Scattering of Phonons by Electrons in Germanium-Silicon Alloys*

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The theory developed by Ziman for the scattering of phonons by electrons is extended to high temperatures using the formalism of Klemens and Callaway. The theory is applied to the experimental results recently published by Dismukes *et al.* on the effect of doping on the thermal conductivity of Ge-Si alloys. After subtracting the electronic contribution from the measured thermal conductivity, the resulting lattice conductivity is analyzed. In describing the effect of doping, the deformation potential is the only free parameter; its value is adjusted for each sample to obtain agreement with the experimental data at 500°K, which is close to the Debye temperature. The theory then predicts the correct temperature dependence of the lattice thermal conductivity. The deformation potentials, derived in this manner, are found to be higher for *n*-type than for *p*-type material, and to increase with carrier concentration. For lightly doped *p*-type and *n*-type material, values of 1.2 and 1.6 eV were obtained, respectively, which compare well with the available literature data.

I. INTRODUCTION

THE high-temperature lattice thermal conductivity of *undoped* Ge-Si alloys has been studied recently both experimentally and theoretically by Abeles *et al.*,[1] Abeles,[2] and Parrott.[3] It was possible to explain the experimental results with the simple phenomenological model developed by Klemens[4] and Callaway[5] by including the contribution of normal processes to the thermal resistance as suggested by Klemens.[6]

This investigation is concerned with the effects of *doping* on the lattice thermal conductivity of Ge-Si alloys at high temperatures. It is known that the addition of donor and acceptor impurities decreases the lattice thermal conductivity of semiconductors.[7-10] It was assumed[7,8] that this is the result of the scattering of phonons by point defects, and it was believed, according to Stratton,[11] that the effect of phonon scattering by the conduction electrons is negligible. Beers *et al.*[9] pointed out that the theory of Stratton is in error due to incorrect combination of the relaxation times. They attributed the observed change in the

lattice thermal conductivity of germanium with doping to phonon-electron scattering. Experimental evidence exists[12] that it is the free charge carriers rather than the ionized impurities which are responsible for the observed decrease in the lattice thermal conductivity of Ge-Si alloys.

Ziman[13] developed a theory of scattering of phonons by electrons at low temperatures. It is the purpose of this paper to extend this theory to high temperatures using the formalism of Klemens and Callaway. This theory is then applied to the experimental results recently published by Dismukes *et al.*[14] on doped Ge-Si alloys. Disordered alloys are of particular interest in this respect because, unlike the situation in elemental[9] or compound semiconductors,[10] the additional point defect scattering introduced by the doping is negligible. Any change in thermal conductivity can therefore be attributed to an interaction of phonons with free charge carriers. It is shown in this paper that this effect quantitatively accounts for the observed decrease in lattice thermal conductivity of Ge-Si alloys with doping.

II. LATTICE THERMAL CONDUCTIVITY OF DEGENERATE SEMICONDUCTORS AT HIGH TEMPERATURES

This treatment applies to semiconductor alloys containing added doping impurities. It is based on an isotropic Debye model for the lattice waves. The contribution of the optical modes to the thermal resistivity[10] is neglected. The assumption is made that the lattice disorder due to alloying can be described by point defect scattering. The following scattering mechanisms are assumed to contribute to the thermal resistivity:

1. Phonon-Phonon Scattering

Only 3-phonon scattering is considered here. We assume that normal (N) and umklapp (U) processes can be characterized by the relaxation times τ_N and τ_U

[1] B. Abeles, D. S. Beers, G. D. Cody, and J. P. Dismukes, Phys. Rev. 125, 44 (1962).

[2] B. Abeles, Phys. Rev. 131, 1906 (1963).

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[4] P. G. Klemens, Proc. Phys. Soc. (London) A208, 108 (1951); A68, 1113 (1955); in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1958), Vol. 7, p. 1; Phys. Rev. 119, 507 (1960).

[5] J. Callaway, Phys. Rev. 113, 1046 (1959), J. Callaway and H. C. von Bayer, *ibid.* 120, 1149 (1960).

[6] P. G. Klemens, G. K. White, and R. J. Tainsh, Phil. Mag. 7, 1323 (1962).

[7] H. J. Goldsmid, Proc. Phys. Soc. (London) A72, 17 (1958).

[8] A. D. Stuckes, Phil. Mag. 5, 84 (1960).

[9] D. S. Beers, G. D. Cody, and B. Abeles, *Proceedings of the International Conference on the Physics of Semiconductors, Exeter* (The Institute of Physics and the Physical Society, London, 1962), p. 41.

