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ELECTRON-PHONON SCATTERING PARAMETERS AND LATTICE THERMAL CONDUCTIVITY OF A DOPED SEMICONDUCTOR AT LOW TEMPERATURES: APPLICATION TO P-DOPED Ge

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The role of electron-phonon scattering parameters (the reduced Fermi energy η^*, the density of states effective mass m^*, the deformation potential constant E_D and the carrier concentration n) in the estimation of the lattice thermal conductivity of the doped semiconductor was studied at low temperatures by calculating the total lattice thermal conductivity of the five samples of P-doped Ge having different carrier concentrations in the temperature range of 1–5 K. The variation of the percentage contribution due to non-peripheral phonons with the parameters η^*, m^*, E_D and n was also investigated at low temperatures.

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1. Introduction

The requirements for the conservation of energy and momentum suggest that the entire phonon can not interact with electrons. The phonons which can not interact with electrons are referred to as peripheral phonons [1] whose wave vectors satisfy the condition $|\bar{q}| > 2|\bar{K}_F|$. The phonons with a wave vector $|\bar{q}| \leqslant 2|\bar{K}_F|$ can interact with electrons and can be referred to as non-peripheral [1] phonons, where $\bar{K}_F$ is the wave vector corresponding to the Fermi surface. In view of the above stated distinction, and following Blewer et al. [1], the author and his co-workers [2–6] studied the lattice thermal conductivity of the doped semiconductors at low temperatures by expressing the total lattice thermal conductivity as a sum of two contributions; $\bar{K}_F$ due to non-peripheral phonons and K_{Ph} due to peripheral phonons, and it is reported that this approach gives a very good response to the experimental data of the lattice thermal conductivity of the doped samples at low temperatures.

Recently, Boghosian and Dubey [3, 4] studied the lattice thermal conductivity of five samples of P-doped Ge having different carrier concentration in the range of $n = 1.2 \times 10^{23} \mathrm{m}^{-3}$ to $1.1 \times 10^{24} \mathrm{m}^{-3}$ in the temperature range of 1–5 K by estimating the separate

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contributions due to peripheral and non-peripheral phonons, and it has been reported that at low temperatures, the lattice thermal conductivity of the P-doped Ge is mainly due to non-peripheral phonons and the electron-phonon scattering relaxation rate [7] plays a very important role in it. From earlier studies, it is also very clear that the reduced Fermi energy η^*, the density of states effective mass m^*, the deformation potential constant E_D and the carrier concentration n are responsible factors to determine the electron-phonon scattering relaxation rate. Therefore, there is a need to study the role of these parameters to estimate the low temperature lattice thermal conductivity of a doped sample.

The aim of the present work is to study the effect of the electron-phonon scattering parameters η^*, m^*, E_D and n on the lattice thermal conductivity of the doped samples at low temperatures and the P-doped Ge sample is taken as an example. The variation of the percentage contribution $\% K_N$ due to non-peripheral phonons toward the total lattice thermal conductivity of P–doped Ge with η^*, m^*, E_D and n has also been studied in the present work.

2. *Phonon conductivity integral*

Considering the separate contributions due to peripheral and non-peripheral phonons, following the earlier work of the author and his co-workers [2, 3], and using the Callaway [8] expression of the lattice thermal conductivity, the total phonon conductivity of a doped sample can be expressed as,

$$K = K_N + K_{Ph}, \tag{1}$$

$$K_N = C \int_0^{\theta^*/T} (\tau_B^{-1} + \tau_{pt}^{-1} + \tau_{ph}^{-1} + \tau_{ep}^{-1})^{-1} F(x) dx, \tag{2}$$

$$K_{Ph} = C \int_{\theta^*/T}^{\theta/T} (\tau_B^{-1} + \tau_{pt}^{-1} + \tau_{ph}^{-1})^{-1} F(x) dx, \tag{3}$$

