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Acoustic-Mode Scattering of Holes

Abstract: Matrix elements are calculated for acoustic-mode scattering of holes in the valence band structure typified by germanium. Whitfield's generalization of the deformation potential theorem is used to calculate the electron-phonon interaction; his method is, however, extended to include the spin-lattice coupling. A general expression for the electron-phonon interaction matrix element is obtained, and calculations are presented for some special directions in k-space.

Introduction

This paper investigates the scattering of holes by acoustic phonons of long wavelength in systems typified by the valence band of germanium. The problem has been dealt with in great detail in two papers by Ehrenreich and Overhauser,[1] who employ the standard theories of electron-phonon interaction.[2] A more comprehensive theory of this interaction, which is essentially a generalization of the Bardeen-Shockley[3] deformation potential theorem, has recently been formulated by Whitfield.[4] The novel feature of the present treatment is the use of this development.

In Section 1 we briefly state Whitfield's results and obtain a general expression for the electron-phonon interaction matrix element. In Sections 2 and 3 this result is applied to the germanium type of valence band structure including spin-orbit interaction, but neglecting the spin-lattice coupling; this coupling is discussed in Section 4. Part II of this paper will deal with application of these results, in particular to transport theory.

1. The deformation potential theorem

Whitfield deduces a generalized deformation potential theorem by adopting a new set of basis states ("Orthogonalized Deformed Bloch" functions) and expanding the one-electron Hamiltonian as a power series in the strains, instead of the usual expansion in the lattice displacements. It is shown in his work that, in nonpolar semiconductors, the principal part of the electron-lattice interaction is given by the matrix elements, taken between combinations of Bloch and phonon states, of the operator[5]

$$E^I = \sum_{i,j} \tfrac{1}{2}(S^{ij}\,\mathfrak{D}^{ji} + \mathfrak{D}^{ji}\,S^{ij}) \,. \tag{1.1}$$

Here S^{ij}, a function of the electron coordinate $\mathbf{x}$ and depending on the lattice variables, is a component of the strain tensor,

$$S^{ij} = \frac{\partial u_j}{\partial x_i} \,, \tag{1.2}$$

where $\mathbf{u}$ is the local lattice displacement[6] from the periodic configuration and is given by

$$\mathbf{u} = \sum_\nu q_\nu \mathbf{V}_\nu \exp(i\mathbf{f}\cdot\mathbf{x}) \,. \tag{1.3}$$

The deformation potential operator[7] is the tensor with components

$$\mathfrak{D}^{ij} = \frac{1}{m}\,(-p_i p_j + \hbar K_i p_j) + U^{ij} \,, \tag{1.4}$$

where $U^{ij}(\mathbf{x})$ is an unknown function with the lattice periodicity, and $\mathbf{K}$ is the diagonal operator in the Bloch representation with the wave vectors as eigenvalues:

$$\mathbf{K}\psi_l = \mathbf{k}\psi_l \,. \tag{1.5}$$

It is shown in Whitfield's work that the diagonal elements of $\mathfrak{D}^{ij}$ are the deformation potentials of the crystal, in the sense that the energies $E_n(\mathbf{k})$ of the Bloch states, when the crystal is subjected to a homogeneous strain ε_{ij}, are given by the eigenvalues of the unstrained Hamiltonian plus $\Sigma_{ij}\varepsilon_{ij}\mathfrak{D}^{ji}$.

Whitfield does not include spin-orbit interaction terms in his one-electron Hamiltonian; if this is done, Eq. (1.4) must be modified to contain the spin-lattice interaction. The additional terms which appear are discussed in the concluding section – at present we proceed with (1.4) as deformation potential operator.

We write the electron-lattice interaction matrix element as

$$M_{ll'} = \langle \phi_l | E^I | \phi_{l'} \rangle \,. \tag{1.6}$$

Here ϕ_l is the usual combination of Bloch functions and lattice wave functions,

$$\phi_l(\mathbf{x}, q) = \psi_{n\mathbf{k}}(\mathbf{x})\chi_{\{N\}}(q)\,, \tag{1.7}$$

with

$$H_e\psi_{n\mathbf{k}} = E_n(\mathbf{k})\psi_{n\mathbf{k}}\,, \tag{1.8}$$

$$H_L\chi_{\{N\}} = \{\sum_\nu (N_\nu + \tfrac{1}{2})\hbar\omega_\nu\}\chi_{\{N\}}\,, \tag{1.9}$$

$$H_e = \sum_i \frac{p_i^2}{2m} + V_0(\mathbf{x})\,, \tag{1.10}$$

$$H_L = \sum_\nu \left\{\frac{|P_\nu|^2}{2M} + \frac{M\omega_\nu^2|q_\nu|^2}{2}\right\}. \tag{1.11}$$

In these equations, m and M are the electron and cell masses respectively, ν refers to both phonon wave number $\mathbf{f}$ and polarization s, and $\chi_{\{N\}}(q)$ is given by

$$\chi_{\{N\}}(q) = \prod_\nu \varphi_{N_\nu}(q_\nu)\,, \tag{1.12}$$

where each of the $\varphi_{N_\nu}(q_\nu)$ satisfies a harmonic oscillator wave equation. $\{N\}$ refers to the entire set of phonon occupation numbers, and q to the whole set q_ν of normal coordinates.

The procedure for obtaining the various transport coefficients is now exactly as usual, with transition probabilities

$$P_{ll'} = \frac{2\pi}{\hbar}\,|M_{ll'}|^2\,\delta(E_{l'} - E_l)\,, \tag{1.13}$$

where

$$E_l = E_n(\mathbf{k}) + \sum_\nu (N_\nu + \tfrac{1}{2})\hbar\omega_\nu\,. \tag{1.14}$$

To apply this formalism, we require the energy eigenvalues and eigenfunctions near the valence band edge, to the lowest nonvanishing order.

2. The valence band

The structure of the germanium type valence band, including the effect of spin-orbit coupling, has been treated by Dresselhaus, Kip and Kittel,[8] Adams,[9] and others.[10] The discussion below is an extension of that of Adams, using the usual methods to obtain the energy, as a function of wave number near $\mathbf{k}=0$, and the eigenfunctions with respect to which the matrix elements of E^l are to be calculated.

The Schrödinger equation for the periodic part of the electron wave function, neglecting spin, is

$$\left\{\frac{p^2}{2m} + V_0(\mathbf{x}) + \frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p}\right\} w_{n\mathbf{k}} = \varepsilon_n(\mathbf{k})w_{n\mathbf{k}}\,, \tag{2.1}$$

where n is a band index, and

$$\varepsilon_n(\mathbf{k}) = E_n(\mathbf{k}) - \frac{\hbar^2k^2}{2m}\,. \tag{2.2}$$

$(\hbar/m)\mathbf{k}\cdot\mathbf{p}$ is now treated as a perturbation on the system

$$\left\{\frac{p^2}{2m} + V_0\right\} w^0 = E^0 w^0\,. \tag{2.3}$$

For the valence band in germanium, (2.3) has a threefold degeneracy, the wave functions transforming under cubic operations like x, y, z. We denote these functions (the "v representation") by v_1, v_2, v_3, and their common energy by E_0. The wave functions for the other bands at $\mathbf{k}=0$ will be denoted by g_i and their energies by E_i^0.

