atomic potentials. It is the purpose of this note to point out that Weaire's calculation is merely a particular example of a more general result[2] proved some years ago.

In Ref. 2., an electron was considered to be moving in a disordered array of identical nonoverlapping potential wells and to obey the Schrödinger equation

$$(-\nabla^2 + V - \epsilon)\psi = 0 , \quad (1)$$

where ψ is a real wave function. The system was then divided into cells, a cell being defined as the region closer to one particular potential well than to any other. Since ψ is continuous at each interface between cells, it follows that with periodic boundary conditions over some large volume we have

$$\sum_{\text{cells}} \int \nabla(\psi^2)\cdot d\vec{S} = 0 , \quad (2)$$

where $d\vec{S}$ is an element of surface area of a cell. It was shown that a gap must exist in the density of states if no cell could be found such that the integral over the cell surface was not positive. If one replaces the Schrödinger Hamiltonian of Eq. (1) by the "lattice gas" Hamiltonian of Ref. 1, then Eq. (2) reduces, in Weaire's notation, to

$$\sum_{\text{cells}} \sum_{i} (v_i^2 - u_i^2) = 0 ,$$

from which that author derived his inequality (9).

It is worth noting that the more general theory is capable of predicting the existence of several different band gaps for suitable potentials, and that it is not necessary that the environment of any atom possess symmetry of any kind.

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Low-Temperature Thermal Conductivity of *n*-Ge

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The measurements of the lattice thermal conductivity of n-Ge from 0.3 to 4.2 °K by Bird and Pearlman are explained satisfactorily by the nonlinear theory of heat transfer in solids given by Kazakov and Nagaev.

I. INTRODUCTION

The lattice thermal conductivity of nonmetals of finite dimensions at low temperatures has drawn considerable attention recently. At low temperatures, the dominant scattering mechanisms are boundary scattering and impurity scattering. The anharmonic interactions (i.e., phonon-phonon interactions) may be neglected at fairly low temperatures. The first attempt to rigorously calculate the phonon conductivity of a finite lattice with defects was undertaken by Erdös.[1] Later, Kazakov and Nagaev (KN)[2] calculated nonlinear heat transfer in a lattice containing impurities using boundary conditions consistent with the experimental situation. It is normally assumed that the system departs slightly from thermodynamical equilibrium which leads to the introduction of local temperature and the linearization of the kinetic equations with respect to the temperature gradient. The KN calculations of the thermal conductivity [see Eqs. (5) and (6)] clearly show that one can calculate the effect of impurity scattering on the lattice thermal conductivity more rigorously than was done with Callaway's phenomenological approach.[3] Callaway's approach is complicated due to the fact that at one temperature there are simultaneously different scattering processes. Recent calculations[4-6] of the thermal conductivity of n-Ge show that the phonon-phonon interaction simply modifies the conductivity integral and itself gives negligible contribution for temperatures below 5 °K. These calculations suggest the use of KN's results to explain the thermal-conductivity measurements of n-Ge between 0.5 and 4.2 °K made by Bird and Pearlman (BP).

KN have considered only the isotopic scattering of the Rayleigh type for impurity scattering processes. However, in certain systems it is observed that resonance phenomenon occurs in the impurity scattering processes. To consider the effect of resonant scattering of phonons at reso-

nance and off-resonance frequencies we can extend the KN calculations. Assuming the validity of the additivity of the inverse of the relaxation times, we can write the relaxation time for the impurity scattering as

$$\tau^{-1}(\vec{k}) = \tau_I^{-1}(\vec{k}) + \tau_{ep}^{-1}(\vec{k}) \quad , \tag{1}$$

