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CONTRIBUTION TO THE LATTICE THERMAL CONDUCTIVITY DUE TO THE THREE PHONON NORMAL PROCESSES IN THE PRESENCE OF CORE DISLOCATIONS IN THE FRAME OF THE CALLAWAY INTEGRAL

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The contribution of the correction term due to the three phonon normal processes has been studied for a sample having core dislocation in the frame of Callaway integral by obtaining an analytical expression for it. To test the applicability of the expression obtained, the contribution of the correction term toward total phonon conductivity has been calculated in the temperature range of 0.2–5 K owing to which a negligible contribution has been found.

1. Introduction

The expression of the lattice thermal conductivity proposed by Callaway [1] was based on the two mode conduction of phonon. The first one gives the lattice thermal conducitivity of an insulator due to the combined scattering relaxation rate, while the second term has a complicated form known as the correction term due to the three phonon normal processes. It was found that the contribution of the correction term (ΔK) is usually small enough compared to the total lattice thermal conductivity [2, 5].

Recently, the lattice thermal conductivity due to the correction term has been studied by several workers [6–8] using the Callaway expression of the correction term in which no distinction is made between transverse and longitudinal phonons. These studies are confined to samples having boundary, point defect and phonon–phonon scattering processes only.

The aim of the present work is to derive an analytical expression for ΔK in the frame of the Callaway integral at very low temperatures in the presence of core dislocations. The contribution of the correction term (ΔK) to the lattice thermal conductivity was calculated also in the frame of Callaway integral for the different values of P which is the ratio of the three phonon normal and umklapp processes scattering strengths.

2. Theory

The generalized Callaway expression of the lattice thermal conductivity is

$$K = c_0 \cdot \int_0^{\theta/T} \left(\tau_N^{-1} + \tau_R^{-1}\right)^{-1} x^4 e^x (e^x - 1)^{-2} dx + \Delta K, \tag{1}$$

where

$$\Delta K = c_0 T_2^2 / T_3, \tag{2}$$

$$T_2 = \int_0^{\theta/T} \tau_N^{-1} \left(\tau_N^{-1} + \tau_R^{-1}\right)^{-1} x^4 e^x (e^x - 1)^{-2} dx, \tag{3}$$

$$T_3 = \int_0^{\theta/T} \tau_R^{-1} \tau_N^{-1} \left(\tau_N^{-1} + \tau_R^{-1}\right)^{-1} x^4 e^x (e^x - 1)^{-2} dx, \tag{4}$$

$$c_0 = (K_B / 2\pi^2 v)(K_B T/\hbar)^3, \quad x = \hbar w / K_B T,$$

where K_B is the Boltzmann constant, $\hbar$ is the Planck constant divided by 2π, θ is the Debye temperature of the specimen under study, v is the average phonon velocity, $\tau^{-1} = B_1 w^2 T^3$ is the three phonon normal process scattering relaxation rate, $\tau_R^{-1} = \tau_B^{-1} + Aw^4 + B_2 w^2 T^3 + aw^3$ is the combined scattering relaxation rate of umklapp processes, τ_B^{-1} is the boundary scattering [9], Aw^4 is the point defect scattering relaxation rate [10], $B_2 w^2 T^3$ is the three phonon umklapp process scattering relaxation rate and aw^3 is the core dislocation relaxation rate [10]. A, a, B_1, B_2 are scattering strengths of point defect, core dislocation and three phonon normal and umklapp processes, respectively. The τ_N^{-1} and τ_R^{-1} can be expressed as

$$\tau_N^{-1} = B_1 w^2 T^3 = b_1 x^2, \tag{5}$$

$$\tau_{pt}^{-1} = Aw^4 = Dx^4, \tag{6}$$

$$\tau_U^{-1} = B_2 w^2 T^3 = b_2 x^2, \tag{7}$$

$$\tau_{cd}^{-1} = aw^3 = cx^3, \tag{8}$$

$$E = b_1 + b_2. \tag{9}$$

It is necessary to mention here that through the numerical analysis of above integral for τ_R^{-1}, it is found that at low temperatures, either τ_{cd}^{-1} dominates over τ_B^{-1} or τ_{cd}^{-1} is dominated by τ_B^{-1}. Therefore, the analytical expressions are obtained under two different approximations, i. e. $\tau_{cd}^{-1} \gg \tau_B^{-1}$ and $\tau_B^{-1} \gg \tau_{cd}^{-1}$.