The first order contribution of the $\mathbf{k}\cdot\mathbf{p}$ term vanishes since inversion is a symmetry operation. The second order contribution is given, in the v representation, by the matrix[11]

$$H = \begin{bmatrix} Mk^2 + (L-M)k_1^2 & Nk_1k_2 & Nk_1k_3 \\ Nk_1k_2 & Mk^2 + (L-M)k_2^2 & Nk_2k_3 \\ Nk_1k_3 & Nk_2k_3 & Mk^2 + (L-M)k_3^2 \end{bmatrix}, \tag{2.4}$$

where

$$L = \frac{\hbar^2}{m^2}\sum_i{}' \frac{(v_1, p_1g_i)(g_i, p_1v_1)}{E_0 - E_i^0}\,, \tag{2.5}$$

$$M = \frac{\hbar^2}{m^2}\sum_i{}' \frac{(v_1, p_2g_i)(g_i, p_2v_1)}{E_0 - E_i^0}\,, \tag{2.6}$$

$$N = \frac{\hbar^2}{m^2}\sum_i{}' \left\{\frac{(v_1, p_1g_i)(g_i, p_2v_2) + (v_1, p_2g_i)(g_i, p_1v_2)}{E_0 - E_i^0}\right\}. \tag{2.7}$$

(The prime on the summations signifies that we are not including the v functions themselves.)

When spin is taken into account, the degeneracy becomes six-fold, the valence band functions being $v_j\alpha$ and $v_j\beta$ where α and β are eigenstates of σ_z with eigenvalues $+1$ and -1. The degeneracy is partially removed by the spin-orbit interaction,[12] $Q = \eta[\nabla V_0 \times \mathbf{p}]\cdot\boldsymbol{\sigma}$, where $\eta = \hbar/4m^2c^2$. The matrix is found to be

$$Q = a\begin{bmatrix} 0 & -i & 0 & 0 & 0 & 1 \\ i & 0 & 0 & 0 & 0 & -i \\ 0 & 0 & 0 & -1 & i & 0 \\ 0 & 0 & -1 & 0 & i & 0 \\ 0 & 0 & -i & -i & 0 & 0 \\ 1 & i & 0 & 0 & 0 & 0 \end{bmatrix}, \tag{2.8}$$

where

$$a = i\eta(v_1, [\nabla V_0 \times \mathbf{p}]_3\, v_2)\,, \tag{2.9}$$

and the ordering of the matrix (2.8) is $v_1\alpha$, $v_2\alpha$, $v_3\alpha$, $v_1\beta$, $v_2\beta$, $v_3\beta$.

The $\mathbf{k}\cdot\mathbf{p}$ contribution is now also given by a 6×6 matrix,

$$H_1 = \begin{bmatrix} H & 0 \\ 0 & H \end{bmatrix}, \tag{2.10}$$

where H is given by (2.4).

It is convenient to transform to a basis in which $\bar{Q}=U^{\dagger}QU$ is diagonal. The transformation matrix used here is

$$U=\begin{pmatrix} -1/\sqrt{2} & 0 & 1/\sqrt{6} & 0 & 0 & 1/\sqrt{3} \\ -i/\sqrt{2} & 0 & -i/\sqrt{6} & 0 & 0 & -i/\sqrt{3} \\ 0 & 2/\sqrt{6} & 0 & 0 & 1/\sqrt{3} & 0 \\ 0 & -1/\sqrt{6} & 0 & 1/\sqrt{2} & 1/\sqrt{3} & 0 \\ 0 & -i/\sqrt{6} & 0 & -i/\sqrt{2} & i/\sqrt{3} & 0 \\ 0 & 0 & 2/\sqrt{6} & 0 & 0 & -1/\sqrt{3} \end{pmatrix} \quad (2.11)$$

and

$$\bar{Q}=a\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 & 0 & -2 \end{pmatrix} \quad (2.12)$$

The new basis states, Z_i $(i=1 \ldots 6)$, are

$$Z_i=\sum_{j=1}^{3}[\alpha U_{ji}+\beta U_{j+3,i}]v_j\,. \quad (2.13)$$

The Z_i are analogous to atomic states with quantum numbers j, m_j. (In the tight-binding limit, we would call this a j, m_j representation.) The correspondence is expressed by

i	1	2	3	4	5	6
j	3/2	3/2	3/2	3/2	1/2	1/2
m_j	3/2	1/2	−1/2	−3/2	1/2	−1/2

Transforming (2.10) to the new representation, we find

$$\bar{H}_1=\begin{pmatrix} \frac{H_{11}+H_{22}}{2} & \frac{-H_{13}+iH_{23}}{\sqrt{3}} & \frac{H_{22}-H_{11}+2iH_{12}}{2\sqrt{3}} & 0 & \frac{-H_{13}+iH_{23}}{\sqrt{6}} & \frac{H_{22}-H_{11}+2iH_{12}}{\sqrt{6}} \\ \frac{-(H_{13}+iH_{23})}{\sqrt{3}} & \frac{H_{11}+H_{22}+4H_{33}}{6} & 0 & \frac{H_{22}-H_{11}+2iH_{12}}{2\sqrt{3}} & \frac{2H_{33}-H_{11}-H_{22}}{3\sqrt{2}} & \frac{H_{13}-iH_{23}}{\sqrt{2}} \\ \frac{H_{22}-H_{11}-2iH_{12}}{2\sqrt{3}} & 0 & \frac{H_{11}+H_{22}+4H_{33}}{6} & \frac{H_{13}-iH_{23}}{\sqrt{3}} & \frac{H_{13}+iH_{23}}{\sqrt{2}} & \frac{H_{11}+H_{22}-2H_{33}}{6/\sqrt{2}} \\ 0 & \frac{H_{22}-H_{11}-2iH_{12}}{2\sqrt{3}} & \frac{H_{13}+iH_{23}}{\sqrt{3}} & \frac{H_{11}+H_{22}}{2} & \frac{H_{11}-H_{22}+2iH_{12}}{\sqrt{6}} & \frac{-(H_{13}+iH_{23})}{\sqrt{6}} \\ \frac{-(H_{13}+iH_{23})}{\sqrt{6}} & \frac{2H_{33}-H_{11}-H_{22}}{6/\sqrt{2}} & \frac{H_{13}-iH_{23}}{\sqrt{2}} & \frac{H_{11}-H_{22}-2iH_{12}}{\sqrt{6}} & \frac{H_{11}+H_{22}+H_{33}}{3} & 0 \\ \frac{H_{11}-H_{22}+2iH_{12}}{-\sqrt{6}} & \frac{H_{13}+iH_{23}}{\sqrt{2}} & \frac{H_{11}+H_{22}-2H_{33}}{6/\sqrt{2}} & \frac{-(H_{13}-iH_{23})}{\sqrt{6}} & 0 & \frac{H_{11}+H_{22}+H_{33}}{3} \end{pmatrix} \quad (2.14)$$

where the H_{ij} denote the elements of the matrix H (Eq. 2.4).

We now measure all energies relative to the top of the valence band (i.e., the $E_{3/2}(0)$ level); then we require the eigenvalues and eigenvectors of $\bar{H}_1+\bar{Q}-a$. It can be shown[13] that it is permissible to neglect those matrix elements connecting states of different j (i.e., the lower left 4×2 and the upper right 2×4) – they contribute only to order k^4/a. The secular determinant then factors into a 4×4 and a 2×2. The 2×2 corresponds to the $j=1/2$ level and, in germanium, it is too far removed in energy[1] (~0.3 ev) from the two degenerate $j=3/2$ levels to be of importance in calculating transition rates. Accordingly, we will not list the energies and wave functions for this band.

