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Influence of internal stress on electron-phonon interaction in n-type germanium and silicon at low temperatures

Mahiradhwaj Singh and G. S. Verma†

Physics Department, Banaras Hindu University, Varanasi-221005, India

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Expressions for resonance scattering of phonons by the bound donor electrons have been obtained for the first time for n-Ge in the presence of strains for the most general situation when, besides the usual valley-orbit splitting of the four-fold degenerate ground state into a singlet state and a triplet state, the triplet state splits into a doublet state and a singlet state due to internal static and dynamic strains present in the crystal. Similarly for n-Si, the most general situation is considered when the degeneracy of the donor-electron ground state is completely removed due to internal strains besides the usual valley-orbit splitting of the six-fold ground state into a singlet state and five-fold degenerate state. The expressions obtained for the resonance scattering relaxation rates of phonons by bound electrons for strained n-Ge are used to explain the phonon conductivity results of Sb-, P-, and As-doped Ge.

I. INTRODUCTION

It is well known that the electron (hole)–phonon interaction has a considerable influence upon the propagation of phonons in semiconductors doped with chemical impurities, particularly those producing shallow impurity states at low temperatures. This has been observed as a strong increase in the thermal resistivity of Ge,[1-10] Si,[11-16] InSb,[17-19] GaAs,[20] GaSb,[21-23] etc.[24] by light doping with n- and p-type impurities. Similar effects were also seen by means of ultrasonic[25,26] and heat-pulse techniques.[29,30] Theoretical investigations of electron (hole)–phonon scattering have been carried out by several authors.[15,31-36] Keyes,[31] Griffin and Carruthers,[32] Kwok,[33] and Suzuki and Mikoshiba[34] have considered the case of an isolated impurity state in n-type germanium and silicon (Ref. 15) and calculated the scattering of phonons arising from virtual transitions of bound electrons between donor levels, namely, the singlet and the next excited state which is triplet in the case of germanium. In the case of silicon (Ref. 37) the lowest state is the fivefold degenerate state and the next excited state is the singlet state. These theories are based on Hasegawa's theory[38] of the donor-electron–lattice interaction. Hasegawa's theory is based on the effective-mass approximation for a donor state[39] and the Herring-Vogt theory[40] for electron-lattice interaction in many-valley semiconductors, and it takes account of intervalley processes only.

It is well known that group-V donors in germanium give rise to a large thermal resistivity. Some years ago Bird and Pearlman[11] measured the phonon conductivity of Sb- and As-doped germanium in the temperature range 0.3 to 4.2 °K. With impurity concentrations varying from 3×10^{14} to 3×10^{16} cm^{-3} they observed resonance dips in the phonon conductivity-vs-temperature curves at about 0.7 °K in Sb-doped Ge samples. The plot of K_D/K_P vs T, where K_D is the phonon conductivity of the doped material and K_P is the same for the pure material, shows also dips at about 2 °K in P- and As-doped Ge samples. They tried to explain their experimental results on the basis of the theories proposed by Keyes[31] and Griffin and Carruthers[32] for the resonant scattering of phonons by donor electrons. However, their analysis of the experimental results does not take into account the inelastic scattering of phonons by bound electrons and the elastic scattering of phonons off the triplet state. Keyes has actually considered the static part of the interaction Hamiltonian which leads to ω^4 dependence for the scattering of phonons due to the bound donor electrons between singlet and triplet states. Besides the above factor there is an additional frequency-dependent part which is known as the cutoff factor. This factor represents the fact that when the phonon wave vector is $q>1/a^*$, where a^* is the Bohr radius, the interaction of the phonon with the donor electron is negligible. Keyes's theory is, however, valid as long as the phonon frequency is small compared to the characteristic frequency with which the electronic wave functions adjust to the phonon perturbation, which is $4\Delta/\hbar$ in the present case. In view of the fact that the resonance temperature $T_r=4\Delta/k_B$ for Sb corresponds to 3.71 °K, which lies in the temperature range in which the heat-conduction measurements are carried out, one has to consider phonon frequencies not only less than $4\Delta/\hbar$ but also greater than $4\Delta/\hbar$. It is thus obvious that static interaction does not give the correct picture of the scattering of phonons by the donor electrons. As a matter of fact one has to consider the dynamic response of the electrons to the strains caused by phonons. Griffin and Carruthers considered this problem in analogy with the resonance fluorescence scattering of phonons in atoms. In the low-frequency limit, this theory gives results analogous to those obtained by Keyes. For low frequencies, the resonance factor $(4\Delta)^2/[(\hbar\omega)^2-(4\Delta)^2]^2$ present in the theory of Griffin and Carruthers simply reduces to unity and one obtains the same ω^4 dependence for the scattering of phonons by the bound donor electrons.

The theory of Griffin and Carruthers, which considered only the resonance scattering of phonons off the singlet state was extended by Kwok[33] for the situation $\hbar w < 4\Delta$ in Ge by taking into account not only elastic scattering from the triplet state but also inelastic scattering as well as phonon-assisted absorption processes. The complete expressions for the scattering relaxation rate, which also included the situation $\hbar w > 4\Delta$, were given by Suzuki and Mikoshiba.[34]

It has, however, been observed[41] that the theories fail to explain the details of the resonance dips in the K_D vs T curves. The discrepancies between theoretical and experimental values are more pronounced at lower temperatures. The reason for the failure of these theories to explain the experimental results lies in the fact that no consideration has been given to the presence of internal static and dynamic strains due to the donor impurities themselves, dislocations, vacancies and lattice defects, and lattice vibrations including the dynamic Jahn-Teller effect. Further removal of the degeneracy of the degenerate states due to the crystal's internal strains leading to new states and additional virtual transitions provides the mechanism for explaining the details of the resonance dips of the phonon conductivity curve and the discrepancies at lower temperatures. However, for such experimental situations, theoretical expressions for the phonon-scattering relaxation rates are not available in the literature. In the present paper we have derived for the first time the expressions for the resonance scattering of phonons by the bound donor electrons in strained n-Ge for the most general situation when besides the usual valley-orbit splitting of the fourfold degenerate ground state into a singlet state and a triplet state, the triplet state splits into a doublet and a singlet state owing to internal static and dynamic strains present in the crystal. Similarly for n-Si the most general situation is considered when the degeneracy of the donor-electron ground state is completely removed owing to interval strains besides the usual valley-orbit splitting of the sixfold ground state into a singlet state and a fivefold degenerate state. The expressions obtained for the resonance scattering relaxation rates of phonons by bound donor electrons for strained n-Ge are used to explain the phonon conductivity results of Sb-, P-, and As-doped Ge.

