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Lattice Thermal Conductivity of p-Type GaSb in the Temperature Range 2–20 °K

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In the present paper the resonance-scattering relaxation rate for the electron-phonon interaction as given by Kumar *et al.* is used in the calculation of the resonance scattering of phonons by bound holes in p-type GaSb in the temperature range 2–20 °K. The present calculations show that with the simplified expressions of Kumar *et al.* for resonance scattering of phonons by bound electrons for $\omega > \omega_r$ and $\omega < \omega_r$, one can explain the anomalous resonance dip in the phonon-conductivity-vs-temperature curves of p-doped GaSb. An excellent agreement between theoretical and experimental values of phonon conductivity is obtained for the entire temperature range 2–20 °K on the basis of Callaway's model of phonon conductivity, provided one incorporates separate conductivity integrals for $0 < \omega < \omega_r$ and $\omega_r < \omega < \omega_D$, where ω_r is the resonance frequency and ω_D is the Debye frequency.

I. INTRODUCTION

Holland[1] measured the phonon conductivity of p-type GaSb in the temperature range 2–20 °K. He observed resonance dips in the phonon-conductivity-vs-temperature curves occurring at 5 °K. He considered the resonance scattering of phonons by the holes on the basis of Carruther's[2] theory but failed to explain his experimental results. Resonance dips in κ-vs-T curves are quite common for doped alkali halides, and they occur both below (in the boundary scattering region) and above the phonon conductivity maximum (phonon-phonon scattering region). However, there are few doped semiconductors for which the resonance dips can be detected, and they usually lie in the boundary scattering region. In Sb-doped Ge the resonance dip occurs at about 0.7 °K. In p-type GaSb Holland observed a very pronounced resonance dip at 5 °K. The slopes of κ-vs-T curves were found to be quite different from each other, both below and above the resonance region. In view of these anomalous features, the experimental results could not be explained consistently. A family of curves were plotted by Holland varying $\delta = r_0^2 \times (k_B/\hbar)^2/4v_s^2$ and $\gamma = G(k_B/4\Delta)^4$, where r_0 is the acceptor-hole radius, k_B is Boltzmann's constant v is average phonon velocity, 4Δ is the energy difference between the acceptor-hole ground state and the next-higher energy state, and G is a constant proportional to the number of scattering centers. With the help of such curves he tried to reach some conclusions regarding different resonance-scattering parameters. It was obvious from these curves that no single curve could explain the experimental results in the entire temperature range.

Recently, Kwok,[3] while discussing acoustic-phonon attenuation in doped Ge, considered both elastic and inelastic scatterings of phonons by bound donor electrons both from the donor-electron ground state and the next-higher energy state. He used perturbation theory as well as the Green's function approach for frequencies close to the resonance region. Kumar *et al.*[4] obtained the simplified expressions from Kwok's theory both for $\hbar\omega_{q\lambda} \gg 4\Delta$ and $k_B T \gg 4\Delta$, and $\hbar\omega_{q\lambda} \ll 4\Delta$ and $k_B T \ll 4\Delta$, where 4Δ is the energy difference between the ground state and the next-higher energy state. These regions correspond to $\omega < \omega_r$ and $\omega > \omega_r$ is the resonance frequency. The resonance-scattering relaxation rate shows different frequency dependences in the different frequency regions. For $\omega < \omega_r$, $\tau_{ep}^{-1} \propto \omega^4$ for scattering off the ground state and $\tau_{ep}^{-1} \propto \omega^2$ for scattering off the next-higher energy state. For inelastic processes τ_{ep}^{-1} is independent of frequency. However, for $\omega > \omega_r$, $\tau_{ep}^{-1} \propto \omega^2$ both for elastic scattering and inelastic scattering processes. It has been found in the present work that if one uses simplified expressions of Kumar *et al.* both for $\omega < \omega_r$ and $\omega > \omega_r$ and expresses the total conductivity as the sum of two integrals for the different frequency regions $\omega < \omega_r$ and $\omega > \omega_r$, it is possible to explain the results in the entire temperature range 2–20°K.

