

and also convert the units of  $a_0$  into angstroms. For this we require the quantities  $\mu_{\perp}$ ,  $\mu_{\parallel}$ ,  $\epsilon_{\perp}$ , and  $\epsilon_{\parallel}$ , which as far as we are aware have not been measured in  $\text{WSe}_2$ . However, the bulk crystal binding energy of the  $A$  exciton in  $\text{WSe}_2$  is known, and using a value of 0.05 eV (Consadori and Frindt<sup>3</sup>) in Eq. (5), we obtain

$$a_0 = 144/(\epsilon_{\perp}\epsilon_{\parallel})^{1/2} \text{ \AA} . \quad (8)$$

The layer structure  $\text{WSe}_2$  is one of the regular  $\text{TX}_2$  transition-metal dichalcogenides and it is grouped in the review by Wilson and Yoffe<sup>7</sup> as belonging to the group-VI trigonal-prism compounds which include  $\text{MoS}_2$ . The spectra of  $\text{WSe}_2$  and  $\text{MoS}_2$  show a number of similarities and we have assumed that the dielectric components are also similar.<sup>8</sup> Using the values given by Evans and Young<sup>9</sup> of  $\epsilon_{\perp} = 6.76$  and  $\epsilon_{\parallel} = 2.74$ , we obtain

$$a_0 = 33.5 \text{ \AA} . \quad (9)$$

For these values of the dielectric components a value of  $W$  of approximately 0.6 would lie midway between the extreme limits for  $W$  (Appendix II in I). By using this value of  $W$ , and choosing  $\beta^2 = 3.2$ , we obtain the results shown in Fig. 2 in comparison with the data taken from Fig. 3 of Consadori and Frindt for  $\text{WSe}_2$ . The original data based on estimated thickness,<sup>10</sup> obtained before conversion to thicknesses which are integer multiples of a single  $\text{WSe}_2$  layer of 6.5 \AA, suggest that a value of  $\beta^2 = 4.5$  may be more suitable.

In conclusion we point out that the theory leads to an energy which closely approaches an inverse-square-law dependence on thickness. By using estimates of the dielectric and reduced-exciton-mass components, we obtain quantitative agreement with data on  $\text{WSe}_2$ .

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<sup>1</sup>G. Jones and J. L. Brebner, *J. Phys. C* **4**, 723 (1971).

<sup>2</sup>B. Bendow, *Phys. Rev. B* **3**, 1999 (1971).

<sup>3</sup>F. Consadori and R. F. Frindt, *Phys. Rev. B* **2**, 4893 (1970).

<sup>4</sup>See I. Essentially this means that results calculated in the transformed coordinate system apply to crystals of half-width  $L = L'/\beta$ , where  $L'$  is the half-width in the transformed coordinate system.

<sup>5</sup>The reason for these values is explained later in the text.

<sup>6</sup>Except for the  $L'$  range near  $a_0$  where the adiabatic approximation makes this difficult to determine—see text.

<sup>7</sup>J. A. Wilson and A. D. Yoffe, *Advan. Phys.* **18**, 193 (1969).

<sup>8</sup>Consadori and Frindt (Ref. 3) use the refractive index of  $\text{MoS}_2$  in their crystal-thickness determination.

<sup>9</sup>B. L. Evans and P. A. Young, *Phys. Status Solidi* **25**, 417 (1968).

<sup>10</sup>F. Consadori (private communication).

## Role of Peripheral Phonons in the Lattice Thermal Conductivity of Doped Semiconductors: Application to $n$ -Ge

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In the present paper we have studied the role of peripheral phonons in the phonon conductivity of doped semiconductors. For this purpose we have taken Callaway's model and we have also separated the contributions of the phonons which are interacting with electrons and of the peripheral phonons. The temperature which differentiates the peripheral phonons from other phonons is given by  $\Theta^* = (2F\hbar v_s/k_B)(\pi^2 n)^{1/3}$ , where the factor  $F$  varies from 3 to 5 for different Sb- and As-doped Ge samples. Excellent agreement between the theoretical and experimental values of phonon conductivity is obtained.