(A) If $\tau_{cd}^{-1} \gg \tau_B^{-1}$:

In the above approximations, the integrals T_2 and T_3 can be reexpressed as follows

$$T_2 = \frac{b_1}{c} \int_0^{\theta/T} \left(1 - \frac{\tau_B^{-1}}{c} x^{-3} - \frac{D}{c} x - \frac{E}{c} x^{-1}\right) x^3 e^x (e^x - 1) dx, \tag{10}$$

which reduces to

$$T_2 = \frac{b_1 I_3}{c}\left(1 - \frac{\tau_B^{-1}}{c} F_3^0 - \frac{D}{c} F_3^4 - \frac{E}{c} F_3^2\right), \tag{11}$$

where

$$F_n^m = I_m / I_n, \qquad I_r = \int_0^{\theta/T} x^r e^x (e^x - 1)^{-2} dx.$$

m, n and r are integers. Similarly

$$T_3 = b_1 I_6 \Bigg(1 - \frac{P A_3}{1+P} F_6^5 - \frac{(2+P)}{(1+P)} A_2 A_3 - A_1^2 F_6^0 - 2 A_1 A_2 F_6^4 - A_2^2 F_6^8 - \\ - A_1 A_3 \frac{(2+P)}{(1+P)} F_6^2 - \frac{A_3^2}{1+P}\Bigg). \tag{12}$$

At low temperatures, the contribution of τ_U^{-1} is very small compared to τ_R^{-1} and it can be ignored in this case, Eq. (2) reduces to

$$K = \frac{c_0 E I_3 F_6^3}{c^2} (1 - 2A_1 F_3^0 - 2A_2 F_3^4 - 2A_3 F_3^2 - A_3 F_6^5), \tag{13}$$

where

$$A_1 = \frac{\tau_B^{-1}}{c}, \quad A_2 = \frac{D}{c}, \quad A_3 = \frac{E}{c} \quad \text{and} \quad P = \frac{b_1}{b_2}.$$

(B) If $\tau_B^{-1} \gg \tau_{cd}^{-1}$:

For this case, the integrals T_2 and T_3 can be expressed as

$$T_2 = b_1 \tau_B I_6 (1 - c\tau_B F_6^9 - D\tau_B F_6^{10} - E\tau_B F_6^8), \tag{14}$$

$$T_3 = b_1 I_6 (1 - b_1 \tau_B F_6^8 - c^2 \tau_B^2 F_6^{12} - 2Dc\tau_B^2 F_6^{10} - (E + b_2) c\tau_B^2 F_6^{11} - \\ - D^2 \tau_B^2 F_6^{12} - (E + b_2) D\tau_B^2). \tag{15}$$

Using these equations ΔK can be approximated as

$$\Delta K = c_0 b_1 \tau_B^2 I_6 \Bigg(1 - 2c\tau_B F_6^9 - 2D\tau_B F_6^{10} - E\tau_B F_6^8 \frac{(2+P)}{(1+P)} - \\ - \frac{2PE}{(1+P)} \tau_B^2 F_6^8 (cF_6^9 - DF_6^{10}) - \frac{2E^2 P}{(1+P)} \tau_B^2 F_6^8 F_6^8 + \\ + c^2 \tau_B^2 F_6^{12} + 2Dc\tau_B^2 F_6^{10} + \frac{(2+P)}{(1+P)} Ec\tau_B^2 F_6^{11} + D^2 \tau_B^2 F_6^{12} + \\ + \frac{(2+P)}{(1+P)} ED\tau_B^2\Bigg). \tag{16}$$

Table I*

Contribution of the correction term ΔK to the total phonon conductivity in the temperature range of 0.2–5 K for different values of P (10^{-3} to 10^{3}), K and ΔK are expressed in Watt/deg/cm

TK	K^*	ΔK						
		10^{-3}	10^{-2}	10^{-1}	1	10	10^{2}	10^{3}
0.2	4.08 10^{-4}	3.02 10^{-16}	2.99 10^{-15}	2.81 10^{-14}	1.51 10^{-13}	2.75 10^{-13}	2.99 10^{-13}	3.02 10^{-13}
0.4	3.26 10^{-3}	7.92 10^{-14}	7.85 10^{-13}	7.21 10^{-12}	3.96 10^{-11}	7.21 10^{-11}	7.85 10^{-11}	7.92 10^{-11}
0.6	1.10 10^{-2}	2.03 10^{-12}	2.01 10^{-11}	1.85 10^{-10}	1.01 10^{-9}	1.84 10^{-9}	2.01 10^{-9}	2.03 10^{-9}
0.8	2.61 10^{-2}	2.03 10^{-11}	2.01 10^{-10}	1.84 10^{-9}	1.01 10^{-8}	1.84 10^{-8}	2.01 10^{-8}	2.03 10^{-8}
1.0	5.09 10^{-2}	1.21 10^{-10}	1.20 10^{-9}	1.01 10^{-8}	1.01 10^{-7}	1.10 10^{-7}	2.20 10^{-7}	1.21 10^{-7}
2.0	4.07 10^{-1}	3.09 10^{-8}	3.06 10^{-7}	2.81 10^{-6}	6.06 10^{-6}	2.80 10^{-5}	3.06 10^{-5}	3.09 10^{-5}
3.0	1.37	7.82 10^{-7}	7.75 10^{-6}	7.12 10^{-5}	1.54 10^{-4}	7.12 10^{-4}	7.75 10^{-4}	7.82 10^{-4}
4.0	3.20	8.27 10^{-6}	8.20 10^{-5}	7.53 10^{-4}	4.14 10^{-3}	7.53 10^{-3}	8.20 10^{-3}	8.27 10^{-3}
5.0	6.14	4.55 10^{-5}	4.51 10^{-4}	4.14 10^{-3}	2.28 10^{-2}	4.14 10^{-2}	4.51 10^{-2}	4.55 10^{-2}