II. THEORY

A. *n-type* Ge

The ground state of the donor electron in Ge is fourfold degenerate in the effective-mass approximation[39] and it is 9.2×10^{-3} eV below the conduction band. However, due to the valley-orbit interaction[42,43] and the central-cell correction, the degeneracy is removed and the ground state is split. The ground state splits into two levels, the lower-energy state being the 1S (A_1) singlet state and the higher-energy one being the 1S (T_2) triply degenerate state. Here A_1 and T_2 are irreducible representations of the T_d point group associated with the site symmetry of the impurity atom. We assume that the triplet state splits into a doublet (E) and singlet (A_1) state due to randomly distributed internal strain. The latter state is the lower state. We further assume that four levels of the ground state are identified by $|n\rangle$. The envelopes of the wave functions are represented by an isotropic (S-like) variational radial function. In order to calculate the strain splitting among the states and the matrix elements for the electron transitions, the following donor-electron–lattice Hamiltonian is used.

$$H_{ep}=\sum_{\alpha,\beta}(E_d\delta_{\alpha\beta}+E_u\hat{e}_\alpha\cdot\hat{e}_\beta)u_{\alpha\beta}\,, \tag{1}$$

where $u_{\alpha\beta}$ is the α,β component of the strain tensor, $\hat{e}$ is unit vector, and E_d and E_u are deformation-potential constants. The matrix elements of donor-electron–phonon interaction between two donor states $|n\rangle$ and $|n'\rangle$ are given by

$$\langle n|H_{ep}|n'\rangle=\sum_{\alpha\beta}\left(\frac{\hbar\omega_{qt}}{2\rho V_t^2}\right)^{1/2}f(q)C_{qt}^{nn'}(a_{qt}+a_{qt}^\dagger)\,, \tag{2}$$

where the donor ground states corresponding to singlet (A_1) and triplet are labeled by $n=0$ and $n=1,2,3$, respectively. ω is the angular frequency and a_{qt} and $a_{qt}^\dagger$ are the destruction and creation operators, respectively, for phonons of wave vector q and in branch t. V_t is the phonon velocity in branch t and p is the crystal density. The factor $f(q)$, is called the cutoff function and is written as

$$f(q)=(1+\tfrac{1}{4}a^{*2}q^2)^{-2}\,. \tag{3}$$

The $C_{qt}^{n'n}$ are referred to as the coupling parameters and are related in the following way:

TABLE I. Quasi-isotropic model for the polarization vector.

Symbol	x	y	z
$\hat{q}$	$\sin\theta\cos\phi$	$\sin\theta\sin\phi$	$\cos\theta$
e_1	$\sin\theta\cos\phi$	$\sin\theta\sin\phi$	$\cos\theta$
e_2	$-\cos\theta\cos\phi$	$-\cos\theta\sin\phi$	$\sin\theta$
e_3	$\sin\phi$	$-\cos\phi$	0

$$C^{00}_{qt}=C^{11}_{qt}=C^{22}_{qt}=C^{33}_{qt}=\begin{cases}D & (t=1),\\ 0 & (t=2,3)\ ,\end{cases}$$

$$C^{01}_{qt}=C^{23}_{qt},\quad C^{02}_{qt}=C^{13}_{qt}\ , \tag{4}$$

$$C^{03}_{qt}=C^{12}_{qt},\quad C^{n'n}_{qt}=C^{nn'}_{qt}\ ,$$

where $D=(E_d+\frac{1}{3}E_u)/\frac{1}{3}E_u$.

In order to obtain analytic expressions for the matrix elements, a quasi-isotropic model for the elastic properties of the crystal has been adopted here. This model results in very simple expressions for the polarization vector $\hat{e}_{qt}$ for the three acoustical modes. These are given in Table I, in terms of conventional polar angles (θ,ϕ), where $(0,0)$ corresponds to the [001] direction, and $(\frac{1}{2}\pi,0)$ to the [100] direction. The coupling parameters can be written in the quasi-isotropic model as shown in Table II. The indices 1, 2, and 3 refer to the longitudinal and the two transverse branches, respectively.

TABLE II. Expressions for C^{nn}_{qt}.

t	1	2	3
C^{01}_t	$\sin2\theta\sin\phi$	$\cos2\theta\sin\phi$	$\cos\theta\cos\phi$
C^{02}_t	$\sin2\theta\cos\phi$	$\cos2\theta\cos\phi$	$-\cos\theta\sin\phi$
C^{03}_t	$\sin2\theta\sin2\phi$	$\frac{1}{2}\sin2\theta\sin2\phi$	$\sin\theta\cos2\phi$

B. Phonon relaxation rates

The thermal phonons in internally strained n-Ge are scattered by various elastic and inelastic processes. The present discussion is limited to the possible second-order processes of which there are two elastic ones in addition to inelastic scattering. The second-order processes all involve transitions of electrons via intermediate states by elastic or inelastic scattering or by thermally assisted phonon absorption.

1. Second-order elastic scattering

Let us calculate the single-mode phonon relaxation rate, $\tau_e^{-1}(qt)$ due to elastic scattering by donor electrons. The first term in the perturbation series for elastic scattering is of second order. Using Eq. (2) and the second-order Born approximation, the elastic scattering rate becomes[33]

$$\tau_e^{-1}(qt)=\frac{\pi\omega_{qt}}{\rho V_t^2}f^2(q)\sum_n N_n(T)\sum_{n'}\sum_{q't'}\frac{\omega_{q't'}}{2\rho V_t^2}f^2(q')\left|\sum_m\left(\frac{C^{n'm}_{q't'}C^{mn}_{qt}}{E_m-E_n-\hbar\omega_{qt}}+\frac{C^{n'm}_{qt}C^{mn}_{qt}}{E_m-E_n+\hbar\omega_{q't}}\right)\right|^2_{E_n=E_{n'}}\delta(\omega_{q't'}-\omega_{qt})\ , \tag{5}$$

where ρ is the density, n, m, and n' are the initial, intermediate, and final states, respectively. $N_n(T)$ is the number of donors per unit volume in the nth level. The average relaxation rate is defined by $\tau_e^{-1}=1/4\pi\int\sin(\theta)\,d\theta\,d\phi\,\tau_e^{-1}(qt)$ and after simplification by means of Eq. (4) can be written as

$$\begin{aligned}\tau_e^{-1}(qt)=\frac{\omega^4_{qt}f^2(\omega_{qt}/V_t)}{64\pi\rho^2V_t^2}\left(\frac{E_u}{3}\right)^4\sum_{t'}\frac{f^2(\omega_{q't'}/V_{t'})}{V^5_{t'}}\left(\frac{\omega_{q't'}}{V_{t'}}\right)\Bigg[N_0(T)\left\langle\left\langle\sum_{n=0}\sum_{n'=0}\left|\sum_m\left(\frac{C^{n'm}_{q't'}C^{mn}_{qt}}{\Delta_{mn}-\hbar\omega}+\frac{C^{n'm}_{qt}C^{mn}_{q't'}}{\Delta_{mn}+\hbar\omega}\right)\right|^2\right\rangle\right\rangle\\+N_1(T)\left\langle\left\langle\sum_{n=1,2}\sum_{n'=1,2}\left|\sum_m\left(\frac{C^{n'm}_{q't'}C^{mn}_{qt}}{\Delta_{mn}-\hbar\omega}+\frac{C^{n'm}_{qt}C^{mn}_{q't'}}{\Delta_{mn}+\hbar\omega}\right)\right|^2\right\rangle\right\rangle+N_3(T)\left\langle\left\langle\sum_{n=3}\sum_{n'=3}\left|\sum_m\left(\frac{C^{n'm}_{q't'}C^{mn}_{qt}}{\Delta_{mn}-\hbar\omega}+\frac{C^{n'm}_{qt}C^{mn}_{q't'}}{\Delta_{mn}+\hbar\omega}\right)\right|^2\right\rangle\right\rangle\Bigg]\ .\end{aligned} \tag{6}$$

