band, where $\varepsilon = \hbar^2 k^2 / (2 m_0^*)$, this gives $\varrho(\varepsilon) = (1/\pi^2) (m_0^* / \hbar^2) k$, whereas for an arbitrary band using definition (1.1) we get $\varrho(\varepsilon) = (1/\pi^2) (m^* / \hbar^2) k$. Thus, both results look the same, with m_0^* for a parabolic band replaced by m^* in the case of general spherical band. The above-mentioned results were summarized by Kołodziejczak and Sosnowski [6], whose procedure was subsequently widely used in interpretation of experimental results in small-gap semiconductors. In particular, using this procedure it was possible to describe all transport coefficients for single scattering modes by generalized Fermi-Dirac integrals [7]. Recently this formalism was extensively quoted by Askerov [8].

However, the non-parabolicity of the band structure affects the relaxation time not only via the density of states but also through the scattering probability $W(\varepsilon)$. In order to calculate properly the electron scattering in the non-parabolic band one should use not only the appropriate $\varepsilon(k)$ relation but also the electron wave functions for the region of the band in question. The first consistent scattering theory for the nonparabolic band structure has been carried out by Ehrenreich [9], who considered scattering of electrons in InSb by heavy holes and optical phonons (polar interaction), solving the Boltzmann transport equation by a variational procedure. Also Haga and Kimura [10] used proper wave functions when calculating the free-carrier optical absorption in n-InSb. A systematic calculation of relaxation times for main scattering modes in the nonparabolic conduction bands of InSb-type materials, as described by the Kane model, has been carried out by Korenblit and Sherstobitov [11]. Unfortunately, this work contains numerous errors and, having in mind wide applications of such a theory, we decided to recalculate this problem. Still, the

general approach follows that of reference [11]. A similar calculation for acoustic and polar scattering for lead-salt band structure has been recently done by Ravich and Morgovskii [12], and for charged impurity scattering in HgSe-type materials by Broerman [13].

In the present paper, we calculate relaxation times for the main elastic scattering mechanisms in InSb-type materials taking consistently into account the non-parabolic structure of the conduction band. Scattering of electrons by ionized impurities and heavy holes as well as by optical (polar), acoustic, and piezo-acoustic interactions with lattice vibrations are considered. Spin-flip scattering and free-carrier screening effects are shown to play an important role in the theory. It is also demonstrated that at higher electron energies the transverse acoustic modes give appreciable contribution to electron scattering. The theory presented here has been recently used by the authors to describe transport phenomena in n-InSb [14]. It has been shown that the consistent calculation of scattering is necessary to explain the behaviour of various transport effects in a wide range of temperatures and electron concentrations. Estimating parameters appearing in the theory we shall mostly refer to InSb as a typical example of III-V compounds.

2. Kane's Band Model — Eigenenergies and Eigenfunctions

In this paragraph we shortly summarize Kane's results [1] on the conduction band structure of some III-V compounds. The model holds particularly well for InSb due to the very narrow gap in this material, but it is believed to describe quite well other compounds of this group, in particular InAs and GaAs.

The initial unperturbed Hamiltonian for an electron is

$$\mathcal{H}_0 = \frac{p^2}{2m_0} + V_0(\mathbf{r}) + \frac{\hbar}{4m_0^2c^2} (\boldsymbol{\sigma} \times \nabla V_0) \cdot \mathbf{p}, \quad (2.1)$$

where $V_0(\mathbf{r})$ is the periodic potential of the lattice and the last term represents the spin-orbit interaction in the standard notation. The eigenvalue problem

$$\mathcal{H}_0 \Psi_{n\mathbf{k}j_z}(\mathbf{r}) = \varepsilon_{n\mathbf{k}j_z}(\mathbf{k}) \Psi_{n\mathbf{k}j_z}(\mathbf{r}) \quad (2.2)$$

is satisfied by the Bloch wave functions, normalized over the crystal volume V :

$$\Psi_{n\mathbf{k}j_z}(\mathbf{r}) = \left(\frac{1}{V}\right)^{1/2} u_{n\mathbf{k}j_z}(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r}). \quad (2.3)$$

Here n denotes the band (being interested in the conduction band alone we shall leave out the band index in the following), $\mathbf{k}$ is the wave vector, j_z the projection of the total angular momentum on the z -direction (j is a good quantum number for non-vanishing spin-orbit interaction). The eigenvalue problem (2.2) is solved by the $\mathbf{k} \cdot \mathbf{p}$ method expanding $\mathbf{k}$ -dependent Bloch amplitudes in terms of $\mathbf{k}$ -independent Luttinger-Kohn amplitudes taken at the band's extremum, i.e. at $\mathbf{k} = 0$ in our case. In the simplified model one takes four bands (eight including spin) neglecting all other bands. Thus we have at $\mathbf{k} = 0$ an s-like conduction band ($j = 1/2$) separated by the energy gap ε_g from degenerate light- and heavy-hole valence bands ($j = 3/2$) and the p-like band ($j = 1/2$) separated from the $j = 3/2$ bands by the energy of the spin-orbit interaction Δ . The $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian is diagonalized exactly for this model, without the usual Luttinger-Kohn canonical transformation. Apart from ε_g and Δ there is one more parameter in the theory: $P = -(i\hbar/m_0) \langle S | p_z | Z \rangle$, which charac-

terizes the interband interaction. S, X, Y, Z denote the Luttinger-Kohn amplitudes, which transform under the tetrahedral group like s, p_x, p_y , and p_z atomic wave functions, respectively. For the Bloch functions in the form (2.3) they are normalized to $(1/\Omega) \langle S|S \rangle = (1/\Omega) \langle Z|Z \rangle = 1$, where the integration is over the volume of the unit cell, Ω . The value of P remains almost constant in different III-V compounds [15], whereas the value of ε_g/Δ varies widely.

In the above model the energy-wave vector relation in the conduction band is isotropic and can be obtained from the following equation:

$$\varepsilon' (\varepsilon' + \varepsilon_g) (\varepsilon' + \varepsilon_g + \Delta) - k^2 P^2 \left(\varepsilon' + \varepsilon_g + \frac{2}{3} \Delta \right) = 0, \quad (2.4)$$

where $\varepsilon' = \varepsilon - \hbar^2 k^2 / 2 m_0$ (the zero of energy is at the bottom of the conduction band). We shall consider the energy range $\varepsilon \ll \varepsilon_g + (2/3) \Delta$ (for higher energies Kane's model is probably not applicable anyway). Moreover we neglect the free electron term, since the effective mass in small-gap materials is just a small fraction of the free electron mass. Under these assumptions equation (2.4) gives for the conduction band (for both spin orientations)

$$\varepsilon(k) = -\frac{\varepsilon_g}{2} + \left[\left(\frac{\varepsilon_g}{2} \right)^2 + \varepsilon_g \frac{\hbar^2 k^2}{2 m_0^*} \right]^{1/2} \quad \text{or} \quad \frac{\hbar^2 k^2}{2 m_0^*} = \varepsilon \left(1 + \frac{\varepsilon}{\varepsilon_g} \right), \quad (2.5)$$

where the effective mass at the bottom of the band is

$$\frac{1}{m_0^*} = \frac{4 P^2}{3 \hbar^2 \varepsilon_g} \frac{\Delta + \frac{3}{2} \varepsilon_g}{\Delta + \varepsilon_g}. \quad (2.6)$$