$$C = (K_B/2\pi^2 v)(K_B T/\hbar)^3, \quad F(x) = x^4 e^x (e^x - 1)^{-2},$$

$$x = (\hbar\omega/K_B T), \quad \theta^* = (2F\hbar v_L/K_B)(\pi^2 n)^{1/3},$$

where K_B is the Boltzmann constant, $\hbar$ is the Planck constant devided by 2π, θ^* is the characteristic temperature [2, 3] which differentiates peripheral phonons from non-peripheral phonons and depends on the carrier concentration n, F is a constant [2, 3], v is the average phonon velocity, v_L is the longitudinal phonon velocity, θ is the Debye temperature of the sample, τ_B^{-1}, τ_{pt}^{-1}, τ_{ep}^{-1} and τ_{ph}^{-1} are the boundary [9], point-defect [10], electron-phonon [7] and phonon-phonon [8] scattering relaxation rates respectively. As stated earlier, our study is confined to low temperatures only. The expression used for these scattering relaxation rates can be expressed as

$$\tau_B^{-1} = v/L,$$

$$\tau_{pt}^{-1} = A\omega^4,$$

$$\tau_{ph}^{-1} = B\omega^2 T^3,$$

$$\tau_{ep}^{-1} = DT \ln \left[\frac{\{1 + \exp \eta^* - (N/T) - PTx^2 + x/2\}}{\{1 + \exp \eta^* - (N/T) - PTx^2 - x/2\}} \right], \tag{4}$$

TABLE I

The constants used in the present study of lattice thermal conductivity of five samples of P-doped Ge in the temperature range of 1–5 K

$T(K)$	Sample I $n = 1.2 \times 10^{23}$ m^{-3} $E_D = -2.40 \times 10^{-19}$ J		Sample II $n = 1.7 \times 10^{23}$ m^{-3} $E_D = -5.09 \times 10^{-19}$ J		Sample III $n = 2.35 \times 10^{23}$ m^{-3} $E_D = -6.30 \times 10^{-19}$ J		Sample IV $n = 5.6 \times 10^{23}$ m^{-3} $E_D = -8.07 \times 10^{-19}$ J		Sample V $n = 1.1 \times 10^{24}$ m^{-3} $E_D = -8.13 \times 10^{-19}$ J	
	η^*	m^*	η^*	m^*	η^*	m^*	η^*	m^*	η^*	m^*
1	25.63	0.24	25.97	0.24	29.30	0.25	30.96	0.27	31.60	0.28
2	21.43	0.32	22.35	0.35	24.30	0.37	25.70	0.39	26.35	0.40
3	19.36	0.38	19.73	0.40	21.15	0.42	22.28	0.44	23.07	0.45
4	18.35	0.40	18.76	0.42	19.50	0.44	20.25	0.45	20.80	0.47
5	17.92	0.41	18.36	0.43	18.90	0.45	19.45	0.47	20.0	0.48

$v = 3.9 \; 10^3$ m/sec, $v_L = 4.92 \; 10^3$ m/sec, $\theta = 376$ K, $\tau_B^{-1} = 7.8 \; 10^5$ sec^{-1}, $A = 2.4 \; 10^{-44}$ sec^3

where

$$D = (E_D^2 m^{*2} K_B)/(4\pi\hbar^2 v_L \varrho),$$

$$\eta^* = E_F/K_B T, \quad N = m^* v_L^2/2K_B, \quad P = K_B/(8m^* v_L^2),$$

ϱ is the density of the sample, L is the Casimir [9] length of the sample, E_F is the Fermi energy level, A and B are the point-defect and phonon-phonon scattering strengths, respectively, and other terms have the same meaning as defined above.

It should be noted that the correction term [8] ΔK due to the three phonon normal processes has been ignored in equation (1) due to its small contribution [11–14]. At the same time, the three phonon scattering relaxation rate τ_{ph}^{-1} has been also ignored in the actual calculation due to its negligibly small contribution compared to other scattering relaxation rates at low temperatures.

