

The right-hand side is symmetric with respect to  $(jp) \leftrightarrow (km)$  and  $(r \leftrightarrow s)$ . The left-hand side is obviously symmetric with respect to  $(jp) \leftrightarrow (km)$ . If it should be symmetric with respect to  $(r \leftrightarrow s)$ ,

$$[\nu l, (km), (rs)] - (\nu s, km)\delta_{lr} - (\nu l, ms)\delta_{rk}$$

must be symmetric with respect to  $(r \leftrightarrow s)$ . This follows from the rotational invariance conditions on third-order coupling parameters.

We can solve for  $d_{pj, mk, rs}$  from (59) by adding the equation obtained by interchanging  $p$  with  $j$  and subtracting the equation obtained by interchanging  $j$  with  $m$ . The expressions for  $c_{jp, km}$  and  $c_{jp, km, rs}$  obtained thus from the long-wave method agree with the expressions (26) and (27) from the method of homogeneous deformation.

The theoretical expressions developed in this paper are being applied to analyze the experimental results on the third-order elastic constants of Ge and Si in terms of the third-order coupling parameters.

#### ACKNOWLEDGMENT

The author wishes to thank Professor G. R. Barsch for suggesting this problem and for the many useful discussions the author had with him.

## Temperature Dependence of Density-of-States Effective Mass and the Electronic and Phonon Contributions to Thermal Resistance of Doped Si-Ge Alloys at High Temperatures

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The electronic polar and dipolar thermal conductivity of both  $n$ - and  $p$ -type Si-Ge alloys with different carrier concentrations are calculated in the temperature range 300 to 1100°K. With carrier concentration remaining constant, the nature of the scattering mechanism is determined from the temperature dependence of the conductivity mobility. The scattering parameter being known, the temperature dependences of the reduced Fermi level and the density-of-states effective mass are determined from thermoelectric measurements on these samples by Dismukes *et al.* These temperature variations are taken into account in the calculation of the contribution of the electron-phonon interaction to the thermal resistance of the doped Si-Ge alloys. The thermal conductivities due to longitudinal phonons and transverse phonons are calculated separately, and there is good agreement between the calculated temperature dependences of the total phonon conductivity and the experimentally obtained values of thermal conductivity minus the electronic thermal conductivity. The dilatational deformation potential is found to increase with the increase in the carrier concentration and the reduced Fermi potential. The dipolar contribution is found to be significant only at temperatures above 700°K and for  $n$ -type alloys, for which the doping is comparatively low.

### I. INTRODUCTION

RECENTLY, it has been observed that doping of Si-Ge alloys<sup>1</sup> reduces the lattice thermal conductivity. This has been interpreted in terms of scattering of phonons by free charge carriers. At high temperatures polar and dipolar contributions to thermal resistance due to electrons and holes also become important. The lattice thermal conductivity at such high temperatures is usually obtained by subtracting the electronic contribution from the experimentally observed total thermal conductivity. In highly doped materials phonons are also scattered by ionized impurities, but this contribution towards thermal resistance is negligible. The influence of phonon-electron

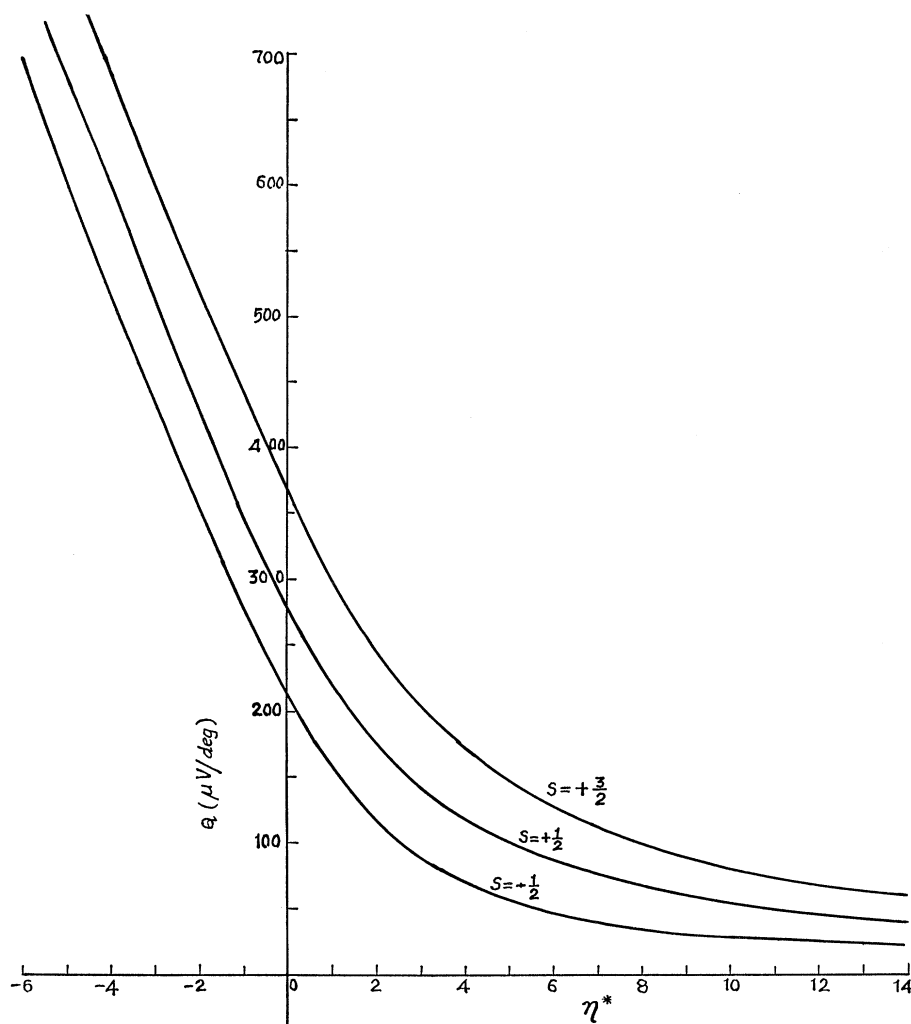
interaction on lattice thermal conductivity has been shown by Steigmeier and Abeles<sup>2</sup> to be substantial in doped Si-Ge alloys. This contribution is estimated by assuming the additivity of reciprocal relaxation times due to different scattering mechanisms of phonons, such as phonon-phonon scattering (umklapp and normal), scattering of phonons by defects, and phonon-electron scattering. The effective relaxation time thus obtained is used to determine the phonon conductivity in the formalism of Callaway.<sup>3</sup> The expression for the phonon-electron relaxation time for the electrons in the parabolic band involves the knowledge of the reduced Fermi potential, the density-of-states effective mass,

<sup>1</sup> J. P. Dismukes, L. Ekstrom, E. F. Steigmeier, I. Kudman, and D. S. Beers, *J. Appl. Phys.* **35**, 2899 (1964).

<sup>2</sup> E. F. Steigmeier and B. Abeles, *Phys. Rev.* **136**, A1149 (1964).

<sup>3</sup> J. Callaway, *Phys. Rev.* **113**, 1046 (1959); J. Callaway and H. C. Von Baeyer, *ibid.* **120**, 1149 (1960).

FIG. 1. Thermoelectric power for different values of the reduced Fermi potential for scattering parameter  $S = -\frac{1}{2}$ ,  $+\frac{1}{2}$ , and  $+\frac{3}{2}$ .



and the deformation potential for the electron-phonon interaction.

In the present paper we have determined the values

of the reduced Fermi potential  $\eta^* = E_F/k_B T$  for doped Si-Ge alloys in the temperature range 300–1200°K from the measured values of thermoelectric power taken from

TABLE I. Temperature dependence of mobility  $\mu_c \propto T^{-\alpha}$ .