Recently Gaur and Verma<sup>1</sup> established that for those semiconductors for which the donor-electron concentration is greater than  $10^{17} \text{ cm}^{-3}$  and for which the donor levels merge with the conduction band, Ziman's scattering of phonons by conduction electrons is the relevant phonon scattering mechanism. This is the explanation of the

drastic reduction in the phonon conductivity of Sb- and As-doped Ge as observed by Goff and Pearlman.<sup>2</sup> However, Gaur and Verma could not explain the results below 10°K. They could improve the agreement between theory and experiment only by lowering  $\tau_{ep}^{-1}$  by a factor of 10 or 30. Recently Singh and Verma<sup>3</sup> have shown that excellent agree-

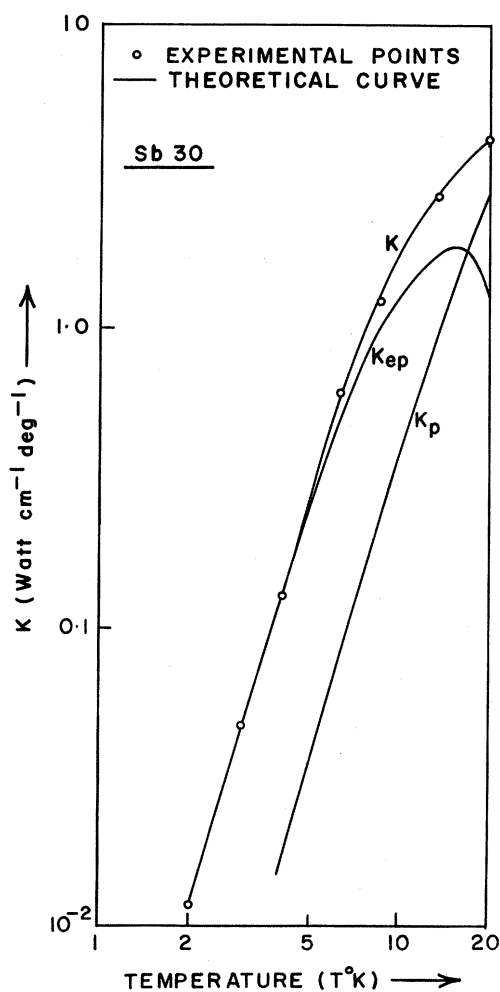


FIG. 1.  $K_p$  is the contribution of peripheral phonons and  $K_{ep}$  is the contribution of those phonons which are interacting with electrons.  $K$  is the total thermal conductivity of Sb-doped Ge sample Sb 30. Circles show the experimental points of Goff and Pearlman (Ref. 2).

ment between theory and experiment is obtained for Sb-doped Ge samples Sb 222, Sb 187, and Sb 30 and the As-doped Ge sample As 226 in the low-temperature range up to 20°K by taking  $m^*$  as an adjustable parameter and keeping the deformation potential constant. The value of  $m^*$  was found to

TABLE I. Values of  $\Theta^*$ , which differentiates peripheral phonons from nonperipheral phonons, for Sb- and As-doped Ge samples.

Sample	$n$ ( $10^{17} \text{ cm}^{-3}$ )	$\Theta^*$ (°K)	$\Theta_{(m)}^*$ (°K)	$F$
Sb 30	25	50	15.6	3.2
Sb 222	11	46	12	3.8
Sb 187	1.2	31.3	5.7	5.5
As 226	8.8	48.4	11.0	4.4

TABLE II. Percentage contribution of peripheral phonons towards phonon conductivity of Sb- and As-doped Ge samples ( $K_p/K \times 100\%$ ).

