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Phonon Conductivity of Ge in the Temperature Range 2–1000 °K*

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The contributions of transverse and longitudinal phonons toward thermal conductivity of undoped Ge have been investigated, both in high- as well as low-temperature regions. Four-phonon processes are also included in the determination of the combined relaxation time τ_c and hence the phonon conductivity. The group velocity of respective phonons in the conductivity integral is obtained on the basis of $\vec{q} = (\omega/\vec{v})(1+\alpha\omega^2)$, where the parameter α is determined from the experimentally obtained dispersion curves for the different acoustic branches in the region $0-\frac{1}{2}q_{max}$ and $\frac{1}{2}q_{max}-q_{max}$. It is observed that the transverse phonons in general make a major contribution toward thermal conductivity in the entire temperature range.

I. INTRODUCTION

Recently Hamilton and Parrott[1] have used a variational treatment to calculate the thermal resistance of Ge in the temperature range 5–300 °K, and have shown that the major contribution toward thermal conductivity is due to transverse phonons. The contribution of transverse phonons on the basis of the variational treatment varies from 80 to 90%. Because the variational treatment gives the nearest approximation to the correct answer, it is desirable to investigate how far one can explain the phonon conductivity results on the basis of transverse phonons alone in the framework of the relaxation-time approach. The calculations of phonon conductivity of Ge due to transverse phonons have been performed in the temperature range 2–1000 °K, both in the presence and absence of four-phonon processes, which play an important role at high temperatures. For the above calculations we have used Holland's[2] model for transverse phonons and appropriate expressions for the different phonon-phonon-scattering relaxation times for the different temperature ranges.

Since the phonon conductivity results of Ge in the temperature range 2–1000 °K cannot be explained on the basis of transverse phonons alone, the aim of the present paper is to investigate the contribution of transverse phonons in the presence of longitudinal phonons as well as four-phonon processes. Holland has not considered the contribution of four-phonon processes in his calculations. Previously Holland replaced v_g/v_p^2 by $1/v_p$, which is a crude approximation. We have used an empirical relation $\vec{q} = (\omega/\vec{v})(1+\alpha\omega^2)$ in order to calculate v_g/v_p^2 for the conductivity integrals. The present approach of calculating v_g/v_p^2 is considered to be quite realistic. Analytical expressions for the various conductivity integrals under different approximations are also obtained. These analytical expressions are quite useful in obtaining the approximate values of the phonon-phonon scattering strenghts which are treated as adjustable parameters.

II. PHONON CONDUCTIVITY DUE TO TRANSVERSE PHONONS

The integral formulation of thermal conductivity as originally suggested by Callaway[3] is divided into two parts[2] according to the two modes of lattice thermal conduction. It leads to

$$\kappa = \kappa_T + \kappa_L . \tag{1}$$

The conductivity due to transverse mode κ_T is further divided[2] into two parts on the basis of angular frequency ranges of transverse phonons,

$$\begin{aligned}\kappa_T &= \kappa_{T1} + \kappa_{T2} \\ &= \frac{2}{3}\frac{k_B}{2\pi^2}\left(\frac{k_B T}{\hbar}\right)^3 \left((v_{T1})_{0<\omega<\omega_1}^{-1} \right. \\ &\quad \times \int_0^{\theta_1/T} \frac{x^4 e^x/(e^x-1)^2}{\tau_B^{-1}+\tau_{pt}^{-1}+B_T \omega T^4}\, dx + (v_{T2})_{\omega_1<\omega<\omega_2}^{-1} \\ &\quad \left. \times \int_{\theta_1/T}^{\theta_2/T} \frac{x^4 e^x/(e^x-1)^2}{\tau_B^{-1}+\tau_{pt}^{-1}+B_{TU}[\omega^2/\sinh(\hbar\omega/k_B T)]}\, dx \right) .\end{aligned} \tag{2}$$

In these integrals which refer to the isotropic case, the phonon velocity (v_{T1} or v_{T2}) of the trans-

verse mode is representative of $(v_g/v_p^2)_T$, where v_g is the group velocity and v_p is the phase velocity of phonons. Actually, replacement of $(v_g/v_p^2)_T$ in the original integrals by $1/v_T$ is a very crude type of approximation. This factor in our calculations is replaced by a more suitable quantity based on simple calculations. Instead of using the acoustic approximation $\vec{q} = \omega/\vec{v}$, we considered $\vec{q} = (\omega/\vec{v}) \times (1+\alpha\omega^2)$, where ω is the angular frequency of the phonon moving with velocity $\vec{v}$, and α is a parameter given by the equation

$$\alpha = \frac{1}{\omega^2}\left[\left(\frac{qv}{\omega}\right) - 1\right] , \tag{3}$$

α is calculated from the phonon dispersion curves[4] at two values of the wave vector $\frac{1}{2}q_{\max}$ and $q_{\max}$. In the present calculations we have considered α in the directions [100] and [111] and then averaged it for further calculations.