Here $\langle\langle\cdots\rangle\rangle$ is called angular average. In the quasi-isotropic Eq. (6) can be written as follows:

$$\begin{aligned}\tau_e^{-1}(q1)&=\frac{B(\omega)f^2(\omega/V_1)}{V_1^2}[32\alpha_1+16\alpha_2+32\alpha_3+16\alpha_4]\ ,\\ \tau_e^{-1}(q2)&=\frac{B(\omega)f^2(\omega/V^2)}{V_2^2}[28\alpha_1+4\alpha_2+28\alpha_3+4\alpha_4]\ ,\\ \tau_e^{-1}(q3)&=\frac{B(\omega)f^2(\omega/V_2)}{V_2^5}[20\alpha_1+20\alpha_2+20\alpha_3+10\alpha_4]\ .\end{aligned} \tag{7}$$

where

$$B(\omega)=[(\tfrac{1}{3}E_u)^4 N_{ex}\omega^4/225\pi\rho^2]\,F(x),\quad F(x)=[f^2(\omega/V_1)/V_1^5+\tfrac{3}{2}f^2(\omega/V_2)/V_2^5],$$

$$\alpha_1=\{N_0(T)+N_1(T)\}\{\Delta_{10}/[\Delta_{10}^2-(\hbar\omega)^2]\}^2,\quad \alpha_2=\{N_0(T)+N_3(T)\}\{\Delta_{30}/[\Delta_{30}^2-(\hbar\omega)^2]\}^2,$$

$$\alpha_3=\{N_1(T)+N_3(T)\}\{\Delta_{13}/[\Delta_{13}^2-(\hbar\omega)^2]\}^2,\quad \alpha_4=\frac{N_1(T)(\Delta_{13}+\Delta_{10})^2[(\hbar\omega)^4+\Delta_{10}^2\Delta_{13}^2+\hbar^2\omega^2(\Delta_{10}^2+\Delta_{13}^2)-4\Delta_{10}\Delta_{13}(\hbar\omega)^2]}{[\Delta_{13}^2-(\hbar\omega)^2]^2[\Delta_{10}^2-(\hbar\omega)^2]^2},$$

and

$$N_1=N_0\exp(-\Delta_{10}/k_BT),$$
$$N_3=N_0\exp(-\Delta_{30}/k_BT),$$
$$N_0+2N_1+N_3=1,$$
$$\Delta_{n'n}=E_{n'}-E_n. \tag{8}$$

Here N_{ex} is the number of donor electrons per unit volume, while the subscripts 1, 2, and 3 stand for the longitudinal and the two transverse modes, respectively.

2. Second-order inelastic scattering

The inelastic scattering in the second order of perturbation falls into two categories. The first is associated with electron transitions from the upper to lower level, and the other involves electron transitions from the lower to the upper level by "thermally assisted" phonon absorption $[\omega<(\Delta/\hbar)]$ or by inelastic scattering $[\omega>(\Delta/\hbar)]$. The corresponding relaxation rates are, respectively,[33]

$$\tau_1^{-1}(qt)=\frac{\pi\omega_{qt}}{\rho V_t^2}f^2(q)[1-\exp(-\hbar\omega/k_BT)]\sum_n N_n(T)\sum_{n'}\sum_{q't'}\left(\frac{\omega_{q't'}}{2\rho V_{t'}^2}\right)f^2(q')(n_{q't'}+1)\,\delta\left(\omega_{q't'}-\frac{\Delta_{n'n}}{\hbar}-\omega_{qt}\right)$$
$$\times\left|\sum_m\left(\frac{C_{q't'}^{n'm}C_{qt}^{mn}}{E_m-E_n-\hbar\omega}+\frac{C_{qt}^{n'm}C_{q't'}^{mn}}{E_m-E_{n'}+\hbar\omega}\right)\right|^2, \tag{9}$$

$$\tau_2^{-1}(qt)=\frac{\pi\omega_{qt}}{\rho V_t^2}f^2(q)\left[1-\exp\left(-\frac{\hbar\omega}{k_BT}\right)\right]\sum_n N_n(T)\sum_{n'}\sum_{q't'}\left(\frac{\omega_{q't'}}{2\rho V_{t'}^2}\right)f^2(q')\left|\sum_m\left(\frac{C_{q't'}^{n'm}C_{qt}^{mn}}{E_m-E_n-\hbar\omega}+\frac{C_{qt}^{n'm}C_{q't'}^{mn}}{E_m-E_{n'}+\hbar\omega}\right)\right|^2$$
$$\times[\epsilon n_{q't'}\,\delta(\omega_{q't'}-\Delta_{nn'}/\hbar+\omega_{qt})$$
$$+(1-\epsilon)(n_{q't'}+1)\,\delta(\omega_{qt}-\Delta_{nn'}/\hbar-\omega_{q't'})], \tag{10}$$

and

$$\tau_{ie}^{-1}(qt)=\tau_1^{-1}+\tau_2^{-1},$$

where ϵ is the step function

$$\epsilon=1 \text{ for } \omega_{qt}<\Delta_{n'n}/\hbar,$$
$$\epsilon=0 \text{ for } \omega_{qt}>\Delta_{n'm}/\hbar.$$

In the isotropic approximation Eq. (9) is written as

$$\tau_1^{-1}(qt)=\frac{\omega_{qt}^2 f^2(\omega_{qt}/V_t)(\tfrac{1}{3}E_u)^4}{64\pi\rho^2V_t^2}\left[1-\exp\left(-\frac{\hbar\omega}{k_BT}\right)\right]N_1(T)\left\langle\left\langle\sum_{n=1,2}\sum_{n'=0}\rho(+n'n)\left|\sum_m\left(\frac{C_{q't'}^{n'm}C_{qt}^{mn}}{\Delta_{mn}-\hbar\omega}+\frac{C_{qt}^{n'm}C_{q't'}^{mn}}{\Delta_{mn}+\hbar\omega}\right)\right|^2\right\rangle\right\rangle$$
$$+N_3(T)\left\langle\left\langle\sum_{n=3}\sum_{n'=0,1,2}P(+n'n)\left|\sum_m\left(\frac{C_{q't'}^{n'm}C_{qt}^{mn}}{\Delta_{mn}-\hbar\omega}+\frac{C_{qt}^{n'm}C_{q't'}^{mn}}{\Delta_{mn}+\hbar\omega}\right)\right|^2\right\rangle\right\rangle, \tag{11}$$

where

$$\rho(+n'n)=\frac{(\Delta_{n'n}+\hbar\omega)^3F(\Delta_{n'n}+\hbar\omega)}{[1-\exp(-\Delta_{nn'}+\hbar\omega/k_BT)]}. \tag{12}$$