[10] E. F. Steigmeier and I. Kudman, Phys. Rev. 132, 508 (1963).

[11] R. Stratton, Phil. Mag. 2, 422 (1957).

[12] B. Abeles and R. Cohen, J. Appl. Phys. 35, 247 (1964).

[13] J. M. Ziman, Phil. Mag. 1, 191 (1956); 2, 292 (1957).

[14] J. P. Dismukes, L. Ekstrom, E. F. Steigmeier, I. Kudman, and D. S. Beers J. Appl. Phys. (to be published).

given by[4,5,15]

$$\tau_N^{-1} = B_1\omega^2, \tag{1}$$

and

$$\tau_U^{-1} = B_2\omega^2, \tag{2}$$

where ω is the phonon frequency and B_1 and B_2 are independent of ω, but functions of temperature. The ratio of N to U processes,

$$\beta = B_1/B_2, \tag{3}$$

is assumed to be temperature-independent. A justification for the use of Eqs. (1) and (2) is given in Sec. IV.

2. Point-Defect Scattering

The relaxation time τ_{PD} for point-defect scattering due to lattice disorder in alloys is given by[4]

$$\tau_{PD}^{-1} = (\delta^3\Gamma/4\pi v^3)\omega^4, \tag{4}$$

where δ is the cube root of the atomic volume. The sound velocity v is assumed to be given by the Debye expression

$$v = (k/\hbar)(6\pi^2)^{-1/3}\Theta\delta, \tag{5}$$

where Θ is the Debye temperature. The disorder parameter Γ, modified[2] for an alloy of two kinds of atoms, differing in mass and atomic volume, is

$$\Gamma = y(1-y)[(\Delta M/M)^2 + \epsilon(\Delta\delta/\delta)^2], \tag{6}$$

where

$$\Delta M = M_{Si} - M_{Ge}, \tag{7}$$

$$\Delta\delta = \delta_{Si} - \delta_{Ge}, \tag{8}$$

and

$$M = yM_{Si} + (1-y)M_{Ge}. \tag{9}$$

Here y is the fraction of silicon content, M is the mean atomic weight, and ϵ is[2] a number of the order 40.

3. Phonon-Electron Scattering

Ziman[13] derived the following expression for the phonon relaxation time τ_{EP} due to phonon-electron interaction with the electrons in a parabolic band:

$$\tau_{EP}^{-1} = \frac{\mathcal{E}^2 m^{*3} v}{4\pi\hbar^4 d}\left\{\frac{kT}{\frac{1}{2}m^*v^2}\right\}\left\{\frac{\hbar\omega}{kT} - \ln\frac{1+\exp[(\frac{1}{2}m^*v^2 - E_F)/kT + \hbar^2\omega^2/8m^*v^2kT + \hbar\omega/2kT]}{1+\exp[(\frac{1}{2}m^*v^2 - E_F)/kT + \hbar^2\omega^2/8m^*v^2kT - \hbar\omega/kT]}\right\}, \tag{10}$$

where $\mathcal{E}$ is the electron-phonon interaction constant or deformation potential, m^* is the density-of-states effective mass, d is the density, and E_F is the Fermi energy. The question as to whether the shear or dilatational deformation potentials or combination of both are to be used will be discussed in Sec. IV. This relaxation time τ_{EP} describes the *intra*valley scattering.

It should be noted that in addition to the *intra*valley scattering, described by Eq. (10), there is also an *inter*valley interaction between electrons and phonons. Experimental evidence exists,[16] however, that *intra*valley scattering is dominant. This is particularly valid for alloys since *inter*valley scattering involves phonons with large wave numbers and these phonons are already efficiently scattered by point defects.

Also, it is known[16–19] that doping changes the elastic properties, and therefore changes the Debye temperature of a solid if measured at ultrasonic frequencies up to 10^8 sec^{-1}. This effect originates in the change of the Fermi level with strain due to the shift of a band or valley with respect to one another. For thermal phonons in silicon ($\omega \approx 4 \times 10^{13}$ sec^{-1}) the condition $\omega\tau_{el} \gg 1$ prevails, since the intervalley electron scattering relaxation

time τ_{el} is 2×10^{-12} sec for p-type silicon,[16] and only slightly lower for n-type germanium.[16] Therefore, it is not possible to establish equilibrium in the electron population of the valleys, and the effect of doping on the elastic constants is greatly reduced for the case considered here. Since the effect is small even at ultrasonic frequencies, it is completely neglected in this work, and the Debye temperature is assumed to be independent of the carrier concentration. Evidence for this is given by Dolling[20] from the measurement of the lattice spectrum of silicon, which is affected less than 1% by adding 3×10^{19} n-type carriers cm^{-3} pure silicon.