It can be shown with the help of the equation $\vec{q} = (\omega/\vec{v})(1+\alpha\omega^2)$ that the group velocity

$$\vec{v}_g = d\omega/d\vec{q} = \vec{v}/(1+3\alpha\omega^2)$$

and phase velocity

$$\vec{v}_p = \omega/\vec{q} = \vec{v}/(1+\alpha\omega^2).$$

Therefore, for the isotropic case

$$\left(\frac{v_g}{v_p^2}\right)_T = \left[\frac{1}{v_p}\left(\frac{(1+\alpha\omega^2)^2}{(1+3\alpha\omega^2)}\right)\right]_T . \tag{4}$$

The term $(1+\alpha\omega^2)^2/(1+3\alpha\omega^2)$ is called the correction factor. Hence, using this correction factor, κ_{T1} and κ_{T2} for the isotropic case can be expressed as

$$\kappa_{T1} = \frac{2}{3}\frac{k_B}{2\pi^2}\left(\frac{k_BT}{\hbar}\right)^3\left[\left(\frac{1}{v_{T1}}\right)_{0<\omega<\omega_1}\int_0^{\theta_1/T}\frac{x^4e^x/(e^x-1)^2}{\tau_B^{-1}+\tau_{pt}^{-1}+B_T\omega T^4}\,\frac{(1+\alpha_1\omega^2)^2}{(1+3\alpha_1\omega^2)}\,dx\right]$$

and

$$\kappa_{T2} = \frac{2}{3}\frac{k_B}{2\pi^2}\left(\frac{k_BT}{\hbar}\right)^3\left[\left(\frac{1}{v_{T2}}\right)_{\omega_1<\omega<\omega_2}\int_{\theta_1/T}^{\theta_2/T}\frac{x^4e^x/(e^x-1)^2}{\tau_{pt}^{-1}+B_{TU}[\omega^2/\sinh(\hbar\omega/k_BT)]}\,\frac{(1+\alpha_2\omega^2)^2}{(1+3\alpha_2\omega^2)}\,dx\right], \tag{5}$$

and the total conductivity κ_T as

$$\kappa_T = \frac{2}{3}\frac{k_B}{2\pi^2}\left(\frac{k_BT}{\hbar}\right)^3\left[\left(\frac{1}{v_{T1}}\right)_{0<\omega<\omega_1}\int_0^{\theta_1/T}\frac{x^4e^x/(e^x-1)^2}{\tau_B^{-1}+Dx^4T^4+\beta_T xT^5}\,\frac{(1+\beta_1x^2T^2)^2}{(1+3\beta_1x^2T^2)}\,dx$$

$$+\left(\frac{1}{v_{T2}}\right)_{\omega_1<\omega<\omega_2}\int_{\theta_1/T}^{\theta_2/T}\frac{x^4e^x/(e^x-1)^2}{Dx^4T^4+\beta_{TU}(x^2T^2/\sinh x)}\,\frac{(1+\beta_2x^2T^2)^2}{(1+3\beta_2x^2T^2)}\,dx\right], \tag{6}$$

where

$$D = A(k_B/\hbar)^4, \quad \beta_T = B_T(k_B/\hbar), \quad \beta_{TU} = B_{TU}(k_B/\hbar)^2,$$
$$\beta_1 = \alpha_1(k_B/\hbar)^2, \quad \beta_2 = \alpha_2(k_B/\hbar)^2.$$

When the boundary scattering is negligible and phonon-phonon scattering dominates the isotope scattering, κ_{T1} is reduced to the following analytical form:

$$\kappa_{T1} = \frac{2}{3}\frac{C_{T1}}{\beta_T}\frac{\theta_1^2}{2T^4}\left(1-\frac{\beta_1\theta_1^2}{2}\right)\left(1-\frac{D}{\beta_TT}\right) , \tag{7}$$

where

$$C_{T1} = \frac{k_B}{2\pi^2}\left(\frac{k_B}{\hbar}\right)^3\frac{1}{v_{T1}} .$$

The analytical expression for κ_{T1}, when dispersion of transverse phonon branches is neglected, is given as

$$\kappa_{T1} = \frac{2}{3}\frac{C_{T1}}{\beta_T}\frac{\theta_1^2}{2T^4}\left[1-\frac{2}{5}\frac{D}{\beta_T}\frac{\theta_1^3}{T^4}\right] .$$

In deriving the above expressions it has been assumed that at high temperatures, when $x = \hbar\omega/k_BT$ is small, $x^2e^x/(e^x-1)^2$ tends to unity.

