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Effect of the anisotropic form factor on the phonon-electron interaction and phonon transport in As-doped Ge

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Usually the phonon-electron relaxation rates in doped semiconductors are calculated by taking a spherical approximation for the conduction-band minima. In the present work we have revoked this approximation and obtained more general expressions for the phonon-electron relaxation rates. Using these expressions, we have calculated the phonon conductivity of As-doped germanium and shown that our approach improves the theoretical value of the phonon conductivity by 30–40 % even at 10 K.

I. INTRODUCTION

Despite the consistent effort of many workers,[1–3] there is no unique quantitative explanation for the phonon conductivity of doped semiconductors at temperatures greater than 4 K. In fact, the phonon transport in doped semiconductors is restricted mainly due to phonon scattering by charge carriers and the usual theory for phonon-electron relaxation rate[4–6] overestimates the phonon conductivity[7,8] beyond this temperature. This happens due to the reason that the form factor appearing in the phonon-electron relaxation rate has a sharp cutoff for high-frequency phonons which consequently cannot be scattered by electrons. This obviously makes it impossible to explain the higher-temperature data of the phonon conductivity. While Singh and Verma[1] assumed the presence of internal strains, Sharma, Roy, and Radhakrishnan,[2] on the other hand, successfully used the Mikoshiba[9] model to interpret the results of phonon conductivity in *p*-type Ge in the whole temperature range. Recently, Puhl, Sigmund, and Mair[3] have shown that the dynamic Jahn-Teller effect also gives rise to an extra time-dependent factor in the phonon relaxation rate which in turn may explain the phonon conductivity at higher temperatures. As reported by the authors, this effect is, however, quantitatively not important in the case of As-doped Ge.

In fact, all the above-referenced models are based on the spherical approximation originally introduced by Hasegawa[10] for the crucial factor called the form factor [Eq. (5)]. According to this approximation the ellipsoidal energy surface of the donor electron is replaced by a spherical one. By doing this the calculation of phonon-electron relaxation rates is very much simplified because the form factor becomes independent of the valley with which it is associated. In the present work, therefore, we wish to investigate the effect of the previous approximation for the form factor on the phonon-electron relaxation rate and then calculate the phonon conductivity on the basis of the corrected form factor in the case of As-doped Ge. We have shown that, due to this correction, the theoretical value of the phonon conductivity can be improved by an amount 30–40 % even at 10 K without using any of the models used in Refs. 1–3.

In Sec. II we have given the relevant modifications in the theory to obtain the general expression for the electron-phonon relaxation rate with desired background. Section III gives the results of the calculations as well as a thorough analysis of the obtained results.

II. THEORY

A. Phonon conductivity

According to Holland,[11] the Callaway model[12] shall be modified to give the following expression for the phonon conductivity:

$$K(T)=\frac{k_B^4 T^3}{6\pi^2\hbar^3}\sum_{\lambda=1}^{3}\frac{1}{v_\lambda}\int_0^{\Theta_{D/T}}\frac{x^4 e^x}{(e^x-1)^2\tau^{-1}(x)}dx \ , \tag{1}$$

where $\lambda=1$ stands for longitudinal and $\lambda=2,3$ are for the transverse modes, $x=(\hbar\omega_{q\lambda}/k_B T)$, k_B is the Boltzmann constant. v_λ, the phonon velocity, $\omega_{q\lambda}$, the phonon frequency, and $\tau^{-1}=\tau_b^{-1}+\tau_{pt}^{-1}+\tau_{e\text{-ph}}^{-1}+\tau_{\text{ph}-\text{ph}}^{-1}$ is the total phonon relaxation rate. $\tau_b^{-1}=v_\lambda/L_c$, L_c is the Casimir length; $\tau_{pt}^{-1}=A\omega_{q\lambda}^4$; $\tau_{\text{ph}-\text{ph}}^{-1}=B_1\omega_{q\lambda}^2T^3$ for longitudinal phonons and $\tau_{\text{ph}-\text{ph}}^{-1}=B_t\omega_{q\lambda}T^4$ for transverse phonons and all these expressions can be found in Ref. 8. Here we will concentrate our discussion only about the phonon-electron relaxation rate, $\tau_{e\text{-ph}}^{-1}$, which is mainly responsible for the decrease of phonon conductivity in the temperature range 2–10 K.

