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Role of compensation in electron-phonon scattering in lightly doped semiconductors

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Low-temperature phonon conductivity results of compensated semiconductors such as Ge(P,Ga), Ge(As,Ga), and Ge(Sb,In) have been for the first time interpreted quantitatively on the basis of the theory proposed by Griffin and Carruthers and extended by Kwok. The compensated Ge samples are designated as Ge(donor impurity, compensating acceptor impurity). The basis of the present interpretations are the complete expressions obtained by Suzuki and Mikoshiba in the light of Kwok's theory for the resonance-scattering relaxation rates of phonons by bound donor electrons in Ge. The elastic and inelastic scatterings, both from the donor-electron singlet ground state and the next higher-energy triplet state, separated by 4Δ, as well as phonon-assisted absorption processes are considered in the present calculations in the temperature range 1–4°K. The effect of compensation by acceptor impurities such as Ga in the case of P- and As-doped (n-type) Ge and by indium in the case of Sb-doped Ge is reflected in the variations of 4Δ and the donor-electron radius a_0. Compensation in the case of P- and As-doped Ge by gallium reduces the values of 4Δ but it almost remains unaffected in the case of Sb-doped Ge when it is compensated by indium. However, the donor-electron radius is reduced in all the cases on compensation.

I. INTRODUCTION

It is now well established that neutral donor impurities cause scattering of phonons in lightly doped semiconductors at temperatures lower than 10 °K. Phonons are scattered by the virtual transitions of the electrons between the donor-electron singlet and triplet states, which are separated by 4Δ. As a matter of fact the donor-electron ground state is fourfold degenerate but the degeneracy is removed partially due to valley-orbit interaction and the fourfold-degenerate state splits up into a singlet state, which is the lower-energy state and a triplet state, which is the next higher-energy state separated by 4Δ. The value of 4Δ in the case of Sb-, P-, and As-doped Ge is 0.32, 2.83, and 4.23 meV, respectively. The resonance scattering of phonons leads to resonance dips in the phonon conductivity κ vs T curve. The temperature T_r, at which the dips occur, corresponds to $4\Delta/5K_B$ or $4\Delta/6K_B$. Still in the off-resonance region, but not very far from the resonance temperature, a drastic reduction in the phonon conductivity persists. The theories of phonon-electron scattering which lead to drastic reduction in the phonon conductivity have been formulated by Keyes,[1] Griffin and Carruthers,[2] and Kwok.[3] Kumar *et al.*[4] considered the approximate expressions of the scattering relaxation rates for off-resonance situations. However, the complete expressions for the scattering relaxation rates have been given by Suzuki and Mikoshiba,[5] and they are based on Kwok's theory for phonon-electron scattering for the acoustical phonons. The scatterings considered are elastic and inelastic scatterings of phonons from both the singlet and triplet states, including phonon-assisted absorption processes.

The phonon-conductivity experiments in compensated samples[6] for low concentrations of doping provide an additional support for the scattering of phonons by neutral-donor electrons. When a n-type sample is compensated by p-type impurities, the concentration of impurities N_I $(=N_A+N_d)$ increases, whereas the concentration of excess electrons, N_{ex} $(=N_d-N_A)$, decreases. It is now experimentally observed that in the off-resonance region, namely, in the temperature range 1 to 5 °K, the phonon conductivity of Sb-doped Ge, instead of decreasing with the increase in the impurity concentration N_I, increases with the increase in the strength of the p-type impurities, which act as compensators in reducing the value of N_{ex}. Thus, the increase in the phonon conductivity is consistent with the decrease in the values of N_{ex}, which should be the case if electron-phonon scattering is responsible for the observed increase in the phonon conductivity. However, the effect of compensation on the increase in the phonon resistivity of Sb-doped Ge is not so much pronounced as in the case of As- and P-doped Ge, where the effect of compensation is much larger. Further, the peculiar aspect of the latter case is that the phonon resistivity of As- and P-doped Ge increases with the compensation. This shows that besides N_{ex}, one has to consider the role of 4Δ and a_0. As far as we are aware of, no attempt has been made to explain the above anomalous results quantitatively. In the present paper we have interpreted quantitatively the phonon-conductivity results for compensated semiconductors such as Ge(P, Ga), Ge(As, Ga), and Ge(Sb, In) on the basis

of the resonance scattering of phonons by bound electrons, for which the complete expressions, based on Kwok's theory, have been obtained by Suzuki and Mikoshiba (SM). In SM's expressions for the relaxation rates for electron-phonon scattering in lightly doped semiconductors, there are two quantities which are susceptible to compensation, namely, the donor-electron radius a_0 and the chemical shift 4Δ. In this paper we also propose to investigate how these quantities characterizing a n-type semiconductor are affected when p-type compensating impurities are introduced.