Similarly when phonon-phonon scattering dominates over isotopic scattering and boundary scattering is negligible, κ_{T2} reduces to the following analytic form:

$$\kappa_{T2} = \frac{2}{3}\frac{C_{T2}}{T}\frac{1}{3\beta_2}\frac{1}{\beta_{TU}}\left\{\left[\frac{1}{3}\ln\frac{\theta_2}{\theta_1}+\frac{5\beta_2}{6}(\theta_2^2-\theta_1^2)\right.\right.$$
$$\left.+\frac{\beta_2^2}{4}(\theta_2^4-\theta_1^4)+\frac{1}{6\beta_2}\left(\frac{1}{\theta_2^2}-\frac{1}{\theta_1^2}\right)\right]$$
$$-\frac{D}{\beta_{TU}T}\left[\frac{1}{9}(\theta_2^3-\theta_1^3)+\frac{\beta_2}{3}(\theta_2^5-\theta_1^5)+\frac{\beta_2^2}{7}(\theta_2^7-\theta_1^7)\right.$$
$$\left.\left.-\frac{1}{3\beta_2}(\theta_2-\theta_1)\right]\right\}. \tag{8}$$

These analytical expressions are very useful in determining the approximate values of the adjustable parameters β_T and β_{TU}. Thus at 1000 °K, when the contribution of κ_{T1} is negligible, one can find the values of β_{TU} from Eq. (8) for the known values of D or A $[D = A(k_B/\hbar)^4]$. Similarly at 100 °K, when the contribution of κ_{T2} may be considered to be small, one can obtain the approximate values of β_T from Eq. (7) for the same values of

D or A.

In the absence of any dispersion in the transverse phonon branch, Eq. (8) reduces to the following simple expression:

$$\kappa_{T2}=\frac{2}{3}\frac{C_{T2}}{2\beta_{TU}}\frac{1}{T}\left[(\theta_2^2-\theta_1^2)-\frac{2}{5}\frac{D}{\beta_{TU}}\frac{1}{T}(\theta_2^5-\theta_1^5)\right],$$

where

$$C_{T2}=(k_B/2\pi^2)(k_B/\hbar)^3(1/v_{T2}).$$

For low temperatures, where phonon-phonon scattering is negligible and boundary scattering dominates over isotope scattering, one obtains the following analytical form:

$$\kappa_{T1}=\frac{2}{3}\frac{4\pi^4}{15}C_{T1}\tau_B T^3(1-16\pi^4 D T^4\tau_B). \tag{9}$$

III. FOUR-PHONON PROCESSES

It has been shown previously[5] that at high temperatures, four-phonon scattering processes also take place. The combined relaxation time τ_c^{-1} in the presence of four-phonon processes is given by

$$\tau_c^{-1}=\tau_B^{-1}+\tau_{pt}^{-1}+\tau_{3ph}^{-1}+\tau_{4ph}^{-1},$$

where

$$\tau_{4ph}^{-1}=B_H\omega^2T^2.$$

The integral expression for phonon conductivity due to transverse phonon becomes

$$\kappa_T=\frac{2}{3}C_{T1}T^3\int_0^{\theta_1/T}\frac{x^4e^x/(e^x-1)^2}{\tau_B^{-1}+Dx^4T^4+\beta_T xT^5}\frac{(1+\beta_1x^2T^2)^2}{(1+3\beta_1x^2T^2)}\,dx$$
$$+\frac{2}{3}C_{T2}T^3\int_{\theta_1/T}^{\theta_2/T}\frac{x^4e^x/(e^x-1)^2}{Dx^4T^4+\beta_{TU}(x^2T^2/\sinh x)+\beta_H x^2T^4}\times\frac{(1+\beta_2x^2T^2)^2}{(1+3\beta_2x^2T^2)}\,dx, \tag{10}$$

where

$$\beta_H=B_H(k_B/\hbar)^2.$$

The effect of four-phonon processes is not included in the first conductivity integral as it is not supposed to operate in the region $0-\frac{1}{2}q_{max}$. At temperatures when four-phonon processes dominate over three-phonon processes and isotopic scattering is negligible, the following analytical expression is obtained for the phonon conductivity:

$$\kappa_{T2}=\frac{2}{3}\frac{C_{T2}}{T^3}\frac{1}{3\beta_2}\frac{1}{\beta_H}\left\{T\left[\left(\frac{1}{\theta_1}-\frac{1}{\theta_2}\right)+\frac{\beta_2^2}{3}(\theta_2^3-\theta_1^3)+\frac{1}{9\beta_2}\left(\frac{1}{\theta_2^3}-\frac{1}{\theta_1^3}\right)+\tfrac{5}{3}\beta_2(\theta_2-\theta_1)\right]\right.$$
$$-\frac{\beta_{TU}}{\beta_H}\left[\frac{1}{6}\left(\frac{1}{\theta_1^2}-\frac{1}{\theta_2^2}\right)+\tfrac{5}{3}\beta_2\ln\frac{\theta_2}{\theta_1}+\frac{\beta_2^2}{2}(\theta_2^2-\theta_1^2)+\frac{1}{12\beta_2}\left(\frac{1}{\theta_2^4}-\frac{1}{\theta_1^4}\right)\right]$$
$$\left.-\frac{D}{\beta_H}\frac{1}{T}\left[\frac{\theta_2-\theta_1}{3}+\frac{5}{9}\beta_2(\theta_2^3-\theta_1^3)+\frac{\beta_2^2}{5}(\theta_2^5-\theta_1^5)+\frac{1}{3\beta_2}\left(\frac{1}{\theta_2}-\frac{1}{\theta_1}\right)\right]\right\}. \tag{11a}$$

At 1000 °K, the contributions due to terms containing β_{TU} and D are negligible and one can determine β_H from the observed value of $\kappa_T=\kappa_{T2}$. As β_H and D are now known, an approximate value of the adjustable parameter β_{TU} may be determined from the above equation at 500 °K by considering all the terms.

The analytical expression of κ_{T2}, when one neglects dispersion of transverse phonon branches, is given by

$$\kappa_{T2}=\frac{2}{3}\frac{C_{T2}}{\beta_H}\frac{1}{T^2}\left[(\theta_2-\theta_1)-\frac{\beta_{TU}}{\beta_H T^2}\ln\left(\frac{\theta_2}{\theta_1}\right)\right.$$
$$\left.-\frac{D}{3\beta_H}\frac{(\theta_2^3-\theta_1^3)}{T^2}\right]. \tag{11b}$$

IV. LONGITUDINAL PHONONS

If one considers the contribution of longitudinal phonons also, the total conductivity due to longitudinal and transverse phonons is given by

$$\kappa=\kappa_{T1}+\kappa_{T2}+\kappa_L.$$

The expressions for phonon conductivity due to transverse phonons have been discussed already. The contribution due to longitudinal phonons κ_L can be expressed as

$$\kappa_L=\frac{1}{3}\frac{k_B}{2\pi^2}\left(\frac{k_BT}{\hbar}\right)^3$$
$$\times\left(\frac{1}{v_{L1}}\int_0^{\theta_4'/T}\frac{x^4e^x/(e^x-1)^2}{\tau_B^{-1}+A\omega^4+B_L\omega^2T^3}\frac{(1+\alpha\omega^2)^2}{(1+3\alpha\omega^2)}\,dx\right.$$
$$\left.+\frac{1}{v_{L2}}\int_{\theta_4'/T}^{\theta_3'/T}\frac{x^4e^x/(e^x-1)^2}{A\omega^4+\tau_{3ph}^{-1}+\tau_{4-ph}^{-1}}\frac{(1+\alpha\omega^2)^2}{(1+3\alpha\omega^2)}\,dx\right). \tag{12}$$

The contribution due to the second integral can be neglected. Since the dispersion curve for longitudinal phonons is almost a straight line, $\alpha=0$, it is not necessary to introduce the correction factor. Thus

TABLE I. Values of the parameters used in the calculation of the phonon conductivity of Ge in the temperature range 2–1000 °K on the basis of transverse phonons.

τ_B^{-1} (expt)	$= 1.45\times10^{6}$ sec^{-1}
τ_B^{-1} (theor)	$= 1.47\times10^{6}$ sec^{-1}
F	$= 1.08$
$(v_{T1})_{0<\omega<\omega_1}$	$= 3.55\times10^{5}$ cm/sec
$(v_{T2})_{\omega_1<\omega<\omega_2}$	$= 1.30\times10^{5}$ cm/sec
$(v_L)_{0<\omega<\omega_4}$	$= 4.92\times10^{5}$ cm/sec
B_T	$= 2.5\times10^{-12}$ deg^{-4}
B_{TU}	$= 5.9\times10^{-18}$ sec
A	$= 2.4\times10^{-44}$ sec^{3}
$\theta_1 = 101$ °K	$\theta_2 = 118$ °K
$[\alpha_1]_{[111]}$ at $\frac{1}{2}q_{max}$	$= 3.7499\times10^{-27}$ sec^2
$[\alpha_1]_{[100]}$ at $\frac{1}{2}q_{max}$	$= 2.15804\times10^{-27}$ sec^2
$[\alpha_1]_{av}$ at $\frac{1}{2}q_{max}$	$= 2.95395\times10^{-27}$ sec^2
$[\alpha_2]_{[111]}$ at q_{max}	$= 10.538\times10^{-27}$ sec^2
$[\alpha_2]_{[100]}$ at q_{max}	$= 6.0246\times10^{-27}$ sec^2
$[\alpha_2]_{av}$ at q_{max}	$= 8.2816\times10^{-27}$ sec^2