B. Phonon-electron relaxation rates

According to Cheung and Barrie,[13] the phonon-electron matrix element for the phonon in the branch λ and wave vector $\mathbf{q}$ can be written as

$$\Omega_{mn}^{q\lambda}=i\left[\frac{\hbar q}{2\rho V v_\lambda}\right]^{1/2}\sum_{j=1}^{4}\theta_{mn}^{j}(\mathbf{q})A_{mn}^{j}(\mathbf{q},\lambda) \ . \tag{2}$$

where j stands for the four valleys of the conduction-band minima in n-type Ge, m and n represent the electronic states. v_λ is the phonon velocity. Also, $A_{mn}^{j}(\mathbf{q},\lambda)$, the deformation-potential matrix, is

$$A^j_{mn}(\mathbf{q},\lambda)=E_d\delta_{\lambda,1}J_{mn}+E_u\mathbf{e}_\lambda(\mathbf{q})\cdot D_{mn}\cdot\mathbf{e}_1(\mathbf{q}) \qquad (3)$$

in which E_d and E_u are the dilatation and shear deformation potentials, $\mathbf{e}_\lambda(\mathbf{q})$ are the phonon polarization vectors defined by Hasegawa,[10] and

$$J_{mn}=\alpha^j_m\alpha^j_n\ ,\quad D_{mn}=\alpha^j_m\alpha^j_n(\hat{\mathbf{k}}^{(j)}:\hat{\mathbf{k}}^{(j)})\ , \qquad (4)$$

where $\hat{\mathbf{k}}^{(j)}$ are the unit vectors pointing towards the bottom of the jth valley of the conduction band. The directions of $\hat{\mathbf{k}}^{(j)}$ and the value of the normalization constants $\alpha^{(j)}$ for Ge have been reported in Ref. 5. Values of the dyad $(\hat{\mathbf{k}}^{(j)}:\hat{\mathbf{k}}^{(j)})$ for different j have been given in Table I. In expression (2), $\theta^j_{mn}(\mathbf{q})$, the form factor, is the most important term in reference to the present work. It depends on the wave function of the impurity electron as well as the wave vector $\mathbf{q}$ of the phonon which causes the transition. Since we are interested in the low-temperature range, the impurity electron is supposed to be in the ground state only and in that case $\theta^{(j)}_{mn}$ takes the following form:

$$\theta^j_{1s,1s}(\mathbf{q})=\left[1+\frac{\chi^2_j}{4}\right]^{-2}\ , \qquad (5)$$

with

$$\chi^2_j=a^2(q^2_{x_j}+q^2_{y_j})+b^2q^2_{z_j}\ ; \qquad (5a)$$

q_{x_j}, q_{y_j}, and q_{z_j} are the components of the vector $\mathbf{q}$ when the z axis is defined as being from the origin to the jth minimum of the valley.

a and b are the longitudinal and transverse Bohr radii. The values of a and b are defined[14] by

$$a=\hbar(2m_tE_0)^{-1/2},\quad b=(m_t/m_l)^{1/2}a\ . \qquad (6)$$

$E_0=0.0127$ eV is the experimental value of the ionization energy for the ls state, m_l and m_t are the longitudinal and transverse effective masses at the conduction-band minima, respectively. For Ge, m_t and m_l are given by $m_t=(0.0813\pm0.002)m_0$ and $m_l=(1.60\pm0.008)m_0$.

The matrix element of Eq. (2) is based on the electron-phonon Hamiltonian initially given by Hasegawa.[10] Here the small intervalley terms have been neglected in comparison to the larger intravalley terms. In order to simplify this matrix element, a spherical approximation for the form factor was introduced[10] with the following assumption:

$$a^*=(a^2b)^{1/3}$$

and

TABLE I. Values of $\hat{\mathbf{k}}^{(j)}:\hat{\mathbf{k}}^{(j)}$ for different values of j in germanium.