$T$ (°K)	Sb 30	As 226	Sb 222	Sb 187
2	0	0	0	0
5	5.8	6.8	8.1	9.0
10	20.0	34.1	40.2	51.6
15	42.5	60.3	62.2	79.8
20	66.7	74.6	79.2	87.4

be sensitive to the variations of temperature but not to the doping. The value of  $m^*$  lies in the range 0.30–0.75 and increases with an increase in temperature. They used the Callaway integral<sup>4</sup> in the Debye approximation

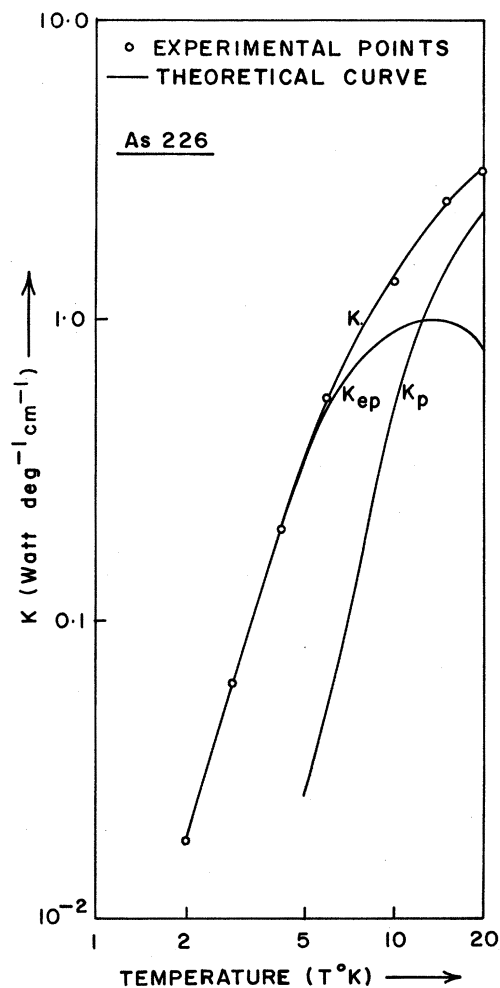


FIG. 2.  $K_p$  is the contribution of peripheral phonons and  $K_{ep}$  is the contribution of those phonons which are interacting with electrons.  $K$  is the total thermal conductivity of As-doped Ge sample As 226. Circles show the experimental points of Goff and Pearlman (Ref. 2).

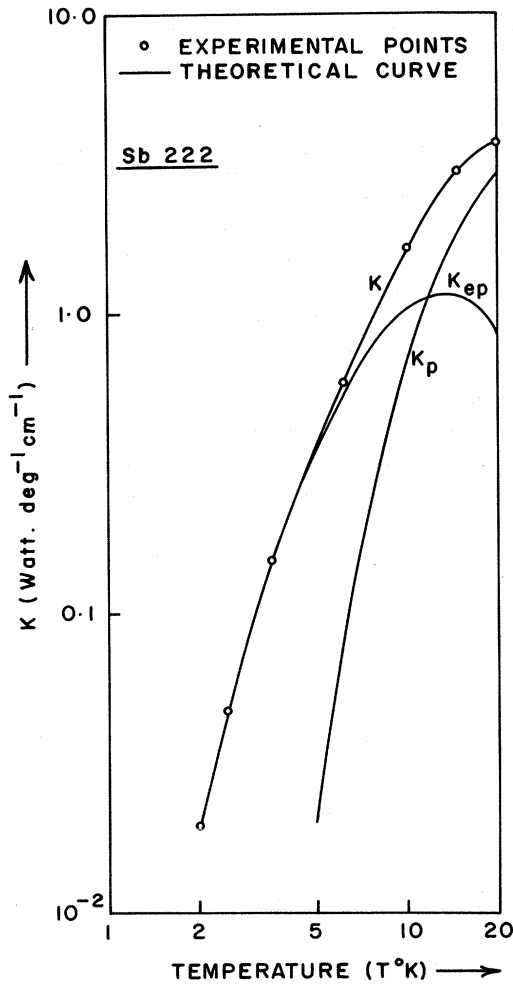


FIG. 3.  $K_p$  is the contribution of peripheral phonons and  $K_{ep}$  is the contribution of those phonons which are interacting with electrons.  $K$  is the total thermal conductivity of Sb-doped Ge sample Sb 222. Circles show the experimental points of Goff and Pearlman (Ref. 2).