II. THEORY

Considering the contribution of the different phonon polarizations, and taking into account different phonon-scattering processes, the temperature dependence of the phonon conductivity of a lightly doped semiconductor ($N_{ex} < 10^{17}\ \mathrm{cm}^{-3}$) can be expressed as

$$\kappa(T) = \frac{K_B^4 T^3}{6\pi^2\hbar^3} \sum_{j=1,2,3} \frac{1}{v_j} \int_0^\infty \frac{x^4 e^x \tau(qj)}{(e^x-1)^2}\, dx$$

$$= \frac{K_B^4 T^3}{6\pi^2\hbar^3 v_1} \int_0^\infty \frac{x^4 e^x (e^x-1)^{-2}\, dx}{D_1(x)} + \frac{K_B^4 T^3}{6\pi^2\hbar^3 v_2} \int_0^\infty \frac{x^4 e^x (e^x-1)^{-2}\, dx}{D_2(x)} + \frac{K_B^4 T^3}{6\pi^2\hbar^3 v_3} \int_0^\infty \frac{x^4 e^x (e^x-1)^{-2}\, dx}{D_3(x)} . \quad (1)$$

Here κ is the phonon conductivity, K_B is the Boltzmann constant, j is the polarization index, v_j is the phonon velocity, $x = \hbar\omega/K_B T$, ω is the phonon frequency, q is the phonon wave vector, $\tau^{-1}(qj)$ is the effective phonon-scattering relaxation rate for the mode (qj) and is given by $\tau^{-1}(qj) = \sum_i \tau_i^{-1}$, where i refers to the ith phonon-scattering process. [Further, $D_j(x) = D_j(q) = \tau^{-1}(qj)$.] In the presence of boundary scattering of phonons, point-defect scattering of phonons, phonon-phonon scattering, and electron-phonon scattering, one can write

$$D_1(x) = [\tau(qj)]_{j=1}^{-1} = (v_1/L) + A(K_B/\hbar)^4 x^4 T^4 + (B_1+B_2)(K_B/\hbar)^2 x^2 T^5 + [\tau_{ep}(qj)]_{j=1}^{-1} , \quad (2)$$

$$D_2(x) = [\tau(qj)]_{j=2}^{-1} = (v_2/L) + A(K_B/\hbar)^4 x^4 T^4 + (B_1+B_2)(K_B/\hbar)^2 x^2 T^5 + [\tau_{ep}(qj)]_{j=2}^{-1} , \quad (3)$$

$$D_3(x) = [\tau(qj)]_{j=3}^{-1} = (v_3/L) + A(K_B/\hbar)^4 x^4 T^4 + (B_1+B_2)(K_B/\hbar)^2 x^2 T^5 + [\tau_{ep}(qj)]_{j=3}^{-1} . \quad (4)$$

Here $\tau_B^{-1} = v_j/L$ is the relaxation rate due to boundary scattering of phonons, $\tau_{pt}^{-1} = A(K_B/\hbar)^4 x^4 T^4$ is the relaxation rate due to point-defect scattering of phonons, $\tau_{ph\text{-}ph}^{-1} = (B_1+B_2)(K_B/\hbar)^2 x^2 T^5$ is the relaxation rate due to phonon-phonon scattering, and $\tau_{ep}^{-1}(qj)$ is the relaxation rate due to electron-phonon scattering.

While considering electron-phonon scattering, the contributions from the elastic and inelastic scattering of phonons as well as phonon-assisted absorption processes are taken into account by putting

$$\tau_{ep}^{-1}(qj) = \tau_{el}^{-1}(qj) + \tau_1^{-1}(qj) + \tau_2^{-1}(qj) , \quad (5)$$

where $\tau_{el}^{-1}(qj)$ represents the relaxation rate due to elastic scattering of phonons both from the triplet as well as the singlet states, $\tau_1^{-1}(qj)$ represents the relaxation rate due to inelastic scattering of phonons from the triplet state, $\tau_2^{-1}(qj)$ represents the relaxation rate due to "thermally assisted" phonon absorption for $\omega_{qj} < 4\Delta/\hbar$ and inelastic scattering by electrons in the singlet states for $\omega_{qj} > 4\Delta/\hbar$.