Specimen	Composition (at.% of Si)	Type	Carrier concentration	$\alpha$	Temperature range (°K)	Scattering parameter $S$
68	73.8	<i>n</i>	$2.2 \times 10^{18}$	0.758	300 to 900	$-\frac{1}{2}$
41	66.8	<i>n</i>	$2.3 \times 10^{19}$	0.730	300 to 1100	$-\frac{1}{2}$
163	70.2	<i>n</i>	$6.7 \times 10^{19}$	0.849	300 to 1200	$-\frac{1}{2}$
162	71.3	<i>n</i>	$1.5 \times 10^{20}$	0.926	300 to 1000	$-\frac{1}{2}$
1834	79.5	<i>n</i>	$1.4 \times 10^{20}$	0.810	300 to 900	$+\frac{1}{2}$
1975	86.8	<i>n</i>	$2.7 \times 10^{20}$	0.684	300 to 1000	$+\frac{1}{2}$
7	72.0	<i>p</i>	$3.4 \times 10^{19}$	0.675	300 to 1100	$+\frac{1}{2}$
42	69.3	<i>p</i>	$8.9 \times 10^{19}$	0.687	300 to 1200	$+\frac{1}{2}$
1941	71.7	<i>p</i>	$1.8 \times 10^{20}$	0.726	300 to 1200	$+\frac{1}{2}$
1970	72.0	<i>p</i>	$2.4 \times 10^{20}$	0.791	300 to 1200	$+\frac{1}{2}$
82	71.0	<i>p</i>	$3.5 \times 10^{20}$	0.669	300 to 1000	$+\frac{1}{2}$
1976	85.3	<i>p</i>	$2.1 \times 10^{20}$	0.736	300 to 1300	$+\frac{1}{2}$
1241	84.6	<i>p</i>	$3 \times 10^{20}$	0.691	300 to 1100	$+\frac{1}{2}$

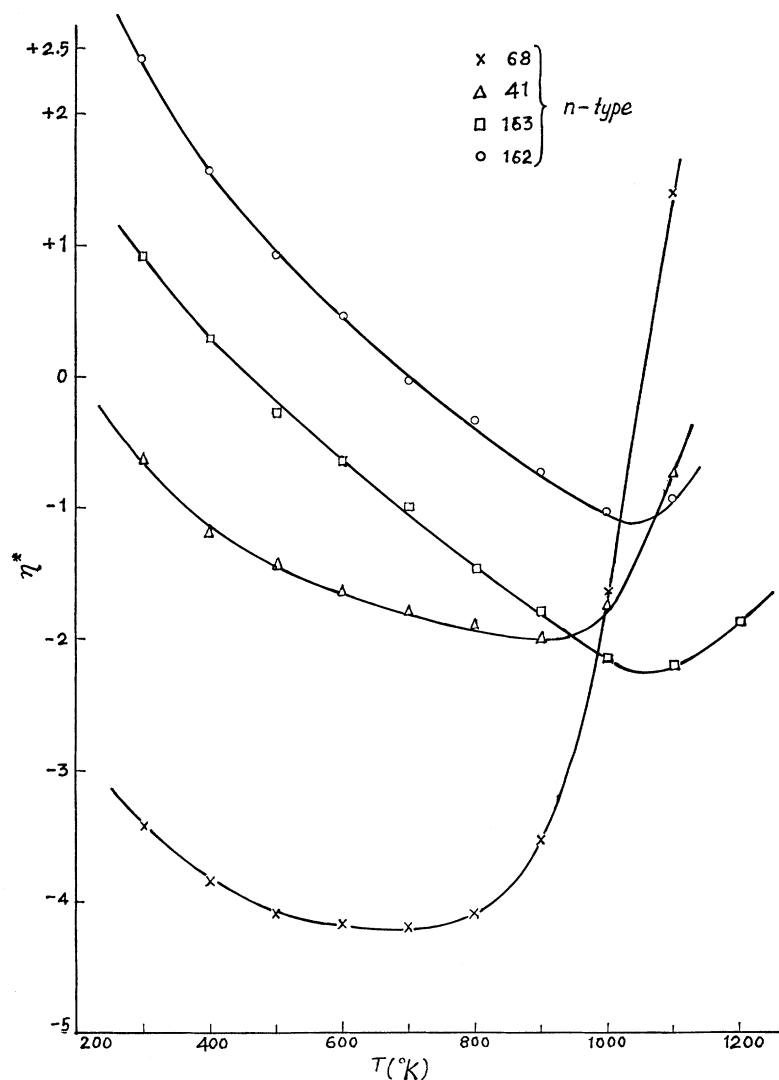


FIG. 2. Temperature dependence of the reduced Fermi potential for *n*-type Si-Ge alloys.

the literature. Assuming that the carrier concentration remains constant with temperature, the values of  $\eta^*$  have been used to determine the temperature dependence of the effective mass. In order to ascertain the nature of the scattering mechanism the temperature dependence of the conductivity mobility has been investigated. Having determined the values of the scat-

tering parameter and the reduced Fermi potential, we then compute the electronic contribution to thermal resistance in doped Si-Ge alloys at high temperatures.

The phonon conductivity of both *n*- and *p*-type Si-Ge alloys with different carrier concentrations has been estimated by calculating separately the contributions of longitudinal phonons and transverse phonons.

TABLE II. Temperature dependence of conductivity mobility  $\mu_c \propto T^x$ .

Specimen	Composition (at. % of Si)	Type	Carrier concentration	$x$	Temperature range ( $^{\circ}\text{K}$ )	Scattering <sup>a</sup> parameter $S$
1975	86.8	<i>n</i>	$2.7 \times 10^{20}$	1.78	1000 to 1300	$+\frac{1}{2}$
68	73.8	<i>n</i>	$2.2 \times 10^{18}$	5.04	900 to 1100	$\frac{3}{2}$
41	66.8	<i>n</i>	$2.3 \times 10^{19}$	1.12	1100 to 1200	$\frac{3}{2}$
162	71.3	<i>n</i>	$1.5 \times 10^{20}$	1.1	1000 to 1200	$-\frac{1}{2}$

<sup>a</sup> It may be noted that for samples 1975 and 162, which represent high levels of doping, the scattering parameter  $S$  is represented better by  $\pm\frac{1}{2}$  rather than  $\frac{3}{2}$ . Sample 1975, which contains a higher content of silicon, gives a better representation with  $S = +\frac{1}{2}$ . In samples which have a lower level of doping, such as 68 and 41,  $S = \frac{3}{2}$ .

This was the approach used by Holland<sup>4</sup> to explain the high-temperature thermal-conductivity data in Si and Ge, which could not be accounted for by Callaway's simplified approach. Although Holland's approach involves a lot of computational labor, it is considered desirable that such an approach should be followed for Si-Ge alloys in order to obtain more reliable information regarding different phonon-scattering processes. In view of the fact that the electron-phonon interaction is important in doped Si-Ge alloys, it has been also incorporated in phonon-conductivity calculations and information has been obtained regarding the deformation potential. These calculations take into account the temperature dependence of the effective mass and the reduced Fermi level.

II. THEORY

The thermoelectric power  $Q$  is given by<sup>5</sup>

$$Q = \pm \frac{k_B}{e} \left( -\eta^* + \frac{K_2}{k_B T K_1} \right), \tag{1}$$

where  $k_B/e = 86.17 \mu\text{V/deg}$  and the reduced Fermi level  $\eta^* = E_F/k_B T$ . The different integrals  $K$  are given by<sup>5</sup>

$$K_\nu = \frac{4(k_B T)^\nu}{3m^*} \int_0^\infty N(\eta) \tau \eta^\nu \frac{\partial f_0}{\partial \eta} d\eta, \tag{2}$$

where  $\eta$  is the reduced carrier energy,  $N(\eta)$  is the density of states,  $\tau$  is the electronic relaxation time for the scattering due to phonons or ionized impurities or both, and  $f_0$  is the Fermi-Dirac distribution function.

The relaxation time due to scattering of electrons by longitudinal acoustical phonons is given by<sup>5</sup>