3. *Results and discussions*

Using the constants reported in Table I, which are taken from the earlier report of Boghosian and Dubey [3], the role of the electron-phonon scattering parameters η^*, m^*, E_D and n in the estimation of the lattice thermal conductivity of the five samples of P-doped

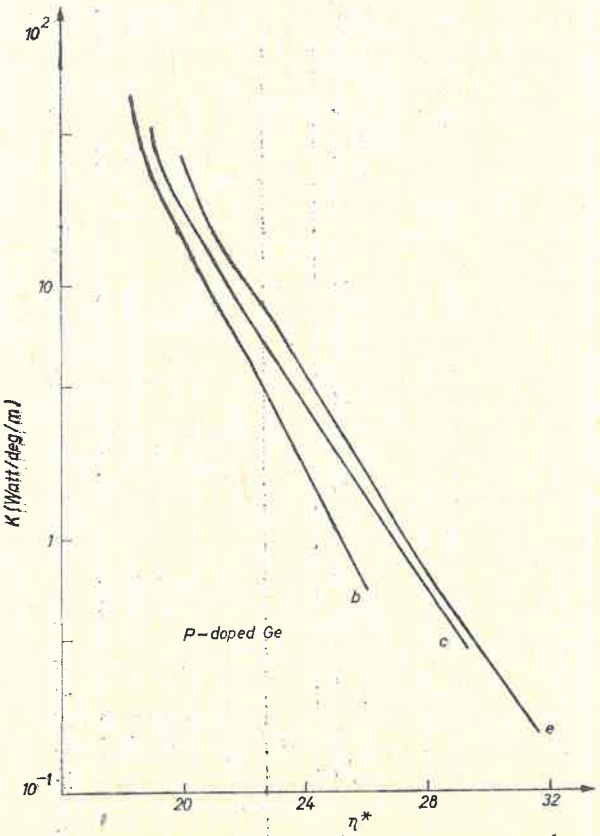

Fig. 1a. The variation of the total lattice thermal conductivity of P-doped Ge samples with η^*. Curves *b*, *c* and *e* correspond to samples having $n = 1.7\times10^{23}$, 2.35×10^{23} and $1.1\times10^{24}\ \mathrm{m^{-3}}$, respectively

Ge having different carrier concentrations have been studied in the temperature range of 1–5 K by calculating the separate contributions of K_{ph} due to peripheral phonons and K_N due to non-peripheral phonons with the help of numerical integration of equations (2) and (3). The variation of the total lattice thermal conductivity K with the reduced Fermi

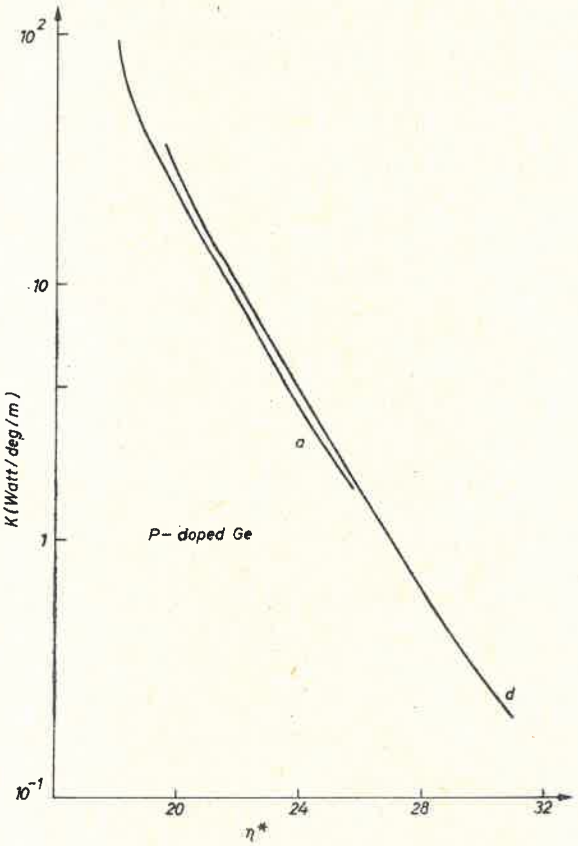

Fig. 1b. The variation of the total lattice thermal conductivity of P-doped Ge samples with η^*. Curve a corresponds to $n = 1.2 \times 10^{23}\ \mathrm{m}^{-3}$ and d corresponds to $n = 5.6 \times 10^{23}\ \mathrm{m}^{-3}$