The effective mass, as defined in (1.1), becomes

$$m^* = m_0^* \left(1 + 2 \frac{\varepsilon}{\varepsilon_g} \right). \quad (2.7)$$

In order to calculate the scattering transition probability one needs to know also the periodic components of the electron Bloch functions for the same range of energies. Under the above assumptions they are found to be²⁾

$$\left. \begin{aligned} u_{\mathbf{k}, 1/2} &= \left(i a S - \frac{b - c \sqrt{2}}{2} \frac{k_+}{k} R_- + \frac{b + c \sqrt{2}}{2} \frac{k_-}{k} R_+ + c \frac{k_z}{k} Z \right) \uparrow - \\ &\quad - b \left(\frac{k_z}{k} R_+ - \frac{k_+}{k} \frac{Z}{\sqrt{2}} \right) \downarrow, \\ u_{\mathbf{k}, -1/2} &= \left(i a S + \frac{b + c \sqrt{2}}{2} \frac{k_+}{k} R_- - \frac{b - c \sqrt{2}}{2} \frac{k_-}{k} R_+ + c \frac{k_z}{k} Z \right) \downarrow + \\ &\quad + b \left(\frac{k_z}{k} R_- - \frac{k_-}{k} \frac{Z}{\sqrt{2}} \right) \uparrow, \end{aligned} \right\} \quad (2.8)$$

where $k_{\pm} = k_x \pm i k_y$ and $R_{\pm} = (X \pm i Y)/\sqrt{2}$ and the arrows $\uparrow$ and $\downarrow$ denote the spin-up and spin-down functions, respectively.

²⁾ The form used in equation (2.8) can be obtained directly from reference [16] by setting the magnetic field strength equal to zero.

The total angular momentum $j = 1/2$ is quantized along the z -direction (in the following we suppress the subscript z). The coefficients a , b , and c are

$$\left. \begin{aligned} a^2 &= \frac{\varepsilon_g + \varepsilon}{\varepsilon_g + 2\varepsilon - \alpha\varepsilon}, & b^2 &= \frac{1}{3} \frac{\varepsilon}{\varepsilon_g + 2\varepsilon - \alpha\varepsilon} \beta^2, \\ c^2 &= \frac{2}{3} \frac{\varepsilon}{\varepsilon_g + 2\varepsilon - \alpha\varepsilon} \gamma^2, \end{aligned} \right\} \quad (2.9)$$

where

$$\left. \begin{aligned} \beta^2 &= \frac{\Delta^2}{(\Delta + \varepsilon_g) \left(\Delta + \frac{3}{2} \varepsilon_g \right)}, \\ \gamma^2 &= \frac{\Delta + \frac{3}{2} \varepsilon_g}{\Delta + \varepsilon_g}, \\ \alpha &= \frac{\Delta \varepsilon_g}{2 \left(\Delta + \frac{3}{2} \varepsilon_g \right) (\Delta + \varepsilon_g)}. \end{aligned} \right\} \quad (2.10)$$

and

Since $\alpha \lesssim 1/10$ for all values of ε_g/Δ ratio, the term $\alpha\varepsilon$ can be neglected in the above expressions. Hence, to a very good approximation

$$a^2 = 1 - L, \quad b^2 = \frac{1}{3} L \beta^2, \quad c^2 = \frac{2}{3} L \gamma^2, \quad (2.11)$$

where $L = \varepsilon/(\varepsilon_g + 2\varepsilon)$. Normalization of the Bloch amplitudes (2.8) is equivalent to the condition $a^2 + b^2 + c^2 = 1$. It can be seen that both Bloch amplitudes are not pure spin functions due to the non-vanishing spin-orbit interaction ($b \neq 0$). It can also be observed that, due to the small forbidden gap, the p-like functions X , Y , and Z mix into the total electron wave function for energies away from the band edge. For small energies this mixing is approximately proportional to $(\varepsilon/\varepsilon_g)^{1/2}$ in agreement with the complete Luttinger-Kohn theory which includes second-order $\mathbf{k} \cdot \mathbf{p}$ terms in the eigenenergies and first-order terms in the eigenfunctions [17]. Namely this fact has to be accounted for in a consistent theory of electron scattering, especially for the nonparabolic region of energies. Very close to the bottom of the band, i.e. for $\varepsilon \ll \varepsilon_g$, there is $a \approx 1$, $b \approx c \approx 0$ and the conduction band wave function contains only the S -component.

In several theories of scattering for the parabolic region of energies (see, e.g., [18]) the perturbing scattering potential is subject to the canonical transformation together with the initial Hamiltonian (2.1) in order to arrive at the decoupled one-band effective mass approximation. It should be emphasized that, using Bloch functions of equations (2.3) and (2.8) for the calculation of scattering, no such transformation of the scattering potential is necessary since, within the adopted model, the Bloch functions (2.3) are *exact* solutions of the unperturbed Hamiltonian and they were obtained without any canonical transformation. Just like in the regular Luttinger-Kohn procedure one has to worry about the interband matrix elements of the perturbing potential with the band

in question; in our case we have to worry about interband elements between 8-band set and all other bands, but these are clearly of no importance in scattering problems.

When calculating matrix elements of perturbing potentials we shall deal with integrals over the crystal volume of slowly varying envelope functions φ and quickly varying periodic amplitudes u . According to common procedure these integrals will be broken into

$$\int_V \varphi(\mathbf{r}) u(\mathbf{r}) d^3r = \frac{1}{\Omega} \int_V \varphi(\mathbf{r}) d^3r \int_{\Omega} u(\mathbf{r}) d^3r_0. \quad (2.12)$$

Transition probabilities for all scattering modes are calculated in the first Born approximation.

3. Charged Impurity Scattering

We shall consider electron scattering by the screened Coulomb potential of a single ion:

$$U(r) = \frac{e^2}{\kappa_0 r} \exp\left(-\frac{r}{\lambda}\right), \quad (3.1)$$

where κ_0 is the static dielectric constant and λ the screening length (see Appendix). We have to calculate the matrix elements of this potential between initial and final electron states. Since in the Bloch amplitudes of (2.8) the spin variables are mixed with the coordinate variables, the spin-flip scattering transitions are also possible. There are four matrix elements

$$\langle \mathbf{k}', j' | U | \mathbf{k}, j \rangle = \frac{1}{V} \int_V e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} U(r) u_{\mathbf{k}'}^* u_{\mathbf{k}} d^3r, \quad (3.2)$$

$\mathbf{k}', j'$ denoting a final electron state. Following equation (2.12) we shall break this integral into two, since the scattering potential extends over many unit cells. The initial $\mathbf{k}$ -vector is taken along the z -direction.³⁾ The resulting scalar product of appropriate Bloch amplitudes gives

$$\left\langle \mathbf{k}', \frac{1}{2} \right| U \left| \mathbf{k}, \frac{1}{2} \right\rangle = \frac{1}{V} [a^2 + (b^2 + c^2) \cos \theta] U(|\mathbf{k}' - \mathbf{k}|), \quad (3.3)$$

$$\left\langle \mathbf{k}', -\frac{1}{2} \right| U \left| \mathbf{k}, \frac{1}{2} \right\rangle = \frac{1}{V} b \left(\frac{1}{2} b - c \sqrt{2} \right) \sin \theta e^{i\varphi} U(|\mathbf{k}' - \mathbf{k}|), \quad (3.4)$$

where θ and φ are the polar angles of $\mathbf{k}'$ in the spherical coordinate system with $\mathbf{k}$ -direction taken as the polar axis. The slowly varying part is just the standard Fourier transform of the screened Coulomb potential,

$$U(|\mathbf{k}' - \mathbf{k}|) = \frac{4\pi e^2}{\kappa_0} \left[4k^2 \sin^2 \frac{\theta}{2} + \lambda^{-2} \right]^{-1}, \quad (3.5)$$

where we have put $k = k'$ (see equation (3.8)). The matrix elements with the initial value of $j_z = -1/2$ are just the complex conjugates of those given by