$$K = \frac{k_B}{2\pi^2 v_s} \left( \frac{k_B T}{\hbar} \right)^3 \int_0^{\Theta_D/T} \frac{x^4 e^x (e^x - 1)^{-2} dx}{\tau_B^{-1} + \tau_{pt}^{-1} + \tau_{pp}^{-1} + \tau_{ep}^{-1}}, \quad (1)$$

where the symbols have their usual meaning. The above treatments, however, make no distinction between peripheral phonons and nonperipheral phonons.<sup>5</sup> Conservation of momentum and energy, however, require that an electron in the state  $\vec{K}$  can only interact with phonons for which  $|\vec{q}| \leq 2|\vec{K}|$ . For a metal it is only necessary to consider electrons with wave vectors at the Fermi surface, i. e.,  $|\vec{K}| = K_F$ . Phonons with wave vector  $\vec{q} > 2K_F = q^*$  do not participate in the electron-phonon scattering. Such phonons are known as peripheral phonons. The characteristic temperature  $\Theta^*$  corresponding to  $q^*$ , which differentiates the peripheral phonons from nonperipheral phonons,

is given by  $\Theta^* = \hbar V_s q^*$ . If one distinguishes between peripheral phonons and nonperipheral phonons, the Callaway integral, in the temperature range where electron-phonon scattering makes an appreciable contribution toward thermal resistance, can be expressed as a sum of two integrals, one from 0 to  $\Theta^*$ , which includes the contribution of nonperipheral phonons, and the other from  $\Theta^*$  to  $\Theta_D$ , which includes the contribution of peripheral phonons.<sup>5</sup> Thus

$$K = \frac{k_B}{2\pi^2 v_s} \left( \frac{k_B T}{\hbar} \right)^3 \left[ \int_0^{\Theta^*/T} \frac{x^4 e^x (e^x - 1)^{-2} dx}{\tau_B^{-1} + \tau_{pt}^{-1} + \tau_{pp}^{-1} + \tau_{ep}^{-1}} \right]$$

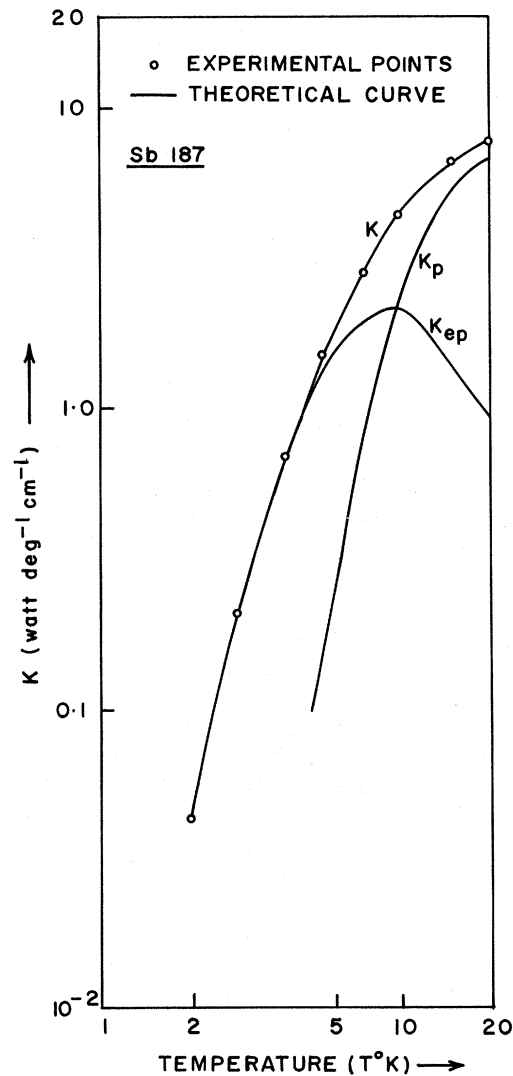


FIG. 4.  $K_p$  is the contribution of peripheral phonons and  $K_{ep}$  is the contribution of those phonons which are interacting with electrons.  $K$  is the total thermal conductivity of Sb-doped Ge sample Sb 187. Circles show the experimental points of Goff and Pearlman (Ref. 2).