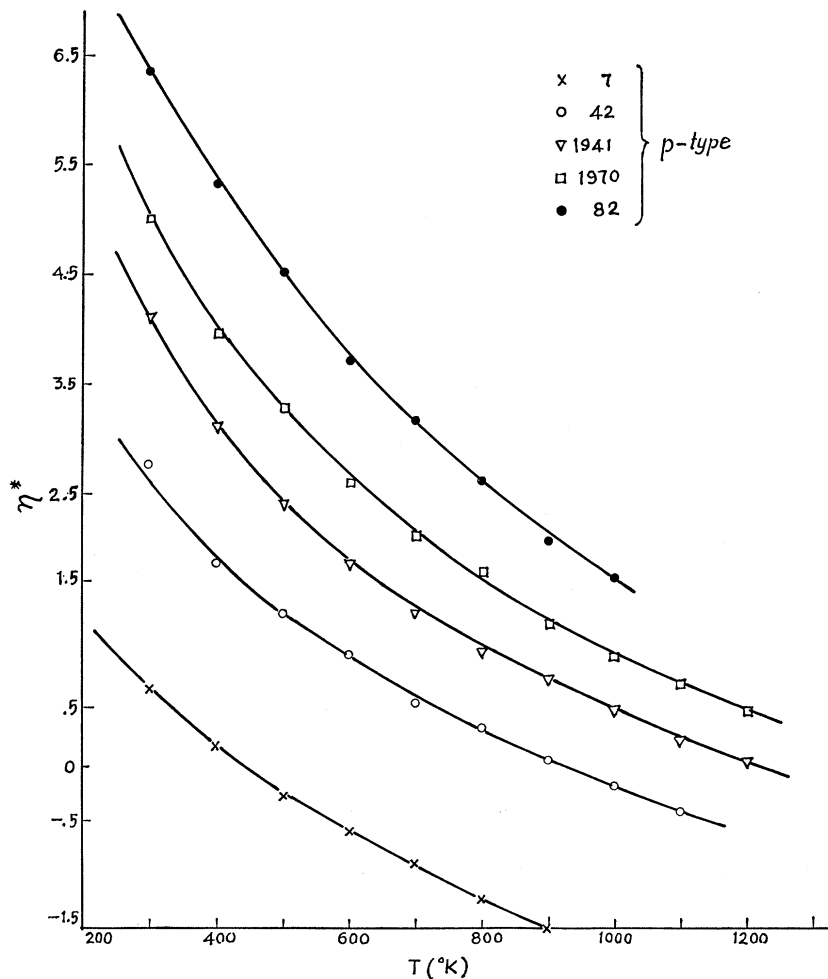
$$\tau_{ac} = A \eta^{-1/2}, \tag{3}$$

where  $A$  is the adjustable energy parameter and is given by

$$A = \frac{h^4 C_{11}}{8\pi^3 (k_B T)^{3/2} 2^{3/2} m_1^{1/2} m_t \mathcal{E}_{eff}^2}. \tag{4}$$

Here  $C_{11}$  is the longitudinal elastic constant,  $m_1$  and

FIG. 3. Temperature dependence of the reduced Fermi potential for  $p$ -type Si-Ge alloys.



<sup>4</sup> M. G. Holland, Phys. Rev. 132, 2461 (1963).

<sup>5</sup> F. J. Blatt, in Solid State Physics, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1957), Vol. 4.

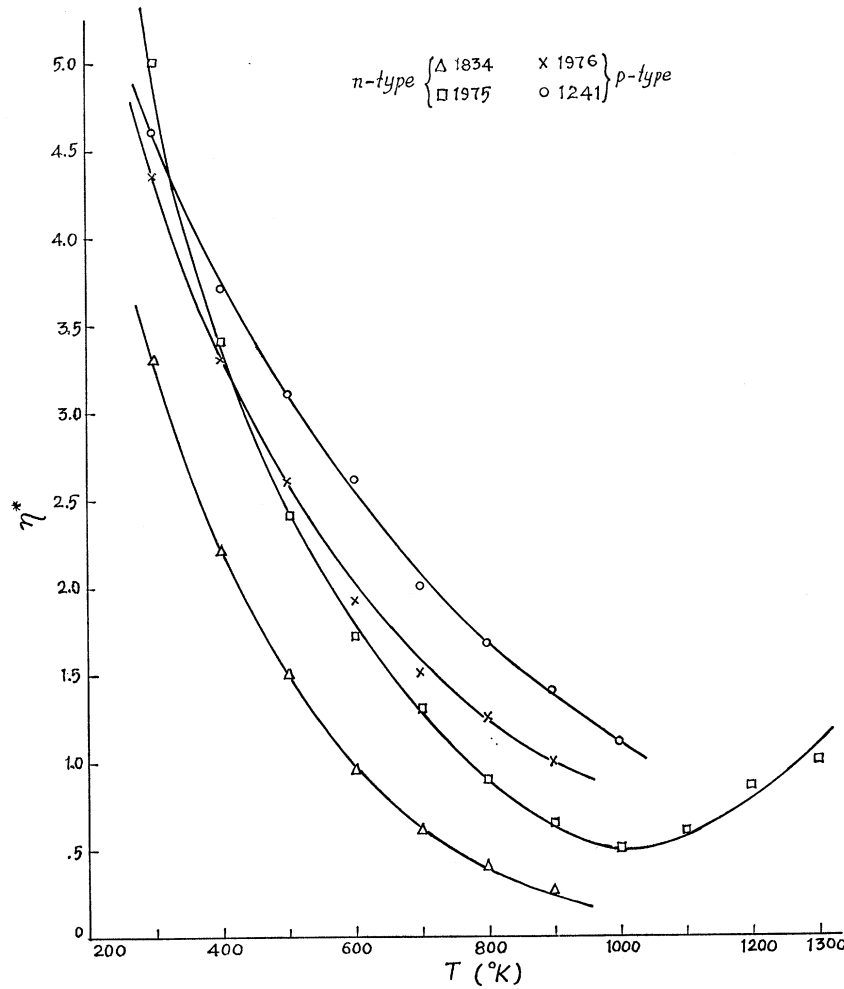


FIG. 4. Temperature dependence of the reduced Fermi potential for Si-Ge alloys.

$m_t$  are the longitudinal and transverse effective masses, and  $\mathcal{E}_{\text{off}}$  is the deformation potential.

The relaxation time due to scattering of electrons by longitudinal optical phonons for  $T \geq \Theta_1$ , where  $\Theta_1$  is the Debye temperature for longitudinal phonons, is given by<sup>6</sup>

$$\tau_{ep} = B\eta^{S(T)}, \quad (5)$$

where  $S$  varies from 0 at  $T = \Theta_1$  to 0.5 at  $T \gg \Theta_1$  and  $B$  is given by

$$B = \left(\frac{T}{\Theta_1}\right)^S \left[ \frac{v_a M (2\pi k_B \Theta_1)^{5/2}}{4\pi (2m^*)^{1/2} e^2 e^* k_B T} \right] \left[ \frac{(e^{\Theta_1/T} - 1) T}{\Theta_1} \right], \quad (6)$$

where  $v_a$  is the volume of unit cell,  $M$  is the reduced atomic mass and  $e^*$  is the effective ionic charge.

The relaxation time due to scattering of electrons by ionized impurities is given by<sup>5</sup>

$$\tau_{ii} = C\eta^{3/2}, \quad (7)$$

<sup>6</sup> H. Ehrenreich, J. Appl. Phys. Suppl. 32, 2155 (1961).

where

$$C = \frac{(2m^*)^{1/2} \epsilon^2 (k_B T)^{3/2}}{\pi N_I e^4 \alpha}. \quad (8)$$

Here  $\epsilon$  is the dielectric constant,  $N_I$  is the concentration of the ionized impurities and  $\alpha$  is given by<sup>7</sup>

$$\alpha = \ln \left[ 1 + \left( \frac{3\epsilon k_B T}{e^2 N_I^{1/3}} \right)^2 \right]. \quad (9)$$

If screening<sup>8</sup> is also taken into account, then

$$\alpha = \ln(1+b) - b/(1+b), \quad (10)$$

where

$$b = \frac{24\pi \epsilon m^* (k_B T)^2}{n e^2 \hbar^2}.$$

The thermoelectric power  $Q$ , when expressed in

<sup>7</sup> E. M. Conwell and V. F. Weisskopf, Phys. Rev. 77, 388 (1950).

<sup>8</sup> H. Brooks, Phys. Rev. 83, 879 (1951); C. Herring (unpublished).

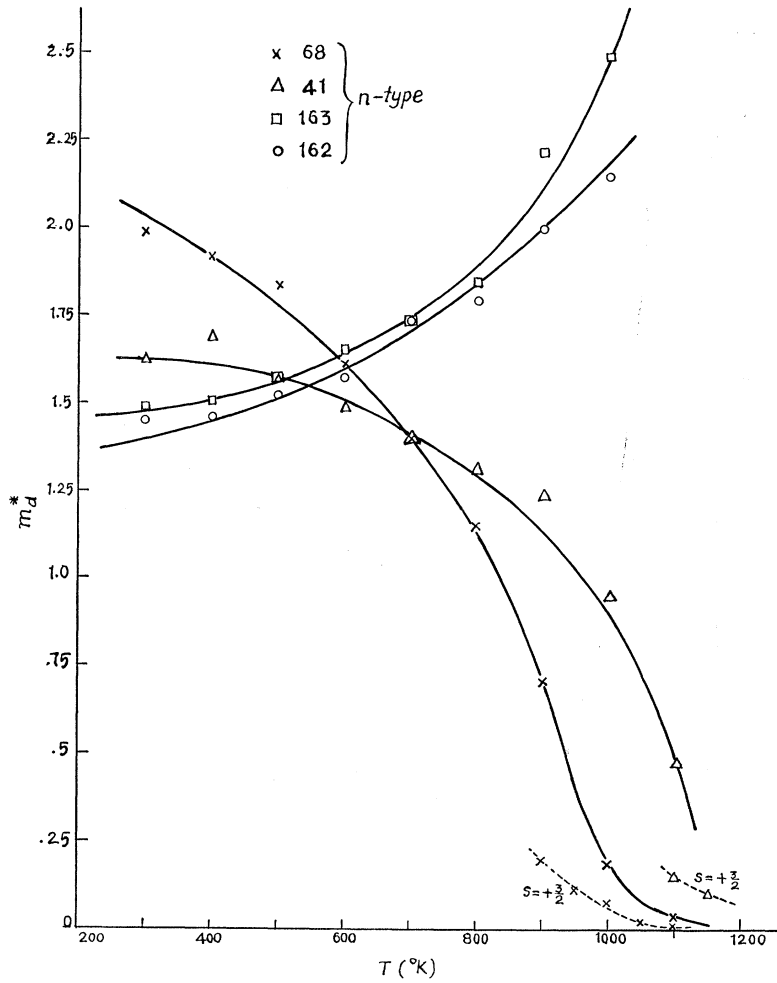


FIG. 5. Temperature dependence of the density-of-states effective mass for different samples of Si-Ge alloys (*n*-type).