The relaxation times given above are combined in the usual manner.

$$\tau_C^{-1} = \tau_N^{-1} + \tau_U^{-1} + \tau_{PD}^{-1} + \tau_{EP}^{-1}. \tag{11}$$

The formalism of Callaway[5] is used to calculate the lattice thermal conductivity κ_l (in cgs units).

$$\kappa_l = 4.67 \times 10^{-2}(\Theta^2/\delta)\{I_1 + I_2^2/I_3\}, \tag{12}$$

where

$$I_1 = \int_0^1 \tau_C x^2 \frac{\alpha^2 x^2 e^{\alpha x}}{(e^{\alpha x}-1)^2}dx, \tag{13}$$

$$I_2 = \beta\int_0^1 \frac{\tau_C}{\tau_U}x^2 \frac{\alpha^2 x^2 e^{\alpha x}}{(e^{\alpha x}-1)^2}dx, \tag{14}$$

and

$$I_3 = \beta\int_0^1 \frac{1}{\tau_U}\left(1 - \frac{\beta\tau_C}{\tau_U}\right)x^2\frac{\alpha^2 x^2 e^{\alpha x}}{(e^{\alpha x}-1)^2}dx. \tag{15}$$

[15] C. Herring, Phys. Rev. 95, 954 (1954).

[16] W. P. Mason and T. B. Bateman, Phys. Rev. Letters 10, 151 (1963).

[17] W. R. Keyes, IBM J. Res. Develop. 5, 266 (1961); L. J. Brunner and R. W. Keyes, Phys. Rev. Letters 7, 55 (1961); C. A. Bryant and P. H. Keesom, Phys. Rev. 124, 698 (1961).

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[20] G. Dolling, Bull. Am. Phys. Soc. 8, 194 (1963).

TABLE I. Properties of Ge-Si alloys used in this investigation.

Speci-men	Composition (at. % Si)	Impurity	Carrier concentration (cm^{-3})	Debye temp. (°K)	Reduced Fermi level at 500°K	κ_{total} (W/cm deg) at 500°K	κ_{el} (W/cm deg) at 500°K	κ_l (W/cm deg) at 500°K	Deformation potential (eV)
68	73.8	As	2.2×10^{18}	532	−3.88	0.055	0.0003	0.055	...
41	66.8	As	2.3×10^{19}	510	−1.41	0.052	0.002	0.050	1.6
163	70.2	P	6.7×10^{19}	521	−0.16	0.048	0.004	0.044	2.8
162	71.3	P	1.5×10^{20}	524	0.96	0.044	0.008	0.036	4.4
1834	79.5	P	1.4×10^{20}	553	0.99	0.046	0.007	0.039	4.9
1975	86.8	P	2.7×10^{20}	581	2.30	0.050	0.011	0.039	6.7
7	72.0	B	3.4×10^{19}	527	0.28	0.053	0.002	0.051	1.3
42	69.3	B	8.9×10^{19}	518	1.15	0.050	0.004	0.046	1.8
1941	71.7	B	1.8×10^{20}	526	2.51	0.050	0.008	0.042	2.5
1970	72.0	B	2.4×10^{20}	527	3.02	0.051	0.011	0.040	2.8
82	71.0	B	3.5×10^{20}	524	4.01	0.053	0.015	0.038	3.1

Here $\alpha=\Theta/T$ and $x=\omega/\omega_D$, where ω_D is the Debye frequency. The contribution of the second term in Eq. (12) to κ_l in alloys is of the order of a few percent.

The relaxation time τ_U contains the parameter B_2 which must be determined. Leibfried and Schloemann[21] used the variational method to calculate the lattice thermal conductivity for 3-phonon processes at high temperatures and obtained (see Ref. 10 for the modification of their formula by a factor 4)

$$\kappa_l=\frac{3}{5}\,4^{1/3}\left(\frac{k}{\hbar}\right)^3\frac{M\delta\Theta^3}{N\gamma^2 T},\qquad(16)$$

where N is Avogadro's number and γ is the anharmonicity parameter. A similar formula, different only in the numerical factor, was derived by Dugdale and McDonald[22] from a dimensional argument.