$$+ \int_{\Theta^*/T}^{\Theta_D/T} \frac{x^4 e^x (e^x - 1)^{-2} dx}{\tau_B^{-1} + \tau_{pt}^{-1} + \tau_{pp}^{-1}} \Big].$$

In view of the fact that  $\Theta^*$  changes with doping and may be different for different doping materials, it has been treated as an adjustable parameter for the best fit between theory and experiment. The values of  $\tau_B^{-1}$ ,  $\tau_{pt}^{-1}$ ,  $\tau_{pp}^{-1}$ , and  $\tau_{ep}^{-1}$  are the same as those used by Singh and Verma.<sup>3</sup> The results of the calculations are shown in Figs. 1–4. Table I gives the values of  $\Theta^*$  and Table II the percentage contribution of peripheral phonons towards the phonon conductivity of Sb- and As-doped Ge in the temperature range 2–20 °K. The adjusted values of  $\Theta^*$  are also compared with the values calculated from

$$\begin{aligned} \Theta_m^* &= (\hbar v_s/k_B)(2k_e) = (2\hbar v_s/k_B)(3\pi^{2/3}n)^{1/3} \\ &= (2\hbar v_s/k_B)(\pi^2 n)^{1/3}, \end{aligned}$$

where  $n$  is the electron concentration. This relation holds for metals with isotropic- and quadratic-energy distribution. One can express  $\Theta^* = F\Theta_m^*$ , where  $F$  is a constant which varies from 3 to 5.

At very low temperatures, say up to 5 °K, all the thermal conductivity is due to those phonons which interact with electrons; i. e., electron-phonon scattering is mainly responsible for the low-temperature phonon conductivity in doped semiconductors. As the temperature increases, the contribution of peripheral phonons increases with it.

<sup>1</sup>N. S. Gaur and G. S. Verma, Phys. Rev. **159**, 610 (1967).

<sup>2</sup>J. F. Goff and H. Pearlman, Phys. Rev. **140**, A2151 (1965).

<sup>3</sup>M. P. Singh and G. S. Verma (private communication).

<sup>4</sup>J. Callaway, Phys. Rev. **113**, 1046 (1959).

<sup>5</sup>R. S. Blewett, N. M. Zebouni, and C. G. Grenier, Phys. Rev. **174**, 700 (1968).

## ERRATA

**Lattice Dynamics of Magnesium for a First-Principles Nonlocal Pseudopotential Approach**, Walter F. King, III and P. H. Cutler [Phys. Rev. B **3**, 2485 (1971)]. The captions of Figs. 3 and 4 should be interchanged.

**Improved Variational Principles for Transport Coefficients**, David Benin [Phys. Rev. B **1**, 2777 (1970)]. The numerical calculations described in Secs. V and VI were performed incorrectly. In fact, the lower bound  $K_1^<$  lies only about 20% higher than the bound  $K_0^<$  at low temperatures, rather than 90% as claimed.

**Shubnikov-de Haas Measurements in Bismuth**, Rodney D. Brown, III [Phys. Rev. B **2** 928 (1970)]. In the discussion of the Dingle temperature (p. 936) the estimates of the cyclotron radii correspond to magnetic fields ten times larger than those indicated. Since the correct radii are larger than the screening length over most of the range of field, the argument leading to Eq. (9) is invalidated, as is the explanation of the Dingle temperature. In addition, in going from Eq. (9) to Eq. (10) the thermal broadening of the level as well as the collision broadening should have been taken into account in estimating  $E_d$ . I am grateful to Dr. M. Springford for pointing out the error in the radii estimates.