The remaining 4×4 results in two twofold degenerate bands. Taking (2.2) into account, we find for the $j=3/2$ band

$$E=Ak^2\pm\mathfrak{R}(\mathbf{k})\,, \quad (2.15)$$

where

$$A=\frac{\hbar^2}{2m}+\frac{L+2M}{3}\,, \quad (2.16)$$

$$\mathfrak{R}(\mathbf{k}) = \left\{ \left(\frac{L-M}{3} \right)^2 k^4 + \left[\frac{N^2-(L-M)^2}{3} \right] [k_1^2 k_2^2 + k_2^2 k_3^2 + k_3^2 k_1^2] \right\}^{1/2} . \tag{2.17}$$

The eigenvectors, referred to the basis Z_i, are found to be:

$$\xi_1 = \mathfrak{N} \begin{pmatrix} \phi \\ 0 \\ -\lambda \\ \chi \end{pmatrix}, \quad \xi_2 = \mathfrak{N} \begin{pmatrix} \chi^* \\ \lambda \\ 0 \\ -\phi^* \end{pmatrix}: \quad E = Ak^2 + \mathfrak{R} .$$

$$\xi_3 = \mathfrak{N} \begin{pmatrix} 0 \\ \phi \\ \chi^* \\ \lambda \end{pmatrix}, \quad \xi_4 = \mathfrak{N} \begin{pmatrix} \lambda \\ -\chi \\ \phi^* \\ 0 \end{pmatrix}; \quad E = Ak^2 - \mathfrak{R} . \tag{2.18}$$

Here

$$\mathfrak{N} = \{ |\phi|^2 + |\chi|^2 + \lambda^2 \}^{-\frac{1}{2}} ,$$

$$\phi = \frac{(L-M)(k_2^2 - k_1^2) + 2iNk_1k_2}{2\sqrt{3}} ,$$

$$\chi = \frac{Nk_3}{\sqrt{3}} (k_1 + ik_2) ,$$

$$\lambda = \frac{(L-M)}{6} (k^2 - 3k_3^2) - \mathfrak{R} . \tag{2.19}$$

The functions ξ_1 and ξ_2 are associated with the larger effective mass, ξ_3 and ξ_4 with the smaller mass.

The ξ_j may all be written in the form

$$\xi_j = \sum_{k=1}^{3} [\alpha a_{jk} + \beta b_{jk}] v_k , \tag{2.20}$$

where the coefficients a_{jk} and b_{jk} contain the $\mathbf{k}$ dependence. Making use of Eqs. (2.13) and (2.18), we obtain for the a's and b's:

$$a_{11} = -\mathfrak{N}\left(\frac{\phi}{\sqrt{2}} + \frac{\lambda}{\sqrt{6}} \right) \qquad a_{12} = -i\,\mathfrak{N}\left(\frac{\phi}{\sqrt{2}} - \frac{\lambda}{\sqrt{6}} \right) \qquad a_{13} = 0$$

$$a_{21} = \frac{-\mathfrak{N}\chi^*}{\sqrt{2}} \qquad a_{22} = \frac{-i\,\mathfrak{N}\chi^*}{\sqrt{2}} \qquad a_{23} = \frac{2\mathfrak{N}\lambda}{\sqrt{6}}$$

$$a_{31} = \frac{\mathfrak{N}\chi^*}{\sqrt{6}} \qquad a_{32} = \frac{-i\,\mathfrak{N}\chi^*}{\sqrt{6}} \qquad a_{33} = \frac{2\mathfrak{N}\phi}{\sqrt{6}}$$

$$a_{41} = \mathfrak{N}\left(\frac{\phi^*}{\sqrt{6}} - \frac{\lambda}{\sqrt{2}} \right) \qquad a_{42} = -i\,\mathfrak{N}\left(\frac{\phi^*}{\sqrt{6}} + \frac{\lambda}{\sqrt{2}} \right) \qquad a_{43} = \frac{-2\mathfrak{N}\chi}{\sqrt{6}}$$

$$b_{11} = \frac{\mathfrak{N}\chi}{\sqrt{2}} \qquad b_{12} = \frac{-i\,\mathfrak{N}\chi}{\sqrt{2}} \qquad b_{13} = \frac{-2\mathfrak{N}\lambda}{\sqrt{6}}$$

$$b_{21} = -\mathfrak{N}\left(\frac{\phi^*}{\sqrt{2}} + \frac{\lambda}{\sqrt{6}} \right) \qquad b_{22} = i\,\mathfrak{N}\left(\frac{\phi^*}{\sqrt{2}} - \frac{\lambda}{\sqrt{6}} \right) \qquad b_{23} = 0$$

$$b_{31} = \mathfrak{N}\left(\frac{\lambda}{\sqrt{2}} - \frac{\phi}{\sqrt{6}} \right) \qquad b_{32} = -i\,\mathfrak{N}\left(\frac{\lambda}{\sqrt{2}} + \frac{\phi}{\sqrt{6}} \right) \qquad b_{33} = \frac{2\mathfrak{N}\chi^*}{\sqrt{6}}$$

$$b_{41} = \frac{\mathfrak{N}\chi}{\sqrt{6}} \qquad b_{42} = \frac{i\,\mathfrak{N}\chi}{\sqrt{6}} \qquad b_{43} = \frac{2\mathfrak{N}\phi^*}{\sqrt{6}} \tag{2.21}$$

3. The electron-phonon interaction matrix element

The matrix element for the electron-phonon interaction is given by Eq. (1.6) which, on account of (1.1), we may write

$$M_{ll'} = \tfrac{1}{2} \sum_{i,j} \langle \psi_{n\mathbf{k}} \chi_{\{N\}} | S^{ij}\, \mathfrak{D}^{ji} + \mathfrak{D}^{ji}\, S^{ij} | \psi_{n'\mathbf{k}'} \chi_{\{N'\}} \rangle . \tag{3.1}$$

We first calculate $(S^{ij}\,\mathfrak{D}^{ji})_{ll'} = \Sigma_{l''} S^{ij}_{ll''} \mathfrak{D}^{ji}_{l''l'}$, where

$$S^{ij}_{ll''} = \int dq d^3\mathbf{x} \chi^*_{\{N\}}(q) \chi_{\{N''\}}(q) \exp[i(\mathbf{k}''-\mathbf{k})\cdot\mathbf{x}] w^*_{n\mathbf{k}} w_{n''\mathbf{k}''} S^{ij} . \tag{3.2}$$

Making use of (1.3) we may write

$$S^{ij}_{ll''} = i \sum_{\nu} V_j(\nu) f_i \langle \chi_{\{N\}} | q\nu | \chi_{\{N''\}} \rangle \times \int \exp[i(\mathbf{f} - (\mathbf{k}-\mathbf{k}''))\cdot\mathbf{x}] w^*_{n\mathbf{k}} w_{n''\mathbf{k}''} d^3\mathbf{x} . \tag{3.3}$$

The last integral is nonzero only if $\mathbf{f} - (\mathbf{k}-\mathbf{k}'') = 2\pi\mathbf{g}$, where $\mathbf{g}$ is any vector of the reciprocal lattice. Since for the situation we are considering here (long-wavelength phonons and small $\mathbf{k}$), Umklapp processes do not occur, we take $\mathbf{g}=0$; then

$$S^{ij}_{ll''} = i \sum_{\nu} V_j(\nu) f_i \langle \chi_{\{N\}} | q\nu | \chi_{\{N''\}} \rangle \delta_{\mathbf{f},\mathbf{k}-\mathbf{k}''} I_{nn''}(\mathbf{k}, \mathbf{k}'') \tag{3.4}$$

where

$$I_{nn''}(\mathbf{k}, \mathbf{k}'') = \int d^3\mathbf{x} w^*_{n\mathbf{k}} w_{n''\mathbf{k}''} . \tag{3.5}$$

The nonvanishing matrix elements of q_ν are

$$\begin{aligned}\langle \chi_{\{N\}} | q_\nu | \chi_{\{N''\}} \rangle &= \left\{ \frac{\hbar(N_\nu+1)}{2nM\omega_\nu} \right\}^{\frac{1}{2}}, \quad N_\nu'' = N_{\nu+1} \\ &= \left\{ \frac{\hbar N_\nu}{2nM\omega_\nu} \right\}^{\frac{1}{2}}, \quad N_\nu'' = N_{\nu-1}\end{aligned} \tag{3.6}$$

with $N''_\mu = N_\mu$ for $\mu \neq \nu$;

where n is the number of unit cells in the crystal.[14] We now set

$$N_\nu = \left\{ \exp\left[\frac{\hbar\omega_\nu}{kT} \right] - 1 \right\}^{-1} \approx \frac{kT}{\hbar\omega_\nu} , \tag{3.7}$$

where the last approximation is valid at all but the very lowest temperatures.