The parameter B_2 in Eq. (2) can be expressed[2] in terms of the anharmonicity parameter γ by assuming that the lattice thermal resistivity caused by pure 3-phonon scattering is the same as derived by Leibfried and Schloemann. After inserting numerical values for the physical constants in Eqs. (1), (2), (4), and (10), and using the reduced temperature α and the reduced frequency x, the following expressions result for the relaxation times (in cgs units):

$$\tau_N^{-1}=\beta\tau_U^{-1},\qquad(17)$$

$$\tau_U^{-1}=3.264\times10^{-2}\left[\frac{1+(5/9)\beta}{1+\beta}\right]\frac{\gamma^2}{M\delta^2\alpha}x^2,\qquad(18)$$

$$\tau_{PD}^{-1}=6.17\times10^{11}\Theta\Gamma x^4,\qquad(19)$$

and

$$\tau_{EP}^{-1}=\lambda\frac{A\mathcal{E}^2}{\alpha}\ln\left\{\frac{1+e^{-\alpha y+\eta-D\alpha x^2+\frac{1}{2}\alpha x}}{1+e^{-\alpha y+\eta-D\alpha x^2-\frac{1}{2}\alpha x}}\right\},\qquad(20)$$

where

$$A=6.76\times10^{26}(m^*/m)^2\delta^2/M,\qquad(21)$$

$$y=3.72\times10^9(m^*/m)\delta^2\Theta,\qquad(22)$$

$$D=1.68\times10^{-11}/(m^*/m)\delta^2\Theta,\qquad(23)$$

where λ denotes the number of valleys and η the reduced Fermi energy.

III. Ge-Si ALLOYS

Dismukes et al.[14] measured the thermal resistivity $1/\kappa$, the absolute Seebeck coefficient Q and the electrical resistivity ρ between 300 and 1300°K of a number of p- and n-type Ge-Si alloys of different composition as a function of doping. The analysis of these thermal conductivity data in terms of phonon-electron scattering is presented in this paper. Table I summarizes the pertinent properties of the specimens investigated. The carrier concentration listed is defined as $n=1/eR_H$, where R_H is the Hall coefficient. The Debye temperatures Θ were computed from the elastic constants. For further details the reader is referred to Ref. 14.

In order to compare the theory given above with the experimental data, first the electronic contribution has to be subtracted from the total measured thermal conductivity. The electronic thermal conductivity κ_{el} of a semiconductor is given by the expression[23]

$$\kappa_{el}=\left(\frac{k}{e}\right)^2\sigma T\left\{\frac{A_n\sigma_n+A_p\sigma_p}{\sigma}+\frac{npb}{(nb+p)^2}\left[\frac{E_g T}{kT}+B_n+B_p\right]^2\right\},\qquad(24)$$

where σ is the electrical conductivity, n and p are the electron and hole concentrations, respectively, b the mobility ratio, and $E_g{}^T$ the band gap at the temperature T. The numbers $A_{n,p}$ and $B_{n,p}$ are determined by the

[21] G. Leibfried and E. Schloemann, Nachr. Akad. Wiss. Göttingen, II Math.-Physik Kl. 4, 71 (1954).

[22] J. S. Dugdale and D. K. C. MacDonald, Phys. Rev. 98, 1751 (1955).

[23] See, e.g., J. R. Drabble and H. J. Goldsmid, Thermal Conduction in Semiconductors (Pergamon Press, Inc., New York, 1961), p. 117.

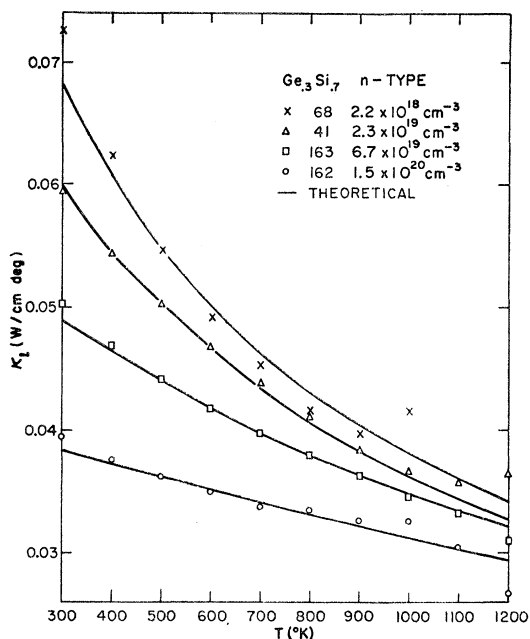FIG. 1. Experimental and theoretical values of the lattice thermal conductivity of n-type $Ge_{0.3}Si_{0.7}$ alloys as a function of the absolute temperature and carrier concentration. The theoretical curves were fitted at 500°K ($\approx\Theta$); this determines the deformation potentials $|\mathcal{E}|$.

scattering mechanism described by a parameter q and the reduced Fermi level η. The quantities q and η were calculated by Amith[24] for the Ge-Si alloys samples given in Table I, from the room-temperature Hall coefficient and the absolute Seebeck coefficient $Q(T)$. By means of the tables of Amith, the Lorenz numbers, $A_{n,p}$ and $B_{n,p}$, were then determined and the electronic thermal conductivity computed using Eq. (24).