³⁾ As demonstrated recently by Vassel et al. [19] this choice does not affect the generality of considerations.

equations (3.3) and (3.4). Thus the transition probability from either $j_z = 1/2$ or $j_z = -1/2$ state is

$$\begin{aligned}
 W(\mathbf{k}, \mathbf{k}') &= \frac{2\pi}{\hbar} \left(\left| \left\langle \mathbf{k}', \frac{1}{2} \right| U \left| \mathbf{k}, \frac{1}{2} \right\rangle \right|^2 + \left| \left\langle \mathbf{k}', -\frac{1}{2} \right| U \left| \mathbf{k}, \frac{1}{2} \right\rangle \right|^2 \right) \delta[\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k})] = \\
 &= \frac{2\pi}{\hbar} \left(\frac{4\pi e^2}{\kappa_0} \right)^2 \frac{1}{V^2} \left(4k^2 \sin^2 \frac{\theta}{2} + \lambda^{-2} \right)^{-2} \delta[\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k})] \times \\
 &\quad \times \left\{ 1 - 4a^2(1 - a^2) \sin^4 \frac{\theta}{2} + \left[2b^2 \left(2c - \frac{b}{\sqrt{2}} \right)^2 - 4(1 - a^2) \right] \times \right. \\
 &\quad \left. \times \sin^2 \frac{\theta}{2} \cos^2 \frac{\theta}{2} \right\}, \quad (3.6)
 \end{aligned}$$

where the δ -function indicates that the scattering is elastic. The total scattering probability is obtained by averaging over the initial states and summing over all possible final states. Since, as we have already observed, the scattering probability from $j_z = 1/2$ state is equal to that from $j_z = -1/2$, the average over the two initial states is equivalent to using just equation (3.6) without any change. In order to calculate the transport scattering transition rate, which is related to the relaxation time, the occupation factors should be introduced in the standard way and one arrives at the following expression for the inverse relaxation time⁴⁾:

$$\frac{1}{\tau(k)} = N \sum_{\mathbf{k}'} W(\mathbf{k}, \mathbf{k}') (1 - \cos \theta) = \frac{V N}{8\pi^3} \int W(\mathbf{k}, \mathbf{k}') (1 - \cos \theta) d^3k', \quad (3.7)$$

where N is a number of charged ions in the volume V . We observe that

$$\delta[\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k})] = \frac{dk}{d\varepsilon} \delta(k' - k) \quad (3.8)$$

which is, of course, directly related to the density of states (1.3). Hence, in the spherical coordinate system the only nontrivial integration is over θ . The final result is

$$\tau_{\text{imp.}}(\varepsilon) = \frac{1}{2} \frac{\kappa_0^2 \hbar}{\pi e^4 N_i} \frac{1}{F_{\text{imp.}}} \frac{d\varepsilon}{dk} k^2, \quad (3.9)$$

where $N_i = N/V$ is the concentration of charged ions. $F_{\text{imp.}}$ is given by

$$\begin{aligned}
 F_{\text{imp.}}(\xi, L) &= \ln(\xi + 1) - \frac{\xi}{\xi + 1} - (4L - fL^2) \left[1 + \frac{1}{\xi + 1} - \frac{2}{\xi} \ln(\xi + 1) \right] + \\
 &\quad + \frac{1}{2} L^2 (4 - f) \left[1 - \frac{4}{\xi} + \frac{6}{\xi^2} \ln(\xi + 1) - \frac{2}{\xi(\xi + 1)} \right], \quad (3.10)
 \end{aligned}$$

⁴⁾ There is some confusion in the solid state literature concerning this point (partly due to following the methods of nuclear physics which uses for Coulomb scattering the concept of cross section rather than the relaxation time). The number of final electron states is $(2/8\pi^3) d^3k'$. However, in the parabolic region of energies, where no spin-flip transitions occur, there is an additional selection rule, usually not written down explicitly, namely the spin conservation, which reduces the number of possible final states by one half. In our case both final spin states are taken into account by the summation of matrix elements squared in (3.6).

where

$$\xi = (2 k \lambda)^2 \quad \text{and} \quad f = \frac{\beta^2}{9} (16 \gamma^2 - 8 \beta \gamma + \beta^2) \quad (3.11)$$

and L , β , and γ are defined in equations (2.10) and (2.11). For $\Delta \gg \varepsilon_g$, $f \approx 1$. In InSb where $\varepsilon_g \approx 0.2$ eV and $\Delta \approx 0.8$ eV, $f \approx 0.8$. For small electron energies, i.e. for $\varepsilon \ll \varepsilon_g$, $L \approx 0$ and only the first two terms are left in (3.10). This represents the well-known result for a parabolic band. In the nonparabolic region of energies, i.e. for higher electron concentrations, $\xi \gg 1$ (in InSb at room temperature it varies from $\xi \approx 20$ for intrinsic samples to $\xi \approx 30$ for $n \approx 10^{19} \text{ cm}^{-3}$). Hence, to a good approximation equation (3.10) may be simplified to the following form:

$$F_{\text{imp.}}(\xi, L) = \ln(\xi + 1) - \frac{\xi}{\xi + 1} - (4L - fL^2) \left[1 - \frac{2}{\xi} \ln(\xi + 1) \right] + \frac{1}{2} L^2 (4 - f) \left(1 - \frac{4}{\xi} \right). \quad (3.12)$$

In InSb at $n \approx 10^{19} \text{ cm}^{-3}$, $L \approx 0.4$ and the last two terms resulting from the mixing of p-like functions reduce the value of $F_{\text{imp.}}$ by about 30% increasing by the same proportion the corresponding mobility. No screening corresponds to $\lambda \rightarrow \infty$, i.e. $\xi \rightarrow \infty$, which gives $\tau_{\text{imp.}} \rightarrow 0$, a well-known result for the unscreened Coulomb potential.

Defining electron mobility with the use of the effective mass (1.1), we have finally

$$u_{\text{imp.}} = \frac{e \tau_{\text{imp.}}}{m^*} = \frac{1}{2 \pi e^3 \hbar N_i} \frac{\kappa_0^2}{F_{\text{imp.}}} \left(\frac{d\varepsilon}{dk} \right)^2 k. \quad (3.13)$$

The above formula can also be applied to the scattering of electrons by heavy holes, with κ_0 replaced by κ_∞ . In III-V compounds the two dielectric constants differ only slightly and it is possible to describe both scattering mechanisms by equation (3.13) with appropriate concentration of scattering centres.