The matrix element is now

$$M_{nn'}(\mathbf{k}, \mathbf{k}') = \frac{i(kT)^{\frac{1}{2}}}{2(2nM)^{\frac{1}{2}}} \sum_{i,j} \frac{f_i V_j(\mathbf{f}, s)}{\omega(\mathbf{f}, s)} B^{ji}_{nn'}(\mathbf{k}, \mathbf{k}') , \tag{3.8}$$

where

$$B^{ji}_{nn'}(\mathbf{k}, \mathbf{k}') = \sum_{n''=1}^{4} \{ I_{nn''}(\mathbf{k}, \mathbf{k}') D^{ji}_{n''n'}(\mathbf{k}') + I_{n''n'} D^{ji}_{nn''}(\mathbf{k}) \} \tag{3.9}$$

and

$$\mathbf{f} = \mathbf{k} - \mathbf{k}' . \tag{3.10}$$

The quantity $D^{ji}_{nm}(\mathbf{k})$ appearing in (3.9) is defined by

$$D^{ji}_{nm}(\mathbf{k}) = \langle \psi_{n\mathbf{k}} | \mathfrak{D}^{ji} | \psi_{m\mathbf{k}} \rangle = \left\langle w_{n\mathbf{k}} \left| \frac{-p_j p_i}{m} + U^{ji} \right| w_{m\mathbf{k}} \right\rangle \tag{3.11}$$

and depends on the deformation potential elements[15]

$$\left.\begin{aligned} F &\equiv \left\langle v_1 \left| \frac{-p_1^2}{m} + U^{11} \right| v_1 \right\rangle , \\ G &\equiv \left\langle v_1 \left| \frac{-p_2^2}{m} + U^{22} \right| v_1 \right\rangle , \end{aligned}\right\} \tag{3.12}$$

and

$$J \equiv \left\langle v_1 \left| \frac{-p_1 p_2}{m} + U^{12} \right| v_2 \right\rangle . \tag{3.13}$$

We have

$$\left.\begin{aligned} D^{11}_{\mu\nu} &= A^{11}_{\mu\nu} F + (A^{22}_{\mu\nu} + A^{33}_{\mu\nu}) G , \\ D^{22}_{\mu\nu} &= A^{22}_{\mu\nu} F + (A^{33}_{\mu\nu} + A^{11}_{\mu\nu}) G , \\ D^{33}_{\mu\nu} &= A^{33}_{\mu\nu} F + (A^{11}_{\mu\nu} + A^{22}_{\mu\nu}) G , \end{aligned}\right\} \tag{3.14}$$

and

$$D^{ij}_{\mu\nu} = (A^{ij}_{\mu\nu} + A^{ji}_{\mu\nu}) J . \qquad (i \neq j) \tag{3.15}$$

Here

$$A^{ij}_{\mu\nu}(\mathbf{k}) = a^*_{\mu i} a_{\nu j} + b^*_{\mu i} b_{\nu j} . \tag{3.16}$$

The sum over bands indicated in (3.9) is restricted, in this treatment, to the two degenerate valence bands. We are calculating matrix elements in the limit $|\mathbf{k}| \to 0$ and $|\mathbf{k}'| \to 0$, and the contributions from the other bands vanish in this limit. The $I_{nm}(\mathbf{k}, \mathbf{k}')$ that appear in the sum over the valence bands may be given explicitly in terms of the parameters ϕ, χ, λ and $\mathfrak{N}$ by making use of (2.20), (2.21) and (2.22); we find that

$$I_{nm}(\mathbf{k}, \mathbf{k}') = \sum_{\mu=1}^{3} (a^*_{n\mu}(\mathbf{k}) a_{m\mu}(\mathbf{k}') + b^*_{n\mu}(\mathbf{k}) b_{m\mu}(\mathbf{k}')) \tag{3.17}$$

which results in:

$$\begin{aligned}
I_{11} &= \mathfrak{N}(\mathbf{k})\mathfrak{N}(\mathbf{k}')\{\phi^*(\mathbf{k})\phi(\mathbf{k}') + \chi^*(\mathbf{k})\chi(\mathbf{k}') + \lambda(\mathbf{k})\lambda(\mathbf{k}')\} \\
I_{22} &= I^*_{11}; \quad I_{33} = I_{22}; \quad I_{44} = I_{11} \\
I_{12} &= \mathfrak{N}(\mathbf{k})\mathfrak{N}(\mathbf{k}')\{\phi(\mathbf{k})\chi(\mathbf{k}') - \chi(\mathbf{k})\phi(\mathbf{k}')\}^* \\
I_{13} &= \mathfrak{N}(\mathbf{k})\mathfrak{N}(\mathbf{k}')\{\chi(\mathbf{k})\lambda(\mathbf{k}') - \lambda(\mathbf{k})\chi(\mathbf{k}')\}^* \\
I_{14} &= \mathfrak{N}(\mathbf{k})\mathfrak{N}(\mathbf{k}')\{\phi(\mathbf{k})\lambda(\mathbf{k}') - \lambda(\mathbf{k})\phi(\mathbf{k}')\}^* \\
I_{34} &= \mathfrak{N}(\mathbf{k})\mathfrak{N}(\mathbf{k}')\{\chi(\mathbf{k})\phi^*(\mathbf{k}') - \phi^*(\mathbf{k})\chi(\mathbf{k}')\} \\
I_{23} &= -I^*_{14} \\
I_{24} &= I^*_{13}
\end{aligned} \tag{3.18}$$

with those not listed here given by

$$I_{mn}(\mathbf{k}, \mathbf{k}') = -I^*_{nm}(\mathbf{k}, \mathbf{k}') .$$

Before concluding this Section, we rewrite the matrix element (3.8) in the form in which we will use it in Part II of this work. For long-wavelength phonons we may replace the frequency spectrum by a simple linear dependence of ω on wave number,

$$\omega(\mathbf{f}, s) = c_s(\mathbf{f}) f , \tag{3.19}$$

where the wave velocity c_s will, in general, be a function of direction of propagation. With this simplification,

$$M_{nn'}(\mathbf{k}, \mathbf{k}') = \frac{i(kT)^{\frac{1}{2}}}{2(2nM)^{\frac{1}{2}}} \sum_{i,j} \frac{V_j(\mathbf{f}, s) \cos\theta_i B^{ji}_{nn'}(\mathbf{k}, \mathbf{k}')}{c_s(\mathbf{f})} \tag{3.20}$$

the angle θ_i being defined by $f_i = f \cos\theta_i$. Although a detailed treatment of the $\mathbf{k}$ and $\mathbf{k}'$ dependence of the $B^{ji}_{nn'}$ will be deferred to Part II, we observe here the important fact that they depend only on the directions of $\mathbf{k}$ and $\mathbf{k}'$ reckoned from the singular zone center point. This is easily seen from (2.19) and (2.21).