II. THEORY

First of all we are interested in reviewing briefly some of the results of Kumar *et al.* based on Kwok's theory of the resonance scattering of phonons by bound electrons. According to them the resonance-scattering relaxation rate is different in the two different frequency regions $\omega < \omega_r$ and $\omega > \omega_r$. These regions correspond to $\hbar\omega_{q\lambda} \ll 4\Delta$ and $\hbar\omega_{q\lambda} \gg 4\Delta$, where 4Δ is known as the chemical shift. Elastic and inelastic processes are also considered separately, and relaxation rates are calculated for such processes. The most simplified expression for τ^{-1}_{ep} in the region $\hbar\omega_{q\lambda} \ll 4\Delta$ is given by

$$\tau^{-1}_{ep,\mathrm{el}} = HF^4(q)\,\omega^2_{q\lambda}\left[f_0(T)\left(\frac{\hbar\omega_{q\lambda}}{4\Delta}\right)^2 + f(T)\right] \qquad (1)$$

for elastic processes, and

$$\tau^{-1}_{ep,\mathrm{in}} = H_1F^4(q)\left(\frac{4\Delta}{k_BT}\right)\left(\frac{4\Delta}{\hbar}\right)^2 f(T) \qquad (2)$$

for inelastic processes. Therefore, the total relaxation rate for electron-phonon scattering is given by

$$\tau^{-1}_{ep,\omega<\omega_r} = \tau^{-1}_{ep,\mathrm{el}} + \tau^{-1}_{ep,\mathrm{in}}\,. \qquad (3)$$

Hence,

$$\tau^{-1}_{ep,\omega<\omega_r} = HF^4(q)\,\omega^2_{q\lambda}\left[f_0(T)\left(\frac{\hbar\omega_{q\lambda}}{4\Delta}\right)^2 + f(T)\right] + H_1F^4(q)\left(\frac{4\Delta}{k_BT}\right)\left(\frac{4\Delta}{\hbar}\right)^2 f(T)\,, \qquad (4)$$

where

$$H = \frac{E_u^4 S}{3^4\pi\rho^2 c_\lambda^7\hbar^2}\,, \quad H_1 = \frac{E_u^4 S_1}{3^4\pi\rho^2 c_\lambda^7\hbar^2}\,.$$

Here S and S_1 depend on the geometrical structure of the conduction band for n-type semiconductors and valence band for p-type semiconductors. The details of S and S_1, which involve angular matrices, are given in Ref. 4 for the conduction band in Ge.

The cutoff factor $F(q)$ is given by

$$F(q) = \left(1 + \frac{r_0^2\,\omega^2}{4c^2}\right)^{-2} = (1+\delta x^2 T^2)^{-2}\,,$$

where r_0 is the effective hole radius,

$$\delta = r_0^2\left(\frac{k_B}{\hbar}\right)^2\frac{1}{4c^2}\,, \quad \text{and} \quad x = \frac{\hbar\omega}{k_BT}\,.$$

The populations of the ground state $f_0(T)$ and that of the next-higher energy state $f(T)$ are given by

$$f(T) = f_0(T)\,e^{-4\Delta/k_BT}$$

and

$$f_0(T) = (1+e^{-4\Delta/k_BT})^{-1}\,.$$

But in the frequency region, i.e., $\omega < \omega_r$, the elastic processes are much more important than inelastic processes. Therefore, for the convenience of the calculations we have neglected the inelastic part of Eq. (4). Thus τ^{-1}_{ep} is given by

$$\tau^{-1}_{ep,\omega<\omega_r} = HF^4(q)\,\omega^2_{q\lambda}\left[f_0(T)\left(\frac{\hbar\omega_{q\lambda}}{4\Delta}\right)^2 + f(T)\right]. \qquad (5)$$

Holland has not given any information about the impurity content of the material, and thus values of the chemical shift 4Δ are not available. For this purpose we have calculated 4Δ from the relation $4\Delta = k_BT_R = k_B(6T_m)$. Here T_m is the tempera-