According to Suzuki and Mikoshiba,[5] the average relaxation rate for the elastic scattering of phonons is given by

$$\tau_{el}^{-1}(qj) = B\omega^4 (4\Delta)^2 \{[(4\Delta)^2 - \hbar^2\omega^2]^2 + 4\Gamma^2(4\Delta)^2\}^{-1} F(\omega) \times \{N_S(T) + N_T(T)[2 + (4\Delta/\hbar\omega)^2]\} , \quad (6)$$

where

$$B = (\pi\rho^2 v_j^2)^{-1} (E_u/3)^4 f^2(\omega/v_j) W_j . \quad (7)$$

Here ρ is the density of the crystal, E_u is the shear deformation potential, and ω is the frequency of the phonon (q, j). The quantity $f^2(\omega/v_j)$ is given by

$$f^2(\omega/v_j) = [1 + (a_0 K_B/2v_j\hbar)^2 x^2 T^2]^{-4} . \quad (8)$$

Here a_0 is the donor-electron radius and $x = \hbar\omega/K_B T$. For n-type Ge, the values of W_j are $W_1 = \frac{48}{225}$, $W_2 = \frac{32}{225}$, and $W_3 = \frac{40}{225}$. The level-width parameter Γ is given by

$$\Gamma=\Gamma_S+\Gamma_T=\frac{1}{15\pi\rho}\left(\frac{E_u}{3}\right)^2\left(\frac{4\Delta}{\hbar}\right)^3\Gamma\left(\frac{4\Delta}{\hbar}\right)\times\left(1+\frac{4}{\exp(4\Delta/K_BT)-1}\right). \quad (9)$$

Here Γ_S and Γ_T are the level widths of the singlet and triplet states.

The quantity $F(\omega)$ is given by

$$F(\omega)=v_1^{-5}f^2(\omega/v_1)+\tfrac{3}{2}v_2^{-5}f^2(\omega/v_2). \quad (10)$$

Further, N_S and N_T are the number of electrons per unit volume in the singlet and triplet states. The quantities $4\Gamma^2(4\Delta)^2$ are usually very small and can be neglected in the off-resonance region.

Writing

$$N_S(T)=N/(1+3e^{-x_0}), \quad (11)$$

$$N_T(T)/N_S(T)=e^{-x_0}, \quad (12)$$

$$\frac{4\Delta}{\hbar\omega}=\frac{4\Delta/K_BT}{\hbar\omega/K_BT}=\frac{x_0}{x}. \quad (13)$$

One can write

$$\tau_{e1}^{-1}(q^j)=\frac{Bx^4}{\hbar^4}(4\Delta)^2(x_0^2-x^2)^{-2}\times F(x)\frac{N}{1+3e^{-x_0}}\left\{1+e^{-x_0}\left[2+\left(\frac{x_0}{x}\right)^2\right]\right\}. \quad (14)$$

Subsituting for B, $F(x)$, and $F^2(x/v_j)$, the final expression for $\tau_{e1}^{-1}(qj)$ can be expressed as

$$\tau_{e1}^{-1}(qj)=\frac{(\frac{1}{3}E_u)^4W_j(4\Delta)^2}{\hbar^4\pi\rho^2v_j^2}\left[1+\left(\frac{a_0K_B}{2v_j\hbar}\right)^2x^2T^2\right]^{-4}\left\{v_1^{-5}\left[1+\left(\frac{a_0K_B}{2v_1\hbar}\right)^2x^2T^2\right]^{-4}+\frac{3}{2}v_2^{-5}\left[1+\left(\frac{a_0K_B}{2v_2\hbar}\right)^2x^2T^2\right]^{-4}\right\}\times\frac{Nx^4}{(1+3e^{-x_0})(x_0^2-x^2)^2}\left\{1+e^{-x_0}\left[2+\left(\frac{x_0}{x}\right)^2\right]\right\}. \quad (15)$$

The relaxation rate due to inelastic scattering of phonons by electrons in the triplet state is given by

$$\tau_1^{-1}(qj)=\frac{(\frac{1}{3}E_u)^4W_jN_{ex}(4\Delta)^2}{2\hbar^4\pi\rho^2v_j^2}\left[1+\left(\frac{a_0K_B}{2v_j\hbar}\right)^2x^2T^2\right]^{-4}\times\left\{v_1^{-5}\left[1+\left(\frac{a_0K_B}{2v_1\hbar}\right)^2(x_0+x)^2T^2\right]^{-4}+\frac{3}{2}v_2^{-5}\left[1+\left(\frac{a_0K_B}{2v_2\hbar}\right)^2(x_0+x)^2T^2\right]^{-4}\right\}\left(\frac{(x_0+x)(1-e^{-x})}{x(3+e^{x_0})(1-e^{-(x_0+x)})}\right). \quad (16)$$