The energy band gap was assumed to be (in eV)

$$E_g{}^T = 1.07 - 4.3 \times 10^{-4} T.$$

for $Ge_{0.3}$ and $Li_{0.7}$ alloys.

This was derived from the results of Braunstein et al.[25] at 296°K, using the same temperature coefficient for the band gap as found for pure silicon by Morin and Maita.[26] The density-of-states effective masses m^* were taken from Busch and Vogt[27]; $m_p{}^* = 1.0m$ was used for the holes and $m_n{}^* = 0.427m$ for the one-valley effective mass of the electrons of $Ge_{0.3}Si_{0.7}$. The mobility ratio $b = 1.5$ was assumed; this is the ratio of the electron mobility in n-type to the hole mobility in p-type Ge-Si.[14]

The values calculated for the electronic thermal conductivity are given in Table I. The experimental points in Figs. 1, 2, and 3 represent the resulting lattice

[24] A. Amith, International Conference on the Physics of Semiconductors, Paris, 1964 (to be published).
[25] R. Braunstein, A. R. Moore, and F. Herman, Phys. Rev. 109, 695 (1958).
[26] F. J. Morin and J. P. Maita, Phys. Rev. 96, 28 (1954).
[27] G. Busch and O. Vogt, Helv. Phys. Acta 33, 889 (1960).

thermal conductivity which is analyzed in the following manner:

Abeles[2] has demonstrated that it is possible to describe the experimental results for *undoped* Ge-Si alloys by means of the phenomenological Eqs. (12) to (19) over the whole system and at all temperatures by adjusting the two parameters β and γ. This step is repeated in this work, since the assumptions[14] on the specific heat at high temperatures had brought about some changes in the experimental data used by Abeles. Moreover, it was decided to fit these parameters at the Debye temperature of the materials rather than at room temperature. The anharmonicity parameter γ was fitted to the experimental results for unalloyed silicon[9] and germanium[9] at their Debye temperatures of 648 and 374°K, respectively; the isotope scattering was taken into account. For both silicon and germanium, a value of $\gamma = 0.91$ was obtained (Abeles had used $\gamma = 0.89$ or, in his notation, $\gamma_1 = 1.77$). Adjusting the parameter β to undoped material is difficult because the true lattice thermal conductivity of an undoped sample is not measurable. A sample with a carrier concentration of 10^{16} to 10^{17} cm^{-3} (e.g., D 171 of Ref. 9) is partially transparent for blackbody radiation and, therefore, exhibits a photon effect.[9] The thermal conductivity of a sample with 2.2×10^{18} cm^{-3} (e.g., sample 68) is already lowered by the doping effect. Therefore, the parameter β was adjusted at 500°K (which is close to the Debye temperature of $Ge_{0.3}Si_{0.7}$), so that $\kappa_l = 0.056$ W/cm deg. This value is slightly higher than that measured on sample 68 by the estimated amount of the doping effect.
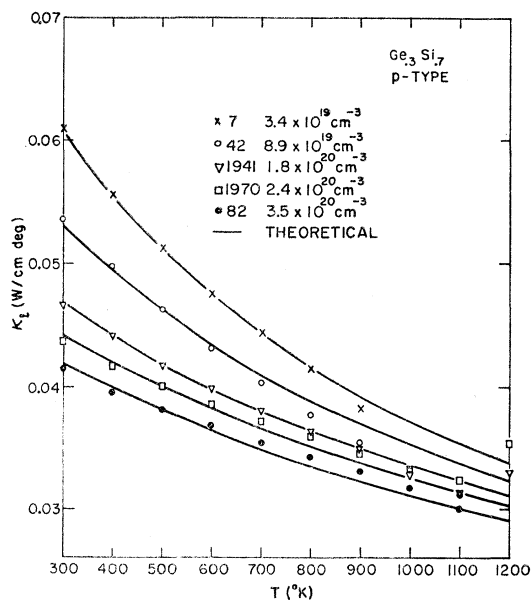

FIG. 2. Experimental and theoretical values of the lattice thermal conductivity of p-type $Ge_{0.3}Si_{0.7}$ alloys as a function of the absolute temperature and carrier concentration. The theoretical curves were fitted at 500°K ($\approx\Theta$); this determines the deformation potentials $|\mathcal{E}|$.