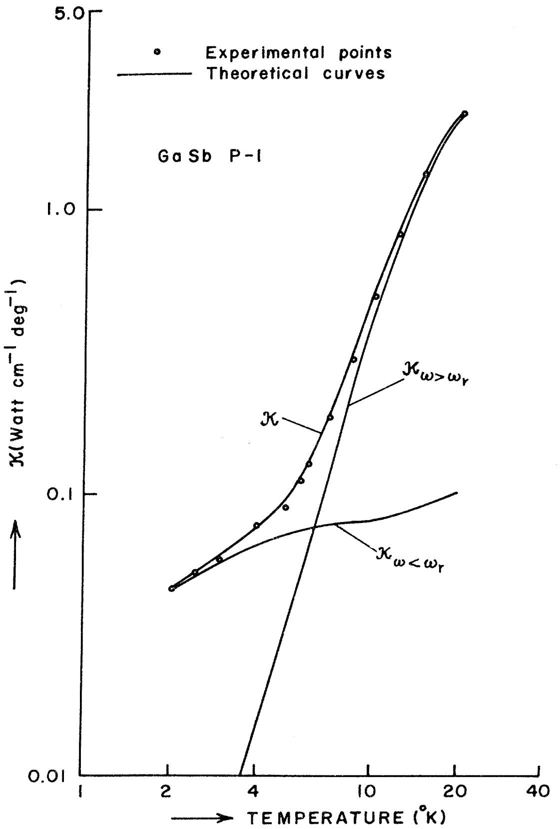

FIG. 1. Comparison of the theoretical values of the phonon conductivity of P-1 GaSb with the experimental values in the temperature range 2–20 °K. κ is the total thermal conductivity. $\kappa_{\omega<\omega_r}$ is the contribution of phonon frequencies ω less than the resonance frequency ω_r. $\kappa_{\omega>\omega_r}$ is the phonon conductivity due to phonons of frequencies $\omega > \omega_r$.

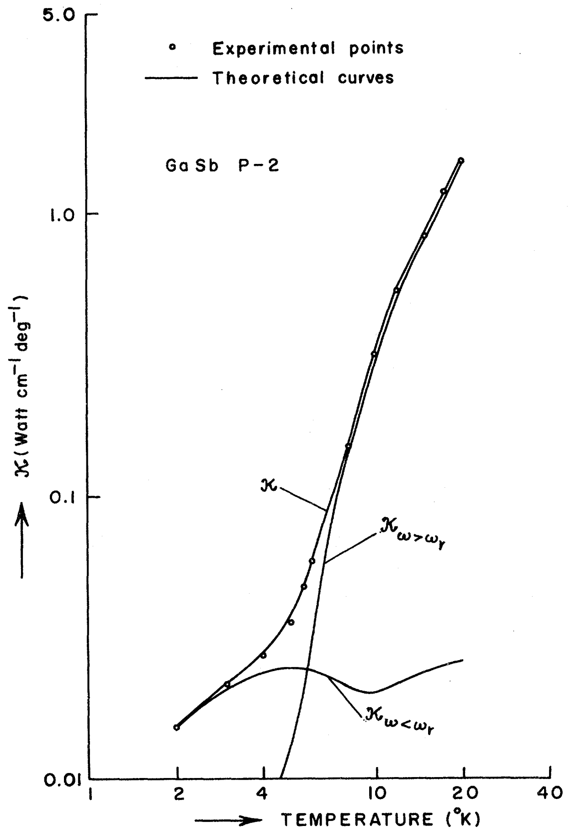

FIG. 2. Comparison of the theoretical values of the phonon conductivity of P-2 GaSb with the experimental values in the temperature range 2–20 °K. κ is the total thermal conductivity. $\kappa_{\omega<\omega_r}$ is the contribution of phonon frequencies ω less than the resonance frequency ω_r. $\kappa_{\omega>\omega_r}$ is the phonon conductivity due to phonons of frequencies $\omega > \omega_r$.