$$\hat{\mathbf{k}}^{(1)}:\hat{\mathbf{k}}^{(1)}=\frac{1}{3}\begin{bmatrix}1&1&1\\1&1&1\\1&1&1\end{bmatrix}$$

$$\hat{\mathbf{k}}^{(2)}:\hat{\mathbf{k}}^{(2)}=\frac{1}{3}\begin{bmatrix}1&-1&-1\\-1&1&1\\-1&1&1\end{bmatrix}$$

$$\hat{\mathbf{k}}^{(3)}:\hat{\mathbf{k}}^{(3)}=\frac{1}{3}\begin{bmatrix}1&-1&1\\-1&1&-1\\1&-1&1\end{bmatrix}$$

$$\hat{\mathbf{k}}^{(4)}:\hat{\mathbf{k}}^{(4)}=\frac{1}{3}\begin{bmatrix}1&1&-1\\1&1&-1\\-1&-1&1\end{bmatrix}$$

$$a^2(q^2_{x_j}+q^2_{y_j})+b^2q^2_{z_j}\longrightarrow(a^*q)^2\ . \qquad (7)$$

a^* is the effective Bohr radius. This approximation reduces the form factor to the simple form $\theta_{1s,1s}(\mathbf{q})=\{1+(qa^*/2)^2\}^{-2}$, which is independent of the valley. Thus in Eq. (2) the form factor can be drawn out of the summation sign and the factor $A^j_{mn}(\mathbf{q},\lambda)$ can be easily summed up over the four valleys. After this, one can smoothly proceed to derive the expressions of phonon-electron relaxation rates for elastic, inelastic, and absorption processes and arrive at the results of Suzuki and Mikoshiba.[6]

In the case of germanium the anisotropy of the form factor, however, is too large and the spherical approximation cannot be very much justified. Therefore we would like to revoke this approximation and keep the general form of the matrix element in Eq. (2) intact. We define

$$M^{\mathbf{q}\lambda}_{mn}=\sum_{j=1}^{4}\theta^j_{mn}(\mathbf{q})A^j_{mn}(\mathbf{q},\lambda)$$

and write

$$\Omega^{\mathbf{q}\lambda}_{mn}=i(\hbar q/2\rho Vv_\lambda)^{1/2}M^{\mathbf{q}\lambda}_{mn}\ . \qquad (8)$$

The general form of the phonon-electron relaxation rates, in which we are basically interested, can now be written for various processes in terms of $M^{\mathbf{q}\lambda}_{mn}$ in the following ways.

1. *Elastic scattering*

In the second-order Born approximation the total transition probability per unit time for the scattering of phonon $\mathbf{q}$ to $\mathbf{q}'$ for this process[4] is

$$\begin{aligned}w(\mathbf{q}\to\mathbf{q}')n_q(1+n_{q'})=\frac{2\pi}{\hbar^2}\delta(\omega_{q'\lambda'}-\omega_{q\lambda})\Bigg[f_0(T)\Bigg|\sum_{m=1}^{3}\left[-\frac{M^{q'\lambda'}_{0m}M^{\mathbf{q}\lambda}_{m0}}{\hbar\omega_{q\lambda}-4\Delta+i\Gamma}+\frac{M^{\mathbf{q}\lambda}_{0m}M^{\mathbf{q}'\lambda'}_{m0}}{\hbar\omega_{q\lambda}+4\Delta-i\Gamma}\right]\Bigg|^2\\ +f_1(T)\sum_{n,n'=1}^{3}\Bigg|\frac{M^{q'\lambda'}_{n'0}M^{\mathbf{q}\lambda}_{0n}}{\hbar\omega_{q\lambda}+4\Delta-i\Gamma}-\frac{M^{\mathbf{q}\lambda}_{n'0}M^{\mathbf{q}'\lambda'}_{0n}}{\hbar\omega_{q\lambda}-4\Delta+i\Gamma}\\ +\sum_{m=1}^{3}\left[\frac{M^{q'\lambda'}_{n'm}M^{\mathbf{q}\lambda}_{mn}}{\hbar\omega_{q\lambda}-i\Gamma}-\frac{M^{\mathbf{q}\lambda}_{n'm}M^{\mathbf{q}'\lambda'}_{mn}}{\hbar\omega_{q\lambda}-i\Gamma}\right]\Bigg|^2\Bigg](a^*_{q'\lambda'}a_{q\lambda})^2q^2q'^2\ . \qquad (9)\end{aligned}$$