Using Eq. (4) and Table II, the Eq. (11) in the quasi-isotropic model becomes

$$
\begin{aligned}
\tau_1^{-1}(q1) &= B_1'(\omega)\{[\rho(+10)(8\beta_1+8\beta_2)+\rho(+13)(8\beta_3+8\beta_2)]N_1(T)+[\rho(+30)(8\beta_4)]N_3(T)\}\,,\\
\tau_1^{-1}(q2) &= B_2'(\omega)\{[\rho(+10)(2\beta_1+7\beta_2)+\rho(+13)(4.5\beta_3+4.5\beta_2)]N_1(T)+\rho(+30)(7\beta_4)N_3(T)\}\,,\\
\tau_1^{-1}(q3) &= B_3'(\omega)\{[\rho(+10)(10\beta_1+5\beta_2)+\rho(+13)(7.5\beta_3+7.5\beta_2)]N_1(T)+\rho(+30)(5\beta_4)N_3(T)\}\,,\\
\beta_1 &= [(\Delta_{30}+\hbar\omega)^{-1}-(\hbar\omega)^{-1}]^2, \quad \beta_2=[(\Delta_{13}+\hbar\omega)^{-1}-(\Delta_{10}+\hbar\omega)^{-1}]^2\,,\\
\beta_3 &= [(\Delta_{30}-\hbar\omega)^{-1}+(\hbar\omega)^{-1}]^2, \quad \beta_4=[(\Delta_{13}-\hbar\omega)^{-1}+(\Delta_{10}+\hbar\omega)^{-1}]^2\,,
\end{aligned}
$$

where

$$\beta_t' = \omega[1-\exp(-\hbar\omega/k_BT)](\tfrac{1}{3}E_u)^4 N_{ex} f^2(q)/225\pi\rho^2\hbar^3 V_t^2\,. \tag{13}$$

Similarly, one can also write the expressions of $\tau_2^{-1}(qt)$

$$
\begin{aligned}
\tau_2^{-1}(q1) &= B_1'(\omega)\{[\rho(-10)(8\delta_1+8\delta_2)+P(-30)(8\delta_4)]N_0(T)+[\rho(-13)(8\delta_2+8\delta_3)]N_3(T)\}\,,\\
\tau_2^{-1}(q2) &= B_2'(\omega)\{[\rho(-10)(2\delta_1+\delta_2)+\rho(-30)(7\delta_4)]N_0(T)+[\rho(-13)(7\delta_2+2\delta_3)]N_3(T)\}\,,\\
\tau_2^{-1}(q3) &= B_3'(\omega)\{[\rho(-10)(10\delta_1+5\delta_2)+\rho(-30)(5\delta_4)]N_0(T)+[\rho(-13)(2\delta_2+10\delta_3)]N_3(T)\}\,,
\end{aligned} \tag{14}
$$

where

$$
\begin{aligned}
\delta_1 &= [(\Delta_{30}-\hbar\omega)^{-1}+(\hbar\omega)^{-1}]^2\,,\\
\delta_2 &= [(\Delta_{13}-\hbar\omega)^{-1}-(\Delta_{10}-\hbar\omega)^{-1}]^2\,,\\
\delta_3 &= [(\Delta_{30}+\hbar\omega)^{-1}-(\hbar\omega)^{-1}]^2\,,\\
\delta_4 &= [(\Delta_{10}-\hbar\omega)^{-1}+(\Delta_{13}+\hbar\omega)^{-1}]^2\,,\\
\rho(-n'n) &= (\Delta_{n'n}-\hbar\omega)^3 F(\Delta_{n'n}-\hbar\omega)[\exp(\Delta_{n'n}-\hbar\omega)-1]^{-1}\,.
\end{aligned} \tag{15}
$$

C. *n*-silicon

In silicon the donor ground state in effective-mass approximation[39,44,45] is sixfold degenerate, reflecting the six equivalent conduction-band minima lying along [100] directions. Valley-orbit interaction splits the sixfold degenerate ground state into a 1*S* (A_1) singlet state and 1*S* ($E+T_2$) fivefold degenerate state. Here A_1, E, and T_2 are irreducible representation of the T_d point group associated with the site symmetry of the impurity atom. In the present paper we have derived expressions for the resonance scattering relaxation rates for phonons in *n*-Si for the situation when the degeneracy of the donor-electron ground state is completely removed due to randomly distributed internal strains. The bound states of donor electrons can be represented by wave packets made up largely of the six Bloch waves chosen from the minima of the conduction band, with appropriate envelope functions to account for their localized hydrogenlike nature. The coupling of phonons to donor electrons and the splitting of the fivefold degenerate ground state by internal stress are dealt with in terms of a strain Hamiltonian. Using the appropriate wave functions for the case of *n*-Si, the matrix elements of the electron-phonon interaction between two donor states $|n\rangle$ and $|n'\rangle$ can be obtained from the general expression (2). The coupling parameters $C_{qt}^{nn'}$ are related in the following way:

$$
\begin{aligned}
C_{qt}^{00} &= \begin{cases} D(t=1), \\ 0(t=2,3)\,, \end{cases}\\
C_{qt}^{11} &= \tfrac{1}{2}(C_{qt}^{00}+C_{qt}^{55})\,,\\
C_{qt}^{22} &= \tfrac{1}{2}(3C_{qt}^{00}-C_{qt}^{55})\,,\\
C_{qt}^{0i} &= C_{qt}^{1i}=C_{qt}^{2i}=C_{qt}^{ij}(i\neq j)=0 \quad (i,j=3,4,5)\,,\\
C_{qt}^{01} &= (C_{qt}^{00}-3C_{qt}^{55})/\sqrt{2}\,,\\
C_{qt}^{12} &= C_{qt}^{02}/\sqrt{2}\,, \quad C_{qt}^{nn'}=(C_{qt}^{n'n})^*\,.
\end{aligned} \tag{16}
$$

The expressions for $C_{qt}^{nn'}$ in the polar coordinates (θ, ϕ) are given in Table III. Here D is E_d/E_u and E_d is the deformation potential.

TABLE III. Expressions for $C_{qt}^{nn'}$.

	$t=1$	2	3
C_{qt}^{02}	$\sqrt{\frac{3}{2}}\sin^2\theta\cos 2\phi$	$-\frac{1}{8}\sqrt{3}\sin 2\theta\cos 2\phi$	$\frac{1}{2}\sqrt{3}\sin\theta\sin 2\phi$
C_{qt}^{33}	$3\sin^2\theta\cos^2\phi$	$\frac{3}{2}\sin 2\theta\cos^2\phi$	$-\frac{3}{2}\sin\theta\sin 2\phi$
C_{qt}^{44}	$3\sin^2\theta\sin^2\phi$	$\frac{3}{2}\sin 2\theta\sin^2\phi$	$\frac{3}{2}\sin\theta\sin 2\phi$
C_{qt}^{55}	$3\cos^2\theta$	$-\frac{3}{2}\sin 2\theta$	0