$$\kappa_L = \tfrac{1}{3}C_L T^3 \int_0^{\theta_4/T} \frac{x^4 e^x/(e^x-1)^2}{\tau_B^{-1} + Dx^4T^4B_L x^2T^5}\,, \qquad (13)$$

where

$$D = A\left(\frac{k_B}{\hbar}\right)^4,\quad \beta_L = B_L(k_B/\hbar)^2,\quad C_B = \frac{k_B}{2\pi^2}(k_B/\hbar)^3\frac{1}{v_L}\,.$$

At temperatures where boundary scattering is negligible and three-phonon scattering dominates over isotope scattering, one can write the analytical expression for the above integral as

$$\kappa_L = \tfrac{1}{3}C_L\frac{\theta^4}{\beta_L T^3}\left(1 - \frac{D\theta_4^2}{3T^3\beta_L}\right)\,. \qquad (14)$$

TABLE II. Values of the parameters[a] used in the calculation of phonon conductivity of Ge in the temperature range 2–1000 °K on the basis of transverse phonons including four-phonon processes also.

$\tau_B^{-1} = 1.5\times10^{6}$ sec^{-1}
$B_T = 0.2\times10^{-11}$ deg^{-4}
$B_T = 5.0\times10^{-18}$ sec
$B_H = 8.2\times10^{-24}$ sec deg^{-2}

[a]Values of other parameters are same as in Table I.

V. RESULTS AND DISCUSSIONS

It has been shown by Hamilton and Parrott on the basis of variational calculations that transverse phonons make a major contribution towards thermal conductivity of Ge in the temperature range 5–300 °K. The contribution of transverse phonons is as high as 80–90%. Using the relaxation time approach, we have investigated the possibility of explaining the phonon conductivity results of Ge in the entire temperature range 2–1000 °K on the basis of transverse phonons alone. For the calculations of phonon conductivity κ_T due to transverse phonons, Eq. (6) is numerically integrated for a given set of parameters β_T and β_{TU}. The values of the various parameters for the best fit between theory and

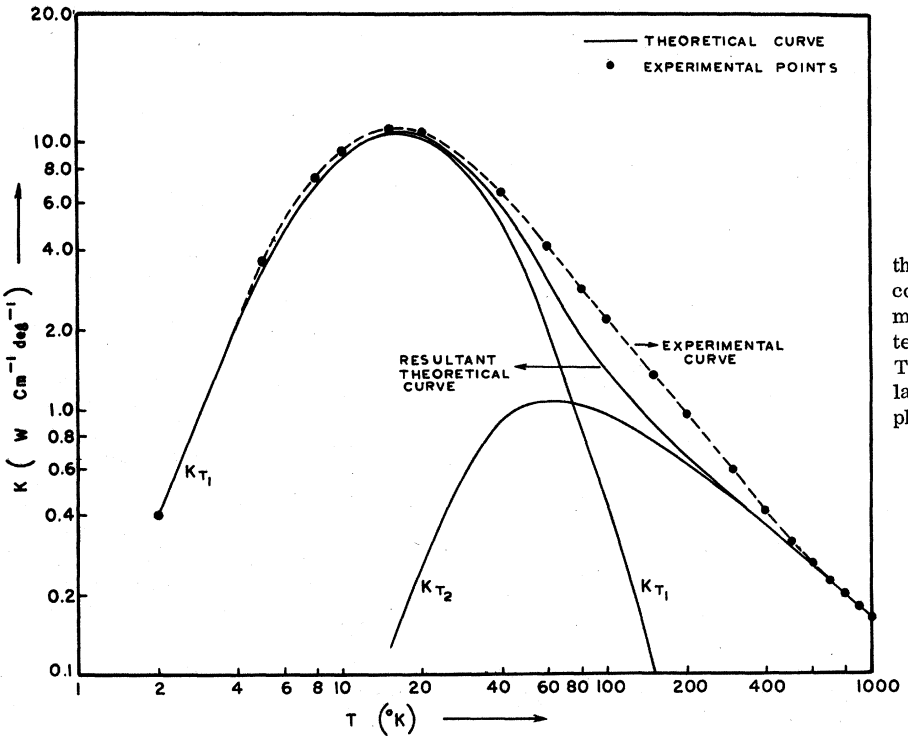

FIG. 1. Comparison of theoretical values of phonon conductivity with the experimental values in Ge in the temperature range 2–1000 °K. Theoretical curve is calculated on the basis of transverse phonons alone.