where $\tau_I(\vec{k})$ and $\tau_{ep}(\vec{k})$ are the relaxation times for isotopic and electron-phonon scattering processes, respectively. We can now study the applicability of the KN calculations for three different cases: (i) $\tau_{ep}^{-1}(\vec{k}) = 0$, (ii) $\tau_{ep}^{-1}(\vec{k}) \neq 0$ and $\omega \neq \omega_{res}$, and (iii) $\tau_{ep}^{-1}(\vec{k}) \neq 0$ and $\omega = \omega_{res}$. The isotopic scattering has always been used in the present calculations. The BP measurements show all the above different cases. These measurements show that Sb donors are strong scatterers resulting in resonant scattering in the temperature range 0.5 to 4.2 °K (the reduction in the thermal resistance at 2 °K is by a factor of 8). As- and P-doped Ge samples, however, do not indicate resonance phenomenon in this temperature range. The values of the chemical splitting 4Δ also suggest that the resonance temperature $T_R (\cong \frac{1}{6} 4\Delta/K_B)$ lies outside of the considered temperature region and corresponds to the frequency condition $\hbar\omega(\vec{k}) < 4\Delta$. In the present work we observe that the KN calculations can explain the thermal-conductivity results remarkably well for the lattices with defects which show no resonance phenomenon. For resonant scattering of phonons, the thermal-conductivity results can be explained by KN calculations for the temperatures where boundary scattering dominates over impurity scattering.

II. THEORY

Following BP, we assume that a pure germanium lattice means a lattice free from electron-phonon interaction. The isotopic phonon scattering process is, however, present in pure germanium and is described by

$$\tau_I^{-1} = A\omega^4(\vec{k}) \quad , \tag{2}$$

where $\omega(\vec{k})$ is the phonon frequency with wave vector $\vec{k}$. In the case of doped germanium, the electron-phonon interaction due to donor ions has been studied[6–13] by a number of authors. The inverse of the electron-phonon relaxation time can be written as

(a) resonance scattering:

$$\tau_{ep}^{-1} = H\omega^4(k)F^4(k)/\{(4\Delta)^2 - [\hbar\omega(k)]^2\}^2 \quad , \tag{3}$$

where

$$H = \tfrac{400}{225} E_u^4 (4\Delta)^2 N_{ex}/4\pi\rho^2 3^4 v^7$$

and

$$F(k) \cong [1 + \tfrac{1}{4} r_0^2 \omega^2(k)/v^2]^{-2} \quad ;$$

(b) nonresonance frequencies $[\hbar\omega(k) < 4\Delta]$[6,13]:

$$\tau_{ep}^{-1} = H_1 F^4(k)\omega^2(k)\,[f_0(T)(\hbar\omega(k)/4\Delta)^2 + f(T)] \quad , \tag{4}$$

where

$$H_1 = \tfrac{400}{225} E_u^4 N_{ex}/4\pi\rho^2 3^4 v^7 \hbar^2 \quad .$$

H and H_1 are adjustable parameters which depend upon the fourth power of the shear deformation potential E_u. 4Δ is the chemical shift. The definitions of the other terms are the same as in Refs. 6 and 11.

It is thus observed that the relaxation time for phonon scattering by defects, $\tau(k)$, is

$$\tau^{-1}(k) = \tau_I^{-1}(k) + \tau_{ep}^{-1} \quad . \tag{2'}$$

$\tau_{ep}^{-1}(k)$ dominates over $\tau_I^{-1}(k)$ only for resonant scattering, otherwise $\tau^{-1}(k)$ is effectively proportional to $\omega^4(k)$. One can, therefore, use $\tau^{-1}(k)$ instead of $\tau_I^{-1}(k)$ given by Eq. (2'). As the scattering is elastic, it does not bring a redistribution of phonons with respect to frequencies, and is merely averaged over the direction $\vec{k}$.

Case (i): $\tau_{ep}^{-1}(\vec{k}) = 0$. Following KN and using Eqs. (1)–(4) we can write the expression for thermal conductivity as follows:

$$K(T) = K_0 \left\{ 1 - \left[\frac{LA}{2v} \left(\frac{K_B T}{\hbar} \right)^4 \frac{I_2}{I_1} + \frac{LH}{2vK_B^4} \left(\frac{K_B T}{\hbar} \right)^4 \frac{I_3}{I_1} \right] \right\} ,$$

where

$$K_0 = 3 \frac{K_B}{2\pi^2 v} \left(\frac{K_B T}{\hbar} \right)^3 \frac{L}{c} I_1 \quad ,$$

$$I_1 = \int_0^\infty \frac{x^3 dx}{e^x - 1} = 6.5 \quad ,$$

$$I_2 = \int_0^\infty \frac{x^7 dx}{e^x - 1} = 7.2 \times 10^2 \quad , \tag{5}$$

$$I_3 = \int_0^\infty \frac{F^4(x) x^7 dx}{(e^x - 1)[(4\Delta/K_B)^2 - (Tx)^2]^2} \quad .$$

