SCATTERING OF PHONONS BY CARRIERS IN THE FIELD OF CHARGED IMPURITIES

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It is shown that if the energy and momentum conservation laws hold for the phonon + carrier system, then the model of scattering of phonons by current carriers cannot explain the experimental results. A new model for scattering in the field of a charged impurity in which the conservation laws do not hold for this system is proposed. It is shown that such a scattering is effective only in semiconductors with sufficiently large carrier effective masses in the presence of impurities producing an attraction field. Agreement between the calculations and the experimental data is obtained.

THE thermal conductivity of semiconductor crystals after acceptor or donor impurities are introduced into them can decrease by several orders of magnitude at low temperatures.[1] To explain the observed increase of the thermal resistance, Ziman[2] proposed a model of phonon scattering by free carriers. For the scattering processes

$$\mathbf{q} + \mathbf{k}' \rightleftarrows \mathbf{k}'' \tag{1}$$

(here $\mathbf{q}$ and $\mathbf{k}$ are the wave vectors of the phonon and of the carrier) he obtained the following relaxation time:

$$\tau_{pe}^{-1} = \frac{\varepsilon_1^2 m^2 T}{2\pi\hbar^4 Ds} \times \ln \frac{1+\exp[\zeta - ms^2/2T - x^2T/8ms^2 + x/2]}{1+\exp[\zeta - ms^2/2T - x^2T/8ms^2 - x/2]}, \tag{2}$$

where ϵ_1—deformation potential, m—effective mass of the carrier, D—crystal density, s—speed of sound, T—temperature in energy units, ζ—reduced chemical potential, and $x = \hbar sq/T$.

The dependence of τ_{pe}^{-1} on x in the case of strong degeneracy is shown in Fig. 1. When $x > x_1 = \sqrt{8ms^2\zeta}/T$ the relaxation time increases with increasing x like $\exp[x^2T/8ms^2]$, i.e., much more rapidly than the decrease of the number of excited phonons, which is proportional to e^{-x}. As a result, when $x > x_1$, the role of the processes (1) decreases rapidly compared with the other scattering processes. A similar limitation of the interaction occurs as a result of the fact that the laws of energy and momentum conservation forbid the processes (1) of phonons with momentum $\hbar q$ larger than double the momentum of the carrier on the Fermi surface $2\hbar k_F$. It will be shown below that the width of the spectrum of the phonons participating in the processes (1) is insufficiently large to make it possible for the Ziman model to explain the experimentally observed decrease of the thermal conductivity. All the estimates that follow below were made for the crystal p-InSb, but it can be shown that analogous estimates hold also for Ge and a number of other semiconductors.

In the purest crystal at sufficiently low temperatures, the phonon scattering is from the boundaries of the sample. The expression for the thermal conductivity of the crystal[3] takes in this case the form

$$\varkappa = \frac{1{,}12 k_0 T^3 L}{24\pi^2\hbar^3}\left(\frac{1}{s_l^2} + \frac{2}{s_t^2}\right)\int_0^\infty \frac{x^4\,dx}{\mathrm{sh}^2(x/2)} \tag{3}$$

(here L is the transverse dimension of the sample, k_0 is the Boltzmann constant, s_l and s_t are the speeds of sound of the longitudinal and transverse modes of the acoustic lattice vibrations). It follows from (3) that the contribution of each branch to κ is inversely proportional to the square of the speed of sound. Therefore to find the average values of the sound speeds of each branch, which enter in (3), it is necessary to average the reciprocal squares of these speeds over the directions, taking into account by the same token the larger weight of the phonons with the smallest speeds. The table shows the sound velocities along the directions of the symmetry axes of the InSb crystal, calculated from the elastic constants.[4] The figure also shows the average values of $\langle s^{-2}\rangle^{-1/2}$, obtained by averaging over the fundamental directions of the reciprocal squares of the velocities of the sound of each branch with allowance for the fact that the cubic crystal has three fourfold axes, four threefold axes, and six twofold axes. With such values of the average velocities of sound, the contribution of the two transverse branches to κ amounts to 88%. Therefore to estimate the decrease in thermal conductivity it is most important to consider the scattering of the transverse phonons. We take values typical of the experimental situations, $T = 1.5\,^\circ K$ and $p = 5 \times 10^{17}\ cm^{-3}$. We then obtain for transverse phonons with a sound velocity $\langle s^{-2}\rangle^{-1/2}$ a parameter $x_1 = 4.6$.