terms of Fermi integrals, is given by

$$Q = \pm \frac{k_B}{e} \left[ -\eta^* + \frac{(S + \frac{5}{2})F_{S+3/2}(\eta^*)}{(S + \frac{3}{2})F_{S+1/2}(\eta^*)} \right], \quad (11)$$

where  $S = -\frac{1}{2}$  for the scattering of electrons due to longitudinal acoustic phonons,  $S = +\frac{1}{2}$  for scattering of electrons due to optical phonons for  $T \gg \Theta_1$ , and  $S = \frac{3}{2}$  for scattering of electrons due to ionized impurities. If the strength of the carriers remains constant, the nature of the scattering mechanism may be known from the temperature dependence of the conductivity mobility, which is proportional to  $\langle \tau \rangle$ .

The Fermi integrals  $F$  are given by

$$F_m(\eta^*) = \int_0^\infty \frac{\eta^m d\eta}{e^{\eta - \eta^*} + 1}. \quad (12)$$

Values of  $F_1$  and  $F_2$  for different values of  $\eta^*$  have been tabulated by Wright.<sup>9</sup>

<sup>9</sup> R. W. Wright, Proc. Phys. Soc. (London) A64, 350 (1951).

$F_3$  and  $F_4$  are tabulated in the Appendix for values of  $\eta^*$  from 0 to  $-4$ . Their values for positive  $\eta^*$  are computed as follows<sup>10</sup>:

$$F_3(+|\eta^*|) = S_3(+|\eta^*|) - F_3(-|\eta^*|), \quad (13)$$

where

$$S_3(+|\eta^*|) = \frac{1}{4}\eta^{*4} + \frac{1}{2}\pi^2\eta^{*2} + (7/60)\pi^4,$$

$$F_3(-|\eta^*|) = 3! \sum_{r=1}^\infty (-1)^{r+1} \frac{e^{-r\eta^*}}{r^4}. \quad (14)$$

Similarly

$$F_4(+|\eta^*|) = S_4(+|\eta^*|) + F_4(-|\eta^*|), \quad (15)$$

where

$$S_4(+|\eta^*|) = \frac{1}{5}\eta^{*5} + \frac{2}{3}\pi^2\eta^{*3} + (7/15)\pi^4\eta^*,$$

and

$$F_4(-|\eta^*|) = 4! \sum_{r=1}^\infty (-1)^{r+1} \frac{e^{-r\eta^*}}{r^5}. \quad (16)$$

Values of  $F_0(\eta^*)$  can be computed from  $F_0 = \ln(1 + e^{\eta^*})$ ,

<sup>10</sup> P. Rhodes, Proc. Roy. Soc. (London) 204, 396 (1951).

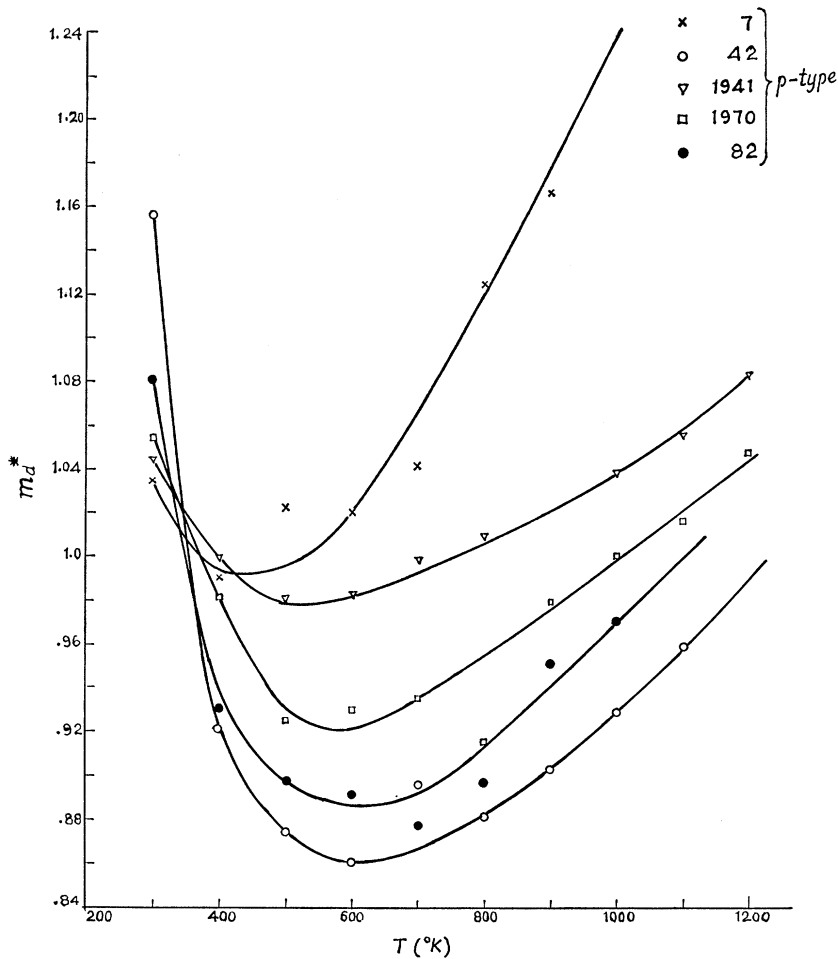


FIG. 6. Temperature dependence of the density-of-states effective mass for different samples of Si-Ge alloys (*p* type).

while values of  $F_{1/2}(\eta^*)$  for different  $\eta^*$  have been tabulated by McDougall and Stoner.<sup>11</sup>

Thus for samples where one of the scattering mechanisms discussed above is the dominant one, the values of the reduced Fermi potential at different temperatures can be obtained from the experimentally measured values of thermoelectric power at different temperatures.

The density-of-states effective mass is given by

$$m_d^* = \frac{m_d}{m_0} = \left(\frac{N}{4\pi}\right)^{2/3} \left(\frac{\hbar^2}{2m_0 k_B T}\right) [F_{1/2}(\eta^*)]^{-2/3}, \quad (17)$$

where  $N$  is the concentration of free carriers, which is known from Hall-coefficient measurements. If  $N$  remains constant with variations in temperature, this relation can be used to study the temperature dependence of the effective mass.