The relaxation rate for "thermally assisted" phonon absorption processes for $\omega_{qj}<4\Delta/\hbar$ and for inelastic scattering of phonons by electrons in a singlet state for $\omega_{qj}>4\Delta/\hbar$ can be written

$$\tau_2^{-1}(qj)=\frac{(\frac{1}{3}E_u)^4W_jN_{ex}(4\Delta)^2}{2\hbar^4\pi\rho^2v_j^2}\left[1+\left(\frac{a_0K_B}{2v_j\hbar}\right)^2x^2T^2\right]^{-4}\times\left\{v_1^{-5}\left[1+\left(\frac{a_0K_B}{2v_1\hbar}\right)^2(x_0-x)^2T^2\right]^{-4}+\frac{3}{2}v_2^{-5}\left[1+\left(\frac{a_0K_B}{2v_2\hbar}\right)^2(x_0-x)^2T^2\right]^{-4}\left(\frac{(x_0-x)(1-e^{-x})}{x(1+3e^{-x_0})(e^{(x-x_0)}-1)}\right)\right\}. \quad (17)$$

III. RESULTS

As mentioned in Sec. I, Mathur and Pearlman have studied the phonon conductivity of compensated samples of Ge extensively. The Ge samples which were initially doped with Sb, P, and As were compensated by indium in the case of antimony and by gallium for arsenic and phosphorous. They compared their experimental results for compensated samples with those for uncompensated samples. They also tried to explain their experimental results qualitatively. Here we have used SM's expressions for the relaxation rates given in Sec. II and used Eq. (1) for evaluating the phonon conductivity of the different samples.

A. Uncompensated samples

The phonon conductivity of the uncompensated samples, Ge(P)-1, Ge(P)-2, and Ge(P)-3, has been calculated in the temperature range 1–5 °K for the different values of a_0, E_u, and 4Δ. In the present calculations an anisotropy factor ϕ has been also considered, $\phi_1=\phi_l=0.81$, whereas $\phi_2=\phi_3=\phi_t=0.24$. It may be mentioned here that Keyes used $\phi_l=0.8$ and $\phi_t=0.6$ for n-type Ge.

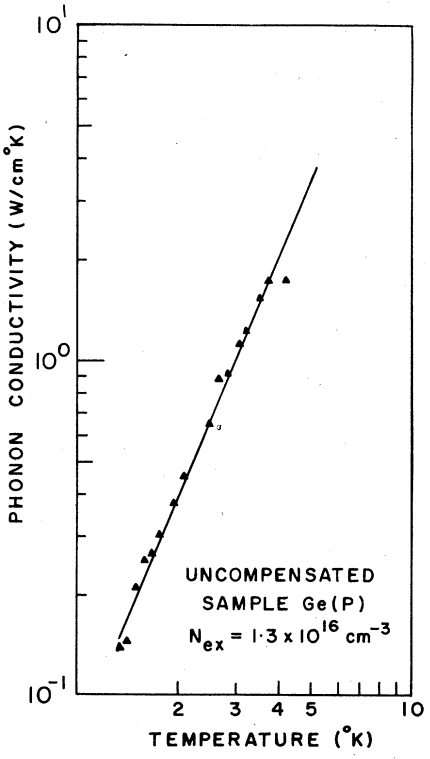

FIG. 1. Phonon conductivity of the uncompensated sample Ge(P)-1 (doped with phosphorous alone, $N_{ex} = 1.3 \times 10^{16}$ cm^{-3}). Experimental points are shown by the symbol ▲. The theoretical curve is shown by a solid line.

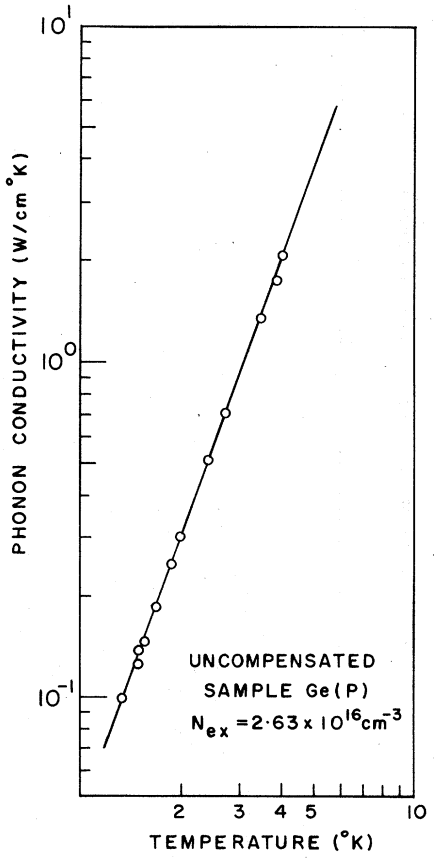

FIG. 2. Phonon conductivity of the uncompensated sample Ge(P)-2 (doped with phosphorous alone, $N_{ex} = 2.63 \times 10^{16}$ cm^{-3}). Experimental points are shown by the symbol ○. The theoretical curve is shown by a solid line.