For the strain term in the expression (6) for the disorder parameter the value $\epsilon = 39$ was used, which was estimated[2] for the Ge-Si alloys assuming the impurity model of Klemens. This strain term, however, contributes less than 7% to the disorder parameter. The value resulting for the ratio of N to U processes is $\beta = 2.0$ (Abeles had used $\beta = 2.5$).

Based on these values of the parameters γ and β which describe the undoped material, we have computed the theoretical lattice thermal conductivity values for the *doped* Ge-Si alloys by using Eqs. (12) to (23). The calculations were based on a one-band model, using the density-of-states effective masses given above. The multivalley structure of the conduction band was taken into account by using $\lambda = 6$ for n-type material. The values[24] of the reduced Fermi level η used here are those used for calculating the electronic thermal conductivity. Figures 1 and 2 show the resulting theoretical curves, which were evaluated by means of a computer, for different samples of p- and n-type $Ge_{0.3}Si_{0.7}$. Figure 3 shows the same for n-type $Ge_{0.2}Si_{0.8}$ and $Ge_{0.15}Si_{0.85}$. The curves were fitted at 500°K ($\approx \Theta$) to the experimental value of each sample by adjusting the deformation potential $|\mathcal{E}|$. As is seen in Figs. 1, 2, and 3, the theoretical curves exhibit the correct temperature dependence of the lattice thermal conductivity. The small deviations for the lightly doped specimens at very high temperatures are probably due to the errors in calculating the large bipolar contribution to the electronic thermal conductivity [Eq. (24)]; it is very likely that
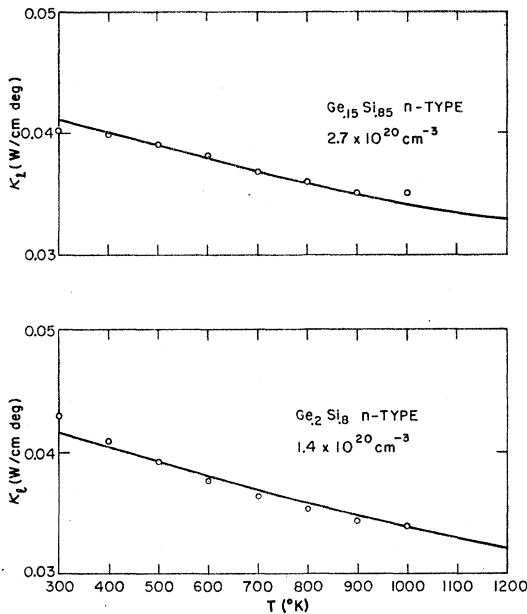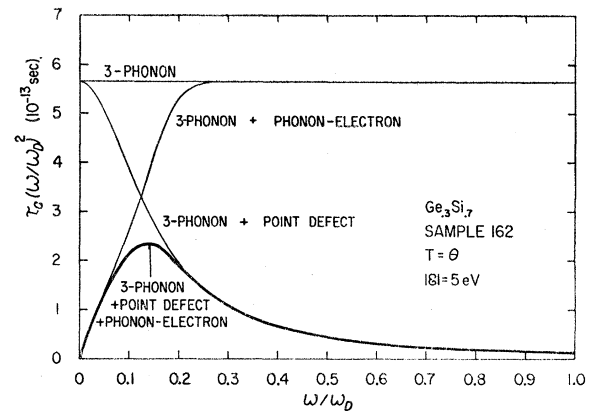

FIG. 4. The quantity $\tau_C x^2$ which determines the lattice thermal conductivity [Eq. (12)], as a function of the reduced phonon frequency x for different scattering mechanisms and their combinations.

Eq. (25), which was established at low temperatures, is inadequate at high temperatures. Some minor deviations occurring in the most heavily doped p-type specimens (1970 and 82 in Fig. 2) at high temperatures are believed to be caused by the influence of the split-off band at these high doping levels (see discussion below).

The values of $|\mathcal{E}|$ required for each sample to fit the experimental points are given in Table I. It is found that $|\mathcal{E}|$ increases with the carrier concentration, and is higher for n- than for p-type material of the same carrier concentration.