The coefficients $f(\mathbf{k}, \mathbf{k}')$, $g(\mathbf{k}, \mathbf{k}')$, $j(\mathbf{k}, \mathbf{k}')$ of the relation

$$B = fF + gG + jJ \tag{3.21}$$

are in general complicated functions, of the wave vector directions $\hat{\mathbf{k}}$ and $\hat{\mathbf{k}}'$, which depend on the constants L, M, N of the energy functions. For certain pairs $\hat{\mathbf{k}}$, $\hat{\mathbf{k}}'$ with

high symmetry, however, f, g, j reduce to simple numbers independent of L, M, and N. This is true when $\hat{\mathbf{k}}$, $\hat{\mathbf{k}}'$ both belong to the "star" of six (1, 0, 0) directions, and is true when $\hat{\mathbf{k}}$, $\hat{\mathbf{k}}'$ both belong to the star of eight (1, 1, 1) directions. One may propose approximate theories of the transport constants involving only the matrix elements for these pairs of star directions, and so representing some interpolation of the matrix elements between the special values of B. In the present work we will simply tabulate, in the Appendix, the coefficients f, g, j for the (1, 0, 0) star and for the (1, 1, 1) star together with the I and D coefficients from which they are derived.

Recently Pikus and Bir have announced a treatment of lattice scattering of holes which, for the acoustic modes, is on the same basis as the work presented here and presumably leads to the same results.[16] In two papers which recently came to our notice, they introduce the same presentation of the effects of strain on the electron Hamiltonian[17] as is used here following Adams,[9] and essentially the same deformation potential tensor-operator[18] as was independently obtained by Whitfield.[4]

4. The spin-lattice interaction

Whitfield's general result is that the electron-lattice interaction part of the Hamiltonian[19] (to be evaluated in the Bloch representation) is $H'-H$ where H is the electron Hamiltonian in the unstrained crystal, and H' is obtained by replacing $\mathbf{p}$, ∇, etc., in H by

$$\mathbf{p}'=T^{\dagger}\mathbf{p}T, \tag{4.1}$$

etc., and V_0 by V_0' as given in Eq. (4.5) below. Here, to first order in strain,

$$T=1-\frac{i}{2\hbar}\sum_j (u_j p_j+p_j u_j)\,. \tag{4.2}$$

We have so far omitted the contribution to $H'-H$ from the spin-orbit term, Q, of H. This contribution is

$$Q'-Q=\eta\boldsymbol{\sigma}\cdot[\nabla' V_0'\times\mathbf{p}'-\nabla V_0\times\mathbf{p}]\equiv\eta\boldsymbol{\sigma}\cdot\mathbf{R}\,. \tag{4.3}$$

Making use of the results[20]

$$\begin{aligned} p_i'&=p_i-\sum_j S^{ij}p_j \\ \nabla_i'&=\nabla_i-\sum_j S^{ij}\nabla_j \end{aligned} \tag{4.4}$$

and the expression[4] for V_0'

$$V_0'=V_0+\sum_{i,j} S^{ij}\,U^{ji}(\mathbf{x})\,, \tag{4.5}$$

we find[19,20]

$$\mathbf{R}=[\sum_{i,j} S^{ij}\,\nabla U^{ji}-\tilde{\nabla}V_0]\times\mathbf{p}-\nabla V_0\times\tilde{\mathbf{p}}\,, \tag{4.6}$$

where

$$\tilde{\nabla}_i=\sum_j S^{ij}\nabla_j \qquad \tilde{p}_i=\sum_j S^{ij}p_j\,. \tag{4.7}$$

The contribution of $\eta\boldsymbol{\sigma}\cdot\mathbf{R}$ to the matrix elements for electron scattering is calculated in the same way as in Section 3 for the operator E^I given by (1.1). It is thus obtained by substituting, for $\mathfrak{D}^{ji}$ in (3.11), the coefficient $\mathfrak{A}^{ji}$ in the expansion

$$\eta\boldsymbol{\sigma}\cdot\mathbf{R}=\sum_{i,j} S^{ij}\mathfrak{A}^{ji}\,. \tag{4.8}$$

It is convenient, however, to compare the matrices for $\mathfrak{D}^{ji}$ and $\mathfrak{A}^{ji}$ not in the representation expressed by $D^{ji}_{nm}(\mathbf{k})$, Eq. (3.11), but in the "Z representation" given by (2.13). For compactness we shall write down a single matrix for

$$\mathfrak{D}(\varepsilon)\equiv\sum_{i,j}\varepsilon_{ij}\mathfrak{D}^{ji} \tag{4.9}$$

(the ε_{ij} are of course c-numbers) and compare it with the matrix of

$$\mathfrak{A}(\varepsilon)\equiv\sum_{i,j}\varepsilon_{ij}\mathfrak{A}^{ji}\,. \tag{4.10}$$

In the Z representation

$$\mathfrak{D}(\varepsilon)=\begin{pmatrix}
(\bar{\varepsilon}_{11}+\bar{\varepsilon}_{22})\left(\frac{F+G}{2}\right)+\bar{\varepsilon}_{33}G & \frac{-2J}{\sqrt{3}}(\bar{\varepsilon}_{13}-i\bar{\varepsilon}_{23}) & 0 & \frac{1}{\sqrt{12}}[(\bar{\varepsilon}_{22}-\bar{\varepsilon}_{11})(F-G)-4i\bar{\varepsilon}_{12}J] \\
\frac{-2J}{\sqrt{3}}(\bar{\varepsilon}_{13}+i\bar{\varepsilon}_{23}) & \frac{1}{3}\left[\bar{\varepsilon}_{33}(2F+G)+\left(\frac{\bar{\varepsilon}_{11}+\bar{\varepsilon}_{22}}{2}\right)(F+5G)\right] & \frac{1}{\sqrt{12}}[(\bar{\varepsilon}_{22}-\bar{\varepsilon}_{11})(F-G)-4i\bar{\varepsilon}_{12}J] & 0 \\
\frac{1}{\sqrt{12}}[(\bar{\varepsilon}_{22}-\bar{\varepsilon}_{11})(F-G)+4i\bar{\varepsilon}_{12}J] & 0 & \frac{1}{3}\left[\bar{\varepsilon}_{33}(2F+G)+\left(\frac{\bar{\varepsilon}_{11}+\bar{\varepsilon}_{22}}{2}\right)(F+5G)\right] & \frac{2J}{\sqrt{3}}(\bar{\varepsilon}_{13}-i\bar{\varepsilon}_{23}) \\
0 & \frac{1}{\sqrt{12}}[(\bar{\varepsilon}_{22}-\bar{\varepsilon}_{11})(F-G)+4i\bar{\varepsilon}_{12}J] & \frac{2J}{\sqrt{3}}(\bar{\varepsilon}_{13}+i\bar{\varepsilon}_{23}) & (\bar{\varepsilon}_{11}+\bar{\varepsilon}_{22})\left(\frac{F+G}{2}\right)+\bar{\varepsilon}_{33}G
\end{pmatrix}, \tag{4.11}$$

and in the v representation

$$\mathfrak{A}(\varepsilon)=\begin{pmatrix} 0 & \alpha & \delta & 0 & \mu & \nu \\ -\alpha & 0 & -\zeta & -\mu & 0 & \pi \\ -\delta & \zeta & 0 & -\nu & -\pi & 0 \\ 0 & -\mu^* & -\nu^* & 0 & -\alpha & -\delta \\ \mu^* & 0 & -\pi^* & \alpha & 0 & \zeta \\ \nu^* & \pi^* & 0 & \delta & -\zeta & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & \rho & 0 & \tau-i\rho & -\omega \\ 0 & 0 & -\tau & -\tau+i\rho & 0 & i\omega \\ -\rho & \tau & 0 & \omega & -i\omega & 0 \\ 0 & \tau+i\rho & -\omega & 0 & 0 & -\rho \\ -(\tau+i\rho) & 0 & -i\omega & 0 & 0 & \tau \\ \omega & i\omega & 0 & \rho & -\tau & 0 \end{pmatrix}, \quad (4.12)$$