energy η^* is shown in Fig. 1 while the variation of K with m^* is shown in Fig. 2. The variation of the total lattice thermal conductivity K with E_D is illustrated in Fig. 3 and the variation of K with n is shown in Fig. 4. The percentage contributions $\% K_N$ due to non-peripheral phonons towards the total lattice thermal conductivity of P-doped Ge for the different values of η^*, m^*, E_D and n have also been studied and the results obtained are given in Tables II and III for the different values of η^* and m respectively. The results obtained for the different values of E_D and n have been given in Table IV.

TABLE II

Variation in the percentage contribution of K_N due to non-peripheral phonons having a reduced Fermi energy η^* for P-doped Ge

$n = 1.2\times10^{23}$ m^{-3}		$n = 1.7\times10^{23}$ m^{-3}		$n = 2.35\times10^{23}$ m^{-3}		$n = 5.6\times10^{23}$ m^{-3}		$n = 1.1\times10^{24}$ m^{-3}	
η^*	% K_N	η^*	% K_N	η^*	% K_N	η^*	% K_N	η^*	% K_N
25.63	100	25.97	100	29.30	100	30.96	100	31.60	100
21.43	98.72	22.35	99.24	24.30	99.30	25.70	99.40	26.35	99.50
19.36	81.38	19.73	87.71	21.15	87.86	22.28	87.89	23.07	88.66
18.35	45.41	18.76	56.09	19.50	57.47	20.25	58.11	20.80	59.46
17.92	15.0	18.36	15.76	18.90	16.34	19.45	16.58	20.0	16.82

3.1. Variation of the lattice thermal conductivity K with the reduced Fermi energy η^*

The variation of the total lattice thermal conductivity of the five samples of P-doped Ge having different carrier concentration with η^* can be studied with the help of Fig. 1a and 1b at a constant carrier concentration n shows that the lattice thermal conductivity of the P-doped Ge decreases with increase of η^* for each value of n. At the same time, it is also very clear that the nature of K vs η^* curve is approximately the same for each value of n in the range $1.2\times10^{23}-1.1\times10^{24}$ m^{-3}. From Table I as well as from the earlier report of Boghosian and Dubey [3], it is very clear that η^* decreases with increasing T. At the same time, K shows an increase with T. Due to these two variables K should decrease with increasing η^* is a way similar to the results shown in these two figures. However, from Table II, it can be seen that the per cent of K_N decreases with the decrease of η^* for each value of n, i.e. for each sample.

3.2. Variation of K with m^*

From Fig. 2, it can be seen that for any value of the carrier concentration i.e., for each sample, K increases with an increase of m^*, and the nature of K vs m^* is nearly the