$s\cdot 10^{-5}$ cm/sec	Direction			Average value
	100	110	111	
s_l	3.46	3.83	3.92	3.8
s_{t_1}	2.32	1.64	2.16	2.0
s_{t_2}	2.32	2.32	2.16	2.0

Let us estimate the maximum possible scattering by the carriers, assuming that all the phonons with the parameter $x < x_1$ are completely scattered. Under this assumption, thermal conductivity will be determined by

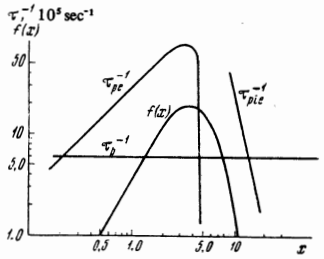

FIG. 1. Reciprocal relaxation times τ_{pe}^{-1}, τ_{pie}^{-1}, τ_b^{-1} and also the function $f(x) = x^4/\sinh^2(x/2)$ against the parameter x.

expression (3), but with the lower limit in the integral replaced by x_1. Figure 1 shows a plot of the integrand $f(x) \equiv x^4/\sinh^2(x/2)$, from which it is seen that x_1 falls in the region of maximum values of this function. Therefore calculation gives a decrease of the thermal conductivity by a factor of approximately 2, whereas experiment gives a factor of about 30.[1] Consequently, interaction of the phonons with the carriers cannot explain the experimental results when the momentum and energy conservation laws are satisfied.

Cases are possible, however, when the conservation laws "do not hold" for the carrier-phonon system. One such possibility was considered by Pyle.[5] He took into account processes of second order of perturbation theory, namely, virtual absorption and emission of phonons: $\mathbf{k}' + \mathbf{q}' \to \mathbf{k}'' \to \mathbf{k}''' + \mathbf{q}''$. Since the energy of the intermediate state is not conserved, the previous limitation $q < 2k_F$ is lifted. However, such scattering turns out to be not very effective.[5]

There exists one more possibility of "violation" of the conservation laws, discussion of which is the object of the present article.

Let us take into account the field of the ionized impurity, in which the interaction of the phonon with the carrier takes place. This violates the condition for the closure of the carrier-phonon system, and again leads to a lifting of the limitation $q < 2k_F$.

A physically analogous situation is known in optics: absorption of light by free carriers in semiconductors within the limits of one band is possible only in the presence of interaction of carriers with phonons or impurities.[6]

Let us consider the scattering of phonons with $q > 2k_F$ by carriers in the Coulomb field of an individual impurity. The experimental situation is characterized by the condition $k_F R_B < 1$ (here R_B is the Bohr radius), in which the Born approximation is not valid. In addition, the Born approximation describes poorly the behavior of the wave function near the impurity center, which, as will be shown below, is important for the given problem. Therefore the behavior of the carrier will be described by the exact wave function of the attracting Coulomb center[7]

$$\psi_k = (2\pi)^{-3/2} e^{\pi/2kR_B} \Gamma\left(1 - \frac{i}{kR_B}\right) e^{ikr} F\left(\frac{i}{kR_B}, 1, i(kr - kr)\right) \qquad (4)$$

(r is the radius vector with origin at the point of location of the impurity ion, F is a hypergeometric function). The wave function of the repelling center is obtained from (4) by replacing R_B by $-R_B$. The characteristic dimensions for the given problem (R_B, $1/q$, $1/k_F$) have values much larger than the lattice constant; therefore it is possible to use the approximation

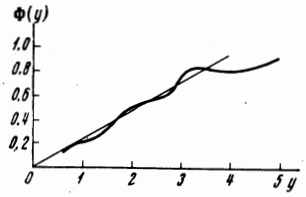

FIG. 2. Dependence of the function $\Phi(y)$ on the argument $y \equiv qR_B$. The straight line shows a plot of the linear function $\chi = 0.23y$.

of the effective mass and the usual theory of the deformation potential. We take the interaction potential in the form

$$U_{pe} = \frac{\varepsilon_1}{\sqrt{G}} \sum_q (\mathbf{q}\mathbf{e}_q) \{a_q e^{iqr} - a_q^+ e^{-iqr}\}, \qquad (5)$$

where G is the number of atoms in the crystal, $\mathbf{e}_q$ is the vector of polarization of the phonon, a_q^+ and a_q are the phonon creation and annihilation operators. In a crystal of cubic symmetry the scalar product $(\mathbf{q} \cdot \mathbf{e}_q)$ for an arbitrarily directed vector $\mathbf{q}$ of the "transverse" phonon differs from zero.