Here as stated earlier m and n are restricted only to the fourfold "impurity-electron ground state," which splits up into a singlet and a triplet state separated by the chemical shift 4Δ. The first term of Eq. (9) represents the elastic scattering off the singlet state and the second term that for the triplet state. Γ is the "level width."[6] $f_0(T)$ and $f_1(T)$ are the occupation probabilities, at temperature T, for the singlet and triplet states, respectively. Taking the angular average of the matrix the above expression can be written in the form

$$\frac{4\pi}{\hbar^2}\delta(\omega_{q'\lambda'}-\omega_{q\lambda})\frac{(4\Delta)^2}{\{(\hbar\omega_{q\lambda})^2-(4\Delta)^2\}^2+4(4\Delta)^2\Gamma^2}$$
$$\times\{2[f_0(T)+f_1(T)][\langle(M_{01}^{q'\lambda'})^2\rangle\langle(M_{10}^{q\lambda})^2\rangle+\langle(M_{02}^{q'\lambda'})^2\rangle\langle(M_{20}^{q\lambda})^2\rangle+\langle(M_{03}^{q'\lambda'})^2\rangle\langle(M_{30}^{q\lambda})^2\rangle]$$
$$+f_1(T)[(4\Delta/\hbar\omega_{q\lambda})^2+1][\langle(M_{01}^{q'\lambda'})^2\rangle\langle(M_{20}^{q\lambda})^2\rangle+\langle(M_{01}^{q'\lambda'})^2\rangle\langle(M_{30}^{q\lambda})^2\rangle+\langle(M_{02}^{q'\lambda'})^2\rangle\langle(M_{10}^{q\lambda})^2\rangle$$
$$+\langle(M_{02}^{q'\lambda'})^2\rangle\langle(M_{30}^{q\lambda})^2\rangle+\langle(M_{03}^{q'\lambda'})^2\rangle\langle(M_{10}^{q\lambda})^2\rangle+\langle(M_{03}^{q'\lambda'})^2\rangle\langle(M_{20}^{q\lambda})^2\rangle]\}\ .$$

In this expression all the cross terms like $\langle(M_{10}^{q\lambda})(M_{20}^{q\lambda})\rangle$ have been neglected in comparison to the squared terms like $\langle(M_{10}^{q\lambda})^2\rangle$. Here $\langle(M_{10}^{q\lambda})^2\rangle=(1/4\pi)\int d\Omega(M_{10}^{q\lambda})^2$. After going through a few steps it is easy to write the single-mode relaxation rate for the elastic process as

$$\tau_e^{-1}=\frac{\omega_{q\lambda}^4}{4\pi\rho^2 v_\lambda^2}\sum_{\lambda'}\frac{1}{v_{\lambda'}^5}\left[\frac{2(4\Delta)^2}{[(\hbar\omega_{q\lambda})^2-(4\Delta)^2]^2+4\Gamma^2(4\Delta)^2}\right.$$
$$\times\{[\langle(M_{01}^{q'\lambda'})^2\rangle\langle(M_{10}^{q\lambda})^2\rangle+\langle(M_{02}^{q'\lambda'})^2\rangle\langle(M_{20}^{q\lambda})^2\rangle+\langle(M_{03}^{q'\lambda'})^2\rangle\langle(M_{30}^{q\lambda})^2\rangle]$$
$$\times 2[C_s(T)+C_t(T)]+[1+(4\Delta/\hbar\omega_{q\lambda})^2]C_t(T)[\langle(M_{02}^{q'\lambda'})^2\rangle\langle(M_{10}^{q\lambda})^2\rangle$$
$$+\langle(M_{03}^{q'\lambda'})^2\rangle\langle(M_{10}^{q\lambda})^2\rangle+\langle(M_{01}^{q'\lambda'})^2\rangle\langle(M_{20}^{q\lambda})^2\rangle+\langle(M_{03}^{q'\lambda'})^2\rangle\langle(M_{20}^{q\lambda})^2\rangle$$
$$\left.+\langle(M_{01}^{q'\lambda'})^2\rangle\langle(M_{30}^{q\lambda})^2\rangle+\langle(M_{02}^{q'\lambda'})^2\rangle\langle(M_{30}^{q\lambda})^2\rangle]\}\right],\qquad(10)$$

where $C_s(T)$ and $C_t(T)$ are the density of donor electrons in the singlet and triplet states, respectively.