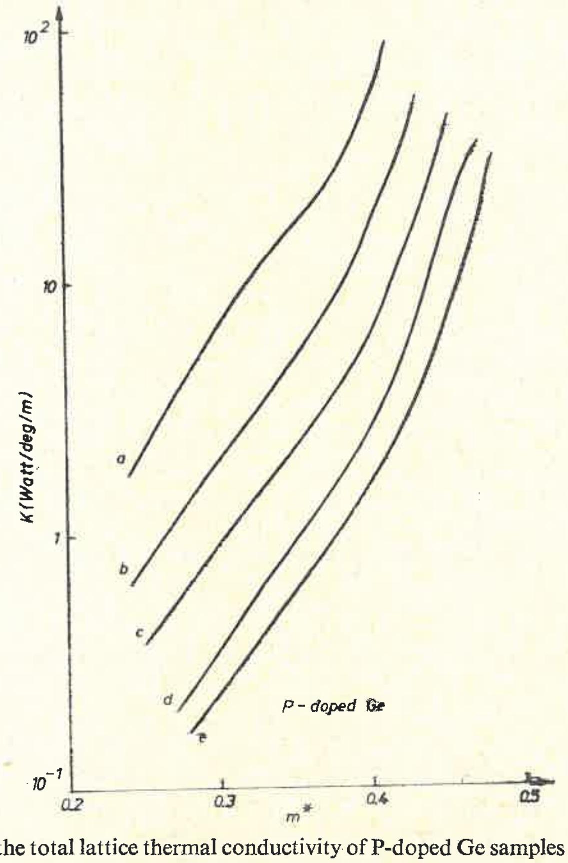

Fig. 2. The variation of the total lattice thermal conductivity of P-doped Ge samples with m^*. Curves a, b, c, d and e correspond to $n = 1.2\times10^{23}$, 1.7×10^{23}, 2.35×10^{23}, 5.6×10^{23} and 1.1×10^{24} m^{-3}, respectively

same for all of the samples of P-doped Ge. The electrons with a lower value of m^* have less energy compared to those with a large m^*. As a result, phonons carrying the heat energy face a smaller resistance in the presence of the electrons having lower value of m^*. In other words, one can also say that the sample has a lower lattice thermal resistivity in the presence of electrons with low m^* compared to electrons with a large m^*. Thus, one can say that the lattice thermal conductivity of a doped sample should increase with an increase in m^*, which is shown in Fig. 2. At the same time, from Table I, it can also be

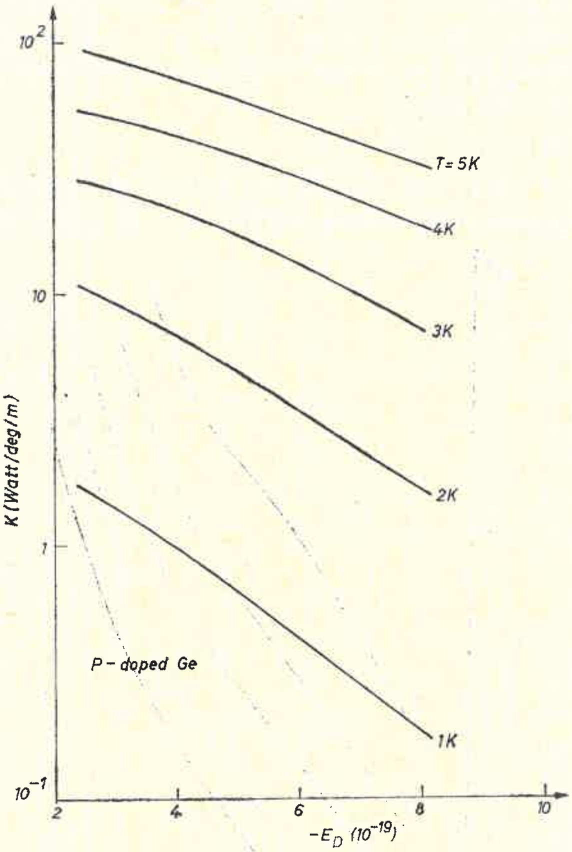

Fig. 3. The variation of the total lattice thermal conductivity of P-doped Ge samples with E_D

seen that m^* increases with increasing temperature and the total lattice thermal conductivity of a doped sample also increases with temperature at low temperatures, hence, K should also increase with increasing m^*.

Using Table III, one can conclude that the per cent of K_N decreases with an increase in m^* for each sample.

TABLE III

Variation of the percentage contribution of K_N due to non-peripheral phonons with the density of states having an effective mass m^* for P-doped Ge

$n = 1.2\times10^{23}$ m^{-3}		$n = 1.7\times10^{23}$ m^{-3}		$n = 2.35\times10^{23}$ m^{-3}		$n = 5.6\times10^{23}$ m^{-3}		$n = 1.1\times10^{24}$ m^{-3}	
m^*	% K_N	m^*	% K_N	m^*	% K_N	m^*	% K_N	m^*	% K_N
0.24	100	0.24	100	0.25	100	0.27	100	0.28	100
0.32	98.72	0.35	99.24	0.37	99.30	0.39	99.40	0.4	99.50
0.38	81.38	0.40	87.77	0.42	87.86	0.44	87.89	0.45	88.66
0.40	45.41	0.42	56.09	0.44	57.47	0.45	58.11	0.47	59.46
0.41	15.0	0.43	15.76	0.45	16.34	0.47	16.58	0.48	16.82