The values of the parameters for the best fit are given in Table I. Comparison between theory and experiment is shown in Figs. 1–3. Table II gives the values of other relevant parameters common to all the samples.

B. Compensated samples

The phonon conductivity of the compensated samples has been evaluated using the procedure adopted for the uncompensated samples. The values of the parameters a_0, 4Δ, and E_u obtained for best agreement between theory and experiment are given in Table III. Figures 4–9 show a comparison between theory and experiment. In Fig. 4 we show the results obtained by varying a_0. Best agreement between theory and experiment is obtained with $a_0 = 28$ Å. In Fig. 6 we show the results obtained by varying 4Δ. Best agreement between theory and experiment is obtained for $4\Delta = 3.69$ MeV.

TABLE I. Values of 4Δ, a_0, and E_u for uncompensated samples.

Sample	N_{ex} (10^{16} cm^{-3})	4Δ (meV)	a_0 (Å)	E_u (eV)
Ge(P)-1	1.3	2.83	33	16
Ge(P)-2	2.63	2.83	33	16
Ge(P)-3	3.0	2.83	33	16

TABLE II. Values of the parameters used in the evaluation of the phonon conductivity.

$V_1 = 5.37 \times 10^5$ cm/sec
$V_2 = 3.28 \times 10^5$ cm/sec
$A = 2.53 \times 10^{-44}$ sec^{-3}
$B_1 + B_2 = 2.80 \times 10^{-23}$ sec K^{-3}

IV. DISCUSSION

The anomalous-phonon-conductivity results of compensated samples of Ge have been interpreted

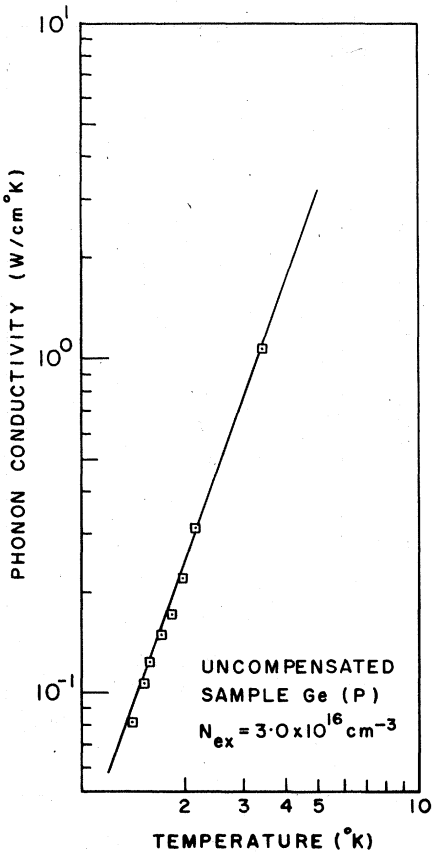

FIG. 3. Phonon conductivity of the uncompensated sample Ge(P)-3 (doped with phosphorous alone, $N_{ex} = 3 \times 10^{16}$ cm^{-3}). Experimental points are shown by the symbol ⊡. The theoretical curve is shown by a solid line.

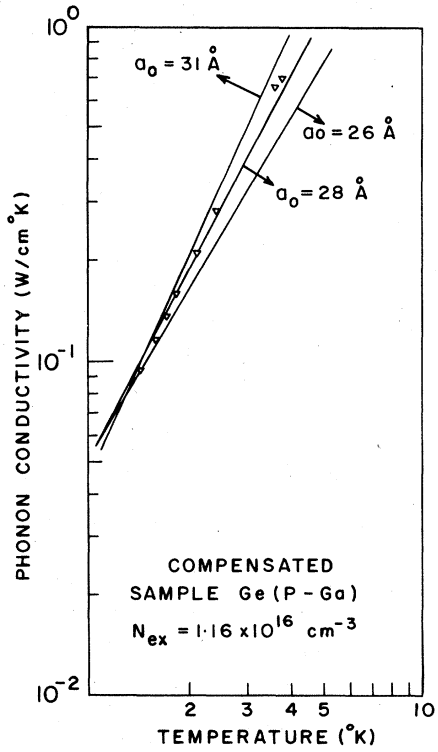

FIG. 4. Phonon conductivity of the compensated sample Ge(P,Ga)-1 (doped with P and Ga, $N_{ex} = N_d - N_A = 1.16 \times 10^{16}$ cm^{-3}). Experimental points are shown by the symbol ∇. The theoretical curves for $a_0 = 28$, 31, and 26 Å are shown by solid lines.