2. *Inelastic scattering*

No resonance occurs in the case of an inelastic process defined by Kowk.[5] Therefore in the denominator of the transition probability level width can be neglected. Thereafter, proceeding in a similar manner as for the elastic process, we can obtain the relaxation rate for the inelastic process by the electrons in the triplet state in the following form:

$$\tau_{ie}^{-1}=\frac{C_t(T)\omega_{q\lambda}}{4\pi\rho^2 v_\lambda^2}\sum_{\lambda'}\frac{(4\Delta/\hbar+\omega_{q\lambda})^3}{v_{\lambda'}^5}\left[\left|\frac{1}{\hbar\omega_{q\lambda}}-\frac{1}{4\Delta+\hbar\omega_{q\lambda}}\right|^2\right.$$
$$\times[\langle(M_{01}^{q'\lambda'})^2\rangle\langle(M_{30}^{q\lambda})^2\rangle+\langle(M_{03}^{q'\lambda'})^2\rangle\langle(M_{10}^{q\lambda})^2\rangle+\langle(M_{02}^{q'\lambda'})^2\rangle\langle(M_{30}^{q\lambda})^2\rangle$$
$$\left.+\langle(M_{03}^{q'\lambda'})^2\rangle\langle(M_{20}^{q\lambda})^2\rangle+\langle(M_{01}^{q'\lambda'})^2\rangle\langle(M_{10}^{q\lambda})^2\rangle+\langle(M_{02}^{q'\lambda'})^2\rangle\langle(M_{20}^{q\lambda})^2\rangle]\right]$$
$$\times\left[1-\exp\left[\frac{-\hbar\omega_{q\lambda}}{k_BT}\right]\right]\left[1-\exp\left[\frac{-4\Delta-\hbar\omega_{q\lambda}}{k_BT}\right]\right]^{-1}.\qquad(11)$$

3. *Thermally assisted phonon absorption scattering*

This kind of phonon scattering process, according to the classification given by Kowk,[5] is due to the electrons in the singlet state. In the off-resonance region, i.e., $\omega_{q\lambda}<4\Delta/\hbar$ and $\omega_{q\lambda}>4\Delta/\hbar$, the following expression for the relaxation rate is obtained.

$$\tau_{ab}^{-1}=\frac{C_s(T)\omega_{q\lambda}}{4\pi\rho^2 v_\lambda^2}\sum_{\lambda'}\frac{|4\Delta/\hbar-\omega_{q\lambda}|^3}{v_{\lambda'}^5}\left[\left|\frac{1}{4\Delta-\hbar\omega_{q\lambda}}+\frac{1}{\hbar\omega_{q\lambda}}\right|^2\right.$$

$$\times[\langle(M_{03}^{\mathbf{q}'\lambda'})^2\rangle\langle(M_{10}^{\mathbf{q}\lambda})^2\rangle+\langle(M_{01}^{\mathbf{q}'\lambda'})^2\rangle\langle(M_{30}^{\mathbf{q}\lambda})^2\rangle+\langle(M_{03}^{\mathbf{q}'\lambda'})^2\rangle\langle(M_{20}^{\mathbf{q}\lambda})^2\rangle$$

$$\left.+\langle(M_{02}^{\mathbf{q}'\lambda'})^2\rangle\langle(M_{30}^{\mathbf{q}\lambda})^2\rangle+\langle(M_{01}^{\mathbf{q}'\lambda'})^2\rangle\langle(M_{10}^{\mathbf{q}\lambda})^2\rangle+\langle(M_{02}^{\mathbf{q}'\lambda'})^2\rangle\langle(M_{20}^{\mathbf{q}\lambda})^2\rangle]\right]$$

$$\times\left[1-\exp\left[-\frac{\hbar\omega_{q\lambda}}{k_BT}\right]\right]\left|\left[\exp\left[\frac{4\Delta-\hbar\omega_{q\lambda}}{k_BT}\right]-1\right]^{-1}\right|. \qquad (12)$$

Near the resonance $\hbar\omega_{q\lambda}\simeq 4\Delta$ we replace Eq. (12) for the absorption process by[5]

$$\tau_\gamma^{-1}=\frac{\omega_{q\lambda}}{\rho v_\lambda^2}\left[1-\exp\left[-\hbar\frac{\omega_{q\lambda}}{k_BT}\right]\right]C_s(T)$$

$$\times\sum_{n=1}^{3}\langle(M_{n0}^{\mathbf{q}\lambda})^2\rangle\frac{\Gamma}{(4\Delta-\hbar\omega_{q\lambda})^2+\Gamma^2}. \qquad (13)$$