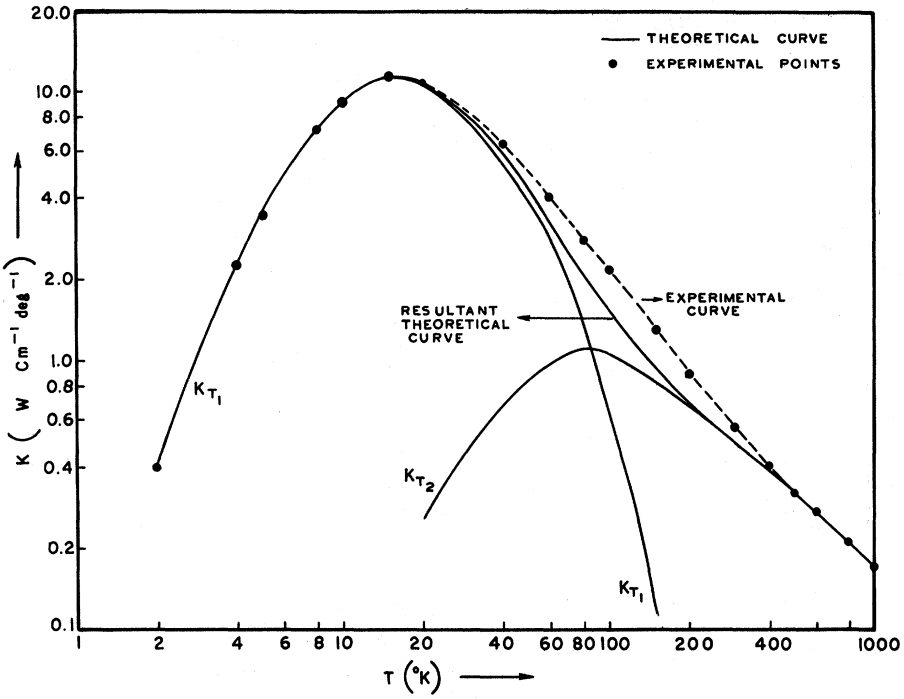

FIG. 2. Comparison of theoretical values of phonon conductivity with the experimental results in Ge in the temperature range 2–1000°K. Theoretical curve is calculated on the basis of transverse phonons alone and it also includes the contribution of four-phonon processes.

experiment are given in Table I. The calculations have been performed with the desk calculating machines. Figure 1 shows the results of the calculation of κ_T at different temperatures. It may be observed that phonon conductivity results cannot be explained in the entire temperature range on the basis of transverse phonons alone. The discrepancy lies in the temperature range 40–300 °K and it can be as high as 36% of the total conductivity at 80 °K.

Next we included four-phonon processes in the conductivity integrals for transverse phonons.

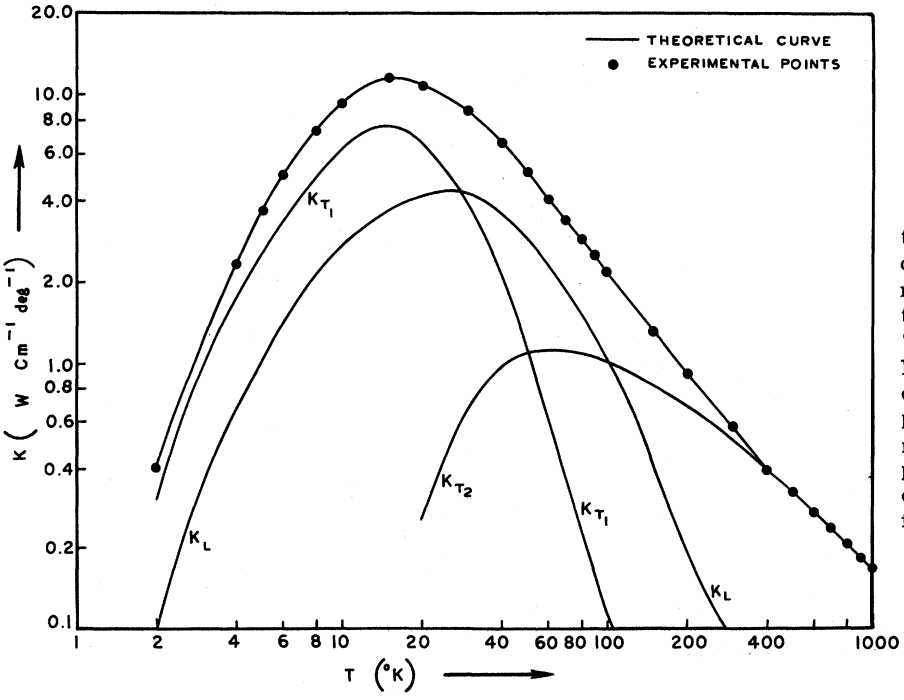

FIG. 3. Comparison of theoretical values of phonon conductivity with the experimental results in Ge in the temperature range 2–1000 °K. Theoretical curve is calculated on the basis of separate contributions of longitudinal phonons and transverse phonons. Contributions of four-phonon processes are also included and the better relation for v_g/v_p^2 is used.