The electronic contribution to thermal conductivity,

$K_{el}$ , is given by<sup>12</sup>

$$K_{el} = \left(\frac{k_B}{e}\right)^2 \sigma T \left\{ \frac{A_n \sigma_n + A_p \sigma_p}{\sigma} + \frac{n p b}{(n b + p)^2} \left[ \frac{E_G^T}{k_B T} + B_n + B_p \right]^2 \right\}, \quad (18)$$

where  $\sigma$  is the electrical conductivity,  $n$  and  $p$  are the electron and hole concentrations,  $E_G^T$  is the energy gap at temperature  $T$ , and  $b$  is the mobility ratio. The coefficients  $A_{n,p}$  and  $B_{n,p}$  are given by

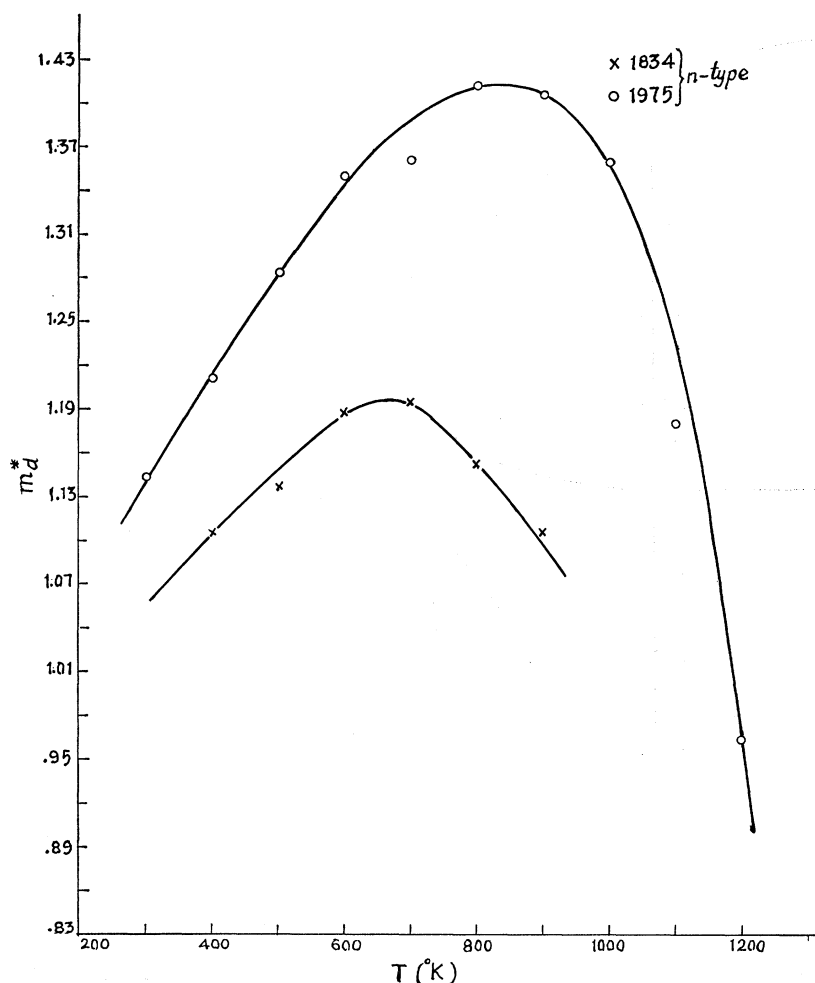
$$\begin{aligned} A_{n,p} &= (k_B T)^{-2} [(K_3/K_1) - (K_2/K_1)^2], \\ B_{n,p} &= (1/k_B T) (K_2/K_1). \end{aligned} \quad (19)$$

These coefficients can be expressed in terms of Fermi

<sup>11</sup> J. McDougall and E. C. Stoner, Phil. Trans. Roy. Soc. London **A237**, 67 (1938).

<sup>12</sup> See, e.g., J. R. Drabble and H. J. Goldsmid, *Thermal Conduction in Semiconductors* (Pergamon Press, Inc., New York, 1961), p. 117.

FIG. 7. Temperature dependence of the density-of-states effective mass for Si-Ge alloys samples 1834 and 1975 (*n* type).



integrals as follows:

$$A_{n,p} = \left[ \frac{S + \frac{7}{2} F_{S+5/2}(\eta^*)}{S + \frac{3}{2} F_{S+1/2}(\eta^*)} - \left\{ \frac{S + \frac{5}{2} F_{S+3/2}(\eta^*)}{S + \frac{3}{2} F_{S+1/2}(\eta^*)} \right\}^2 \right], \quad (20)$$

$$B_{n,p} = \frac{S + \frac{5}{2} F_{S+3/2}(\eta^*)}{S + \frac{3}{2} F_{S+1/2}(\eta^*)}. \quad (21)$$

### III. DENSITY-OF-STATES EFFECTIVE MASS

Dismukes *et al.*<sup>1</sup> have measured the thermoelectric power  $Q$ , the electrical resistivity, the Hall coefficient, and the thermal resistivity of doped Si-Ge alloys in the temperature range 300 to 1300°K. If the impurities are fully ionized and the intrinsic carrier concentration remains negligible up to the highest temperatures at which the measurements have been made, the temperature dependence of the mobilities is the inverse of that of the measured electrical resistivities. Tables I and II give the temperature dependence of the conductivity mobility for the samples mentioned there, and the value of the scattering parameter  $S$ .

In Fig. 1 are plotted the values of the thermoelectric power  $Q$  for different values of  $\eta^*$  with  $S = -\frac{1}{2}$ ,  $+\frac{1}{2}$ , and  $\frac{3}{2}$ . This graph is used to find the temperature dependence of  $\eta^*$  from the experimentally measured values of  $Q$ ; the results of calculation for different samples are shown in Figs. 2 to 4. It may be seen from these figures that in both *n*- and *p*-type samples  $\eta^*$  increases with the increase in the carrier concentrations and that  $\eta^*$  decreases rapidly with increase in temperature. In Figs. 5 to 7 is shown the temperature dependence of density-of-states effective mass. For samples 68 and 41, for which arsenic is the doping material and the concentration of carriers is low compared with other *n*-type samples, the effective mass decreases with temperature. For samples 163 and 162, phosphorus is the doping material and the carrier concentration is high; the effective mass increases with temperature. For samples 1834 and 1975, the effective mass first increases with temperature and then decreases with further increase in temperature.

For *p*-type samples 7, 42, 1941, 1970, and 82, the density-of-states effective mass first decreases very



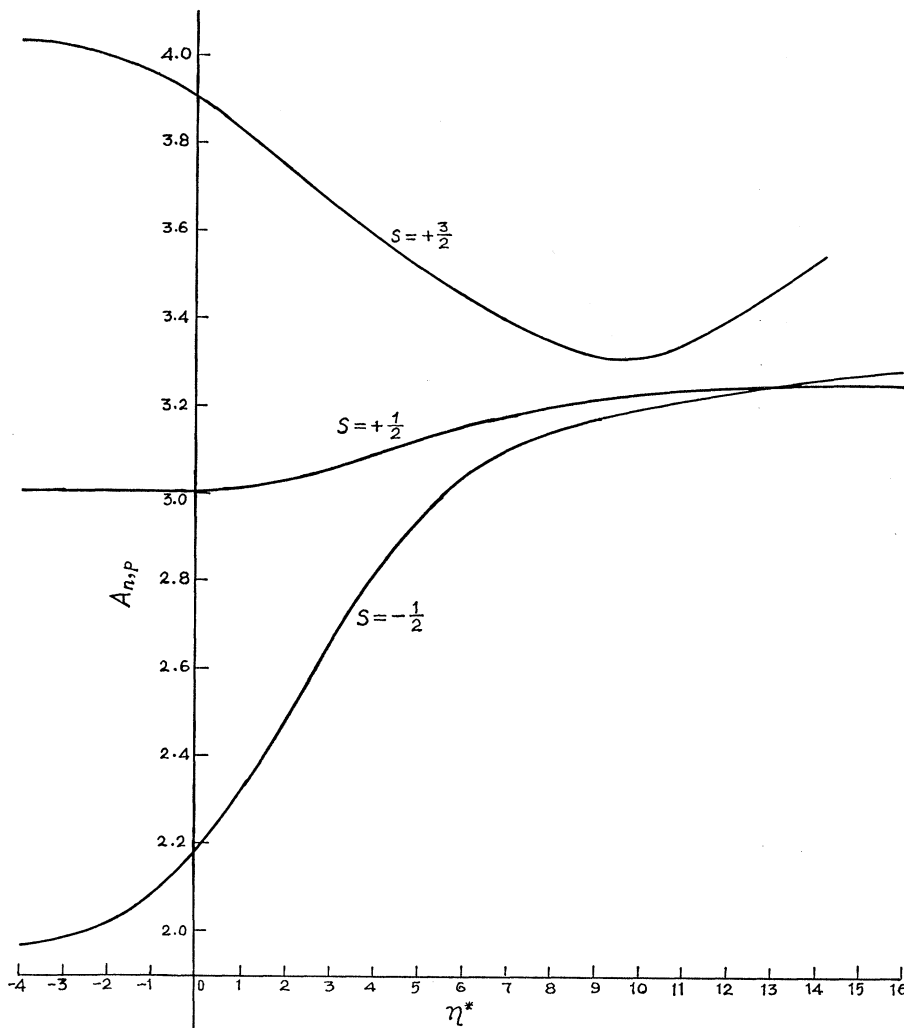


FIG. 8. Variation of the electronic thermal conductivity parameter  $A_{n,p}$  with the reduced Fermi potential  $\eta^*$  for scattering parameter  $S = -\frac{1}{2}$ ,  $+\frac{1}{2}$ , and  $+\frac{3}{2}$ .

rapidly with increasing temperature, reaches a minimum in the temperature range 400–600°K, and then increases with temperature. A comparison of samples 7, 42, 1941, and 82, which are  $p$  type and are listed in increasing order of atomic percentage of silicon as well as carrier concentration, reveals that density-of-states effective mass is decreased with the increase of the content of silicon and strength of carriers. For samples 7 and 1970, which have the same atomic percentage of silicon, the effective mass is lower for the latter sample, which has greater carrier concentration.

