TABLE I. Structure factor for the diamond structure.

hkl	$\lvert S_{hkl}\rvert$
111	$4\sqrt{2}$
200	0
220	8
222	0
311	$4\sqrt{2}$

experiment of WP measures the shape of the Jones zone, modified by the fact that the contribution of each quantum state is weighted by its respective Fourier amplitude. This interpretation is supported by Fig. 1(a), in which it is seen that the region of high contour density roughly follows the boundary of the Jones zone. The deviation along the ⟨100⟩ directions will be due to the above-mentioned weighting, and to the fact that the truncation at $l = 8$ of the expansion in cubic harmonics will cause some smearing of the angular variations in the momentum density. Figure 1(b) shows that the maxima in the ⟨100⟩ and ⟨111⟩ directions are necessary to fill up the corners of the Jones zone, while the negative areas along the ⟨110⟩ directions serve to compress the distribution in these directions. For a more quantitative comparison of experiment and theory a band computation of the wave functions would be needed, which is outside the scope of this note.

One final question may be asked, namely, why the reconstructed momentum density exhibits anisotropy for momenta larger than 1.6 a.u., while the observed profiles are isotropic from $p_z = 1.6$ a.u. upwards (cf. Table II of Ref. 1). The answer must be sought in the limited accuracy of the profiles. It is possible to show on general grounds that, if the measured Compton profiles are expanded[3] in a series of lattice harmonics F_l according to

$$J_{\beta,\alpha}(p_z) = \sum_l F_l(\beta, \alpha) g_l(p_z), \tag{3}$$

where (β, α) denote, respectively, the polar and azimuthal angles of the x-ray scattering vector with respect to the crystal axes, the $g_l(p_z)$ *must* satisfy

$$\int_0^\infty g_l(z) P_l''(z/p)\, dz = 0 . \tag{4}$$

Here p is an arbitrary quantity and $P_l''(x)$ denotes the second derivative of the lth-order Legendre polynomial. Equation (4) forms a rather stringent requirement on the experimental data, which is not quite met by the profiles of WP. Consequently, although at $p_z > 1.6$ a.u. the $g_l(p_z)$ $(l \neq 0)$ have vanished, this is not true of the expansion coefficients in the expansion of the momentum density, which results in the anisotropy extending beyond $p = 1.6$ a.u.

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Deformation-Potential Constants in the Acceptor-Hole–Phonon Interaction in Germanium

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It is shown that the values of the deformation-potential constants D_u^a and $D_{u'}^a$ in the interaction of acceptor holes with thermal phonons in Ge are larger than those in the interaction with static strains.

In a recent paper[1] we have calculated the low-temperature thermal conductivity of In-doped Ge and obtained good agreement with experiment. However, the values of the deformation-potential constants, $D_u^a = 4.2$ eV and $D_{u'}^a = 4.9$ eV, employed in our numerical calculations are considerably

larger than those obtained from the effect of uniaxial compression on the excitation spectra of acceptors[2] ($D_u^a = 2.1 \pm 0.3$ eV and $D_{u'}^a = 2.51 \pm 0.35$ eV). Since the strength of phonon scattering by acceptor holes depends strongly on the values of D_u^a and $D_{u'}^a$, such a difference is serious and should be theoretically explained. The purpose of this paper is to show that the values of D_u^a and $D_{u'}^a$ in the interaction of acceptor holes with thermal phonons in Ge are in general larger than those in the interaction with static strains.

The strain Hamiltonian at the valence band edge is given by[3]

$$\mathcal{H}_s = \tfrac{2}{3} D_u[(J_x^2 - \tfrac{1}{3}J^2)e_{xx} + \mathrm{CP}] + \tfrac{1}{3} D_{u'}[(J_x J_y + J_y J_x)e_{xy} + \mathrm{CP}] \ , \quad (1)$$