The matrix element $\langle \bar{\psi}_{k'} | U_{pe} | \psi_{k''} \rangle$ is calculated analytically using the inequalities $q > 2k_F$ and $k_F R_B \ll 1$ (see the Appendix). The square of the modulus of the matrix element, averaged over the directions of the vectors $\mathbf{k}'$ and $\mathbf{k}''$ is equal to

$$|\langle \bar{\psi}_{k'} | U_{pe} | \psi_{k''} \rangle|^2 = \frac{\varepsilon_1^2 (\mathbf{q}\mathbf{e}_q)^2 \hbar N_q \Phi(qR_B)(1 - e^{-2\pi/k'' R_B})^{-1}}{2DVk'k''(q/2)^8 R_B^4 (1 - e^{-2\pi/k'R_B})\omega} \qquad (6)$$

(here $\omega = sq$, V is the volume of the crystal, $\Phi(qR_B)$ is the function represented in Fig. 2, and N_q is the number of phonons having an energy $\hbar\omega$).

Expression (6) is given for the case of an attraction field, when the exponential functions in the parentheses can be neglected. The matrix element calculated for a repulsion field turns out to be small because of the positive arguments of these exponentials. Thus, for the considered scattering mechanism only the attraction field plays an important role. Physically this is explained by the fact that in the given scattering, the probability of absorption of the phonon q is determined by the probability of finding the carrier near the impurity at a distance $1/q$; the latter probability, however, is large in attraction fields and small in repulsion fields.

The phonon relaxation time is calculated in the usual manner:[2]

$$\tau_{pie}^{-1} = \frac{2\pi}{\hbar} \int |\langle \bar{\psi}_{k'} | U_{pe} | \psi_{k''} \rangle|^2 (n_{k'} - n_{k''}) \times \delta(\varepsilon_{k'} + \hbar\omega - \varepsilon_{k''}) d^3k' d^3k'' = \frac{\pi \varepsilon_1^2 (\mathbf{q}\mathbf{e}_q)^2 m^2 N_i \Phi(qR_B) T}{\hbar^4 D\omega (q/2)^8 R_B^4} \ln \frac{1 + e^{\zeta}}{1 + e^{\zeta - x}} \qquad (7)$$

(here n_k is the distribution function with respect to the carrier energy ϵ_k, N_i is the concentration of the attracting centers). In the case of strong degeneracy, when $\zeta \gg x$, the logarithmic function in (7) is close to x. If $qR_B < 3$, then, as is seen from Fig. 2, the function Φ is close to a linear function of χ and the expression for the relaxation time of the phonons greatly simplifies:

$$\tau_{pie} = \frac{\hbar^3 D R_B^3 q^7}{59\pi \varepsilon_1^2 (\mathbf{q}\mathbf{e}_q)^2 m^2 N_i}. \qquad (8)$$

Since $R_B \sim m^{-1}$, it follows that $\tau_{pie} \sim m^{-5}$. Therefore in semiconductors with small effective mass, for exam-

ple n-InSb, the considered mechanism of scattering is not effective.

From a comparison with experiment we can estimate the product of the constant ϵ_1 by the cosine of the angle between $\mathbf{q}$ and $\mathbf{e_q}$, quadratically averaged over the directions $\mathbf{q}$:

$$\varepsilon_1 \langle (\mathbf{q}\mathbf{e}_q)^2 \rangle^{1/2} / q \approx 0.3 \text{ eV}.$$

The dependence of τ_{pie}^{-1} with such a parameter on x is shown in Fig. 1. We see that τ_{pie} complements Ziman's τ_{pe} for $x > x_1$. The same figure shows, for comparison, the relaxation time τ_b for the scattering of the phonons by the boundaries of a sample with transverse dimensions 3×3 mm. With increasing x, the time τ_{pie} increases rapidly and becomes equal to τ_b at the point $x_2 = 14$. The total relaxation time $\tau = (\tau_b^{-1} + \tau_{pie}^{-1})^{-1}$ at $x > x_2$ is close to τ_b. Therefore only phonons with $x < x_2$ are important for the discussed scattering mechanism. The condition $qR_B < 3$, which is used in (8), is satisfied for these phonons both at $T = 1.5°K$ and at higher temperatures.

Thus, phonons in the entire region of the maximum of the function f(x) are effectively scattered by the carriers. The considered phonon scattering mechanism makes it possible to explain the experimental results and gives a reasonable estimate of the deformation potential in p-InSb.

In conclusion I take the opportunity to thank S. S. Shalyt for suggesting the topic and L. E. Gurevich for very useful discussions.