4. Lattice Scattering — General

In III-V compounds which have two different ions in a unit cell and no inversion symmetry, an electron can interact with lattice vibrations in a number of different ways. Of these we shall consider three modes of main importance, but it is useful to bear in mind the neglected interactions and simplifying assumptions. First, we assume that all longitudinal and transverse modes can be exactly decoupled, which is usually true only for propagation directions along the main crystal axes. Secondly, for acoustic modes the transverse and longitudinal sound velocities will be considered independent of the propagation direction. In the lattice with two atoms per unit cell the lattice waves have neither pure optical nor acoustic branches. The acoustic branch has an admixture of optical displacement and *vice versa*. In particular in acoustic wave, due to the small phase difference for the two ions within one cell, there appears a non-vanishing dipole moment which in principle gives rise to the polar interaction with electrons. The admixing modes are of higher order in the $a q$ expansion for long wavelengths (a lattice constant), and they will be neglected com-

pared to the main modes.⁵⁾ The optical lattice wave can interact with electrons in two ways: via the polar interaction considered below and via the nonpolar interaction, similar to that in mono-atomic crystals. We do not consider the latter as it is believed to be much less important in polar crystals than the polar interaction, although, to our knowledge, the detailed discussion of this problem has not been carried out. We employ static screening by free electrons for the long-range interactions. The limitations of this approach are discussed for polar optical mode by Ehrenreich [20] and for piezo-acoustic mode by Hutson and White [21].

5. Polar Optical Scattering

Again, the first thing is to establish the form of the perturbing potential. We do not quote the derivation of the Fröhlich Hamiltonian for the polar interaction between electrons and optical phonons, as it is rather standard (see, e.g., [22] and [23]). The final expression for the unscreened perturbing potential in the continuum approximation is

$$U' = i \frac{4\pi e^* e}{\Omega} \left(\frac{\hbar}{2NM\omega} \right)^{1/2} \sum_{\mathbf{q}} \frac{1}{q} (b_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}} - b_{\mathbf{q}}^* e^{-i\mathbf{q}\mathbf{r}}), \quad (5.1)$$

where $\mathbf{q}$ is the phonon wave vector, ω the frequency of longitudinal phonons, N the number of unit cells in the volume V , M the reduced mass of the ions ($1/M = 1/m_1 + 1/m_2$), and e^* is the effective ionic charge defined, according to Callen [24], as

$$(e^*)^2 = \frac{\Omega M \omega^2}{4\pi} \left(\frac{1}{\kappa_{\infty}} - \frac{1}{\kappa_0} \right), \quad (5.2)$$

where κ_{∞} and κ_0 are the high-frequency and the static dielectric constants, respectively. Only the longitudinal branch of optical phonons couples to the electron motion in this approximation. According to Ehrenreich [20] the screening of the initial interaction (5.1) by other free carriers in the band introduces two effects. First, there appears the following dispersion in the $\omega(q)$ dependence:

$$\omega^2(q) = \omega^2 \frac{1 + \frac{\kappa_{\infty}}{\kappa_0} \frac{1}{q^2 \lambda^2}}{1 + \frac{1}{q^2 \lambda^2}} \quad (5.3)$$

and, secondly, screening weakens the initial interaction according to the relation

$$U = U' \left(1 + \frac{1}{q^2 \lambda^2} \right)^{-1}, \quad (5.4)$$

where λ is again the screening length, the same which appeared in the Coulomb interaction. In III-V compounds we get the ratio $0.8 < \kappa_{\infty}/\kappa_0 < 1$ (see, e.g., [25]), so that to a good approximation $\omega(q) \approx \omega$, i.e., the effect of screening in the phonon dispersion can be neglected. Still, we are left with the modified screened interaction (5.4) which will be used in the following derivations.

Next we have to calculate the matrix element between the initial and final states $|\mathbf{k}, j, N_{\mathbf{q}}\rangle$ and $|\mathbf{k}', j', N'_{\mathbf{q}}\rangle$, where $N_{\mathbf{q}}$ is the number of phonons charac-

⁵⁾ Estimates of scattering by the mixed-in components included in [11] are very rough and cannot be used for comparison with effects due to the main modes.

terized by q . There are two non-vanishing matrix elements of the potential between phonon states:

$$\left. \begin{aligned} \langle N_q - 1 | b_q | N_q \rangle &= N_q^{1/2} & \text{for } N'_q = N_q - 1, \\ \langle N_q + 1 | b_q^* | N_q \rangle &= (N_q + 1)^{1/2} & \text{for } N'_q = N_q + 1, \end{aligned} \right\} \quad (5.5)$$

corresponding to phonon absorption and emission, respectively. Using equation (2.3) for the initial and final electron states, the matrix element is obtained in the form

$$\begin{aligned} \langle \mathbf{k}', j', N'_q | U | \mathbf{k}, j, N_q \rangle &= i \frac{4\pi e^* e}{\Omega} \left(\frac{\hbar}{2NM\omega} \right)^{1/2} \frac{1}{q} \times \\ &\times [\delta_{\mathbf{k}', \mathbf{k}+\mathbf{q}} N_q^{1/2} - \delta_{\mathbf{k}', \mathbf{k}-\mathbf{q}} (N_q + 1)^{1/2}] \frac{1}{1 + \frac{q^2 \lambda^2}{2}} I_{jj'}(q), \end{aligned} \quad (5.6)$$

where the integral over the crystal volume has been broken into the sum of integrals over unit cells and the relation

$$\frac{1}{N} \sum_{n=1}^N \exp [i (\mathbf{k} - \mathbf{k}' \pm \mathbf{q}) \mathbf{r}_n] = \delta_{\mathbf{k}', \mathbf{k} \pm \mathbf{q}} \quad (5.7)$$

has been used. Choosing as before $\mathbf{k} = (0, 0, k)$, which gives $\mathbf{k} \pm \mathbf{q} = (\pm q_1, \pm q_2, k \pm q_3)$, one obtains

$$I_{1/2, 1/2}(q) = \frac{1}{\Omega} \int_{\Omega} u_{\mathbf{k} \pm \mathbf{q}, 1/2}^* u_{\mathbf{k}, 1/2} d^3 r_0 = 1 - (b^2 + c^2) \frac{q^2}{2k^2} \quad (5.8)$$

and

$$I_{1/2, -1/2}(q) = \frac{1}{\Omega} \int_{\Omega} u_{\mathbf{k} \pm \mathbf{q}, -1/2}^* u_{\mathbf{k}, 1/2} d^3 r_0 = \pm b \left(\frac{b}{2} - c \sqrt{2} \right) \frac{q}{k} \left(1 - \frac{q^2}{4k^2} \right)^{1/2} e^{i\varphi}, \quad (5.9)$$

where, slightly anticipating (see (5.12)), we have put $\cos \theta = \mp q/2k$ for phonon absorption and emission, respectively. Hence the transition probability for the both processes is

$$\left. \begin{aligned} W_{\mathbf{k}, \mathbf{k}+\mathbf{q}} &= w(k, q) N_q \delta [\varepsilon(|\mathbf{k} + \mathbf{q}|) - \varepsilon(|\mathbf{k}|) - \hbar \omega] \\ W_{\mathbf{k}, \mathbf{k}-\mathbf{q}} &= w(k, q) (N_q + 1) \delta [\varepsilon(|\mathbf{k} - \mathbf{q}|) - \varepsilon(|\mathbf{k}|) + \hbar \omega], \end{aligned} \right\} \quad (5.10)$$

where

$$w(k, q) = \frac{2\pi}{\hbar} \left(\frac{4\pi e^* e}{\Omega} \right)^2 \frac{\hbar}{2NM\omega} \left(\frac{\lambda^2 q}{1 + \lambda^2 q^2} \right)^2 (|I_{1/2, 1/2}|^2 + |I_{1/2, -1/2}|^2). \quad (5.11)$$