where J_α is the αth component of the angular momentum operator for $J = \frac{3}{2}$, $e_{\alpha\beta}$ is the conventional strain component,[4] and CP denotes the cyclic permutation with respect to the indices x, y, and z. Following Hasegawa's method,[5] we shall calculate the coupling parameter $C(q)$ in the interaction of acceptor holes with the phonon with wave vector $\vec{q}$ in the t branch within the effective-mass approximation. Using Eq. (1) and Schechter's four-component acceptor wave functions,[6] we obtain the expressions for $C^1(q)$ for the longitudinal phonon propagating along [001] and $C^2(q)$ for the transverse phonon propagating along [001] and polarized in the [100] direction:

$$C^1(q) \equiv D_u \langle F^{(3/2)} | (J_z^2 - \tfrac{1}{3}J^2) e^{iqz} | F^{(3/2)} \rangle$$

$$= D_u\{c_1^2 \pi r_1^3 f_1 + c_2^2 \pi r_2^3 f_2 (45X_1 - 63X_2 + 45X_3 + 15X_4) + c_3^2 \pi r_2^3 f_2 (21X_1 - 27X_2 + 15X_3)$$

$$- c_1 c_2 \pi a^3 f_a [6q^{-2} - 6(1 - 0.75q^2a^2) f_a^{1/2} q^{-2} - 6a^2(1 - 0.25q^2a^2) f_a]\} \ , \quad (2)$$

$$C^2(q) \equiv (1/\sqrt{3}) D_{u'} \langle F^{(3/2)} | (J_z J_x + J_x J_z) e^{iqz} | F^{(1/2)} \rangle$$

$$= D_{u'}[c_1^2 \pi r_1^3 f_1 - c_2^2 \pi r_2^3 f_2 (63X_1 - 81X_2 + 45X_3 + 15X_4) - 3c_3^2 \pi r_2^3 f_2 (X_1 - X_2)] \ , \quad (3)$$

where

$$F^{(3/2)} = c_1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} e^{-r/r_1} + c_2 \begin{pmatrix} z^2 - (x^2+y^2)/2 \\ 0 \\ (\sqrt{3}/2)(x^2 - y^2) \\ 0 \end{pmatrix} e^{-r/r_2} + c_3 \begin{pmatrix} 0 \\ xz + iyz \\ ixy \\ 0 \end{pmatrix} e^{-r/r_2} \ , \quad (4)$$

$$F^{(1/2)} = c_1 \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} e^{-r/r_1} + c_2 \begin{pmatrix} 0 \\ -z^2 + (x^2+y^2)/2 \\ 0 \\ (\sqrt{3}/2)(x^2 - y^2) \end{pmatrix} e^{-r/r_2} + c_3 \begin{pmatrix} xz - iyz \\ 0 \\ 0 \\ ixy \end{pmatrix} e^{-r/r_2} \ , \quad (5)$$

$$J_x = \frac{1}{2} \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}, \quad J_y = \frac{i}{2} \begin{pmatrix} 0 & -\sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & -2 & 0 \\ 0 & 2 & 0 & -\sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}, \quad J_z = \frac{1}{2} \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix} , \quad (6)$$

$$X_1 = q^{-4}[1 - (1 - 0.75q^2 r_2^2) f_2^{1/2}] \ , \quad (7)$$

$$X_2 = r_2^2 (1 - 0.25q^2 r_2^2) f_2 q^{-2} \ , \quad (8)$$

$$X_3 = r_2^2 (0.4 - q^2 r_2^2 + 0.125 q^4 r_2^4) f_2^{3/2} q^{-2} \ , \quad (9)$$

$$X_4 = r_2^4 (1.5 - 1.25q^2 r_2^2 + 3q^4 r_2^4/32) f_2^2 \ , \quad (10)$$

$$f_i = (1 + \tfrac{1}{4} q^2 r_i^2)^{-2} \quad (i = 1, 2) \ , \quad (11)$$

$$f_a = (1 + \tfrac{1}{4} q^2 a^2)^{-2}, \quad a = 2r_1 r_2/(r_1 + r_2) \ , \quad (12)$$

and the numerical values of c_1, c_2, c_3, r_1, and r_2 are given in Ref. 6.