quantitatively for the first time. For the electron-phonon scattering we have used the expressions given by Suzuki and Mikoshiba, which are based on Kwok's theory. These relaxation rates take into account both elastic and inelastic scatterings of phonon from the donor electrons in both the ground state and in the next higher-energy state separated by 4Δ. Phonon-assisted absorption processes are also taken into account. Considering all these phonon scattering processes, it is possible to account for the low-temperature phonon-conductivity results for uncompensated samples of Ge in the temperature range 1–5 °K. Comparisons between theoretical and experimental values of the phonon conductivity are shown

TABLE III. Values of 4Δ, a_0, and E_u for compensated samples.

Sample	N_{ex} (10^{16} cm^{-3})	4Δ (meV)	a_0 (Å)	E_u (eV)
Ge(P, Ga)-1[a]	1.16	2.30	31	19
Ge(P, Ga)-2[a]	2.41	2.30	31	19
Ge(As, Ga)-1[b]	1.5	3.69	26.3	25
Ge(As, Ga)-2[b]	2.6	3.69	26.3	25
Ge(Sb, In)-1[c]	3.1	0.33	33	20
Ge(Sb, In)-2[c]	5.35	0.33	33	20

[a] For Ge(P), $4\Delta = 2.83$ meV, $a_0 = 33$ Å (our calculations).
[b] For Ge(As), $4\Delta = 4.23$ meV, $a_0 = 32$ Å (Mathur and Pearlman).
[c] For Ge(Sb), $4\Delta = 0.32$ meV, $a_0 = 44.2$ Å (Mathur and Pearlman).

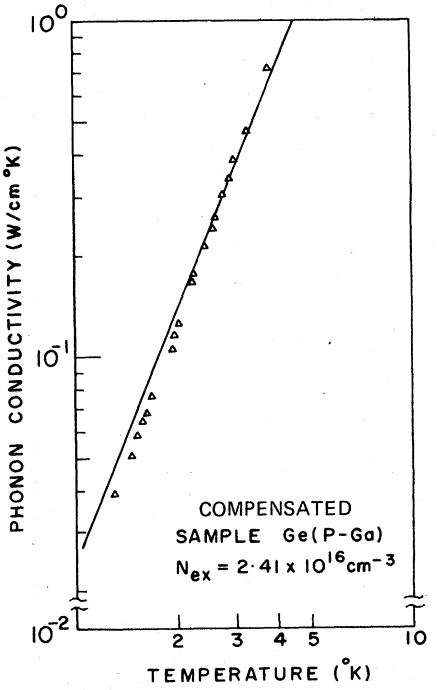

FIG. 5. Phonon conductivity of the compensated sample Ge(P,Ga)-2 (doped with P and Ga, $N_{ex}=N_d-N_A = 2.41\times10^{16}$ cm^{-3}). Experimental points are shown by the symbol Δ. The theoretical curve is shown by a solid line.

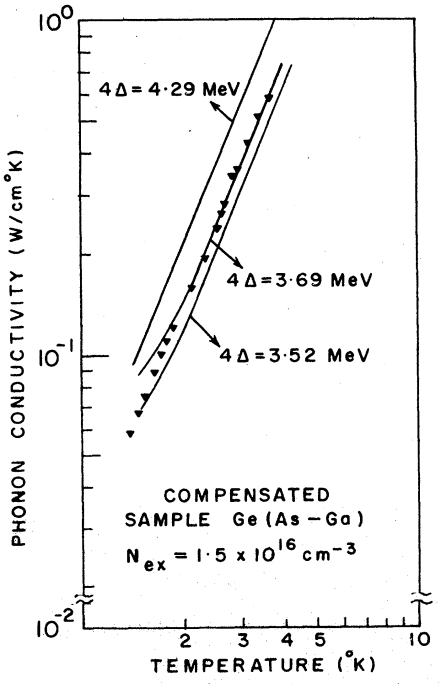

FIG. 6. Phonon conductivity of the compensated sample Ge(As,Ga)-1 (doped with As and Ga, $N_{ex}=N_d-N_A = 1.5\times10^{16}$ cm^{-3}). Experimental points are shown by the symbol ▼. The theoretical curves for $4\Delta = 3.69$, 4.29, and 3.52 meV are shown by solid lines.