The relaxation rate of elastic scattering of phonons by bound electrons can be written as

$$\tau_e^{-1}(qt) = Bx^4 F(x) T^2 f^2(x) W_t \,, \tag{17}$$

where

$$W_1 = (32\alpha_1 + 32\alpha_2)N_0 + (32\alpha_1 + 8\alpha_3)N_1 + 16\alpha_2 + 8\alpha_3)N_2 \,,$$

$$W_2 = (48\alpha_1 + 8\alpha_2)N_0 + (48\alpha_1 + 2\alpha_3)N_1 + (4\alpha_2 + 2\alpha_3)N_2 \,,$$

$$W_3 = (40\alpha_2)N_0 + (10\alpha_3)N_1 + (20\alpha_2 + 10\alpha_3)N_2 \,,$$

and

$$\begin{aligned}
&F(x) = v_1^{-5} f^2(x/v_1) + \tfrac{3}{2} v_2^{-5} f^2(x/v_2) \,,\\
&B = (\tfrac{1}{3}E_u)^4 N_{ex} k_B^2 / 200\pi\rho^2 v_t^2 \hbar^4 \,,\\
&\alpha_1 = x_{01}^2/(x^2 - x_{01}^2)^2 \,, \quad \alpha_2 = x_{02}^2/(x^2 - x_{02}^2)^2 \,,\\
&\alpha_3 = x_{12}^2/(x^2 - x_{12}^2)^2 \,.
\end{aligned} \tag{18}$$

$$\begin{aligned}
&N_1 = N_0 \exp(\Delta_{01}/k_B T) = N_0 \exp(x_{01}/T) \,,\\
&N_2 = N_0 \exp(\Delta_{02}/k_B T) = N_0 \exp(x_{02}/T) \,,\\
&N_3 = N_0 \exp(\Delta_{03} | k_B T) = N_0 \exp(x_{03}/T) \,,\\
&N_4 = N_0 \exp(\Delta_{04} | k_B T) \,, \quad N_5 = N_0 \exp(\Delta_{05} | k_B T) \,,\\
&N_0 = N_{ex}[1 + \exp(x_{01}) + \exp(x_{02}) + \exp(x_{03})\\
&\qquad + \exp(x_{04}) + \exp(x_{05})]^{-1} \,,\\
&(E_{n'} - E_n)/k_B T = \Delta_{n'n}/k_B T = x_{n'n} \,,\\
&N_0 + N_1 + N_2 + N_3 + N_4 + N_5 = N_{ex} \,.
\end{aligned}$$

The unphysical divergencies in Eq. (17) can be removed by taking into account the finite linewidths of the donor states. This corresponds to replacing $(\Delta_{n'n}^2 - \hbar^2\omega^2)^{-2}$ by $[(\Delta_{n'n}^2 - \hbar^2\omega^2)^2 + 4\Gamma^2\Delta_{n'n}^2]^{-1}$. It is interesting to note that the contribution due to triplet state into Eq. (17) is zero.

The inelastic scattering in the second order of perturbation falls into two categories. The first (τ_1^{-1}) is associated with electron transitions from the upper to the lower level and the other (τ_2^{-1}) involves electron transition from the lower to the upper level by "thermally assisted" phonon absorption $(w < \Delta/\hbar)$ or by inelastic scattering $(w > \Delta/\hbar)$. The relaxation rates are, respectively,

$$\tau_1^{-1}(qt) = B'x[1 - \exp(-x)] T^2 f^2(x/vt) W_t \,, \tag{19}$$

where

$$\begin{aligned}
W_1 = {} & [\{\rho + 01)(4\beta_1 + 4\beta_2) + \rho(+02)(4\beta_3 + 4\beta_2)\} N_0(T)\\
& + \{\rho(+12)(q\beta_3 + q\beta_4)\} N_1(T)] \,,
\end{aligned}$$

$$\begin{aligned}
W_2 = {} & \{[\rho(+01)(\beta_1 + 6\beta_2) + \rho(+02)(4\beta_3 + 4\beta_2)] N_0(T)\\
& + [\rho(+12)(12\beta_3 + 2\beta_4)] N_1(T)\} \,,
\end{aligned}$$

$$\begin{aligned}
W_3 = {} & [\{\rho(01)(5\beta_1) + \rho(02)(5\beta_3)\} N_0(T)\\
& \times \{\rho(+12)(10\beta_4)\} N_1(T) \,,
\end{aligned}$$

and

$$\begin{aligned}
&B' = (\tfrac{1}{3}Eu)^4 N_{ex} k_B^2 / 200\pi\rho^2 v_t^2 \hbar^3 \,,\\
&\beta_1 = [(x_{02} + x)^{-1} - (x_{12} + x)^{-1}]^2 \,,\\
&\beta_2 = [(x_{01} + x)^{-1} - (x)^{-1}]^2 \,,\\
&\beta_3 = [(x_{12} + x)^{-1} - (x_{02} + x)^{-1}]^2 \,,\\
&\beta_4 = [(x_{01} - x)^{-1} + (x)^{-1}]^2 \,,\\
&\rho(+n'n) = (x + x_{n'n})^3 F(x + x_{n'n}) \{1 - \exp[-(x + x_{n'n})]\}^{-1} \,.
\end{aligned} \tag{20}$$

A similar expression is also obtained for $\tau_2^{-1}(qt)$ and is given by

$$\tau_2^{-1}(q\,t) = B'x[1 - \exp(-x)] T^2 f^2(x/v_t) W_t \,, \tag{21}$$

where

$$\begin{aligned}
W_1 = {} & \{[\rho(-01)(4\delta_1 + 4\delta_2)] N_1(T)\\
& + [\rho(-02)(4\delta_3 + 4\delta_2) + \rho(-12)(8\delta_3 + 8\delta_1)] N_2(T)\} \,,\\
W_2 = {} & \{[\rho(-01)(\delta_1 + 6\delta_2)] N_1(T)\\
& + [\rho(-02)(\delta_3 + 6\delta_2) + \rho(-12)(2\delta_3 + 12\delta_1)] N_2(T)\} \,,\\
W_3 = {} & \{[\rho(-01)(5\delta_1)] N_1(T)\\
& + \{\rho(-02)(5\delta_3) + \rho(-12)(10\delta_3)\} N_2(T)\} \,.
\end{aligned}$$

Here

$$\begin{aligned}
&\delta_1 = [(x_{02} - x)^{-1} + (x_{12} + x)^{-1}]^2 \,,\\
&\delta_2 = [(x_{01} - x)^{-1} + (x)^{-1}]^2 \,,\\
&\delta_3 = [(x_{02} - x)^{-1} - (x_{12} - x)^{-1}]^2 \,,\\
&\delta_4 = [(x_{01} + x)^{-1} - (x)^{-1}]^2 \,,\\
&\rho(-n'n) = (x - x_{n'n})^3 [\exp(x_{n'n} - x) - 1]^{-1} F(-x + x_{n'n}) \,.
\end{aligned} \tag{22}$$

As mentioned before, the contribution due to the transitions from the triplet state denoted by 3, 4, and 5 vanish.