APPENDIX

We introduce a polar system of coordinates with a radius vector $\mathbf{r}$ and polar angles ϑ and φ in such a way that the origin coincides with the point of location of the impurity atom and x is directed parallel to the vector $\mathbf{q}$. Then the vectors $\mathbf{k}'$ and $\mathbf{k}''$ are specified by the polar coordinates (k', α', β') and (k'', α'', β''). We introduce also the parabolic coordinates

$$\xi = r(1 + \cos\vartheta), \quad \eta = r(1 - \cos\vartheta). \tag{9}$$

The calculation of the matrix element of the operator U_{pe} (5) with the wave functions $\psi_{\mathbf{k}}$ (4) for the absorption of a phonon $\mathbf{q}$ reduces to the calculation of $\langle \bar{\psi}_{\mathbf{k}''} | e^{i\mathbf{q}\mathbf{r}} | \psi_{\mathbf{k}'} \rangle$:

$$\langle \Psi_{\mathbf{k}''} | U_{pe} | \psi_{\mathbf{k}'} \rangle = \frac{\varepsilon_1 (\mathbf{q}\mathbf{e}_q) \sqrt{\hbar N_q}}{\sqrt{2DV\omega}} \langle \Psi_{\mathbf{k}''} | e^{i\mathbf{q}\mathbf{r}} | \psi_{\mathbf{k}'} \rangle. \tag{10}$$

When $kR_B \ll 1$ we can use the transition to the limit from the hypergeometric function which enters into $\psi_{\mathbf{k}}$ to the Bessel function:[8]

$$\lim_{kR_B \to 0} F(i/kR_B, 1, ik\tilde{\eta}) = J_0(\sqrt{4\eta/R_B}). \tag{11}$$

The argument of these functions $\tilde{\eta} \equiv r - \mathbf{r}\mathbf{k}/k$ is given in parabolic coordinates by

$$\tilde{\eta} = \xi \sin^2\frac{\alpha}{2} + \eta \cos^2\frac{\alpha}{2} - 2\sqrt{\xi\eta} \sin\frac{\alpha}{2}\cos\frac{\alpha}{2}\cos(\varphi - \beta). \tag{12}$$

The matrix element (10) is calculated with the aid of the theorem for the addition of Bessel functions:[8]

$$J_0(\sqrt{4\tilde{\eta}/R_B}) = \sum_{n=-\infty}^{\infty} J_n(2\sqrt{\xi/R_B}\sin(\alpha/2)) J_n(2\sqrt{\eta/R_B}\cos(\alpha/2)) e^{in(\varphi-\beta)}. \tag{13}$$

After integrating with respect to φ from 0 to 2, only terms with $n' = n''$ remain in the double sum over $n' = n''$, which appears when (11) and (13) are substituted in (10). The integrals with respect to ξ and π reduce to tabular forms. Then the series is again summed with the aid of the theorem (13) and we finally obtain

$$\langle \Psi_{\mathbf{k}''} | e^{i\mathbf{q}\mathbf{r}} | \psi_{\mathbf{k}'} \rangle = \frac{1}{A} \exp\left[\frac{2i(\cos\alpha' + \cos\alpha'')}{qR_B}\right] \left\{ J_0\left(\frac{4\sqrt{\mu}}{qR_B}\right) + i\sqrt{\mu} J_1\left(\frac{4\sqrt{\mu}}{qR_B}\right) \right\}, \tag{14}$$

$$A = 4\pi (q/2)^4 \sqrt{k'k''} R_B^2 [1 - \exp(-2\pi/k'R_B)]^{1/2} [1 - \exp(-2\pi/k''R_B)]^{1/2},$$

where the parameter μ, which contains the entire dependence on the angles α and β, is equal to

$$\mu = \sin^2\left(\frac{\alpha'}{2}\right)\sin^2\left(\frac{\alpha''}{2}\right) + \cos^2\left(\frac{\alpha'}{2}\right)\cos^2\left(\frac{\alpha''}{2}\right) + \frac{1}{2}\sin\alpha' \sin\alpha'' \cos(\beta'' - \beta'). \tag{15}$$

Thus, in the expression for the square of the modulus of the matrix element, the only function that depends on the angles is

$$\varphi = J_0^2\left(\frac{4\sqrt{\mu}}{qR_B}\right) + \mu J_1^2\left(\frac{4\sqrt{\mu}}{qR_B}\right). \tag{16}$$

This function is positive and changes little when the parameter μ changes from 0 to 1 upon integration with respect to the angles. Therefore the averaging over the directions k' and k'' can be approximately replaced by averaging over the parameter μ:

$$\int \varphi(\mu) d\Omega' d\Omega'' \approx 16\pi^2 \int_0^1 \varphi(\mu) d\mu = 16\pi^2 \left\{ J_0^2\left(\frac{4}{qR_B}\right) + \frac{4}{3} J_1^2\left(\frac{4}{qR_B}\right) + \frac{1}{3} J_2^2\left(\frac{4}{qR_B}\right) \right\}, \tag{17}$$

where $d\Omega = \sin\alpha \, d\alpha \, d\beta$. The function in the curly brackets is denoted by $\Phi(qR_B)$, and its plot is shown in Fig. 2.

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