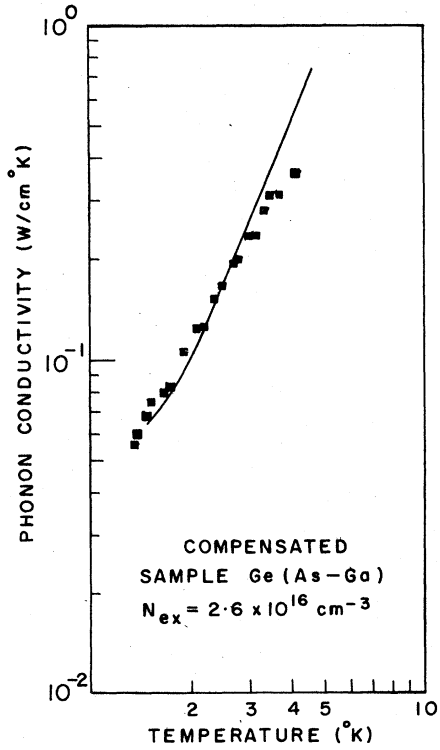

FIG. 7. Phonon conductivity of the compensated sample Ge(As,Ga)-2 (doped with As and Ga, $N_{ex}=N_d-N_A = 2.6\times10^{16}$ cm^{-3}). Experimental points are shown by the symbol ■. The theoretical curve is shown by a solid line.

in Figs. 1–3. From the good agreement between theory and experiment, it can be concluded that electron-phonon scattering involving virtual transitions between donor-electron singlet and triplet states can account very well for the observed phonon conductivity of n-type Ge in the temperature range 1–5 °K.

Compensation of n-type Ge, namely, P-, As-, and Sb-doped Ge, is brought about by doping the n-type samples with p-type impurities. As defined earlier, N_{ex} $(=N_d - N_A)$ decreases with compensation. For P- and As-doped Ge, gallium has been used as the compensator, whereas In has been used for Sb-doped Ge. Besides N_{ex}, other quantities such as donor-electron radius a_0 and the chemical shift 4Δ also change on compensation. Taking all these factors into account for electron-phonon scattering, it has been possible to account for the variation with compensation in the phonon conductivity of n-type Ge, a variation which is not expected with the increase in the strength of the impurities, but follows consistently the decrease in the value of N_{ex} and variations of other parameters such as a_0 and 4Δ. Thus, if it is assumed that the SM expres-

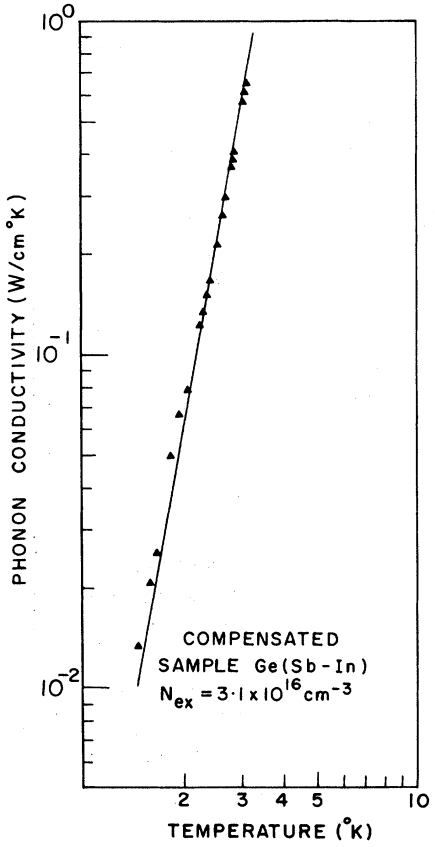

FIG. 8. Phonon conductivity of the compensated sample Ge(Sb, In)-1 (doped with Sb and In, $N_{ex}=N_d-N_A = 3.1 \times 10^{16}$ cm^{-3}). Experimental points are shown by the symbol ▲. The theoretical curve is shown by a solid line.

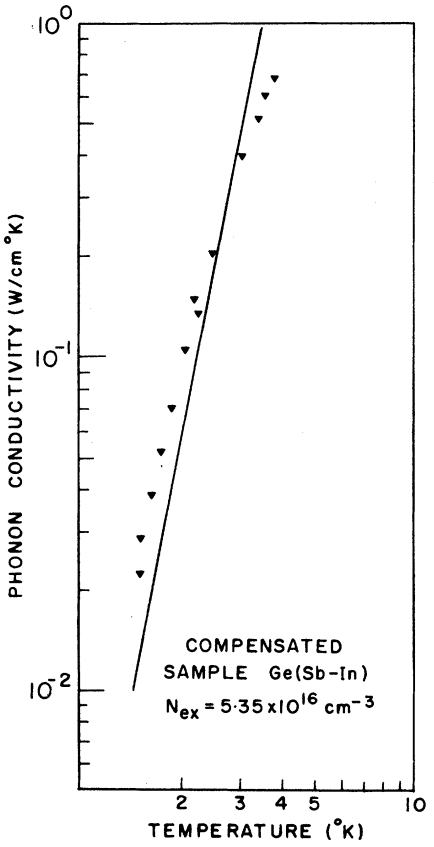

FIG. 9. Phonon conductivity of the compensated sample Ge(Sb, In)-2 (doped with Sb and In, $N_{ex}=N_d-N_A = 5.35 \times 10^{16}$ cm^{-3}). Experimental points are shown by the symbol ▼. The theoretical result is shown by a solid line.