The expressions for bound-electron–phonon relaxation rates for the case of D_{3d} symmetry[46] are also derived. In the D_{3d} symmetry fivefold state $(A_{2u} + E_g + E_u)$ is the lower state. We have considered the splitting of a fivefold degenerate state into five states denoted by 1, 2, 3, 4, and 5. The A_{2u} state corresponds to 3, the E_g state to 1 and 2, and the state E_u to 4 and 5. The following relations among coupling constants are used in the evaluation of different relaxation rates

$$\begin{aligned}
&C_{qt}^{11} = C_{qt}^{44} = C_{qt}^{00} - (1/\sqrt{2}) C_{qt}^{02} \,,\\
&C_{qt}^{22} = C_{qt}^{55} = C_{qt}^{00} + (1/\sqrt{2}) C_{qt}^{02} \,,\\
&C_{qt}^{12} = C_{qt}^{45} = (1/\sqrt{2}) C_{qt}^{02} \,,\\
&C_{qt}^{n'n} = 0 (i = 0, 1, 2, \;\; j = 3, 4, 5) \,.
\end{aligned} \tag{23}$$

The values of C_{qt}^{33}, C_{qt}^{02}, C_{qt}^{55}, and C_{qt}^{44} are given in the Table III. The following expressions are obtained for elastic, inelastic, and phonon-assisted scattering, respectively.

$$\tau_e^{-1} = Bx^4T^2f^2(x/v_t)F(X)W_t \,, \tag{24}$$

where

$$W_1 = (32\alpha_1 + 32\alpha_2)N_0(T) + (32\alpha_1 + 16\alpha_3)N_1(T) + (32\alpha_2 + 16\alpha_3)N_2(T) + 16\alpha_4(N_4 + N_5) \,,$$

$$W_2 = (48\alpha_1 + 8\alpha_2)N_0(T) + (48\alpha_1 + 4\alpha_3)N_1(T) + (8\alpha_2 + 4\alpha_3)N_2 + 4\alpha_4(N_4 + N_5) \,,$$

$$W_3 = (40\alpha_2)N_0(T) + (20\alpha_3)N_1(T) + (40\alpha_2 + 20\alpha_3)N_2(T) + 20\alpha_4(N_4 + N_5)$$

where

$$\alpha_1 = (x_{01}/x_{01}^2 - x^2)^2 \,, \quad \alpha_3 = (x_{12}/x_{12}^2 - x^2)^2 \,,$$

$$\alpha_2 = (x_{02}/x_{02}^2 - x^2)^2 \,, \quad \alpha_4 = (x_{45}/x_{45}^2 - x^2)^2 \,. \tag{25}$$

$$\tau_1^{-1}(qt) = BT^2x[1 - \exp(-x)]f^2(\omega/v_t)W_t \,,$$

where

$$W_1 = \{[\rho(+01)(4\beta_1 + 4\beta_2) + \rho(+02)(4\beta_3 + 4\beta_1)]N_0(T)[\rho(+12)(8\beta_3 + 8\beta_4)]N_1(T) + [\rho(+45)(8\beta_5 + \beta_6)]N_4\} \,,$$

$$W_2 = \{[\rho(+01)(6\beta_1 + \beta_2) + \rho(+02)(\beta_3' + 6\beta_1)]N_0(T) + [\rho(+12)(12\beta_3 + 2\beta_4)]N_1(T) + [\rho(+45)(2\beta_5 + 12\beta_6)]N_4(T)\} \,, \tag{26}$$

$$W_3 = \{[\rho(+01)(5\beta_2) + \rho(+02)(5\beta_3)]N_6(T) + [\rho(+12)(10\beta_4)]N_1(T) + [\rho(+45)(10\beta_5)]N_4(T)\} \,.$$

Here

$$\beta_1 = \left(\frac{x_{01}}{x(x + x_{01})}\right)^2 \,, \quad \beta_2 = \left(\frac{x_{12} + x_{02}}{(x + x_{02})(x - x_{12})}\right)^2$$

$$\beta_3 = \left(\frac{x_{02} - x_{12}}{(x + x_{12})(x + x_{02})}\right)^2 \,, \quad \beta_4 = \left(\frac{x_{01}}{x(x_{01} - x)}\right)^2 \tag{27}$$

$$\beta_5 = \left(\frac{1}{x + x_{45}}\right)^2 \,, \quad \beta_6 = \left(\frac{1}{x}\right)^2 .$$

Similarily the relaxation rate $\tau_2^{-1}(qt)$ is given by

$$\tau_2^{-1}(qt) = BxT^2[1 - \exp(-x)]f^2\left(\frac{x}{v_t}\right)W_t \,, \tag{28}$$

where

$$W_1 = \{[\rho(-01)(4\delta_1 + 4\delta_2)]N_1(T) + [\rho(-02)(4\delta_3 + 4\delta_1) + \rho(-12)(8\delta_4 + 8\delta_3)]N_2 + [\rho(-45)(8\delta_5 + 8\delta_6)]N_5\} \,,$$

$$W_2 = \{[\rho(-01)(6\delta_1 + \delta_2)]N_1(T) + [\rho(-02)(\delta_3 + 6\delta_4) + \rho(-12)(2\delta_4 + 12\delta_3)]N_2(T) + [\rho(-45)(2\delta_5 + 12\delta_6)]N_5\} \,,$$

$$W_3 = \{[\rho(-01)(5\delta_2)]N_1 + [\rho(-02)(5\delta_3) + \rho(-12)(10\delta_4)]N_2(T) + [\rho(-45)(10\delta_5)]N_5(T)\} \,.$$

Here

$$\delta_1 = \left(\frac{x_{01}}{x(x_{01} - x)}\right)^2 \,, \quad \delta_2 = \left(\frac{x_{12} + x_{02}}{(x + x_{12})(x - x_{02})}\right)^2 \,,$$

$$\delta_3 = \left(\frac{x_{12} - x_{02}}{(x - x_{12})(x - x_{02})}\right)^2 \,, \quad \delta_4 = \left(\frac{x_{01}}{x(x_{01} + x)}\right)^2 \,, \tag{29}$$

$$\delta_5 = (x - x_{45})^{-2} \,, \quad \delta_6 = x^{-2} \,.$$

It is interesting to note that transitions from states denoted by 4 and 5 make nonvanishing contributions, whereas transitions involving state 3 do not contribute. It may be further noted that the scattering strength of phonons for the D_{3d} symmetry is stronger than that for the T_d symmetry.

III. THERMAL CONDUCTIVITY

Bird and Pearlman[11] have carried out an extensive study of phonon conductivity of Sb-, As-, and P-doped Ge in the temperature range 0.3 to 4.2 °K. Besides the usual plot of K_D vs T, they have also plotted K_D/K_P vs T, where K_D is the phonon conductivity of the doped sample and K_P is the same for the pure material. The latter plots show very conclusively the resonance nature of the scattering of phonons and the temperatures at which resonance dips occur. For example, in the Sb-doped Ge sample resonance dip occurs at 0.7 °K. For As- and P-doped Ge samples, resonance dips are much less pronounced and occur at about 2 °K. These materials provide suitable illustrations for the application of the theory developed in the present paper for strained n-Ge crystals.