#### IV. ELECTRONIC THERMAL CONDUCTIVITY

The electronic contribution to thermal conductivity is calculated with the help of Eqs. (18) and (19). The parameters  $A_{n,p}$  and  $B_{n,p}$  are known from Eqs. (20) and (21). These parameters are shown as functions of  $\eta^*$  in Figs. 8 and 9. Thus one can find the values of the parameters  $A_{n,p}$  and  $B_{n,p}$  at a given temperature corre-

sponding to the reduced Fermi potential at that temperature. Using these values of  $A_{n,p}$  and  $B_{n,p}$  and the experimentally determined values of the electrical conductivity of these doped Si-Ge alloys by Dismukes *et al.*, one can determine the electronic polar and dipolar contributions to the thermal conductivity.

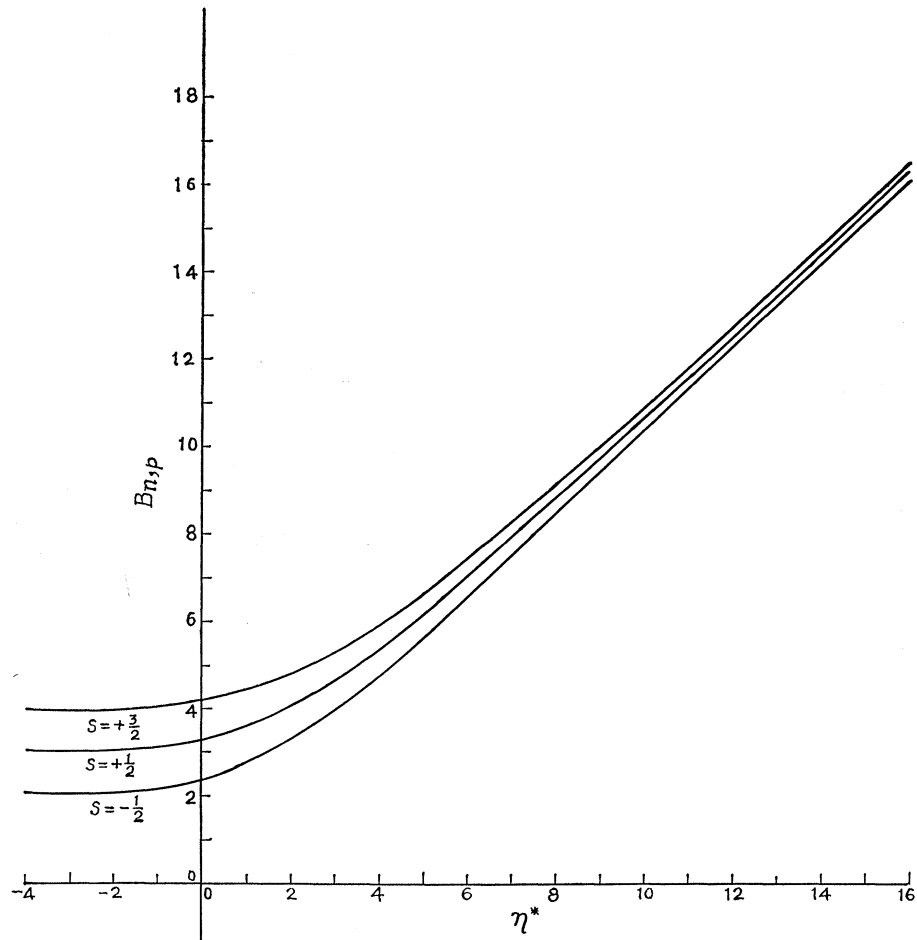
The present calculations reveal that electronic dipolar contributions also become important in the doped alloys at high temperatures. However, such a calculation requires the knowledge of both electron and hole concentrations and the energy gap at different temperatures. The energy gap at different temperatures can be calculated with the help of the following relation given by Morin and Maita<sup>13</sup>:

$$E_G(T) = 1.07 - 4.3 \times 10^{-4}T, \quad (22)$$

where  $E_G$  is given in eV. The values of the carrier con-

<sup>13</sup> F. J. Morin and J. P. Maita, Phys. Rev. 96, 28 (1954).

FIG. 9. Variation of the electronic thermal conductivity parameter  $B_{n,p}$  with the reduced Fermi potential  $\eta^*$  for scattering parameter  $S = -\frac{1}{2}$ ,  $+\frac{1}{2}$ , and  $+\frac{3}{2}$ .



centration for  $n$ -type (electrons) and  $p$ -type (holes) Si-Ge alloys are given by Dismukes *et al.* and are taken to be independent of temperature.<sup>2</sup> Using  $m_e m_h = 4.5$  for  $n$ -type alloys and  $m_e m_h = 1.56$  for  $p$ -type alloys, which is consistent with the effective-mass determinations of the majority-carrier concentrations in  $n$ - and  $p$ -type alloys, one can determine the concentration of the minority carrier for the calculations of dipolar thermal conductivity with the help of the well-known expression for the product  $np$ :

$$np = 4(2\pi k_B T / h^2)^3 (m_e m_h)^{3/2} \exp(-E_G / k_B T). \quad (23)$$

It may be seen from Eq. (18) that the dipolar contribution to thermal conductivity is proportional to  $npb / (nb + p)^2$ . At comparatively low temperatures (below 800°K) the concentrations  $n$  and  $p$  differ significantly and the term  $npb / (nb + p)^2$  is small, resulting in a low contribution to the dipolar thermal conductivity. With increase in temperature  $n$  and  $p$  tend to become equal, thus increasing the term  $npb / (nb + p)^2$ , which acquires a maximum value  $b / (1 + b)^2$  for  $n = p$ . The mobility ratio  $b$  is taken to be 1.5, as used by Steigmeier and Abeles.<sup>2</sup> The results of these calculations are shown

in Figs. 10 and 11. It may be noticed that dipolar contribution to thermal conductivity is significant only for  $n$ -type alloys at temperatures above 700°K, and is insignificant for  $p$ -type alloys. This is due to comparatively low doping in  $n$ -type samples.

## V. PHONON THERMAL CONDUCTIVITY

It has been shown by Holland, who studied the thermal conductivity of Si from 1.7 to 1300°K and Ge from 1.7 to 1000°K, that it was not possible to explain the entire temperature dependence of thermal conductivity on the basis of Callaway's formulation. In order to explain the high-temperature data it became necessary to divide the heat flow into that carried by transverse phonons and by longitudinal phonons. This approach, which requires the knowledge of the phonon vibration spectra, could explain the high-temperature as well as the low-temperature data simultaneously. In our present analysis of Si-Ge alloys we have followed this approach, which holds very well for Si or Ge. This approach was also followed for undoped Si-Ge alloys.<sup>14</sup>

<sup>14</sup> C. M. Bhandari and G. S. Verma, Phys. Rev. **138**, A288 (1965).