The relaxation time may be introduced for the region of temperatures where $k_0 T \gg k_0 \theta_1 = \hbar \omega$. Then the electron energy is much larger than the phonon energy, the collisions may be regarded as quasi-elastic, and the term $\hbar \omega$ may be neglected in the argument of the δ -functions. Using the reasoning analogous to that of equation (3.8), we get for any spherical energy band

$$\delta [\varepsilon(|\mathbf{k} \pm \mathbf{q}|) - \varepsilon(|\mathbf{k}|)] = \frac{1}{q} \frac{dk}{d\varepsilon} \delta \left(\frac{q}{2k} \pm \cos \theta \right), \quad (5.12)$$

where θ is the angle between $\mathbf{k}$ - and $\mathbf{q}$ -vectors. Next the transport scattering transition rate between $\mathbf{k}$ - and $\mathbf{k}'$ -states is to be found and summed over all possible final states, which is equivalent to summation over $\mathbf{q}$. This procedure can be found in reference [23], giving in case of a spherical band the following general result for the relaxation time:

$$\frac{1}{\tau(\mathbf{k})} = \frac{V}{8\pi^2} \frac{1}{k^2} \frac{dk}{d\varepsilon} \int_0^{2k} w(\mathbf{k}, \mathbf{q}) (2N_q + 1) q^3 dq. \quad (5.13)$$

For $T \gg \theta_1$ there is $2N_q + 1 \approx 2k_0 T / (\hbar \omega)$ and after the integration we obtain

$$\tau_{\text{op.}}(\varepsilon) = \frac{1}{8\pi} \frac{\Omega M \hbar \omega^2}{(e e^*)^2 k_0 T} \frac{1}{F_{\text{op.}}} \frac{d\varepsilon}{dk}, \quad (5.14)$$

where

$$F_{\text{op.}} = A - \frac{1}{2} (4L - fL^2) B + \frac{1}{3} (4 - f) L^2 C \quad (5.15)$$

with

$$\left. \begin{aligned} A &= 1 - \frac{2}{\xi} \ln(\xi + 1) + \frac{1}{\xi + 1}, \\ B &= 1 - \frac{4}{\xi} + \frac{6}{\xi^2} \ln(\xi + 1) - \frac{2}{\xi(\xi + 1)}, \\ C &= 1 - \frac{3}{\xi} + \frac{9}{\xi^2} - \frac{12}{\xi^3} \ln(\xi + 1) + \frac{3}{\xi^2(\xi + 1)}. \end{aligned} \right\} \quad (5.16)$$

f and ξ are defined in (3.11). Replacing $\hbar \omega$ by $k_0 \theta_1$ the final formula describing electron mobility for polar optical scattering is

$$u_{\text{op.}} = \frac{1}{8\pi} \frac{M \Omega (k_0 \theta_1)^2}{\hbar^3 e (e^*)^2 k_0 T} \frac{1}{F_{\text{op.}}} \left(\frac{d\varepsilon}{dk} \right)^2 k^{-1}. \quad (5.17)$$

Using the previous approximations ($\xi \gg 1$), $F_{\text{op.}}$ can be simplified to the form

$$F_{\text{op.}} = 1 - \frac{2}{\xi} \ln(\xi + 1) - \frac{1}{2} (4L - fL^2) \left(1 - \frac{4}{\xi} \right) + \frac{1}{3} (4 - f) L^2 \left(1 - \frac{3}{\xi} \right). \quad (5.18)$$

As before, the terms containing L are directly due to the mixing of p-like functions into the conduction band wave function, so that for very small electron energies only the first two terms are left. $\xi \rightarrow \infty$ corresponds to no screening effects. To give some idea about the numbers involved we again consider InSb at room temperature and $n = 10^{19} \text{ cm}^{-3}$. For the previously quoted values of L and ξ both screening and non-parabolicity increase the theoretical value of mobility by the factor of 3.5, as compared to the procedure taking into account only the proper density of states (i.e. giving $F_{\text{op.}} = 1$).

6. Acoustic Scattering

We shall describe scattering of electrons by acoustic phonons on the basis of the deformable-ion model of Bloch [26]. Using the initial Hamiltonian (2.1) the

interaction between electrons and acoustic phonons can be written as

$$U = \delta V_0 + \frac{\hbar}{4 m_0^2 c^2} (\boldsymbol{\sigma} \times \nabla \delta V_0) \cdot \mathbf{p}, \quad (6.1)$$

where δV_0 is the change of the periodic potential of the crystal due to acoustic wave propagation. In the deformable-ion model this change is assumed to be given by

$$\begin{aligned} \delta V_0 &= V - V_0 = -\mathbf{u} \cdot \nabla V_0 = \\ &= - \sum_{\mathbf{q}, \nu} \left(\frac{\hbar}{2 N m \omega_q} \right)^{1/2} (\mathbf{e}_{\text{ac.}}^\nu \cdot \nabla V_0) (b_q e^{i\mathbf{q}\mathbf{r}} + b_q^* e^{-i\mathbf{q}\mathbf{r}}), \end{aligned} \quad (6.2)$$

where $\mathbf{u}$ is the displacement, $\mathbf{e}_{\text{ac.}}^\nu$ denotes the polarization of the wave, and $m = m_1 + m_2$. The summation is over the wave vectors $\mathbf{q}$ and the three possible polarizations ν (one longitudinal and two transverse branches). Again, we have to calculate the matrix element of U between initial and final electron and phonon states. Using a directional derivative $\mathbf{e}_{\text{ac.}}^\nu \cdot \nabla V_0 = \partial V_0 / \partial S_\nu$ and equations (2.3) and (5.5), the matrix element is obtained in the form

$$\begin{aligned} \langle \mathbf{k}', j', N_q' | U | \mathbf{k}, j, N_q \rangle &= \\ &= - \sum_{\mathbf{q}, \nu} \left(\frac{\hbar}{2 N m \omega_q} \right)^{1/2} [\delta_{\mathbf{k}', \mathbf{k}+\mathbf{q}} N_q^{1/2} + \delta_{\mathbf{k}', \mathbf{k}-\mathbf{q}} (N_q + 1)^{1/2}] I_{jj'}^\nu(\mathbf{q}), \end{aligned} \quad (6.3)$$

where

$$I_{jj'}^\nu(\mathbf{q}) = \frac{1}{\Omega} \int_{\Omega} u_{\mathbf{k} \pm \mathbf{q}, j'}^* \left[\frac{\partial V_0}{\partial S_\nu} + \frac{\hbar}{4 m_0^2 c^2} \left(\boldsymbol{\sigma} \times \nabla \frac{\partial V_0}{\partial S_\nu} \right) (\mathbf{p} + \hbar \mathbf{k}) \right] u_{\mathbf{k}, j} d^3 r_0. \quad (6.4)$$