*From the earlier report of Dubey [11]

Neglecting τ_U^{-1} as well as the term of lower values, Eq. (16) becomes

$$\Delta K = c_0 b_1 \tau_B^2 I_6 \left(1 - 2c\tau_B F_6^9 - 2D\tau_B F_6^{10} - b_1 \tau_B F_6^8\right). \tag{17}$$

Due to the very low value of temperature and the large value of θ, one can evaluate integral I's with the help of the Riemann zeta function, and one gets an expression for ΔK

$$\Delta K = 720 \rightarrow c_0 b_1 \tau_B^2 (1 - 1008c\tau_B - 10080D\tau_B - 56b_1\tau_B).$$

In the absence of dislocations, the expression for ΔK stated in Eq. (17) becomes

$$\Delta K = c_0 b_1 \tau_B^2 I_6 (1 - 2D\tau_B F_6^{10} - b_1 \tau_B F_6^8), \tag{18}$$

which is the same as obtained by Dubey [4] for a pure sample.

3. Results and discussion

Using the above expression, ΔK is calculated in the temperature range of 0.2–5 K for a sample having core dislocations for different values of P (10^3 to 10^{-3}) as shown in Table I. The values of constants τ_B^{-1}, A and a are taken from the earlier report of Dubey [11], but an approximate value of E has been calculated as $E = 1.0 \times 10^{-23}$s. deg^{-3}. To test the applicability of the analytical expressions, the value of ΔK has been calculated in the temperature range of 0.2–5 K.

From Table I, it is clear that the contribution of ΔK to the total phonon conductivity is very small in comparison with K, thus we can neglect its contribution, which is similar to the earlier finding of [2–5]. With the help of Table II, the values of ΔK obtained in the frame of the analytical expression are very close to those obtained using numerical integrations.

Table II

Phonon conductivity correction term ΔK in the frame of Callaway integral, $(\Delta K)_{\text{anal.}}$ is the value of ΔK obtained in the frame of analytical expression, $(\Delta K)_{\text{num. int.}}$ is the value of ΔK based on numerical integration

T K	$(\Delta K)_{\text{anal.}}$		$(\Delta K)_{\text{num. int.}}$		Percentage difference*	
0.2	2.819	10^{-14}	2.819	10^{-14}	0	
0.4	7.217	10^{-12}	7.218	10^{-12}	1.385	10^{-2}
0.6	1.849	10^{-10}	1.850	10^{-10}	5.405	10^{-2}
0.8	1.847	10^{-9}	1.849	10^{-9}	0.108	
1.0	1.099	10^{-8}	1.102	10^{-8}	0.272	
2.0	2.786	10^{-6}	2.816	10^{-6}	1.065	
3.0	6.910	10^{-5}	7.125	10^{-5}	3.017	
4.0	6.389	10^{-4}	7.532	10^{-4}	15.175	
5.0	3.237	10^{-3}	4.148	10^{-3}	21.962	

*Percentage difference = $\frac{(\Delta K)_{\text{num. int.}} - (\Delta K)_{\text{anal.}}}{(\Delta K)_{\text{num. int.}}} \cdot 100$.

With the help of Eq. (17), it can be concluded that for $\tau_B^{-1} \gg \tau_{cd}^{-1}$, $\Delta K \propto b_1 \tau_B^2$, which indicates that ΔK mainly depends on τ_B^{-1} and $\tau_{3Ph,N}^{-1}$. The present results are in good accord with the findings of previous works [4, 12]. At the same time, with the help of Eq. (13), it is clear that for $\tau_{cd}^{-1} \gg \tau_B^{-1}$, $\Delta K \propto B_1/c^2$, which shows that ΔK is mainly governed by $\tau_{3Ph,N}^{-1}$ and τ_{cd}^{-1}.

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