We shall use Callaway's[47] expression for the calculation of the lattice thermal conductivity

$$K(T)=\frac{K_B^4T^3}{6\pi^2\hbar^3}\sum_t\frac{1}{v_t}\int_0^{(\Theta_D/T)}\frac{x^4[\exp(x)-1]^{-2}}{\tau_c^{-1}(qt)}dx, \qquad (30)$$

where Θ_D is the Debye temperature and k_B is the Boltzmann constant. The most important parameter in the theory is the combined relaxation time for phonons $\tau_c^{-1}(qt)$. In the presence of several phonon-scattering processes, τ_c^{-1} can be expressed as

$$\tau_c^{-1}=\tau_B^{-1}+\tau_{pt}^{-1}+\tau_{pp}^{-1}+\tau_{ep}^{-1}, \qquad (31)$$

where τ_B^{-1} is the relaxation time for the boundary scattering of phonons and expressed as[48]

$$\tau_B^{-1}=V_t/L. \qquad (31')$$

L is the characteristic length of the specimen and is given by $L=1.12\sqrt{s}$ for the rectangular cross section S. τ_{pt}^{-1} is the relaxation time for the scattering of phonons by point defects and is written as[49]

$$\tau_{\text{pt}}^{-1}=\frac{V_0}{2\pi V^3}\sum_i\left(f_i\left[1-\frac{m_i}{\overline{m}}\right]^2\right)\omega^4=A\omega^4, \qquad (32)$$

where V_0 is the atomic volume, f_i is the fractional concentration of the ith species, m_i is the mass of the ith species, and $\overline{m}$ is the average mass. τ_{pp}^{-1} is the phonon-phonon relaxation rate. Callaway[47] assumed that both three-phonon normal and umklapp processes have the same frequency and temperature dependence. Actually he writes

$$\tau_{pp}^{-1}=[\tau_{pp}^{-1}]_N+[\tau_{pp}^{-1}]_U=(B_1+B_2)\omega^2T^3, \qquad (33)$$

where U and N denote umklapp and normal processes, respectively. Equation (33) corresponds to Herring's[50] expression for the low-frequency phonon-phonon scattering for longitudinal phonons and normal processes,

$$[\tau_{pp}^{-1}]_N\propto[\tau_{pp}^{-1}]_U\propto\omega^jT^{5-j}. \qquad (34)$$

Here $j=2$ for longitudinal phonons in a cubic cyrstal. With this phenomenological expression Callaway was able to account for the phonon conductivity results of normal and isotope-enriched Ge very well. The usual procedure of investigating the role of additional phonon scattering mechanisms in doped Ge is to use Callaway's results for undoped Ge as the basis. In the temperature range where phonon-phonon scattering is relevant, the analysis of phonon conductivity resulting in doped Ge is to some extent handicapped due to the uncertainty in the temperature and the frequency dependence of τ_{pp}^{-1}. However, in the present analysis we are interested in the region 0.3 to 4.2 °K where the phonon-phonon scattering make no appreciable contribution to the phonon conductivity. Thus the investigation of the role of resonance scattering of phonons by bound electrons is not handicapped due to the uncertainties regarding τ_{pp}^{-1}. Thus the relaxation rates for the doped and undoped samples are written, respectively, as

$$\tau_c^{-1}(qt)=\tau_{pp}^{-1}+\tau_{pt}^{-1}+\tau_B^{-1}+\tau_{ep}^{-1}, \qquad (35)$$

$$\tau^{-1}(qt)=\tau_{pp}^{-1}+\tau_{pt}^{-1}+\tau_B^{-1}. \qquad (36)$$

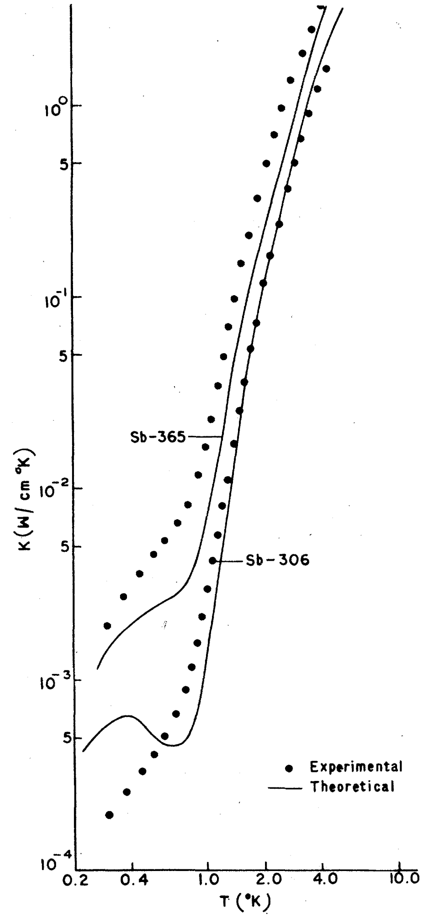

FIG. 1. Plot of the thermal conductivity vs temperature for Sb-doped sample Sb-365. Theoretical curves are calculated with the help of SM theory.

IV. RESULTS AND DISCUSSION

The experimental results of Bird and Pearlman are very interesting in the sense that they cover the temperature range both below and above the temperature at which the resonance dips are observed. They have not only given the results in the usual form of K vs T curves, but also plotted K_D/K_P vs T. These plots show clearly the resonance nature of phonon scattering by bound donor electrons in doped germanium. They have tried to explain their experimental results in doped germanium with the theories proposed by Keyes[31] and Griffin and Carruthers.[32] However, they failed to explain their experimental results in the temperature range 0.3 to 4.2 °K. Their analysis does not take into account the inelastic scattering of phonons by bound electrons and the elastic scattering of phonons off the triplet state. Suzuki and Mikoshiba (SM)[34] have taken into account the above scattering processes in their paper. As a first step we have used expressions of SM to analyze the above experimental results of n-type Ge in the temperature range 0.3 to 4.2 °K. The theoretical results along with the experimental values are shown in the Figs. 1 and 2 only for Sb-306 and Sb-365. One can see from Figs. 1 and 2, that the Suzuki and Mikoshiba theory is also unable to explain the details of the resonance dips in the case of Sb-306 and Sb-365 samples.[41]

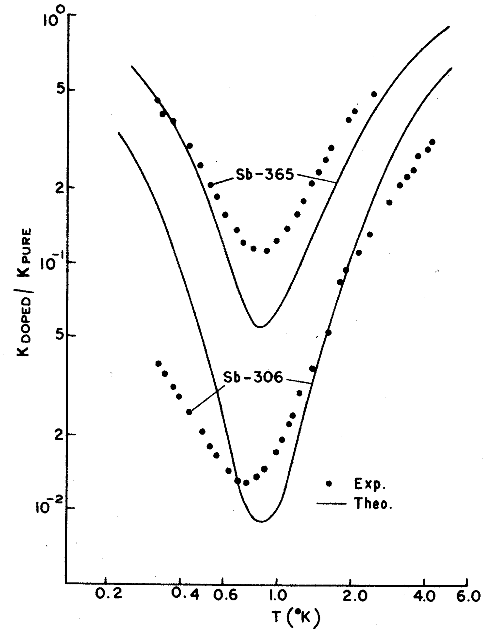

FIG. 2. Plot of the k_D/K_P vs temperature for Sb-doped sample. K_D is the phonon conductivity of the doped material and K_P is the same for pure. Theoretical curves are calculated with the help of SM theory.