We shall now transform equation (6.4) according to the well-known procedure [11, 23]. Using the unperturbed Hamiltonian $\mathcal{H}_0$ of equation (2.1) the last equation can be written as

$$I_{jj'}^\nu(\mathbf{q}) = \frac{1}{\Omega} \int_{\Omega} u_{\mathbf{k} \pm \mathbf{q}, j'}^* \left(\frac{\partial}{\partial S_\nu}, \mathcal{H}_0 + \frac{\hbar}{m_0} \mathbf{k} \cdot \boldsymbol{\pi} \right) u_{\mathbf{k}, j} d^3 r_0, \quad (6.5)$$

where $\boldsymbol{\pi} = \mathbf{p} + (\hbar/4 m_0 c^2) (\boldsymbol{\sigma} \times \nabla V_0)$ and (A, B) denotes the commutator. Observing that $[\mathcal{H}_0 + (\hbar/m_0) \mathbf{k} \cdot \boldsymbol{\pi}] u_{\mathbf{k}j} = [\varepsilon(\mathbf{k}) - \hbar^2 k^2/(2 m_0)] u_{\mathbf{k}j}$ and neglecting the value of $\varepsilon(\mathbf{k}) - \varepsilon(|\mathbf{k} + \mathbf{q}|) - (\hbar^2/2 m_0) (k^2 - |\mathbf{k} + \mathbf{q}|^2)$ as compared to $(\hbar/m_0) (\mathbf{q} \cdot \boldsymbol{\pi})$, equation (6.4) is finally transformed into

$$I_{jj'}^\nu(\mathbf{q}) = \frac{\hbar^2}{m_0} \frac{i}{\Omega} \int_{\Omega} (\mathbf{q} \cdot \nabla u_{\mathbf{k} \pm \mathbf{q}, j'}^*) (\mathbf{e}_{\text{ac.}}^\nu \cdot \nabla u_{\mathbf{k}, j}) d^3 r_0, \quad (6.6)$$

where we have approximated the operator $\boldsymbol{\pi}$ by $\mathbf{p}$.

Regarding periodic parts of the Bloch functions, as given by (2.8), it can be seen that there are five different non-vanishing integrals (and their cyclic equivalents) in the matrix element (6.6), namely

$$\varepsilon_0 = \frac{\hbar^2}{m_0} \frac{1}{\Omega} \int_{\Omega} (\nabla S)^2 d^3 r_0, \quad \varepsilon_1 = \frac{\hbar^2}{m_0} \frac{1}{\Omega} \int_{\Omega} \left(\frac{\partial X}{\partial x} \right)^2 d^3 r_0, \quad \varepsilon_2 = \frac{\hbar^2}{m_0} \frac{1}{\Omega} \int_{\Omega} \left(\frac{\partial X}{\partial y} \right)^2 d^3 r_0, \quad (6.7)$$

$$D = \frac{\hbar^2}{m_0} \frac{1}{\Omega} \int_{\Omega} \frac{\partial X}{\partial x} \frac{\partial Y}{\partial y} d^3 r_0, \quad E = \frac{\hbar^2}{m_0} \frac{1}{\Omega} \int_{\Omega} \frac{\partial X}{\partial y} \frac{\partial Y}{\partial x} d^3 r_0. \quad (6.8)$$

Values of these integrals cannot be directly calculated since the explicit form of S -, X -, Y -, and Z -functions is not known. These values can be estimated by considering on one end the atomic limit, i.e. taking for S , X , Y , and Z the hydrogen functions of s - and p -states, and on the other using the empty-lattice approximation. The real values of the integrals lie somewhere in between. In the hydrogenic approximation we have $\varepsilon_1/\varepsilon_0 = 9/20$ and $\varepsilon_2/\varepsilon_0 = 3/20$, whereas in the empty-lattice approximation $\varepsilon_1/\varepsilon_0 \approx 1$ and $\varepsilon_2/\varepsilon_0 \approx 0$. Due to lack of something better we shall use in the following estimations the averages of these values, i.e. $\varepsilon_1/\varepsilon_0 = 29/40$ and $\varepsilon_2/\varepsilon_0 = 3/40$.

Polarizations of the three phonon branches were chosen in the following way. We denote the directional cosines of $\mathbf{q}$ as $\mathbf{e}$. Thus $\mathbf{q} = q(e_1, e_2, e_3)$. Hence for the longitudinal acoustic wave there is $\mathbf{e}_{ac.}^{\parallel} = (e_1, e_2, e_3)$. First transverse polarization is chosen to be perpendicular to both $\mathbf{q}$ and z -directions. This gives $\mathbf{e}_{ac.}^{\perp 1} = (e_1^2 + e_2^2)^{-1/2} (-e_2, e_1, 0)$. Second transverse mode must be perpendicular to the above two. This gives for the unit polarization vector

$$\mathbf{e}_{ac.}^{\perp 2} = (e_1^2 + e_2^2)^{-1/2} (-e_3 e_1, -e_3 e_2, e_1^2 + e_2^2).$$

There are six different matrix elements of equation (6.6): spin-conserving and spin-flip transitions for the three branches. The main contribution to acoustic scattering is given by the longitudinal spin-conserving transition, although the others are not negligible. After choosing, as before, the initial $\mathbf{k}$ -vector in the z -direction and calculating the matrix elements (6.6) it turns out that in five cases, namely in longitudinal spin-flip and four transverse processes there appear terms which in the spherical coordinate system depend on the azimuthal angle φ . In principle this fact would prevent rigorous introduction of the relaxation time; fortunately, however, the troublesome terms are very small. They are proportional to $L^2(\varepsilon_1 \varepsilon_2/\varepsilon_0^2)$ and $L^2(\varepsilon_2^2/\varepsilon_0^2)$ and so, even for the highest achievable energies, they do not exceed the value of 0.01, which can be simply neglected as compared to the terms of the order of unity. Furthermore, in order to simplify the calculations we have assumed $D = \varepsilon_1$ and $E = \varepsilon_2$, which are good approximations since the quantities involved represent the same types of integrals.

With the above simplifications the squares of the matrix elements for the longitudinal mode are

$$|I_{1/2, 1/2}^{\parallel}(q)|^2 = \varepsilon_0^2 q^2 \left\{ a^2 + \frac{\varepsilon_1}{\varepsilon_0} \frac{b^2}{2} + \frac{\varepsilon_2}{\varepsilon_0} \left(c^2 + \frac{b^2}{2} \right) - \frac{q^2}{4 k^2} \left[\frac{\varepsilon_1}{\varepsilon_0} \left(c^2 + \frac{b^2}{2} \right) + \frac{\varepsilon_2}{\varepsilon_0} \left(5 c^2 + \frac{b^2}{2} \right) \right] + \frac{q^4}{4 k^4 \varepsilon_0} \left(c^2 - \frac{b^2}{2} \right)^2 \right\}, \quad (6.9)$$

$$|I_{1/2, -1/2}^{\parallel}(q)|^2 = \varepsilon_1^2 \frac{q^4}{4 k^2} \left(1 - \frac{q^2}{4 k^2} \right) b^2 c^2, \quad (6.10)$$

where in equation (6.9), after squaring, the terms proportional to $\varepsilon_1 \varepsilon_2$ and ε_2^2 are to be neglected. For the transverse modes we have

$$|I_{1/2, 1/2}^{\perp 1}(q)|^2 = \varepsilon_1^2 \frac{q^2}{4} \left(1 - \frac{q^2}{4 k^2} \right) \left[b^2 - \frac{q^2}{k^2} \left(\frac{b c}{\sqrt{2}} + \frac{b^2}{2} \right) \right]^2, \quad (6.11)$$

$$|I_{1/2, -1/2}^{\perp 1}(q)|^2 = \varepsilon_1^2 \frac{q^4}{4 k^2} \left(1 - \frac{q^2}{4 k^2} \right) \left[\left(b^2 + \frac{b c}{\sqrt{2}} \right) - \frac{q^2}{2 k^2} \left(\frac{b^2}{2} + \frac{b c}{\sqrt{2}} \right) \right]^2, \quad (6.12)$$

$$|I_{1/2, 1/2}^{\perp 2}(q)|^2 = \varepsilon_1^2 \frac{q^4}{4 k^2} \left(1 - \frac{q^2}{4 k^2}\right) \left(c^2 + \frac{b^2}{2}\right)^2, \quad (6.13)$$

$$|I_{1/2, -1/2}^{\perp 2}(q)|^2 = \varepsilon_1^2 \frac{q^2}{2} \left(1 - \frac{q^2}{2 k^2}\right)^2 b^2 c^2. \quad (6.14)$$