III. RESULTS AND DISCUSSION

Using Eq. (1) we have calculated the phonon conductivity in As-doped Ge for As samples No. 1, No. 2,[17] and No. 3,[18] with donor electron density 2.1×10^{16}, 6.3×10^{16}, and $2.7\times10^{16}\text{cm}^{-3}$, respectively. The values used for the various physical constants and parameters are as follows: $\rho=5.35$ g/cm^3, $\bar{v}_1=5.37\times10^5$ cm/sec, $\bar{v}_2=3.28\times10^5$ cm/sec, $A=2.40\times10^{-44}$ sec^3, $B_l=6.89974\times10^{-24}$ sec, $B_t=1.0\times10^{-11}$ K^{-4}, $4\Delta=4.23$ meV, $E_d=-2.0$ eV, $L_C=0.4592$ cm for As sample Nos. 1 and 2 and is 0.428 cm for sample No. 3. E_u has been taken to be 19.0 15.0, and 18.0 eV for sample Nos. 1, 2, and 3, respectively.

These calculations show the effect of the anisotropy of impurity-electron wave functions on the phonon-electron relaxation rate as well as the phonon conductivity. The three phonon and the point defect scattering strength parameters have been taken to be the same[8,15] as that in the case of pure samples. The value of the chemical shift 4Δ has been experimentally determined by Reuszer and Fisher[16] in As-doped Ge. The only parameter used for the adjustment of theoretical and experimental results is the deformation-potential constants. This parameter is adjusted at $T=2$ K and then calculations are performed at other temperatures. The angular average for the matrix element is done over the solid angle $d\Omega$ by numerical methods as it is not possible to do this analytically. Figure 1 shows the phonon conductivity obtained from the experimental measurements,[17,18] the present calculation, and the calculations based on the Suzuki and Mikoshiba (SM) model.[6] Figure 2 shows the comparison of the phonon relaxation rates obtained from the present calculation and the SM model for the typical value of the shear deformation-potential constant. It is observed that while, on the one hand, the spherical approximation for the form factor overestimates the elastic relaxation rate for low-frequency phonons, on the other hand, it underestimates the same for phonons of higher frequency. This can be explained by comparing the exact form of the form factor with the one obtained through the spherical approximation. This comparison can be easily seen if we write the exact form factor as

$$\theta_{mn}^{j}(\mathbf{q})=\left[1+\frac{q^2a^2}{4}-(a^2-b^2)\left[\frac{\mathbf{q}\cdot\hat{\mathbf{k}}_j}{2}\right]^2\right]^{-2}. \qquad (14)$$

The above-written form can be obtained from Eq. (5) and (5a) by taking the z axis along the direction of $\hat{\mathbf{k}}_j$.

As expected from the behavior of the relaxation rates Fig. 1 shows the present approach improves the theoretical interpretation of the experimental data both in the lower- and higher-temperature regions. We have been able to explain the thermal-conductivity data exactly in between 1.5 and 5 K. Even at 10 K the theoretical values are improved by 30–40 % over the theoretical values obtained by the SM model which could successfully[1] explain the experimental data only in the temperature range 2–4 K. This is a considerable improvement and permits us to conclude that the spherical approximation is not a good approximation due to the large anisotropy of the form factor in doped germanium. The discrepancy still remaining in between the theoretical and the experimental data above 6 K can be because of any of the following reasons.

(i) First of all, we would like to comment that the exact wave function for the impurity electron is not known. In the presence of the stress due to impurity, the anisotropy of the impurity wave function may became larger than that it is expected from the usual effective-mass theory. A larger anisotropy will improve the results further.

(ii) The donor impurity may give rise to different force constants for the nearest neighbors resulting in a new point defect scattering of phonons. Some authors[19,20] have tried to explain the phonon conductivity data on the basis of this type of scattering. According to our information, no quantitative theory has been given for the justification of the added point defect scattering so far. Since the aim of the present paper is to investigate the effect of the form factor only, we have not made any attempt to find out how much increase in the anisotropy of the hydrogenic wave function of the impurity electron due to the internal stress or the addition of point defect scattering will explain the experimental data.