TABLE III. Values of the parameters[a] used in the calculation of phonon conductivity of Ge in the temperature range 2–1000 °K considering the separate contributions of transverse phonons and longitudinal phonons. Four-phonon processes are also included.

$\theta_4 = 1.92$ °K, $\theta_3 = 333$ °K
$\tau_B^{-1} = 1.96 \times 10^6$ sec^{-1}
$B_T = 1.0 \times 10^{-11}$ deg^{-4}
$B_{TU} = 5.0 \times 10^{-18}$ sec
$B_H = 8.2 \times 10^{-24}$ sec deg^{-2}
$B_L = 6.7 \times 10^{-24}$ sec deg^3

[a]Values of other parameters are in Table I.

The values of the parameters used in this case are given in Table II and the results of calculation are shown in Fig. 2. Here again we find that the discrepancy, though to a lesser extent, still exists in the temperature range 60–200 °K. However, if we include the contribution of longitudinal phonons, it is possible to explain the phonon conductivity results in the entire temperature range. The values of the various parameters used in this case are given in Table III and the results of calculation are shown in Fig. 3. Figure 4 shows the plot of κ_T/κ and κ_L/κ at different temperatures in the range 2–1000 °K, respectively. Thus Fig. 4 shows that in the temperature range 30–100 °K the contribution of longitudinal phonons towards thermal conductivity dominates over that of the transverse phonons. The maximum difference between the two contributions, i.e., $\kappa_L - \kappa_T$ can be as high as 20% of the total conductivity κ. This appears to be the reason for the discrepancy between theory and experiment in the temperature range 30–100 °K in Figs. 1 and 2, where we tried to explain the phonon conductivity results on the basis of transverse phonons alone.

At very low temperatures, where boundary scattering is the only relevant scattering of phonons, one can write

$$\kappa_{T1}/\kappa_L = 2(v_L/v_{T1})(\tau_B)_T/(\tau_B)_L = 2(v_L/v_{T1})^2,$$

where $(\tau_B)_T = L_{eff}/v_{T1}$, $(\tau_B)_L = L_{eff}/v_L$, and L_{eff} is the effective scattering length. Since $v_L/v_T = 1.386$, the contribution of transverse phonons dominates over that of longitudinal phonons. The same situation (i.e., $\kappa_{T1} > \kappa_L$) prevails up to about 20 °K in the presence of isotopic scattering of phonons. However, in the presence of three-phonon scattering processes, which become relevant at 20 °K, the situation changes. The limit of the conductivity integral for longitudinal phonons is

$$x_{\max} = \frac{\hbar\omega_{\max}}{k_B T} = \frac{\theta_4}{T} = \frac{319}{T},$$

whereas the similar limit for transverse phonons for the conductivity integral κ_{T1} is $\theta_1/T = 101/T$. Thus at temperatures beyond the conductivity maximum, $\kappa_L > \kappa_{T1}$. However, both of them decrease very rapidly with temperature. κ_{T1} at 100 °K becomes about 5% of the observed value of κ. Similarly, κ_L is reduced to about 10% of the observed value of κ at about 200 °K. The rapid decrease of κ_L and κ_{T1} with temperature is due to the high exponent of the temperature dependences of three-phonon relaxation times, i.e., $\tau_{3ph,L}^{-1} \propto \omega^2 T^3$ and $\tau_{3ph,T}^{-1} \propto \omega T^4$. At still higher temperatures, three-phonon umklapp processes are more effective and the contribution of κ_{T2} due to the transverse phonons dominates over κ_L and κ_{T1}. As a matter of fact, in the temperature range 400–1000 °K, the phonon conductivity results are explained by κ_{T2} alone, which includes three-phonon umklapp processes and also four-phonon processes. Thus, except for a small temperature range 30–80 °K, the transverse phonons make a major contribution toward thermal conductivity in the entire temperature range 2–1000 °K.