where

$$\bar{\varepsilon}_{ij}=\tfrac{1}{2}(\varepsilon_{ij}+\varepsilon_{ji})$$

$$\alpha=(\varepsilon_{11}+\varepsilon_{22})[C_1-C_2]+\varepsilon_{33}C_3$$

$$\delta=-\bar{\varepsilon}_{23}(C_2+2C_4)$$

$$\zeta=-\bar{\varepsilon}_{13}(C_2+2C_4)$$

$$\mu=(\bar{\varepsilon}_{13}-i\bar{\varepsilon}_{23})(C_2+2C_4)$$

$$\nu=i(\varepsilon_{11}+\varepsilon_{33})[C_1-C_2]+i\varepsilon_{22}C_3-\bar{\varepsilon}_{12}(C_2+2C_4)$$

$$\pi=(\varepsilon_{22}+\varepsilon_{33})(C_1-C_2)+\varepsilon_{11}C_3-i\bar{\varepsilon}_{12}(C_2+2C_4)$$

$$\rho=(\varepsilon_{32}-\varepsilon_{23})C_2$$

$$\tau=(\varepsilon_{31}-\varepsilon_{13})C_2$$

$$\omega=(\varepsilon_{21}-\varepsilon_{12})C_2$$

$$C_1=\langle v_1|(\nabla U^{11}\times\mathbf{p})_3|v_2\rangle$$

$$C_2=\langle v_1|(\nabla V_0\times\mathbf{p})_3|v_2\rangle$$

$$C_3=\langle v_1|(\nabla U^{33}\times\mathbf{p})_3|v_2\rangle$$

$$C_4=\langle v_1|(\nabla U^{32}\times\mathbf{p})_2|v_2\rangle\,. \quad (4.13)$$

Transforming (4.12) to the Z representation, we find that $\mathfrak{A}(\varepsilon)$ has precisely the same form[21] as (4.11), but with F, G, J replaced by

$$F_s=i[2(C_1-C_2)-C_3]$$

$$G_s=iC_3 \quad (4.14)$$

$$J_s=-i(C_2+2C_4)\,.$$

It is clear from these results that (4.12) may be combined with (4.11) by introducing new constants

$$F_*=F+F_s\,,$$

$$G_*=G+G_s\,, \quad (4.15)$$

$$J_*=J+J_s\,.$$

The contributions from (4.14) are small.

5. Acknowledgments

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Appendix

It is not necessary to derive f, g, j for all pairs of directions $\hat{\mathbf{k}}$, $\hat{\mathbf{k}}'$ belonging to the (1, 0, 0) and (1, 1, 1) stars, because a pair of directions is physically equivalent to a second pair into which it is transformed by a cubic symmetry operation. So we take only the pairs [(1, 0, 0), (1, 0, 0)], [(1, 0, 0), (0, 0, 1)], and [(1, 0, 0), ($\bar{1}$, 0, 0)] for the (1, 0, 0) star, and the pairs [(1, 1, 1), (1, 1, 1)], [(1, 1, 1), ($\bar{1}$, $\bar{1}$, $\bar{1}$)], [(1, 1, 1), (1, $\bar{1}$, 1)], and [(1, 1, 1), ($\bar{1}$, 1, $\bar{1}$)] for the (1, 1, 1) star. The number of I's, D's, and hence B's, to be evaluated is further reduced by some general relations among them. For the I's, these have been given in Section 3. For the D's, the following relations hold for all $\hat{\mathbf{k}}$ and $\hat{\mathbf{k}}'$:

$$D_{12}=D_{34}=0;\ D_{22}=D_{11};\ D_{44}=D_{33};\ D_{24}=D_{13}^*;$$

$$D_{23}=-D_{14}^*\,. \quad (A.1)$$

Furthermore, since D is a hermitian operator, the D's satisfy $D_{\nu\mu}=D_{\mu\nu}^*$, so that for a given pair of superscripts we need list at most four independent D's.

For both the (1, 0, 0) and (1, 1, 1) stars the B's satisfy

$$B_{22}=B_{11}^*;\ B_{44}=B_{33}^*;\ B_{23}=-B_{14}^*;\ B_{32}=-B_{41}^*;$$

$$B_{24}=B_{13}^*;\ B_{42}=B_{31}^*;\ B_{21}=-B_{12}^*\ B_{43}=-B_{34}^*\,, \quad (A.2)$$

while the following relationships hold for the (1, 0, 0) star, but not for the (1, 1, 1) star:

$$B_{31}=B_{13}^*;\ B_{42}=B_{24}^*;\ B_{34}=B_{12}^*\,. \quad (A.3)$$

The absence of some expected symmetry relations in (A.2) is accounted for by the choice of eigenvectors as given in Eq. (2.18). By choosing suitable linear combinations of the two eigenstates for a given energy, one can introduce additional symmetries; the form (2.18) was chosen because it involves the smallest number of parameters.

From Eq. (2.19) it is evident that the D's and I's, and hence the B's, are unchanged if $\hat{\mathbf{k}}$ is changed to $-\hat{\mathbf{k}}$. This means that the B's are exactly the same for the transition (1, 0, 0)→($\bar{1}$, 0, 0) as for the transition (1, 0, 0)→(1, 0, 0); hence we list only the latter in

Tables 1-6. Likewise $(1, 1, 1)\rightarrow(\bar{1}, \bar{1}, \bar{1})$ has the same B's as $(1, 1, 1)\rightarrow(1, 1, 1)$, and $(1, 1, 1)\rightarrow(1, \bar{1}, 1)$ has the same B's as $(1, 1, 1)\rightarrow(\bar{1}, 1, \bar{1})$.

For the $(1, 0, 0)\rightarrow(1, 0, 0)$ and $(1, 1, 1)\rightarrow(1, 1, 1)$ transitions, we find that $I_{nm}=\delta_{nm}$, so that $B^{ij}_{nm}=2D^{ij}_{nm}$; therefore we list only the B's for these transitions. For $(1, 1, 1)\rightarrow(1, \bar{1}, 1)$ we find:

$$I_{11}=\frac{1-i}{3}\,;\ I_{33}=\frac{1+i}{3}\,;\ I_{34}=-I_{12}=\frac{i}{3}\,;$$

$$I_{13}=I_{14}=\frac{i}{\sqrt{3}}\,;\quad I_{mn}=I_{nm}\,, \tag{A.4}$$

while for $(1, 0, 0)\rightarrow(0, 0, 1)$,

$$I_{14}=-I_{23}=I_{32}=-I_{41}=\sqrt{3}/2\,;$$

$$I_{ii}=\tfrac{1}{2}\,. \tag{A.5}$$

All other I's are zero. Furthermore, the tensor components of the form $C^{nn}_{\mu\nu}$ have $j=0$ while those of the form $C^{nm}_{\mu\nu}$ $(n\neq m)$ have $f=g=0$; these entries are therefore omitted in the tables.