(iii) We would also like to discuss the role of E_d, the dilatation deformation potential in electron-phonon relaxation rates. In the SM model E_d does not appear in the final expression of the phonon relaxation rate because in the spherical approximation the first term of the deformation-potential matrix becomes zero when summa-

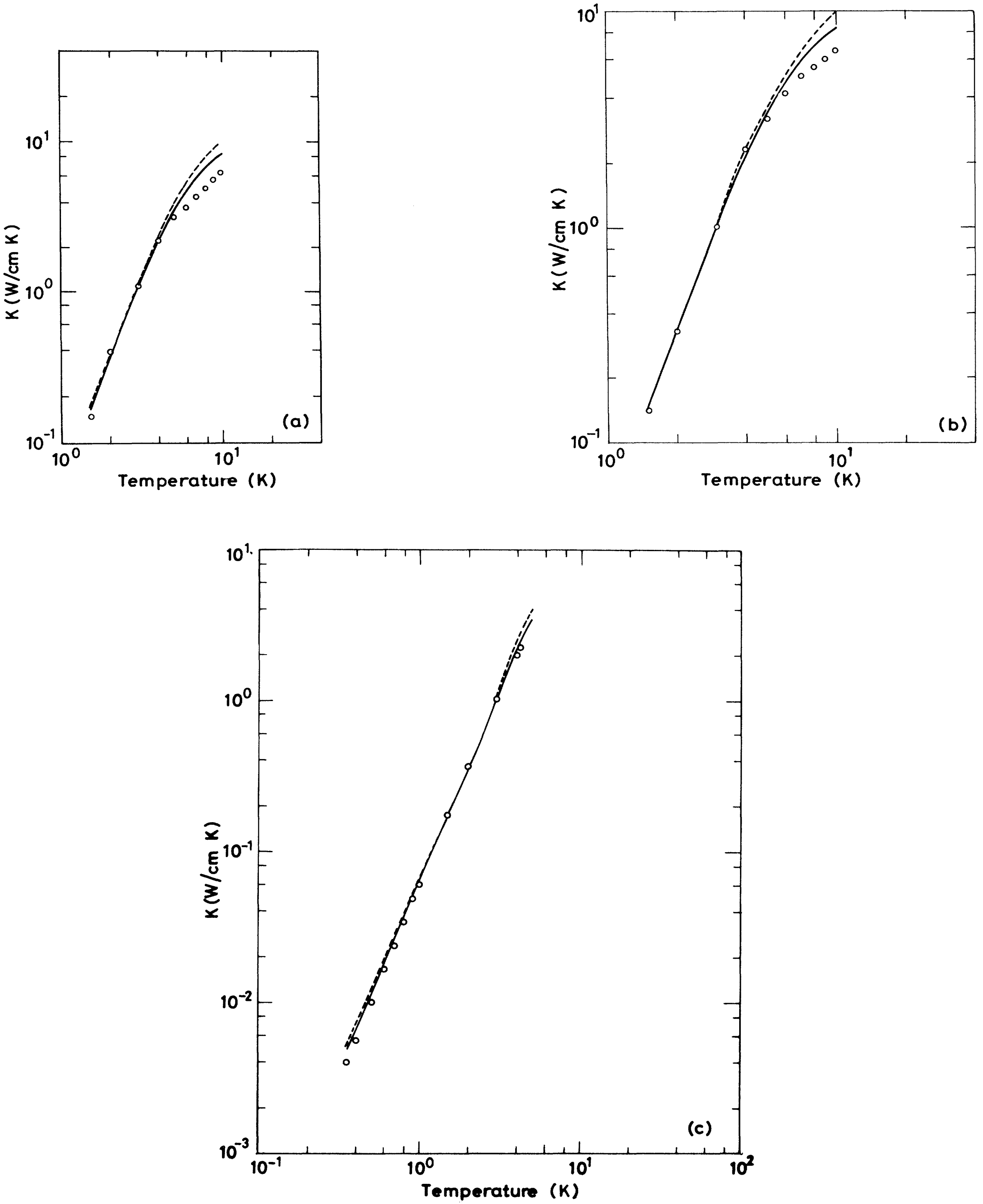

FIG. 1. Lattice thermal conductivity K obtained by the present calculations, SM model, and the experiment for As samples (a) No. 1, (b) No. 2, and (c) No. 3. Solid line shows the present calculations: dashed line is for the SM model with $E_u = 16.5$. 13.5, and 15.5 eV for sample Nos. 1, 2, and 3, respectively and $a^* = 36.69$ Å.