ture at which the dip in the κ-vs-T curve is observed experimentally. Using these values, we have the final expression for τ_{ep}^{-1} as

$$\tau^{-1}_{ep,\,\omega<\omega_r} = M_1\,[f_0(T)\,(T/T_R)^2\,x^2 + f(T)]\,x^2T^2 \times (1+\delta x^2T^2)^{-8}\ , \quad (6)$$

where

$$M_1 = H\,(k_B/\hbar)^2\,S \quad .$$

The expression for τ_{ep}^{-1} for the frequency region, i.e., $\omega < \omega_r$ is given by

$$\tau^{-1}_{ep,\,\mathrm{el}} = HF^4(q)\,\omega^2_{q\lambda} f(T) \qquad (7)$$

for elastic scattering processes and

$$\tau^{-1}_{ep,\,\mathrm{in}} = H_1 F^4(q)\,\omega^2_{q\lambda} f(T) \qquad (8)$$

for inelastic-scattering processes. Therefore, the total relaxation rate for electron-phonon scattering in the frequency region $\omega > \omega_r$ is given by

$$\tau^{-1}_{ep,\,\omega>\omega_r} = (H+H_1)\,F^4(q)\,\omega^2_{q\lambda} f(T)\ , \qquad (9)$$

which can be expressed as

$$\tau^{-1}_{ep,\,\omega>\omega_r} = M_2\,x^2\,T^2 f(T)(1+\delta x^2T^2)^{-8} \quad . \qquad (10)$$

Here $M_2 = (H_1+H)\,(k_B/\hbar)^2$ and the other symbols have been already defined in the case of $\tau^{-1}_{ep,\,\omega<\omega_r}$.

Using the above relaxation rates for the electron-phonon interaction [Eqs. (6) and (10)] the phonon conductivity of doped semiconductors can be calculated on the basis of Callaway's model.[5] The phonon conductivity κ is given by

$$\kappa = \frac{k_B}{2\pi^2}\left(\frac{k_BT}{\hbar}\right)^3 \frac{1}{v_s}\int_0^{\Theta_D/T} \frac{x^4e^x(e^x-1)^{-2}dx}{\tau_B^{-1}+\tau_{pt}^{-1}+\tau_{3ph}^{-1}+\tau_{ep}^{-1}} \ . \qquad (11)$$

Since we have different expressions for τ_{ep}^{-1} in the different regions $\omega<\omega_r$ and $\omega>\omega_r$ the conductivity integral is separated into two parts:

$$\kappa = \frac{k_B}{2\pi^2}\left(\frac{k_BT}{\hbar}\right)^3 \frac{1}{v_s}\left(\int_0^{T_R/T} \frac{x^4e^x(e^x-1)^{-2}dx}{\tau_B^{-1}+\tau_{pt}^{-1}+\tau_{3ph}^{-1}+\tau^{-1}_{ep,\,\omega<\omega_r}} + \int_{T_R/T}^{\Theta_D/T} \frac{x^4e^x(e^x-1)^{-2}dx}{\tau_B^{-1}+\tau_{pt}^{-1}+\tau_{3ph}^{-1}+\tau^{-1}_{ep,\,\omega>\omega_r}}\right) . \qquad (12)$$

Here,

$$\tau_B^{-1} = \frac{v_s}{L}, \qquad \tau_{pt}^{-1} = A\omega^4 = Dx^4T^4\ ,$$

$$\tau_{3ph}^{-1} = B\omega^2T^3 = \beta\,x^2\,T^5\ , \qquad x = \hbar\,\omega/k_BT\ ,$$

and hence the final form of integral can be written as

$$\kappa = \left(\frac{k_B}{2\pi^2}\right)\left(\frac{k_BT}{\hbar}\right)^3 \frac{1}{v_s}\left(\int_0^{T_R/T} \frac{x^4e^x\,(e^x-1)^{-2}dx}{\tau_B^{-1}+Dx^4T^4+\beta x^2T^5+M_1x^2T^2(1+\delta x^2T^2)^{-8}[f_0(T)\,(T/T_R)^2x^2+f(T)]} + \int_{T_R/T}^{\Theta_D/T} \frac{x^4e^x\,(e^x-1)^{-2}dx}{\tau_B^{-1}+Dx^4T^4+\beta x^2T^5+M_2x^2T^2f(T)\,(1+\delta x^2T^2)^{-8}}\right) . \qquad (13)$$

In the present calculations the values of τ_B^{-1} and A are taken from Holland's paper. T_R is calculated from the experimental curve of Holland. M_1 and M_2, which contain the shear deformation potential E_u and angular matrices, are treated as adjustable parameters. On the assumption that the angular

TABLE I. Values of the various parameters used in the analysis of phonon conductivity of GaSb.