3.3. Variation of K with E_D

From studies of earlier workers, it is clear that the deformation potential constant E_D differs among samples and this depends mainly on the carrier concentration. From Fig. 3, it is clear that K decreases with an increase in the absolute value of E_D at each temperature in the range of 1–5 K. The decreasing value of K can be understood with the expression of the electron–phonon scattering relaxation rate as stated in equation (4). This shows that the electron–phonon scattering relaxation time $\tau_{ep} \propto E_D^{-2}$. As a result, K shows a decrease with an increase of the absolute value of E_D.

TABLE IV

Variation of the percentage contribution of K_N due to non-peripheral phonons with the carrier concentration n and the deformation potential, E_D for P-doped Ge at different temperatures

$n(10^{23})$	$\%K_N\,(T=1)$	$\%K_N\,(T=2)$	$\%K_N\,(T=3)$	$\%K_N\,(T=4)$	$\%K_N\,(T=5)$	$E_D(10^{-19}J)$
1.2	100	98.72	81.38	45.41	15.0	−2.40
1.7	100	99.24	87.77	56.09	15.76	−5.09
2.35	100	99.30	87.86	57.47	16.34	−6.30
5.6	100	99.40	87.89	58.11	16.58	−8.07
11.0	100	99.50	88.66	59.46	16.82	−8.13

The variation of the % of K_N with E_D can be studied with the help of Table IV which shows the increasing value of the % of K_N with increase of the absolute value of E_D at each temperature, but the variation is very slow.

3.4. Variation of K with n

The carrier concentration n is one of the most important parameters to estimate the lattice thermal conductivity of a doped sample. However, the expression for the electron–phonon scattering relaxation rate as stated in equation (4) does not have the term n. But, the parameters, η^*, m^*, and E_D which are responsible for τ_{ep}^{-1}, are measured with the help of the carrier concentration n. Thus, it is interesting to study the variation of K with n.

From Fig. 4, it can be seen that the total lattice thermal conductivity of P-doped Ge decreases with an increase of the carrier concentration n at each temperature in the range of 1–5 K. From this figure, it is also clear that for a low value of n, the variation in K is much faster than same for large n value. The decreasing nature of the lattice thermal conductivity with n can be understood considering the electron as an extra scatterer of phonons. Increasing the carrier concentration in a sample number of collisions increases, and as a result of this the electron–phonon scattering relaxation rate increases which results in a reduction in the lattice thermal conductivity.

The variation of the % K_N with n can be seen in Table IV which shows that the % of K_N increases with n at each temperature which is similar to the increasing value of the % of K_N with E_D.