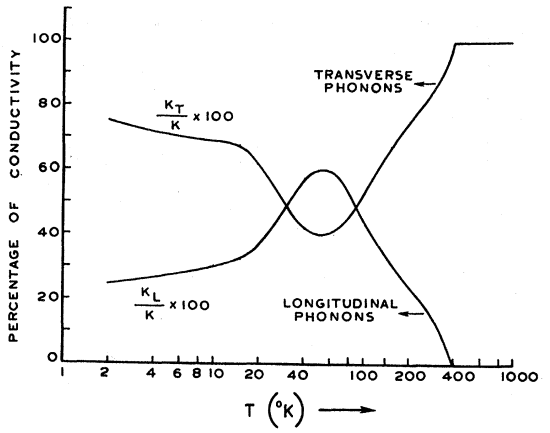

FIG. 4. Percentage contribution of longitudinal phonons and transverse phonons towards thermal conductivity.

It may be mentioned that the present calculations (see Fig. 3) differ from Holland's calculations in two important respects. First, four-phonon scattering processes are included in the determination of the combined relaxation time τ_c and second, in the replacement of the factor (v_g/v_p^2) by $(1/v_p) \times [(1+\alpha\omega^2)^2/(1+3\alpha\omega^2)]$ on the basis of the relation $\vec{q} = (\omega/\vec{v})(1+\alpha\omega^2)$, which is more realistic.

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Small-Polaron Propagators

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The diagrammatic expansion in the real-time domain of the one-electron and electron-hole propagators for the small-polaron problem is presented. For this purpose, special graphs consisting of fermion lines, multiphonon interaction lines, and migration vertices are used. The spectral function of the small-polaron propagator is calculated for two cases. First, the interaction with a narrow band of optical modes, and second, the interaction with longitudinal acoustic modes, is considered. The expressions for the small-polaron mobility in the hopping region are also derived for both models.

I. INTRODUCTION

Since the publication in 1959 of Holstein's fundamental paper[1] on small polarons, the problem of the very low electron mobility in the case of strong electron-phonon interaction has been the subject of several theoretical investigations.[2-7] In this paper the field-theoretic techniques are applied to the small-polaron problem. Propagators for small polarons are introduced and their properties are investigated. The theory presented leads to some new results concerning the small-polaron mobility. One-electron propagators have been studied in some detail already in the previous paper by the author and Choi.[8]

Small-polaron theory deals with the motion of electrons in narrow bands. Therefore in calculations we use the tight-binding approach and the corresponding Wannier representation. In this representation the complete set of states for the particular band is given by the localized states $|i\rangle$ at the individual cells i of the crystal. The small-polaron Hamiltonian may be written as

$$H=\epsilon_0\sum_i c_i^\dagger c_i+\sum_{i,j} w_{ij}c_i^\dagger c_j+\sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda - N^{-1/2}\sum_{i,\lambda}\omega_\lambda\eta^{1/2}e^{i\vec{q}\cdot\vec{R}_i}c_i^\dagger c_i(a_\lambda+a_{-\lambda}^\dagger),\quad \hbar=1 \qquad (1)$$

where $c_i^\dagger$ and c_i are, respectively, the creation and annihilation operators for electrons in the localized states $|i\rangle$, and where ϵ_0 is the local electron energy and w_{ij} the intercell transfer or resonance integral. $a_\lambda^\dagger$ and a_λ denote the creation and annihilation operators, respectively, for a phonon in the phonon mode λ. The parameter λ includes the wave vector $\vec{q}$ and the branch p of the phonon spectrum. The normal modes λ and $-\lambda$ belong to the same branch, the corresponding wave vectors being $\vec{q}$ and $-\vec{q}$, respectively. ω_λ is the phonon frequency and η_λ the electron-phonon coupling constant. N is the number of cells in the crystal and $\vec{R}_i$ the lattice vector of the ith cell. Additionally, w_{ij} and η_λ are real, and $w_{ij}=w_{ji}$.

The electron-phonon interaction is assumed to be linear in phonon operators and diagonal with respect to the localized states $|i\rangle$. If the phonon frequency is greater than the width of the electron band, only the diagonal coupling terms are important. This fact justifies the use of (1) in the case of narrow bands. In the small-polaron theory, the transfer integrals w_{ij} are considered as a small perturbation.

In Sec. II one-electron propagators are introduced and their properties are studied. Section III deals with the electron-hole propagators. Small-polaron mobility is calculated in Sec. IV.

II. ONE-ELECTRON PROPAGATORS

We would like to formulate the theory of propagators for a single polaron. We define the propagator for the small polaron by

$$g_{ij}(t)=-i\langle T\underline{c}_i(t)\underline{c}_j^\dagger(0)\rangle, \qquad (2)$$

where T is a time-ordering operator and $\langle\ \rangle$ denotes the canonical ensemble average over the states of the crystal with no electrons. The underlined operators are Heisenberg operators. It is easy to realize that the diagrammatic expansion of $g_{ij}(t)$ in the real-time domain is possible. We consider the second and also the last term of (1) as the per-