sions for the relaxation rate with the altered values of 4Δ and a_0 are valid for the compensated samples, when the concentration of p-type impurities is comparable but less than that of n-type impurities, one obtains the values of a_0, 4Δ, and E_u, etc., for the compensated samples.

For the three P-doped uncompensated samples of Ge of dopant comcentrations 1.3×10^{16}, 2.63×10^{16}, and 3.0×10^{16} cm^{-3}, the values of 4Δ, a_0, and E_u remain same, see Table I. Thus, in the range $N_{ex} = (1.3\text{–}3.0)\times10^{16}$ cm^{-3}, the variations in the phonon conductivity of As-doped Ge are due to variations in N_{ex} alone. When the P-doped Ge is compensated by Ga, the 4Δ and the donor-electron radius are decreased for $N_{ex} = 1.16\times10^{16}$ and 2.4×10^{16} cm^{-3}. In both cases 4Δ decreases from 2.83 to 2.30 meV and a_0 from 35 to 31 Å. A similar behavior is also observed in the case of compensation of As-doped Ge samples by gallium. Both a_0 and 4Δ are decreased considerably (a_0 from 32 to 26.3 Å and 4Δ from 4.23 to 3.69 meV). The deformation potentials are also higher in this case. In the case of the compensated samples Ge(Sb, In) both 4Δ and the deformation potentials increase slightly but a_0 is decreased considerably from 40 to 32 Å for $N_{ex} = 3.1\times10^{16}$ and 5.35×10^{16} cm^{-3}. Thus, in all the compensated samples, a_0 decreases on compensation whereas 4Δ decreases for the Ge(PGa) and Ge(As, Ga) samples but increases slightly for the Ge(Sb, In) samples. The variations of a_0 and 4Δ for the different compensated samples are summarized in Table III.

The presence of negative acceptor ions affects the donor-impurity atom ground-state wave function. As mentioned in the Introduction, the fourfold-degenerate donor-electron ground state is split into a singlet state and a higher-energy triplet state separated by 4Δ. This result follows from effective-mass theory in which besides the Coulomb potential, a correction

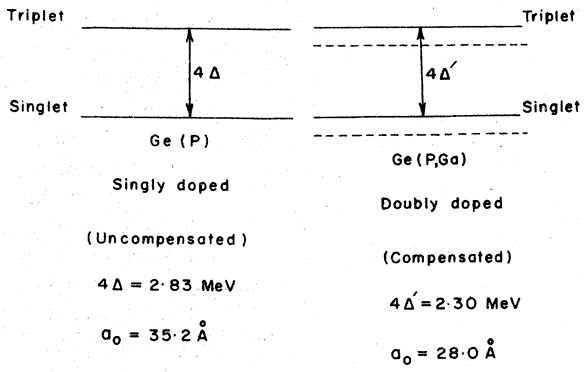

FIG. 10. Donor-electron ground-state energy-level scheme in compensated and uncompensated samples.

potential $U(r)$ is included, which is large in the vicinity of the lattice cell containing the impurity atom. In the presence of the acceptor ions, the original correction potential $U(r)$ for the donor-impurity atoms is modified and affects the wave functions. As the explicit calculations of the wave functions are not available for compensated samples, one can conclude that the lowering of 4Δ and hence a_0 in the compensated samples may be due to the different behavior of singlet-state and triplet-state wave functions. The singlet amplitude is much larger within the cell containing the donor atom than is the triplet's, since the latter vanishes at the center of the cell. Thus, the triplet wave function with its amplitude concentrated away from the center of the cell is affected most in the presence of acceptor ions (compensator impurities). So when the extent of the wave function a_0 is reduced, there is an increase in energy in both the singlet and triplet state, but for the latter state the increase is smaller. This results in lower values of 4Δ as a_0 is decreased. This situation is depicted in Fig. 10, which also applies to the Ge(As, Ga) system.

However, the case of compensation by indium of Sb-doped Ge is different. Here, although a_0 is lowered from 44.2 to 35 Å, both levels are affected to the same extent and in the same direction so that 4Δ practically remains the same or may increase very slightly.

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