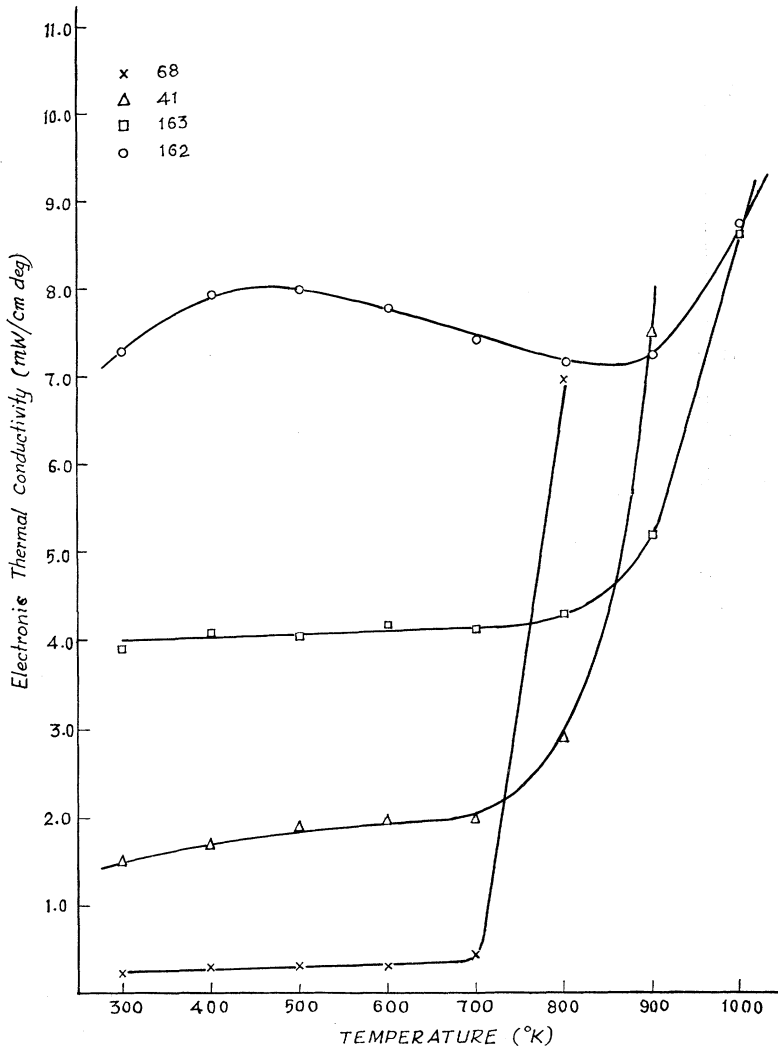


FIG. 10. Electronic thermal conductivity of  $n$ -type  $\text{Ge}_{0.3}\text{Si}_{0.7}$  alloys plotted against temperature. The electronic conductivity includes both polar and dipolar contributions.

The present analysis covers  $\text{Ge}_{0.3}\text{Si}_{0.7}$  alloys, both  $n$ - and  $p$ -type, containing different amounts of carrier concentration. The thermal conductivity of the samples under investigation has been studied by Dismukes *et al.* The present analysis incorporates the influence of the phonon-electron interaction on the phonon thermal conductivity. The phonon-electron scattering relaxation time is given by

$$\tau_{ep}^{-1} = DT \ln \frac{1 + \exp[\eta^* - N/T - PTx^2 + x/2]}{1 + \exp[\eta^* - N/T - PTx^2 - x/2]}, \quad (24)$$

where

$$D = \frac{\mathcal{E}^2 m^* k_B \delta^3}{2\pi \hbar^4 M v_1}, \quad N = \frac{m^* v_1^2}{2k_B}, \quad P = \frac{k_B}{8m^* v_1^2}.$$

Here  $\mathcal{E}$  is the electron-phonon interaction constant,  $m^*$  is the density-of-states effective mass,  $k_B$  is Boltzmann's constant,  $\delta^3$  is the atomic volume,  $M$  is the mean atomic weight,  $v_1$  is the longitudinal phonon velocity,  $\eta^* = E_F/k_B T$  where  $E_F$  is the Fermi energy, and

$$x = \frac{\hbar\omega}{k_B T}.$$

Assuming the additivity of reciprocal relaxation times and following Holland's approach of considering the separate contributions of longitudinal phonons and transverse phonons, one can express the phonon conductivity as

$$K_{ph} = K_{ph-T} + K_{ph-L} = \frac{2}{3} T^3 C_t \int_{\Theta_1/T}^{\Theta_2/T} \frac{x^2 e^x (e^x - 1)^{-2} dx}{ax^2 T^2 + b' x^2 T^2 / \sinh x} + \frac{1}{3} T^3 C_l \int_0^{\Theta_3/T} \frac{x^4 e^x (e^x - 1)^{-2} dx}{ax^4 T^4 + bx^2 T^5 + DT \ln X(\eta^*, N, P, T; x)},$$

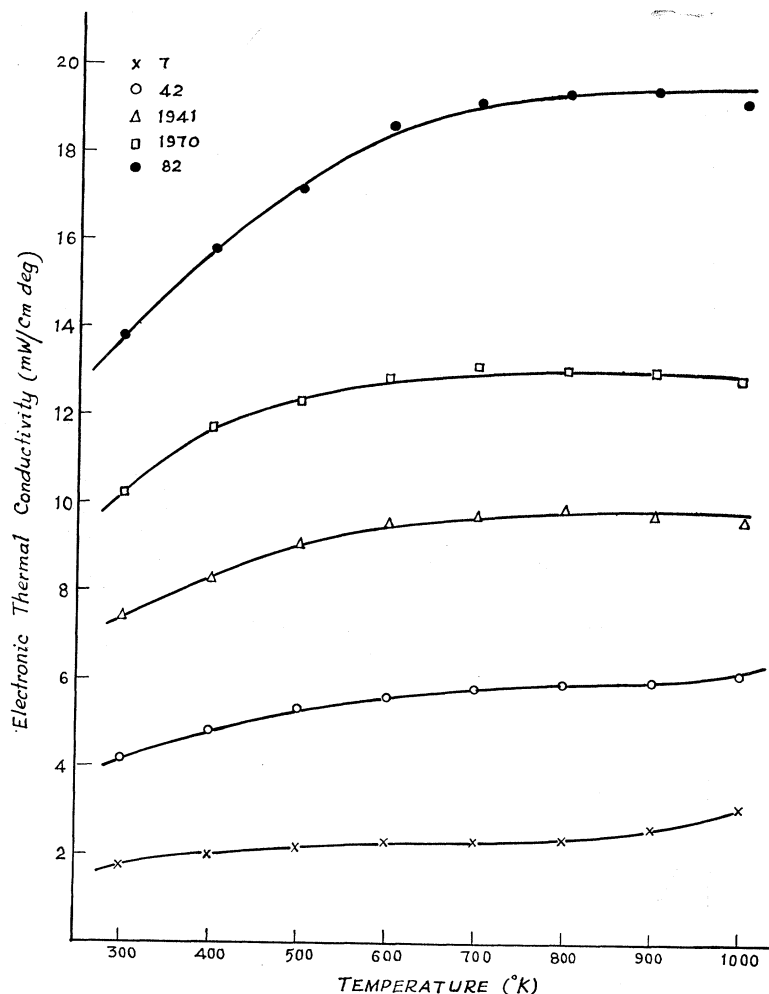


FIG. 11. Electronic thermal conductivity of *p*-type  $\text{Ge}_{0.3}\text{Si}_{0.7}$  alloys versus temperature.

where

$$X(\eta^*, N, P, T; x) = \frac{1 + e^{\eta^* - N/T - PTx^2 + x/2}}{1 + e^{\eta^* - N/T - PTx^2 - x/2}}; \quad (25)$$

$$C_i = \frac{k_B}{2\pi^2 v_i} \left( \frac{k_B}{\hbar} \right)^3, \quad i=1, t; \quad a = A \left( \frac{k_B}{\hbar} \right)^4; \quad b' = B_{tu} \left( \frac{k_B}{\hbar} \right)^2; \quad b = B_1 \left( \frac{k_B}{\hbar} \right)^2;$$

and the other symbols have been explained in Ref. 14.

For calculating the integrals corresponding to the contribution due to longitudinal phonons, the temperature dependence of  $m^*$  and  $\eta^*$  is taken into account. By plotting  $\tau_{ep}x^2$  versus  $x$  (see Fig. 12) it can be shown that phonon-electron scattering is strongly dependent upon frequency, and that the low-frequency phonons are scattered most effectively. As the contribution of transverse phonons involves phonons of frequencies which are close to zone-boundary frequencies for the transverse-phonon branch, the influence of electron-phonon scattering on conductivity due to transverse phonons is negligible. At high temperatures the lower

limit of the integral for the transverse phonons is lowered, but at such temperatures the dominant scattering processes are phonon-phonon scattering and the scattering of phonons by impurities.