Table 1 $\mathbf{k}=(0, 0, 1)$

	n	n'	f	g		n	n'	j
D^{11}	1	1	1/6	5/6	D^{12}	1	1	0
	3	3	1/2	1/2		3	3	0
	1	3	0	0		1	3	0
	1	4	$1/2\sqrt{3}$	$-1/2\sqrt{3}$		1	4	$i/\sqrt{3}$
D^{22}	1	1	1/6	5/6	D^{13}	1	1	0
	3	3	1/2	1/2		3	3	0
	1	3	0	0		1	3	$-1/\sqrt{3}$
	1	4	$-1/2\sqrt{3}$	$1/2\sqrt{3}$		1	4	0
D^{33}	1	1	2/3	1/3	D^{23}	1	1	0
	3	3	0	1		3	3	0
	1	3	0	0		1	3	$i/\sqrt{3}$
	1	4	0	0		1	4	0

Table 2 $\mathbf{k}=(1, 0, 0)$; $\mathbf{k}'=(0, 0, 1)$

	n	n'	f	g		n	n'	j
B^{11}	1	1	2/3	1/3	B^{12}	1	1	$-i$
	3	3	0	1		3	3	i
	1	2	0	0		1	2	0
	1	3	0	0		1	3	0
	1	4	$2/\sqrt{3}$	$1/\sqrt{3}$		1	4	$i/\sqrt{3}$
	3	2	0	$\sqrt{3}$		3	2	$-i/\sqrt{3}$
B^{22}	1	1	$-1/3$	4/3	B^{13}	1	1	0
	3	3	1	0		3	3	0
	1	2	0	0		1	2	-1
	1	3	0	0		1	3	$-1/\sqrt{3}$
	1	4	$1/\sqrt{3}$	$2/\sqrt{3}$		1	4	0
	3	2	$1/\sqrt{3}$	$2/\sqrt{3}$		3	2	0
B^{33}	1	1	2/3	1/3	B^{23}	1	1	0
	3	3	0	1		3	3	0
	1	2	0	0		1	2	i
	1	3	0	0		1	3	$i/\sqrt{3}$
	1	4	0	$\sqrt{3}$		1	4	0
	3	2	$2/\sqrt{3}$	$1/\sqrt{3}$		3	2	0

References and footnotes

1. H. Ehrenreich and A. W. Overhauser, *Phys. Rev.* **104,** 331 (1956); *Phys. Rev.* **104,** 649 (1956).
2. The standard theories of electron-phonon interaction are discussed in a number of books and articles. See, for example, F. J. Blatt, *Theory of Mobility of Electrons in Solids,* in *Solid State Physics,* ed. F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1957), Vol. 4; J. M. Ziman, *Electrons and Phonons* (Oxford, 1960). Ehrenreich and Overhauser employ the rigid ion model for optical modes, but they use both the deformable and rigid ion models for acoustic modes.
3. J. Bardeen and W. Shockley, *Phys. Rev.* **80,** 72 (1950). This work was restricted to compressional waves and crystals with a band edge point at the center of the Brillouin zone. The theorem has, however, been used (before Whitfield's work) for all modes and an arbitrary band edge point. See, for example, W. P. Dumke, *Phys. Rev.* **101,** 531 (1956); C. Herring and E. Vogt, *Phys. Rev.* **101,** 944 (1956).
4. G. D. Whitfield, *Phys. Rev. Letters* **2,** 204 (1959); *Phys. Rev.* **121,** 720 (1961).
5. In this paper all summations are explicitly indicated. Also we do not distinguish between covariant and contravariant quantities, so that subscripts and superscripts will be used for notational convenience.
6. If $\mathbf{R}_n$ is the lattice vector from the origin to the center of mass of the n^{th} unit cell, then $\mathbf{u}(\mathbf{R}_n)$ is the displacement of the center of mass of this cell. Letting $\mathbf{u}_{nj}$ be the displacement of the lattice point which belongs in the j^{th} place of the n^{th} unit cell, we may write $\mathbf{u}_{nj}=\Sigma_\nu q_\nu \mathbf{V}_j(\nu)\exp(i\mathbf{f}\cdot\mathbf{R}_n)$, where $\mathbf{V}_j(\nu)$ is the usual polarization vector. This then implies that $\mathbf{V}_\nu=\Sigma_j M_j\mathbf{V}_j(\nu)/\Sigma_j M_j$. For the diamond structure, where there are two atoms per unit cell, $\mathbf{V}_\nu=\frac{1}{2}(\mathbf{V}_1(\nu)+\mathbf{V}_2(\nu))$.
7. See Ref. 4 for a discussion of other possible definitions of a deformation potential operator. The expression used here has the advantage that its matrix elements approach zero in the limit of vanishing coupling.
8. Dresselhaus, Kip and Kittel, *Phys. Rev.* **98,** 368 (1955).
9. E. N. Adams, Chicago Midway Laboratories Report CML-TN-P8, September 1954 (unpublished).

Table 3 $\mathbf{k}=(1,0,0)$; $\mathbf{k}'=(1,0,0)$

	n	n'	f	g		n	n'	j
B^{11}	1	1	4/3	2/3	B^{12}	1	1	0
	3	3	0	2		3	3	0
	1	2	0	0		1	2	0
	1	3	0	0		1	3	0
	1	4	0	0		1	4	$2i/\sqrt{3}$
B^{22}	1	1	1/3	5/3	B^{13}	1	1	0
	3	3	1	1		3	3	0
	1	2	0	0		1	2	0
	1	3	0	0		1	3	$-2/\sqrt{3}$
	1	4	$1/\sqrt{3}$	$-1/\sqrt{3}$		1	4	0
B^{33}	1	1	1/3	5/3	B^{23}	1	1	0
	3	3	1	1		3	3	0
	1	2	0	0		1	2	0
	1	3	0	0		1	3	$2i/\sqrt{3}$
	1	4	$-1/\sqrt{3}$	$1/\sqrt{3}$		1	4	0

Table 4 $\mathbf{k}=(1,\bar{1},1)$

	n	n'	f	g		n	n'	j
D^{11}	1	1	1/3	2/3	D^{12}	1	1	$-1/3$
	3	3	1/3	2/3		3	3	1/3
	1	3	$\frac{-(1+i)}{6\sqrt{3}}$	$\frac{1+i}{6\sqrt{3}}$		1	3	$\frac{-(1+i)}{3\sqrt{3}}$
	1	4	$\frac{3-i}{6\sqrt{3}}$	$\frac{-(3-i)}{6\sqrt{3}}$		1	4	$\frac{2i}{3\sqrt{3}}$
D^{22}	1	1	1/3	2/3	D^{13}	1	1	1/3
	3	3	1/3	2/3		3	3	$-1/3$
	1	3	$\frac{-(1+i)}{6\sqrt{3}}$	$\frac{1+i}{6\sqrt{3}}$		1	3	$\frac{i-2}{3\sqrt{3}}$
	1	4	$\frac{-(3+i)}{6\sqrt{3}}$	$\frac{3+i}{6\sqrt{3}}$		1	4	$\frac{i}{3\sqrt{3}}$
D^{33}	1	1	1/3	2/3	D^{23}	1	1	$-1/3$
	3	3	1/3	2/3		3	3	1/3
	1	3	$\frac{1+i}{3\sqrt{3}}$	$\frac{-(1+i)}{3\sqrt{3}}$		1	3	$\frac{2i-1}{3\sqrt{3}}$
	1	4	$\frac{i}{3\sqrt{3}}$	$\frac{i}{3\sqrt{3}}$		1	4	$\frac{-i}{3\sqrt{3}}$