IV. DISCUSSION

In order to determine which phonons contribute dominantly to the thermal conductivity, it is useful to plot the quantity $\tau_C x^2$ against the reduced phonon frequency x; the contribution of the second term in Eq. (12) is small. This is shown in Fig. 4 for the different scattering mechanisms involved and their combinations. The lattice thermal conductivities are, according to Eq. (12), proportional to the areas under the curves. It is seen that the addition of phonon-electron scattering to phonon-phonon and point-defect scattering reduces the area by an appreciable amount. Point-defect scattering cuts out the high-frequency phonons, while phonon-electron scattering reduces the mean free path of the low-frequency phonons. Most of the heat is carried, therefore, by phonons of frequency $\omega \approx 0.15\omega_D$. This provides some justification for the use of a Debye spectrum. Herring[15] has pointed out that the longitudinal phonons undergo much less scattering by other phonons than transverse phonons in the long-wave-length limit, and that for the N processes, Eq. (1) is valid. If this limit still applies in our case, then the heat is predominantly carried by the long-wavelength phonons and the use of Eq. (1) is justified. Moreover, since the combination of phonon-electron and phonon–

FIG. 3. Experimental and theoretical values of the lattice thermal conductivity of n-type $Ge_{0.2}Si_{0.8}$ and $Ge_{0.15}Si_{0.85}$ alloys as a function of the absolute temperature. The theoretical curves were fitted at 500°K ($\approx \Theta$); this determines the deformation potentials $|\mathcal{E}|$.

TABLE II. Information on deformation potentials.

Type	Material	$\mathcal{E}_1$ (eV)	$\mathcal{E}_2$ (eV)	Method
n	$Ge_{0.3}Si_{0.7}$	± 1.6[a]	$\cdots$	Thermal conductivity
	Si	-1.80[b]	9.57	Theory[c]
	Si	$\cdots$	8.3 ± 0.3	Piezoresistance, piezo-Hall effect[d]
	Si	$\cdots$	8.7	Piezoresistance[e]
	Si	$\cdots$	11.3 ± 1.3	Piezobirefringence[f]
	Si	$\cdots$	8–11	Older values[g]
	Si	$\cdots$	± 11	Elastic constants[h]
	Si	-3.9[i]	$\cdots$	Mobility[j]
	Si	-1.7[k]	$\cdots$	Mobility anisotropy[d]
p	$Ge_{0.3}Si_{0.7}$	± 1.2[l]	$\cdots$	Thermal conductivity
	Si	-2.09	3.74/4.92	Theory[c]
	Si	$\cdots$	2.04/2.68	Piezo-cyclotron resonance[m]
	Si	$\cdots$	± 5	Elastic constants[n]
$dE_g/d \ln V$	$Ge_{0.3}Si_{0.7}$	± 0.4 or 2.8	$\cdots$	Thermal conductivity
	Si	$+0.3$	$\cdots$	Theory[c]
	Si	$+1.5$	$\cdots$	Optical absorption[o]

[a] For the most lightly doped sample $n = 2.3 \times 10^{19}$ cm^{-3}.
[b] Calculated for the symmetry point X, not for Δ.
[c] Reference 31.
[d] Reference 33.
[e] M. Asche and W. Möhling, Phys. Stat. Sol. 3, K225 (1963).
[f] K. J. Schmidt-Tiedemann, *Proceedings of the International Conference on the Physics of Semiconductors, Exeter* (The Institute of Physics and the Physical Society, London, 1962), p. 191.
[g] References given in Ref. 33.

[h] Reference 18.
[i] Assuming $\mathcal{E}_2 = 8.3$ eV and using Fig. 6 top of Ref. 29 (1957).
[j] Reference 32.
[k] Assuming $\mathcal{E}_2 = 8.3$ eV and using Fig. 6 bottom of Ref. 29 (1957).
[l] Extrapolated for a lightly doped sample of $n = 2.3 \times 10^{19}$ cm^{-3}.
[m] J. C. Hensel and G. Feher, Phys. Rev. 129, 1041 (1963).
[n] Reference 19.
[o] Reference 34.

point-defect scattering dominate at all frequencies the results are not sensitive to the assumptions made for τ_N and τ_U.

It is attempted now to determine the physical meaning of the deformation potential as deduced from the thermal conductivity measurements. In a cubic crystal the deformation potential tensor has two independent components[28]: $\mathcal{E}_1$, the dilatation deformation potential, governing longitudinal mode scattering and $\mathcal{E}_2$, the shear deformation potential, governing transverse mode scattering. Electrons interact both with longitudinal and transverse phonons.[29] If, however, as indicated above, the phonons with the longest mean free path are the longitudinal phonons, then it is sufficient to use Ziman's[13] expression for the phonon-electron relaxation time, which was derived for the case of longitudinal mode interaction only, and the deformation potential given in Table I is the dilatation deformation potential $|\mathcal{E}_1|$.