In all the above equations we have put, anticipating slightly, $e_3 = \cos \theta = -q/2 k$ for phonon absorption (see equation (5.12)). Now the scattering probability with absorption and emission of a phonon can be calculated in analogy to equation (5.10), where now

$$w^r(k, q) = \frac{2 \pi}{\hbar} \left(\frac{\hbar}{2 N m \omega_q^r} \right) \sum_{j'} |I_{j' j}^r(q)|^2. \quad (6.15)$$

For acoustic phonons of small energies $\omega_q^{\parallel} = v_{\parallel} q$ and $\omega_q^{\perp} = v_{\perp} q$, i.e., one must make a distinction between the velocities of longitudinal and transverse modes. It can be readily shown by standard methods that the acoustic phonon energy in (5.10) is negligible compared to electron energies for all temperatures above few degrees of Kelvin, so that equations (5.12) and (5.13) may be used without any change. For the same condition there is $2 N_q + 1 \approx 2 k_0 T / (\hbar v_{\parallel} q)$. The integration indicated in (5.13) can now be performed to give finally for the longitudinal mode (the crystal density $\varrho = m N/V$)

$$\tau_{\text{ac.}}^{\parallel} = -\frac{\pi \hbar v_{\parallel}^2 \varrho}{k_0 T \varepsilon_0^2} \frac{1}{F_{\text{ac.}}^{\parallel}} \frac{d\varepsilon}{dk} k^{-2}, \quad (6.16)$$

where, to a very good approximation,

$$F_{\text{ac.}}^{\parallel} = \left[1 - L \left(1 + \frac{7}{18} \frac{\varepsilon_1}{\varepsilon_0} \varphi_1 + \frac{5}{18} \frac{\varepsilon_2}{\varepsilon_0} \varphi_2 \right) \right]^2 \quad (6.17)$$

with

$$\varphi_1 = \frac{8 \gamma^2 - \beta^2}{7} \quad \text{and} \quad \varphi_2 = \frac{4 \gamma^2 + \beta^2}{5}. \quad (6.18)$$

The relaxation time $\tau_{\text{ac.}}^{\perp}$ for both transverse modes can also be expressed by (6.16) with $v_{\parallel}^2$ replaced by $v_{\perp}^2$, and $F_{\text{ac.}}^{\parallel}$ replaced by $F_{\text{ac.}}^{\perp}$, where

$$F_{\text{ac.}}^{\perp} = \frac{17}{72} \left(\frac{\varepsilon_1}{\varepsilon_0} \right)^2 L^2 \varphi_3 \quad (6.19)$$

with

$$\varphi_3 = \frac{3 \beta^4 + 32 \beta^2 \gamma^2 + 16 \gamma^4}{51}. \quad (6.20)$$

For $\Delta \gg \varepsilon_g$ there is $\varphi_1 \approx \varphi_2 \approx \varphi_3 \approx 1$. The mobility due to all the three modes of acoustic scattering can be defined as

$$u_{\text{ac.}} = \frac{\pi v_{\parallel}^2 \varrho}{\hbar k_0 T \varepsilon_0^2} \frac{1}{F_{\text{ac.}}} \left(\frac{d\varepsilon}{dk} \right)^2 k^{-3} \quad (6.21)$$

with

$$F_{\text{ac.}} = F_{\text{ac.}}^{\parallel} + \frac{v_{\parallel}^2}{v_{\perp}^2} F_{\text{ac.}}^{\perp}. \quad (6.22)$$

In InSb $v_{||}^2/v_{\perp}^2 \approx 2.2$ and at highest achievable energies the transverse modes contribute more than 20% to the total acoustic scattering. At these energies, equations (6.21) and (6.22) give the theoretical values of mobility of about 3.7 times higher than those obtained by taking into account only the proper density of states (which gives $F_{ac.} = 1$).

The constant ϵ_0 , both by its definition (6.8) and its place in the formula for mobility (6.21), plays the role of the deformation potential constant. It should be emphasized, however, that the deformation potential method is not directly applicable to the case considered above, since it can be used only for the electron states describable by the decoupled band scheme of the one-band effective mass approximation.

Another approach to acoustic scattering is usually made by means of the rigid-ion model of Nordheim [27]. For long phonon wavelengths this model differs from the Bloch model by a term which is of the first order in q . For small electron energies, i.e. for electron states which can be described by Luttinger-Kohn amplitudes, both procedures do not differ significantly leading only to somewhat different definitions of the deformation potential (cf. the paper of Pikus [28]). In our case, however, the two models lead not only to different definitions of ϵ_0 , but also to different values of other integrals in (6.7) and (6.8), thus giving different energy dependences of the relaxation time for acoustic scattering.

7. Piezo-Acoustic Scattering

In III-V compounds this mode is possible due to lack of inversion symmetry and it becomes of importance at low temperatures where in pure samples it competes with the regular acoustic scattering. It has been shown by Harrison [29] that the two modes can be considered independently. Calculating piezo-acoustic scattering we shall follow in general the approach of Hutson [30].

First, we have to determine the scattering potential due to piezo-effect associated with acoustic wave deformation. In an ideal dielectric (no movable charge) the electric induction is zero, i.e.

$$4\pi \mathbf{e} \mathbf{S} + \kappa_0 \mathbf{E} = 0, \quad (7.1)$$

where $\mathbf{e}$ is the piezo-electric tensor of the third order, $\mathbf{S}$ the deformation tensor $S_{ij} = (1/2)(\partial u_i/\partial x_j + \partial u_j/\partial x_i)$, and $\mathbf{u}$, as before, denotes the displacement connected with the acoustic wave. Using equation (6.2) we have

$$S_{ij} = \frac{i}{2} \sum_{\mathbf{q}, \nu} \left(\frac{\hbar}{2 N m \omega_q^{\nu}} \right)^{1/2} (e_{ac. i}^{\nu} q_j + e_{ac. j}^{\nu} q_i) (b_q e^{i \mathbf{q} \mathbf{r}} - b_q^* e^{-i \mathbf{q} \mathbf{r}}). \quad (7.2)$$