Table 5 $\mathbf{k}=(1,1,1)$; $\mathbf{k}'=(1,1,1)$

	n	n'	f	g		n	n'	j
B^{11}	1	1	2/3	4/3	B^{12}	1	1	2/3
	3	3	2/3	4/3		3	3	$-2/3$
	1	3	$\frac{i-1}{3\sqrt{3}}$	$\frac{-(i-1)}{3\sqrt{3}}$		1	3	$\frac{2(1-i)}{3\sqrt{3}}$
	1	4	$\frac{3+i}{3\sqrt{3}}$	$\frac{-(3+i)}{3\sqrt{3}}$		1	4	$\frac{4i}{3\sqrt{3}}$
B^{22}	1	1	2/3	4/3	B^{13}	1	1	2/3
	3	3	2/3	4/3		3	3	$-2/3$
	1	3	$\frac{i-1}{3\sqrt{3}}$	$\frac{1-i}{3\sqrt{3}}$				$\frac{-2(2+i)}{3\sqrt{3}}$
	1	4	$\frac{i-3}{3\sqrt{3}}$	$\frac{3-i}{3\sqrt{3}}$		1	4	$\frac{-2i}{3\sqrt{3}}$
B^{33}	1	1	2/3	4/3	B^{23}	1	1	2/3
	3	3	2/3	4/3		3	3	$-2/3$
	1	3	$\frac{2(1-i)}{3\sqrt{3}}$	$\frac{2(i-1)}{3\sqrt{3}}$		1	3	$\frac{2(2i+1)}{3\sqrt{3}}$
	1	4	$\frac{-2i}{3\sqrt{3}}$	$\frac{2i}{3\sqrt{3}}$		1	4	$\frac{-2i}{3\sqrt{3}}$

10. E. O. Kane, *Intern. J. Phys. Chem. Solids* **1**, 82 (1956); Ehrenreich and Overhauser, Ref. 1. See also Pikus and Bir, Ref. 17.
11. The parameters L, M, N that appear in the Shockley matrix (2.4) are the usual ones found in the literature. Adams denotes them respectively by A, B, C. It is possible for confusion to arise here since Adams' A, B, and C are not equivalent to the A, B, C that appear in the standard equation
$E=Ak^2\pm[B^2k^4+C^2(k_1^2k_3^2+k_2^2k_3^2+k_3^2k_1^2)]^{\frac{1}{2}}$.
The constants in the latter are given by:
$A=\hbar^2/2m+\frac{1}{3}(L+2M)$; $B=\frac{1}{3}(L-M)$;
$C^2=\frac{1}{3}[N^2-(L-M)^2]$.
12. We are neglecting a term $\hbar\eta\nabla V_0\times\mathbf{k}\cdot\boldsymbol{\sigma}$ here; this approximation is discussed in E. O. Kane, Ref. 10, where it is concluded that the term is negligible. See also Pikus and Bir, Ref. 17.

Table 6 $\mathbf{k}=(1,1,1)$; $\mathbf{k}'=(1,\bar{1},1)$

	n	n'	f	g
B^{11}	1	1	0	$\frac{2}{3}(1-i)$
	3	3	$\frac{2}{9}(2-i)$	$\frac{2}{9}(1+4i)$
	1	2	$\frac{-2i}{3}$	0
	1	3	$\frac{3i-1}{3\sqrt{3}}$	$\frac{3i+1}{3\sqrt{3}}$
	1	4	$\frac{i+1}{3\sqrt{3}}$	$\frac{5i-1}{3\sqrt{3}}$
	3	4	$\frac{4i}{9}$	$\frac{2i}{9}$
	3	1	$\frac{3i-1}{3\sqrt{3}}$	$\frac{3i+1}{3\sqrt{3}}$
	4	1	$\frac{i+1}{3\sqrt{3}}$	$\frac{5i-1}{3\sqrt{3}}$
B^{22}	1	1	$\frac{-2i}{3}$	$\frac{2}{3}$
	3	3	$\frac{4}{9}(1+i)$	$\frac{2}{9}(1+i)$
	1	2	0	$\frac{-2i}{3}$
	1	3	$\frac{i-1}{3\sqrt{3}}$	$\frac{5i+1}{3\sqrt{3}}$
	1	4	$\frac{3i-1}{3\sqrt{3}}$	$\frac{3i+1}{3\sqrt{3}}$
	3	4	$\frac{-2i}{9}$	$\frac{8i}{9}$
	3	1	$\frac{i-1}{3\sqrt{3}}$	$\frac{5i+1}{3\sqrt{3}}$
	4	1	$\frac{3i-1}{3\sqrt{3}}$	$\frac{3i+1}{3\sqrt{3}}$
B^{33}	1	1	$\frac{2}{3}$	$\frac{-2i}{3}$
	3	3	$\frac{2}{9}(2i-1)$	$\frac{2}{9}(4+i)$
	1	2	0	$\frac{-2i}{3}$
	1	3	$\frac{2(1+i)}{3\sqrt{3}}$	$\frac{2(2i-1)}{3\sqrt{3}}$
	1	4	$\frac{2i}{3\sqrt{3}}$	$\frac{4i}{3\sqrt{3}}$
	3	4	$\frac{4i}{9}$	$\frac{2i}{9}$
	3	1	$\frac{2(1+i)}{3\sqrt{3}}$	$\frac{2(2i-1)}{3\sqrt{3}}$
	4	1	$\frac{2i}{3\sqrt{3}}$	$\frac{4i}{3\sqrt{3}}$

	n	n'	j
B^{12}	1	1	0
	3	3	0
	1	2	$\frac{2}{3}$
	1	3	$\frac{2i}{3\sqrt{3}}$
	1	4	$\frac{2(2i+1)}{3\sqrt{3}}$
	3	4	$-\frac{2}{3}$
	3	1	$\frac{-2i}{3\sqrt{3}}$
	4	1	$\frac{-2(2i+1)}{3\sqrt{3}}$
B^{13}	1	1	$\frac{2}{3}(1-i)$
	3	3	$\frac{-2}{3}(1+i)$
	1	2	$\frac{-2i}{3}$
	1	3	0
	1	4	0
	3	4	$\frac{-2i}{3}$
	3	1	0
	4	1	0
B^{23}	1	1	0
	3	3	0
	1	2	$\frac{-2}{3}$
	1	3	$\frac{4i}{3\sqrt{3}}$
	1	4	$\frac{2(i-1)}{3\sqrt{3}}$
	3	4	$\frac{2}{3}$
	3	1	$\frac{-4i}{3\sqrt{3}}$
	4	1	$\frac{-2(i-1)}{3\sqrt{3}}$

13. Dresselhaus, Kip and Kittel, Ref. 8; E. O. Kane, Ref. 10.
14. See, for example, R. E. Peierls, *Quantum Theory of Solids* (Oxford, 1956), Eq. (1.63).
15. The parameters F, G, J, defined in Eqs. (3.12) and (3.13) correspond to Adams' constants E_{11}, E_{12}, $E_{44}/2$. Also observe that in (3.13) interchanging v_1 and v_2 leaves the integral unaltered. The form of Eq. (3.15) is a consequence of this invariance.
16. G. E. Pikus and G. L. Bir, *Abstracts for the International Conference on Semiconductor Physics,* Prague 1960; and to be published.
17. G. E. Pikus and G. L. Bir, *Soviet Physics – Solid State,* **1,** 1502 (1960). See also **1,** 1675 (1960).
18. G. E. Pikus and G. L. Bir, *Soviet Physics – Solid State,* **1,** 136 (1959).
19. These results include terms only up to first order in the strain; higher order terms have been discarded.
20. In Eq. (4.4), we have neglected a term in ∇S^{ij}; this gives a negligible contribution to the matrix element for acoustic modes.
21. We are not neglecting the contribution from the antisymmetric part of ε_{ij}; it makes a nonvanishing contribution to the matrix elements in the v representation, but when one transforms to the Z representation the resulting matrix is identically zero.

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