When $q = 0$ for static strains, we obtain

$$C^1(0) = 0.569 D_u = D_{us}^a \ , \quad (13)$$

$$C^2(0) = 0.613 D_{u'} = D_{u's}^a \ . \quad (14)$$

The relations similar to Eqs. (13) and (14) were obtained by Bir *et al.*,[7] and by Suzuki *et al.*[8] who calculated D_{us}^a and $D_{u's}^a$ by using the six-component acceptor wave functions.[9]

Although it is desirable to use the acceptor wave

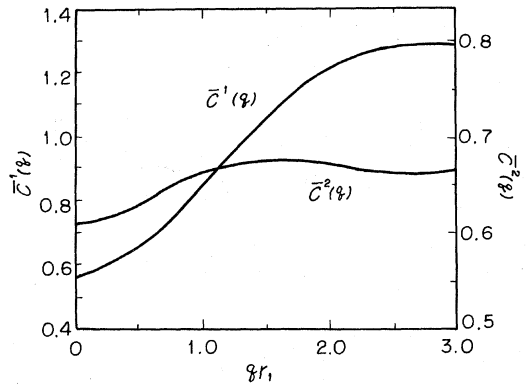

FIG. 1. Ratios of the coupling parameters in Eqs. (2) and (3) to those in Eqs. (15) and (16).

functions containing a d-like part as well as an s-like part in the calculation of the acceptor-hole–phonon interaction, such calculations for phonons with $\tilde{q}$ propagating in arbitrary directions are very complicated. Therefore, in calculating the thermal conductivity of p-Ge, [1] we have made the approximation that the acceptor wave functions consist of only the s-like part, i.e., $c_1=1$, $c_2=c_3=0$ in Eqs. (4) and (5), and regarded D_u^a and $D_{u'}^a$ as adjustable parameters. In this approximation we obtain

$$C^{1'}(q)=D_u f_1, \qquad D_u \to D_u^a \ , \tag{15}$$

$$C^{2'}(q)=D_{u'} f_1, \qquad D_{u'} \to D_{u'}^a \ . \tag{16}$$

Let us now consider the ratios of the coupling parameters in Eqs. (2) and (3) to those in Eqs. (15) and (16), i.e.,

$$\bar{C}^1(q)=C^1(q)/C^{1'}(q) \ , \tag{17}$$

$$\bar{C}^2(q)=C^2(q)/C^{2'}(q) \ . \tag{18}$$

In Fig. 1 we have plotted $\bar{C}^1(q)$ and $\bar{C}^2(q)$ as a function of qr_1. It is seen from Fig. 1 that the coupling parameters for finite values of q are considerably larger than those for $q=0$. Therefore, in the approximate calculations of the phonon relaxation rates, [1] we should use the values of D_u^a and $D_{u'}^a$ larger than the values of D_{us}^a and $D_{u's}^a$. However, if we assume that $D_{u'}=4.9$ eV, the value of the effective deformation potential $\bar{C}^2(q)D_{u'}$ becomes smaller than $D_{u'}^a=4.9$ eV employed in the previous paper. [1] We have tried to recalculate the thermal conductivity by taking account of Fig. 1 and the experimental data of D_u and $D_{u'}$ in In-doped Ge. [2] By putting $D_u^a=4.53$ eV $=1.074 D_{u'}$, $D_u^a=3.5$ eV $=0.734 D_{u'}$, and $r_1(=a^*)=33$ Å in Eq. (2.11) of Ref. 1, we could obtain a good agreement between the theory and experiments in the region of 1 to 5 K. The values of D_u and $D_{u'}$ used are the largest ones within the experimental error. [2]

Finally, we would like to make two comments. First, we have carried out the numerical calculation of the effect of the uniaxial stress on the low-temperature thermal conductivity of p-Ge, by using the same values of D_u^a and $D_{u'}^a$ for both static strains and thermal phonons. [10] For static strains, however, we should use the values of D_{us}^a and $D_{u's}^a$ given in Ref. 2 or in Eqs. (13) and (14). Next, the difference between D_u^a and $D_{u'}^a$ for $q\neq 0$ and D_{us}^a and $D_{u's}^a$ for $q=0$ in the approximate calculation has been recently confirmed by Ishiguro *et al.* [11] in the analysis of heat-pulse propagation in p-Ge under uniaxial stresses.

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