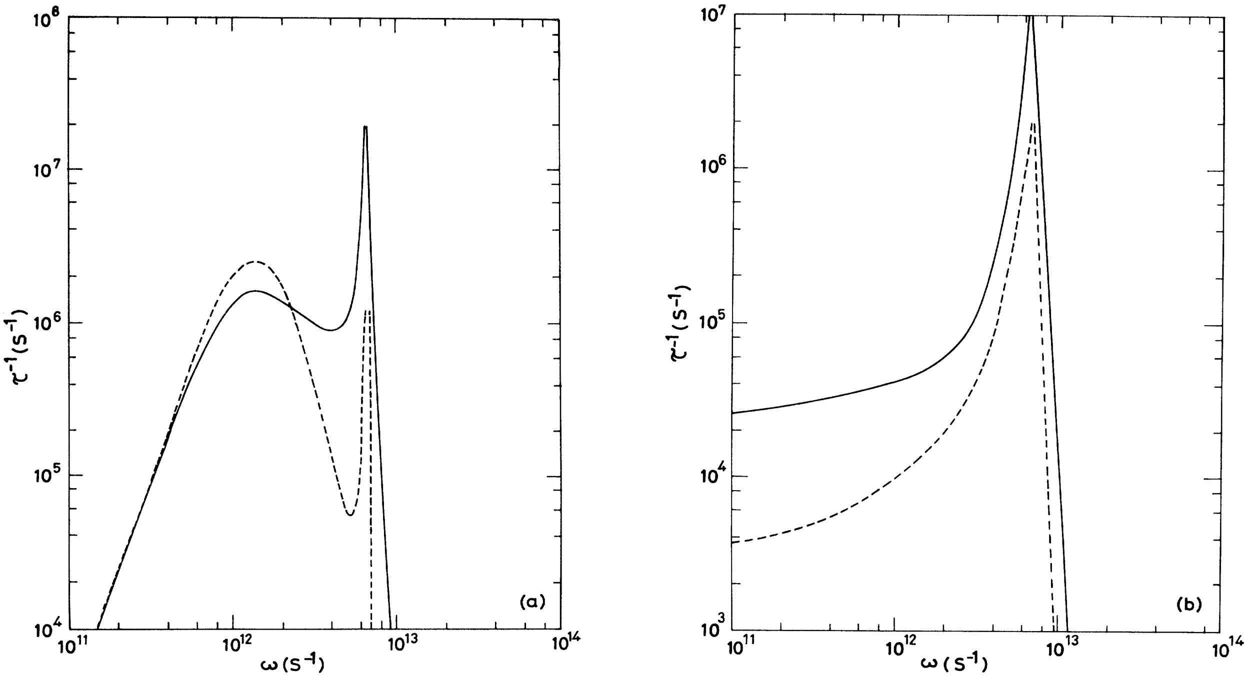

FIG. 2. Relaxation rates of the incoming longitudinal phonon as a function of angular frequency ω in As sample No. 1. Solid line represents the present calculations: the dashed line is for the SM model (a) $T=7.0$ K, elastic process: (b) $T=7.0$ K, absorption process with $E_u=16.0$ eV, $E_d=-6.0$ eV.

tion over all the valleys is done. In the present case, this term has to exist because this has to be multiplied first with the valley-dependent form factor and then summed up over all the valleys. In our calculations for the thermal conductivity we have chosen $E_d=-2$ eV. This value is larger than that reported earlier.[21,22] According to Markiewicz,[23] however, the value of E_d should be larger than that reported in the literature because of the screening effect. A positive value of E_d would give a still better explanation to the phonon conductivity results. It is interesting to note that Cheung and Barrie[13] have also taken a positive value of E_d in n-type Si in order to explain the shift of the donor energy levels with temperature. They have not given any theoretical justification for such a choice.

(iv) Further, as suggested by Sota, Suzuki, and Fortier,[24] phonon frequency dependent values of E_d and E_u can also remove the remaining discrepancy in between the theoretical and experimental values of the phonon conductivity. Such an exercise will not be illogical as the deformation-potential approximation had never been supposed to be a very sophisticated technique. However, in the absence of any quantitative justification for the variation of E_d and E_u with phonon frequency, right now we have not made any attempt to explain the experimental result on the basis of this idea.

We would, however, in the end, like to emphasize that for the calculation of electron-phonon relaxation rate the use of the correct form factor is essential in those cases wherever the conduction-band minima are highly anisotropic. After the correct form factor has been used, the remaining discrepancy can be explained on the basis of one or more effects described either in the previous models or in the text of this discussion. It would be interesting to see which of the above-mentioned reasons are proved to be most suitable for explaining the phonon conductivity in the entire temperature range.

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