Information about the deformation potentials in Ge-Si alloys is not available. Since we are dealing with alloys high in silicon content, and since the band structure of these alloys is very similar[25,30] to the band structure of silicon, a comparison is made in Table II with the available deformation potentials for silicon. The agreement among the different literature values given for $\mathcal{E}_2$ is excellent; the elastic constant measurements[18,19] result in slightly higher values. Less reliable

values are available, however, for $\mathcal{E}_1$, due to the difficulty of direct experimental determination of this quantity. In view of this, the agreement of our values with the theory,[31] and with the values derived from mobility[32] and mobility anisotropy[33] by using the curves given by Herring and Vogt[29] and assuming[33] $\mathcal{E}_2 = 8.3$ eV, is satisfactory. It is, of course, not possible to determine the sign of $\mathcal{E}_1$.

By combining the dilatation deformation potentials of n- and p-type material, the volume dependence of the energy gap,

$$dE_g/d \ln V = \mathcal{E}_{1n} - \mathcal{E}_{1p}, \qquad (26)$$

can be obtained. This quantity is accessible from optical measurements; the value determined by Paul[34] is compared in Table II with the values derived by combining $\mathcal{E}_{1n}$ and $\mathcal{E}_{1p}$ given in Table II.

The advantage in the use of alloys over that of elemental or compound semiconductors has to be stressed. The strong point-defect scattering of short-wave phonons in the alloys reduces the problem to the long-wavelength limit. This has very desirable consequences: A number of assumptions are better fulfilled [Debye spectrum, the use of Eq. (1)], the additional point-defect scattering introduced by the dopant can be neglected, and finally, it is possible to determine the dilatation deformation potential $\mathcal{E}_1$.

The increase of the deformation potential with doping is shown in Fig. 5. It is seen that $|\mathcal{E}|$ increases as $n^{0.4}$

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and $n^{0.5}$ for p-type and n-type alloys, respectively. The slope seems to be independent of alloy composition; the result for $Ge_{0.2}Si_{0.8}$ and $Ge_{0.15}Si_{0.85}$ follow quite closely the curve for $Ge_{0.3}Si_{0.7}$. No values of $|\mathcal{E}|$ can be obtained for carrier concentrations smaller than 2×10^{19} cm^{-3}, but it is expected that in this region $|\mathcal{E}|$ is independent of n. An indication of the carrier concentration dependence of $|\mathcal{E}|$ shown in Fig. 5 can also be found in the analysis[24] of the change in mobility with doping. Furthermore, a similar effect with a similar power of n was observed by Csavinszky and Einspruch[19] for the shear deformation potential in p-type silicon from measurements of the elastic constants. The explanation offered by these authors is likely to apply also for the dilatation deformation potential, namely: (a) warping of the bands and (b) change in the band structure with doping. An additional possibility (c) is the dependence of the deformation potential on wave vector; this means that the deformation potential approximation, which assumes all states of a particular band to shift by the same amount under strain, is not valid any more for high-carrier concentrations.

The effective masses used for the calculation in this paper are based on the single-band model for the valence band, and no attempt was made to include the change of m^* with doping. This, however, does not affect seriously the observed increase of $|\mathcal{E}|$ with doping (Fig. 5). In the n-type material estimates were made on the sensitivity of the results on m^*. It turns out that the changes of m^* with doping[35] are not able by far to account for the observed effect. The same probably holds for p-type material. Csavinszky and Einspruch[19] have allowed for a 3-band model in p-type silicon and have modified the effective masses to take into account the nonparabolicity of the bands. However, this did not

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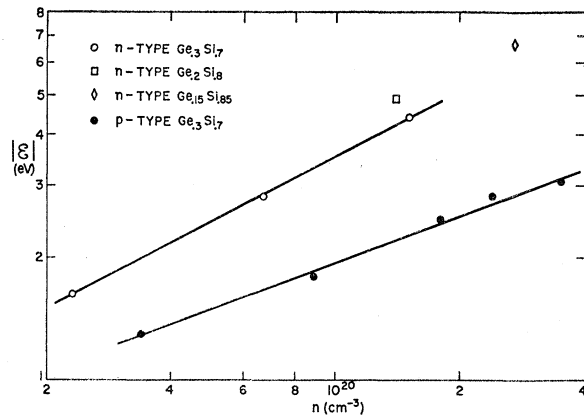

FIG. 5. The deformation potential required to fit the theoretical curves in Figs. 1, 2, and 3, as a function of the carrier concentration.

change significantly the apparent dependence of $|\mathcal{E}|$ on n. It seems that at least in n-type material the dependence of the deformation potential on wave vector (c) is the dominant mechanism for the observed effect, because of the weak dependence of m^* on doping.[35] A breakdown of the deformation potential approximation should also show up in the measurements of physical properties under applied strain. Further studies in this direction are in progress.

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