Case (ii): $\omega(k) \neq \omega_{resonance}$. We find

$$K(T) = K_0 \left(1 - \left\{ \frac{LA}{2v} \left(\frac{K_B T}{\hbar} \right)^4 \frac{I_2}{I_1} + \frac{LH_1}{2v} \left(\frac{K_B T}{\hbar} \right)^2 \left[2f_0(T) \left(\frac{K_B T}{4\Delta} \right)^2 \frac{I_4}{I_1} + \frac{3}{2} f(T) \frac{I_5}{I_1} \right] \right\} \right) \quad , \tag{6}$$

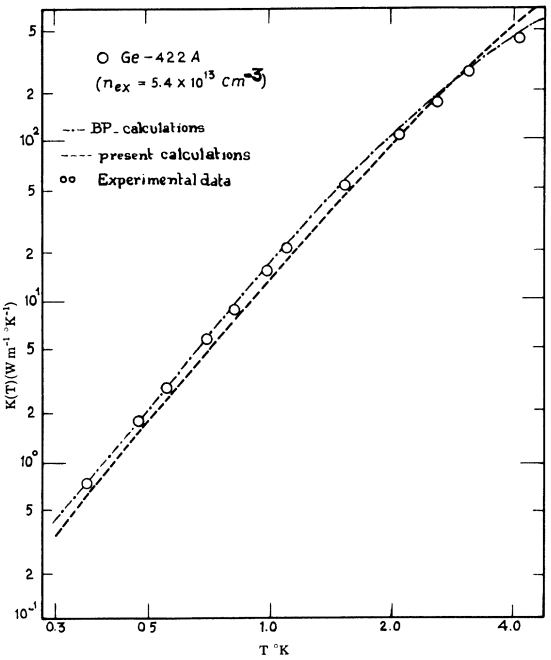

FIG. 1. Plot of the phonon-conductivity curve for the Ge-422A sample. The dashed curve is the calculated phonon-conductivity curve [using Eq. (7)]. BP calculations are shown as a chained curve.

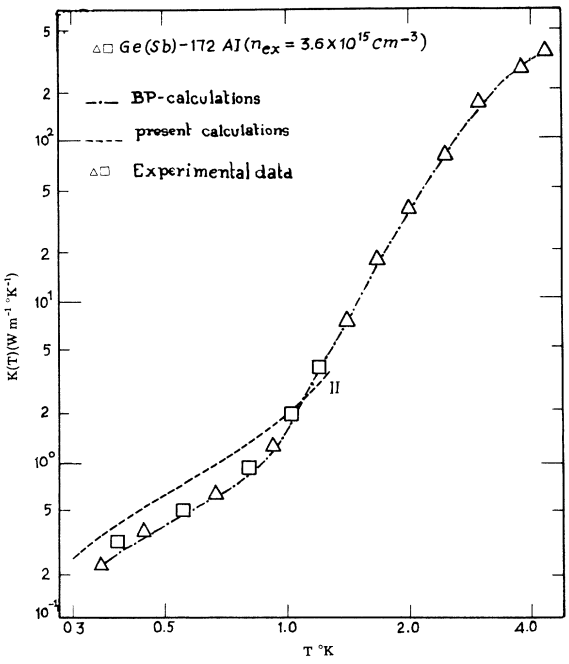

FIG. 2. Plot of $K(T)$ vs T for the Ge(As) 200A sample with $N_{ex} = 5.3 \times 10^{15}$ cm^{-3}. The present calculations [using Eq. (6)] are represented by the dashed curve. BP calculations are shown as a chained curve.

where

$$I_4 = \int_0^\infty \frac{F^4(x) x^7 dx}{e^x - 1}$$

(for off-resonance frequency).

Here K_0 [see Eq. (5)] is the phonon conductivity when there is only boundary scattering.