In cubic crystals of InSb type there is one non-vanishing component of the piezo-electric tensor: $e_{123} = e_{132} = e_{231} = e_{213} = e_{312} = e_{321} = P/2$. Hence, using equations (7.1) and (7.2) to obtain components of the electric field and next employing the Poisson equation, we get for the unscreened perturbing potential energy

$$U' = - \frac{4\pi P e}{\kappa_0} \sum_{\mathbf{q}, \nu} \left(\frac{\hbar}{2 N m \omega_q^{\nu}} \right)^{1/2} K_{\nu} (b_q e^{i \mathbf{q} \mathbf{r}} - b_q^* e^{-i \mathbf{q} \mathbf{r}}) \quad (7.3)$$

with

$$K_{\nu} = e_{ac. 1}^{\nu} e_2 e_3 + e_{ac. 2}^{\nu} e_1 e_3 + e_{ac. 3}^{\nu} e_1 e_2, \quad (7.4)$$

where, as before, $e_{ac.}^{\nu}$ is the unit polarization vector of the acoustic wave and $\mathbf{e}$ the unit vector along its propagation direction. It can be seen that U' is strongly

anisotropic. For instance, it vanishes for $e = (1, 0, 0)$ for both longitudinal and transverse modes, and for $e = (1, 1, 0)$ for the longitudinal mode. If there are movable carriers in the band one does not deal with a perfect dielectric and the screening effects come into play in this long-range interaction. According to Hutson [30] the screened piezo-acoustic interaction takes the form

$$U = U' \left(1 + \frac{1}{q^2 \lambda^2} \right)^{-1}. \quad (7.5)$$

In other words, the effect of screening is the same as for polar optical interaction. The matrix element between initial and final states is

$$\begin{aligned} \langle k', j', N'_q | U | k, j, N_q \rangle = & - \frac{4 \pi P e}{\kappa_0} \left(\frac{\hbar}{2 N m \omega_q^2} \right)^{1/2} \times \\ & \times [\delta_{k', k+q} N_q^{1/2} - \delta_{k', k-q} (N_q + 1)^{1/2}] K_v \frac{1}{1 + \frac{1}{q^2 \lambda^2}} I_{jj'}(q), \end{aligned} \quad (7.6)$$

where $I_{jj'}(q)$ are defined in (5.8) and (5.9). In principle, due to the strong anisotropy of the scattering, the usual relaxation time cannot be introduced in a rigorous way. However, following the common procedure, we shall introduce the relaxation time averaging over the angles. Making use of $\omega_q^2 = q v_s$, where v_s is the sound velocity depending on the direction of propagation and the mode in question, $v_s^2 = c/\rho$ with c representing an appropriate combination of elastic constants. Following equation (5.13) and performing the integration as in the case of polar optical scattering, the final formula for the relaxation time is obtained in the form

$$\frac{1}{\tau_{p.a.}} = 8 \pi \frac{P^2 e^2 k_0 T}{\kappa_0^2 \hbar} \left(\frac{K_v}{c} \right)_{av.} \frac{dk}{d\varepsilon} F_{p.a.}, \quad (7.7)$$

where $F_{p.a.} = F_{op.}$ of equation (5.18). We do not elaborate on the averaging procedure, since it has been done by Meijer and Polder [31], Hutson [30], and Zook [32]. In order to avoid all misunderstanding we note that equation (7.7) was obtained by simply taking out (K_v/c) in front of the integral sign, as if it did not depend on q - or e'_{ac} -directions. The electron mobility can now be defined to give

$$u_{p.a.} = \frac{1}{8 \pi} \frac{\kappa_0^2}{P^2 e} \frac{1}{\hbar k_0 T} \left(\frac{K_v}{c} \right)^{-1}_{av.} \frac{1}{F_{p.a.}} \left(\frac{d\varepsilon}{dk} \right)^2 k^{-1}. \quad (7.8)$$

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Appendix

We shall derive now an expression for the screening length λ due to screening by free electrons in an arbitrary spherical energy band. This quantity appears in the long-range interactions considered above. It is not accidental that in all

three cases (see equations (3.5), (5.4), and (7.5)) the screening in the Fourier transforms is represented by the term $[1 + (1/q^2 \lambda^2)]^{-1}$ since this is a general result, whose derivation requires only a slow variation of the initial potential (see, e.g., [33]).

The Poisson equation for the self-consistent statically screened potential is

$$\nabla^2 \varphi = \frac{4 \pi e}{\kappa_0} (n' - n), \quad (\text{A } 1)$$

where n is the equilibrium electron concentration and n' is the concentration in the presence of the potential φ . n' can be calculated by adding to the electron energy $\varepsilon(k)$ the potential energy $-e \varphi$, which is equivalent to replacing the Fermi level ζ in the distribution function f_0 by $\zeta + e \varphi$. The equilibrium concentration in a spherical energy band is (cf. Kołodziejczak [2])

$$n = \frac{2}{8 \pi^3} \int f_0 d^3 k = \frac{1}{3 \pi^2} \langle 1 \rangle, \quad (\text{A } 2)$$

where, in general,

$$\langle A \rangle = \int_0^\infty -\frac{\partial f_0}{\partial z} A k^3(z) dz \quad (\text{A } 3)$$

with $z = \varepsilon/k_0 T$. A is in general an operator (cf. Zawadzki [2]). n' can be calculated using (A 2) but replacing $\eta = \zeta/(k_0 T)$ by $\eta + u$, where $u = e \varphi/(k_0 T)$. For $e \varphi \ll \zeta$ one can expand n' in a Taylor series around n . Restricting ourselves to the linear approximation in u and observing (upon integrating by parts) that $\partial \langle 1 \rangle / \partial \eta = \langle d/dz \rangle$ one obtains equation (A 1) in the form

$$\nabla^2 \varphi = \frac{1}{\lambda^2} \varphi, \quad (\text{A } 4)$$

where

$$\frac{1}{\lambda^2} = \frac{4}{3 \pi \kappa_0 k_0 T} \left\langle \frac{d}{dz} \right\rangle, \quad (\text{A } 5)$$

λ being the screening length. For the nondegenerate electron gas $\langle d/dz \rangle = \langle 1 \rangle$ and the well-known result $(1/\lambda^2) = 4 \pi e^2 n/(\kappa_0 k_0 T)$ is obtained. For the strongly degenerate gas $n = (1/3 \pi^2) k^3(\eta)$, and upon using equation (1.1) we get

$$\frac{1}{\lambda^2} = \left(\frac{3 n}{\pi} \right)^{1/3} \frac{4 m^* e^2}{\kappa_0 \hbar^2} \quad (\text{A } 6)$$

which is again the well-known result, except that in our case the effective mass m^* depends on the Fermi level and, hence, on electron concentration.

The general result (A 5) can be specialized for the energy band described by (2.5). The electron concentration (A 2) becomes (Kołodziejczak [34])

$$n = \frac{1}{3 \pi^2} \left(\frac{2 m_0^* k_0 T}{\hbar^2} \right)^{3/2} {}^0 L_0^{3/2}(\eta, \beta) \quad (\text{A } 7)$$

and the screening length is now

$$\frac{1}{\lambda^2} = \frac{2}{\pi} \frac{e^2}{\kappa_0 k_0 T} \left(\frac{2 m_0^* k_0 T}{\hbar^2} \right)^{3/2} {}^0 L_1^{1/2}(\eta, \beta), \quad (\text{A } 8)$$

where

$${}^kL_m^l(\eta, \beta) = \int_0^\infty -\frac{\partial f_0}{\partial z} z^k (z + \beta z^2)^l (1 + 2\beta z)^m dz \quad (\text{A } 9)$$

are the generalized Fermi integrals ($\beta = k_0 T/\varepsilon_g$). Their properties have been discussed in [7]. A similar expression in terms of a series of the usual Fermi integrals has been derived by Ehrenreich [9]. In InSb, at room temperature for $n = 10^{18} \text{ cm}^{-3}$ the screening length is about 70 Å and for $r \geq \lambda/10$ the condition $e\varphi \ll \zeta$ is well satisfied.

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