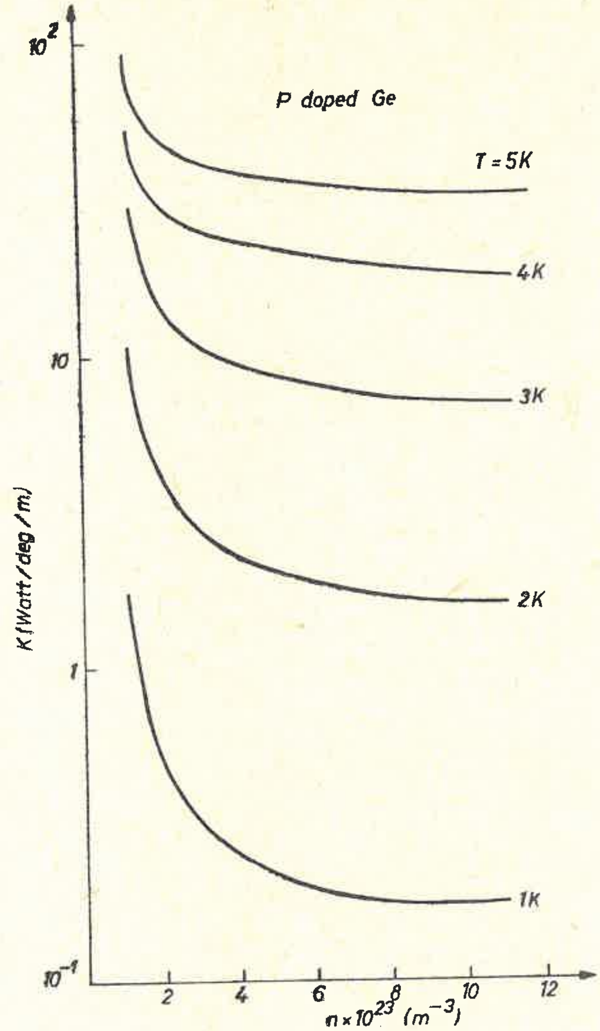

Fig. 4. The variation of the total lattice thermal conductivity of P-doped Ge samples with n

3.5. Conclusions

To test the reliability of the electron-phonon scattering parameters used in the present analysis, the total lattice thermal conductivities of two samples of P-doped Ge having carrier concentrations of 1.2×10^{23} and 1.1×10^{24} m^{-3}, are also illustrated in Fig. 5. They are in good agreement with the calculated and experimental values of the lattice thermal conductivity of these two samples in the entire temperature range of 1–5 K. Therefore, one can conclude that the values of the electron-phonon scattering parameters used in the present analysis are correct and give a very good response to the experimental data

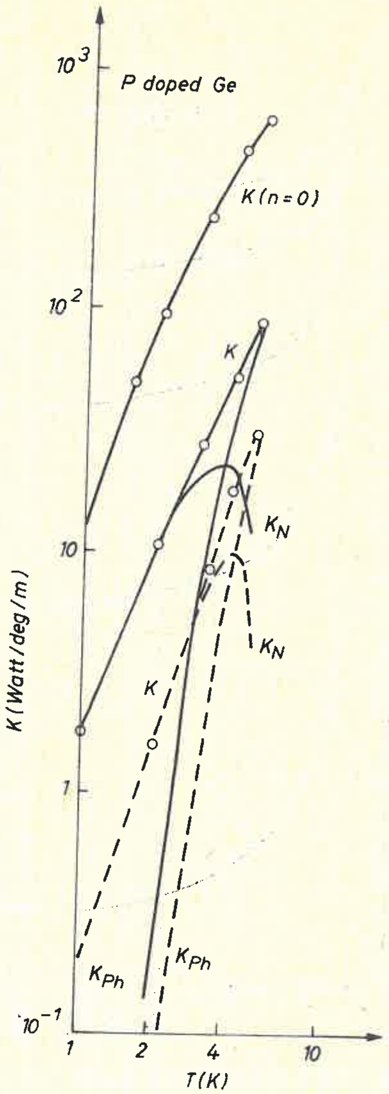

Fig. 5. The lattice thermal conductivity of P-doped Ge samples. Solid and dashed lines correspond to the sample having $n = 1.2 \times 10^{23}$ and $1.1 \times 10^{24}\ m^{-3}$, respectively. $K(n = 0)$ represents the lattice thermal conductivity of the undoped sample. Circles are the experimental points

for lattice thermal conductivity of the samples studied. The lattice thermal conductivity of the pure sample is also shown in Fig. 5.

Finally, with the help of results stated above one can conclude the following:

1. The total lattice thermal conductivity of P-doped Ge decreases with an increase in the reduced Fermi energy η^* while it also shows an increase with an increase in the density of states having an effective mass m^*.

2. The total lattice thermal conductivity of P-doped Ge increases with an increase of the carrier concentration n at each temperature while it decreases with an increase of the absolute value of the deformation potential constant E_D.

3. The percentage contribution K_N due to non-peripheral phonons shows an increase with the carrier concentration n as well as with the absolute value of the deformation potential constant E_D at each temperature.

4. The percentage contribution K_N increases with an increase of the reduced Fermi energy η^* while it shows decrease with an increase in the density of states effective mass m^*.

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