Sample	τ_B^{-1} (sec^{-1})	A(sec^3)	B[(°K)$^{-3}$ sec]	M_1[sec^{-1}(°K)$^{-2}$]	M_2[sec^{-1}(°K)$^{-2}$]
GaSb P-1	1.28×10^6	0.813×10^{-44}	0.8×10^{-22}	2.82×10^7	1.8×10^{10}
GaSb P-2	1.16×10^6	0.813×10^{-44}	0.8×10^{-22}	1.19×10^8	4.0×10^{10}

$\Theta_D=270\,°K$ $T_R=30\,°K$ $V_s=3.09\times10^5$ cm/sec $r_0=12.5$ Å $T_m=5\,°K$

matrices are constant quantities and the second part of Eq. (13) is negligible at very low temperatures, we adjusted M_1 at 2 °K. Having adjusted M_1, M_2 is adjusted at 10 °K. Further, B is adjusted at 20 °K. Here we have not considered the separation of the transverse phonons and longitudinal phonons. As the temperature range of our calculation is quite low, the distinction between longitudinal phonons and transverse phonons is not important. We have also neglected three-phonon umklapp processes due to the fact that Umklapp processes are negligible in the low-temperature range. Holland has stated that r_0 lies between 10 and 15 Å. We have taken $r_0=12.5$ Å. T_m is observed at 5 °K in both of the samples.

III. RESULTS

The values of the various parameters used in the calculation of the phonon conductivity of p-type GaSb are given in Table I. The present calculations show excellent agreement between the theoretical and experimental values of the phonon conductivity, as shown in Figs. 1 and 2 for the samples P-1 and P-2. This indicates that such results can be explained using the simplified expressions of Kumar *et al.* for the resonance scattering of phonons by bound electrons. It may be further noted that for $\omega>\omega_r$, $\tau_{ep}^{-1}\propto\omega^2 f(T)$ and for $\omega<\omega_r$, $\tau_{ep}^{-1}\propto[f_0(T)\,\omega^4+f(T)\,\omega^2]$, where $f_0(T)$ is the population of the acceptor-hole ground state and $f(T)$ is the population of the next-higher energy state. The value of 4Δ, which is the energy difference between the two states, is inferred from the temperature at which the resonance dip in the κ-vs-T curve is observed. The mechanism of the resonance scattering of phonons is due to the virtual transitions of the acceptor hole between the two states. For $\omega>\omega_r$ the scattering off the higher-energy state dominates that of the ground state and $\tau_{ep}^{-1}\propto\omega^2$. For $\omega<\omega_r$ the elastic scattering dominates the inelastic scattering. For the elastic scattering of phonons off the ground state, the relaxation rate is proportional to ω^4, whereas for the elastic scattering off the higher-energy state it is proportional to ω^2. With the above frequency dependences of τ_{ep}^{-1} both for $\omega<\omega_r$ and $\omega>\omega_r$, it has been possible to explain the anomalous resonance dip in the thermal conductivity vs temperature of p-type GaSb. There are some discrepancies near the resonance frequency due to the fact that the expressions used for τ_{ep}^{-1} are valid only for $\omega<\omega_r$ and $\omega>\omega_r$, but invalid at $\omega=\omega_r$. One can improve the agreement at $\omega=\omega_r$ by incorporating τ_{ep}^{-1} obtained by Kwok's Green's-function approach. In view of the fact that the resonance is of very narrow width, its influence over phonon conductivity κ is the negligible for the frequencies in the off-resonance region.

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