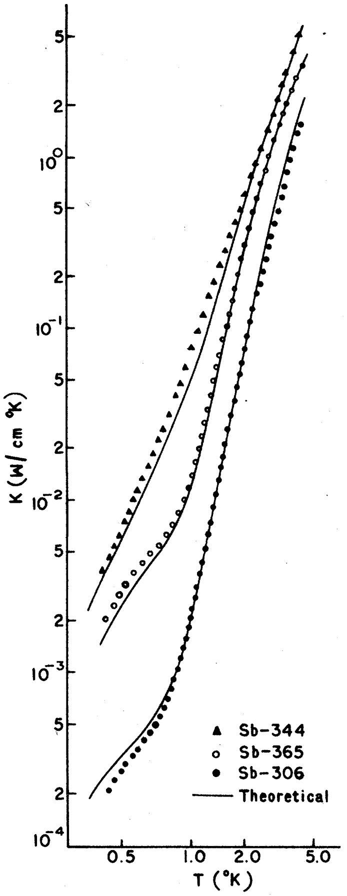

FIG. 3. Plot of the experimental and theoretical conductivity vs temperature for Sb-doped samples (Sb-344, Sb-365, Sb-306).

The reason for the failure of the theory to explain the experimental results lies in the fact that no consideration is given to the presence of internal strains. We have taken into account the effect of the internal strain in our expressions for the relaxation rates which are given by Eqs. (7), (12), and (14). Therefore, we have used our expressions in the calculation of K_D. K_D is calculated by using the Eqs. (30) and (35), K_P is calculated by using the Eqs. (30) and (36). The theoretical results are shown in the Figs. 3–6 along with the experimental results. The theoretical parameters used in the calculations are given in Table IV. We have used no adjustable parameters except $\Delta_{n'n}$.

One can see from the Figs. 3–6 that our theory can explain fairly well the experimental data of Sb-, P-, and As-doped germanium. Some discrepancies are observed between the theoretical and experimental results. These discrepancies can be removed[12] by taking into account the concentration dependence with energy-level splitting,

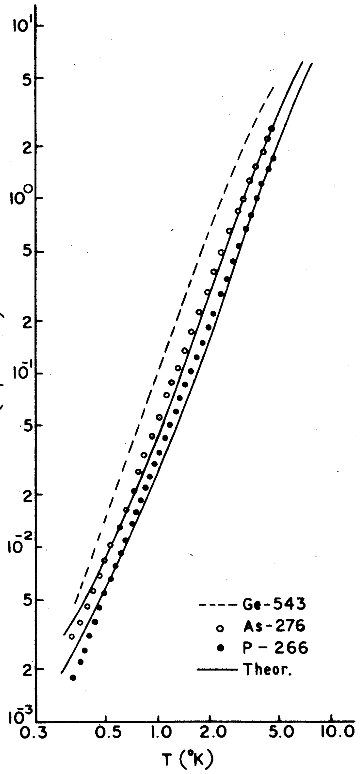

FIG. 4. Experimental and theoretical thermal conductivity for and As-doped germanium.

of the deformation potential and Bohr radius, respectively.

Recently[51] Halbo has used SM theory to explain the magnetothermal conductivity of n-type germanium by considering the magnetic dependence of the donor-ground-state effective Bohr radius a^* and the chemical shift 4Δ. However, he has failed to explain his experimental results. Our theory can be used in place of SM theory to explain the magnetothermal conductivity of n-type germanium.

TABLE IV. Physical parameters used in the calculations of doped germanium.

	Sb	P	As
ρ(g/cm^3)	5.35	5.35	5.35
V_1(cm/sec)	3.37	5.37	5.37
V_2(cm/sec)	3.28	5.28	5.28
A (10^{-44}sec^{-3})	2.4	2.4	2.4
E_u (eV)	19	16	16
a^* (Å)	65	40	45
Δ_{10}/k_B(°K)	5.0	32.8	49.1
Δ_{30}/k_B(°K)	3.71	8.0	10.0
Δ_{13}/k_B(°K)	1.0	25.0	35.0

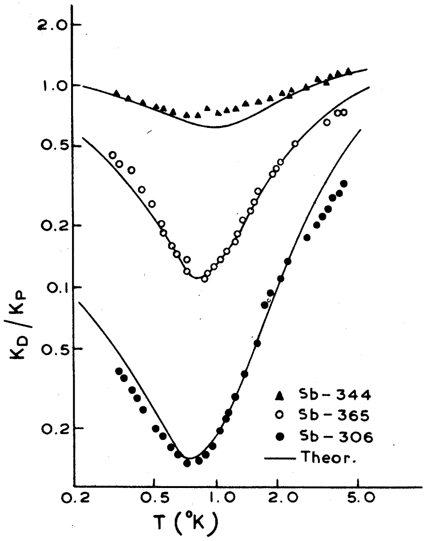

FIG. 5. Plot of K_D/K_P vs temperature for samples Sb-344, Sb-365, and Sb-306. K_D is the phonon conductivity of doped material and K_P is the same for pure material.

To display the contributions of elastic and inelastic scatterings the theoretical curves of K_D/K_P vs T for elastic scattering and for inelastic scattering as a function of temperature are shown in Figs. 4 for the Sb-365 sample. K_D/K_P for elastic scattering is calculated only by taking elastic phonon scattering, i.e., $\tau_{ep}^{-1}=\tau_e^{-1}$ in Eq. (36). Similarly K_D/K_P for inelastic scattering is calculated taking only inelastic scattering, i.e., $\tau_{ep}^{-1}=\tau_{ie}^{-1}$ in Eq. (36). It is seen from these curves that elastic scattering is important between 0.3 and 0.6 °K, but the contributions of elastic and inelastic scattering to the K_D/K_P-vs-T curve are approximately equal for $T>0.6$ °K.

The deviation between experimental and theoretical results at higher temperatures is due

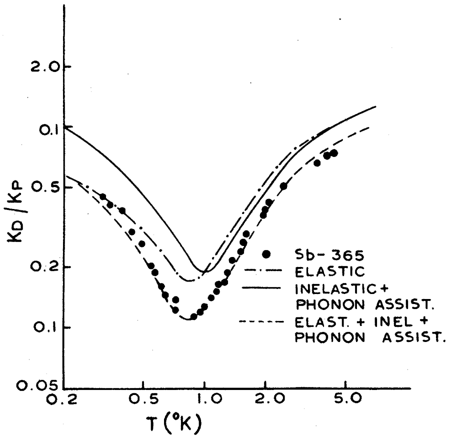

FIG. 6. Plot of K_D/K_P vs temperature for sample Sb-365.

partly to the form of the donor wave function used in the calculations. The population of the phonons with frequency $\omega > V_t/a^*$ is increasing with temperature. For these phonons the strength of the coupling to the donor depends strongly on the donor wave function, and, as a consequence, in the calculation of $K(T)$ we should use the true wave function which is not known for strained crystals.

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†Present address: Physics Dept., Nottingham University, Nottingham, U.K.

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