Values of the parameters needed in the analysis of the phonon conductivity, which is obtained by subtracting the electronic thermal conductivity from the experimentally measured thermal conductivity, are given in Table III. The procedure for calculating the phonon conductivity is outlined in Ref. 14. The results of calculations are shown in Figs. 13 and 14, where good agreement between theory and experiment is found. However, there is a slight systematic deviation

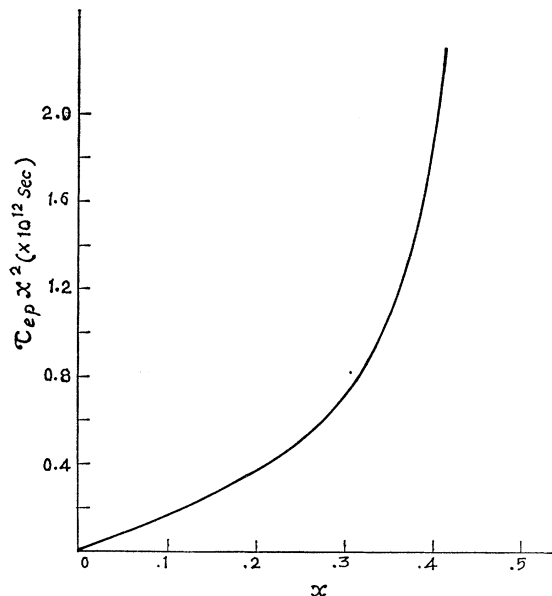


FIG. 12.  $\tau_{ep} x^2$  versus  $x$ , where  $\tau_{ep}$  is the electron-phonon relaxation time and  $x = \hbar\omega/k_B T$ . The curve refers to  $T = 500^\circ\text{K}$ ,  $D = 13.2 \times 10^8 \text{ sec}^{-1} \text{ deg}^{-1}$ ,  $P = 0.03926 \text{ deg}^{-1}$ ,  $N = 1.592 \text{ deg}$  and  $\eta^* = +2.4$ .

TABLE III. Parameters used in the analysis of thermal conductivity data of doped Si-Ge alloys.

$a = 250 \text{ sec}^{-1} \text{ deg}^{-4}$
$b' = 0.1 \times 10^6 \text{ sec}^{-1} \text{ deg}^{-2}$
$b = 0.04 \text{ sec}^{-1} \text{ deg}^{-5}$
$V_1 = 7.017 \times 10^5 \text{ cm/sec}$
$V_2 = 4.841 \times 10^5 \text{ cm/sec}$
$V_3 = 1.652 \times 10^5 \text{ cm/sec}$
$M = 41.44$
$a = 5.488 \times 10^{-8} \text{ cm}$
$\rho = 3.24 \text{ gm cm}^{-3}$
$Q_1 = 124^\circ\text{K}$
$Q_2 = 145^\circ\text{K}$
$Q_3 = 508^\circ\text{K}$

at high temperatures, and it may be due to the approximate estimate of electronic thermal conductivity. The variation in the thermal conductivity of Si-Ge alloys with doping is explained by the variation in the deformation potential, whose measure is the parameter  $D$ , which is proportional to the square of the deformation potential. The information regarding the deformation potential, which has been obtained in the present,

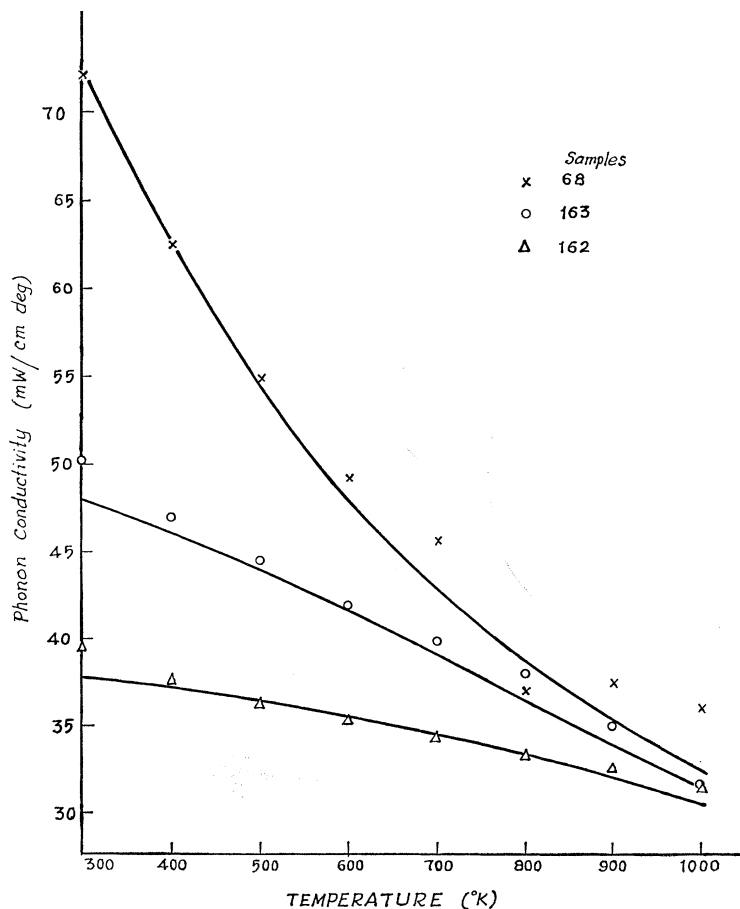
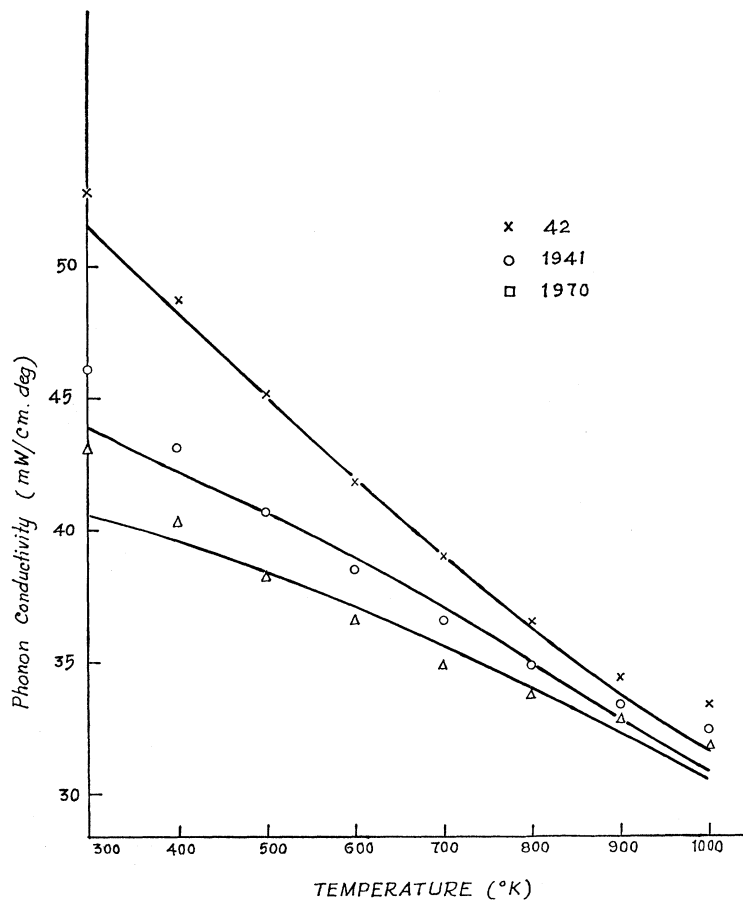


FIG. 13. The phonon thermal conductivity of  $n$ -type  $\text{Ge}_{0.3}\text{Si}_{0.7}$  alloys versus temperature. Solid lines represent theoretical curves. Points represent the experimental thermal conductivity minus the electronic contribution to the thermal conductivity.

FIG. 14. Phonon thermal conductivity of *p*-type  $\text{Ge}_{0.3}\text{Si}_{0.7}$  alloys versus temperature.



analysis of thermal-conductivity data, refers to the dilatation deformation potential corresponding to longitudinal-mode scattering. Values of the deformation potential for *n*- and *p*-type Si-Ge alloys with different amounts of doping are given in Table IV. It may be

TABLE IV. Deformation potential as obtained from the analysis of the thermal conductivity of different samples of Si-Ge alloys.

	Sample					
	42	1941	1970	68 <sup>a</sup>	163	162
$D \times 10^{-8}$	5.0	132	24.0	...	12.6	83.0
$\epsilon$ (eV)	6.4	9.3	12.98	...	2.34	6.17

<sup>a</sup> The electron-phonon interaction term is negligible compared with other scattering terms.

noted from this table that the deformation potential increases with the increase in carrier concentration.

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#### APPENDIX

TABLE V. Fermi integrals  $F_3$  and  $F_4$ .

$\eta^*$	$F_3(\eta^*)$	$F_4(\eta^*)$
1	14.3894	60.9684
2	34.2984	153.1895
3	74.8299	363.7653
4	154.2115	808.1692
5	290.9440	1674.8492
6	512.9455	3249.0045
7	853.3046	5936.6241
8	1351.1581	10286.2679
9	2051.2093	17014.9203
10	3004.7597	27034.5759
11	4268.61	41468.2325
12	5905.96	61681.8900
13	7985.51	89299.5475
14	10582.56	126251.2050
15	13777.61	174756.8625
16	17658.36	237392.5200