III. RESULTS AND DISCUSSIONS

We now use Eqs. (5) and (6) to calculate the thermal conductivity of n-Ge. The calculated results are compared with the recent BP measurements and calculations.[1]

Case (i): $\tau_{ep}^{-1}(k) = 0$, Ge 422A. Figure 1 represents the phonon-conductivity curve for pure Ge sample 422A where we consider $\tau_{ep}^{-1}(k) = 0$. In this case, the phonon conductivity can be described as

$$K(T) = K_0 \left[1 - \frac{LA}{2v} \left(\frac{K_B T}{\hbar} \right)^4 \frac{I_2}{I_1} \right] . \qquad (7)$$

The values for normal germanium were found by Callaway,[3] i.e., $A = 2.57 \times 10^{-44}$ sec^3, $v = 3.5 \times 10^5$ cm/sec, $L/v = 1.106 \times 10^{-6}$ sec^{-1}. Using these values and Eq. (7), we calculate the thermal conductivity as shown by dotted curve in Fig. 1. It is observed that the agreement is reasonable as compared with the BP calculations and the measurements. However at temperature $T > 2.5$ °K there is a deviation between the two calculations. This is due to the fact that we have not considered phonon-phonon scattering processes, which lower

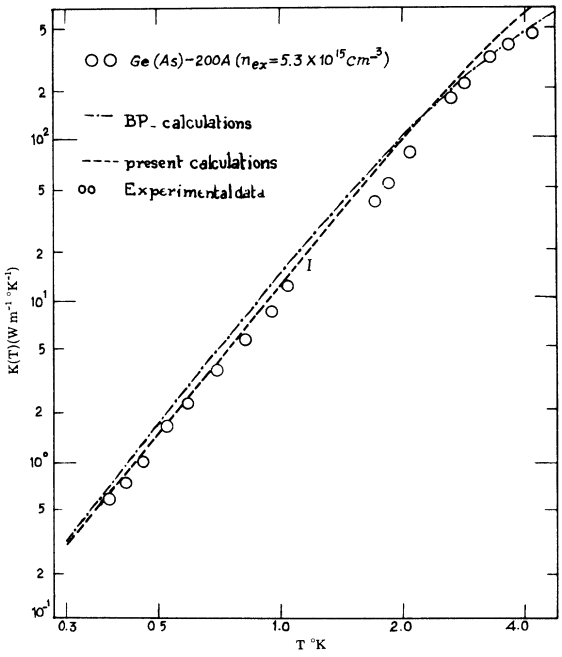

FIG. 3. Plot of $K(T)$ vs T for Ge(Sb) 172AI with $N_{ex} = 3.6 \times 10^{15}$ cm^{-3}. The dashed curve is calculated by using Eq. (5). BP calculations are shown as chained curve.

the values of phonon conductivity at these temperatures.

Case (ii): $\tau_{ep}^{-1}(\vec{k}) \neq 0$, $\omega \neq \omega_{res}$. We present here only the calculations of the Ge(As 200A)-doped sample. The calculations for the Ge(P 229A)-doped sample will be similar except for the value of 4Δ. The phonon conductivity is calculated by using Eq. (6) and by assuming $r_0 = 32$ Å and $4\Delta = 4.23 \times 10^{-3}$ eV, in addition to other values like A, v, L/v as suggested in Case (i) (see Fig. 2). The agreement between theory, experiment, and BP calculations is good at low temperatures. There is a deviation between the two calculated results at and above 2.5 °K. It is because of the fact that we have neglected phonon-phonon interaction, which reduces the value of the conductivity integral at these temperatures. The shear deformation potential E_u obtained from the calculations is 9.8 eV.

Case (iii): $\tau_{ep}^{-1}(\vec{k}) \neq 0$, $\omega \simeq \omega_{res}$. In Fig. 3 the phonon conductivity of Ge(Sb) 172AI-doped sample has been calculated assuming $4\Delta = 0.32 \times 10^{-3}$ eV and $r_0 = 44$ Å as suggested by BP. The phonon conductivity can be calculated only up to the temperature 1.2 °K assuming Eq. (5), i.e., up to the temperature where boundary scattering dominates resonant scattering. The resonant scattering dominates boundary scattering after 1.2 °K which give a negative value for the factor in square bracket in Eq. (5). The phonon conductivity calculated up to 1.2 °K, however, agrees remarkably well with experimental data. The BP calculations, however, agree with the experimental results in a reasonably good manner.

IV. CONCLUSIONS

It is concluded that the analysis of Kazakov and Nagaev can explain the experimental results quite well for lattices with defects where resonant phonon scattering is absent. However in the presence of resonant scattering of phonons, we can explain the phonon conductivity only up to the temperature where boundary scattering dominates over the resonant scattering.

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