NONLINEAR HEAT TRANSFER IN A LATTICE HAVING DISLOCATION CORE

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ABSTRACT

A simple expression for the lattice thermal conductivity for a sample having dislocation core together with isotopic impurities has been obtained in the frame of the nonlinear heat transfer theory at low temperatures.

The lattice thermal conductivity of an insulator of finite dimension at low temperature is of recent importance. At these temperatures, the important scatterers of phonons are the boundary walls of the crystal and various kinds of defects present in the crystal lattice. Erdos[1] first studied such a system to obtain an analytical expression for the lattice thermal conductivity. It is normally assumed that the system deviates slightly from its thermodynamical equilibrium which leads to the concept of local temperature and the linearization of kinetic equation with respect to the temperature gradient. Following Erdos and using the boundary conditions consistent with the experimental situation, Kazakov and Nagaev[2] (KN) calculated the nonlinear heat transfer in a lattice having isotopic defects alone, by reformulating the Erdos expression for the lattice thermal conductivity of such samples and they obtained a simple expression for it, based on the relaxation time approach. Due to its simplicity, it was applied by several workers[3-8] to study the lattice thermal conductivity of samples having various types of defects (such as electrons, substitutional impurities, etc.) in the frame of the nonlinear heat transfer theory. The aim of the present note is to extend the KN theory for a sample having dislocation cores together with isotopic defects by obtaining an analytical expression for the lattice thermal conductivity of such sample in the frame of the nonlinear heat transfer theory.

Assuming the additivity of the inverse of relaxation times due to the different scattering processes, the combined scattering relaxation time due to the crystal lattice defects (dislocation cores and isotopic impurities only) can be expressed as

$$\tau^{-1}(k) = \tau^{-1}_{iso}(k) + \tau^{-1}_{dis,c}(k) \qquad (1)$$

where $\tau^{-1}(k)$ is the combined scattering relaxation rate, $\tau^{-1}_{iso}(k)$ and $\tau^{-1}_{dis,c}(k)$ are the scattering relaxation rates due to point-defects and dislocation core respectively. The respective scattering relaxation rates[9] are given by

$$\tau^{-1}_{iso}(k) = Aw^4(k) \text{ and } \tau^{-1}_{dis,c}(k) = cw^3(k) \qquad (2)$$

where $w(k)$ is the phonon frequency as a function of the phonon wave vector k, A and c are the scattering strengths due to the respective scattering processes. Thus, the combined scattering relaxation rate is given by

$$\tau^{-1}(k) = Aw^4(k) + cw^3(k). \qquad (3)$$

Following KN as well as Dubey[3] and using eqn. (3), an expression for the lattice thermal conductivity can be obtained in the frame of the nonlinear heat transfer theory as

$$K = K_0 [1 - (Lc/2v)(k_B T/\hbar)^3 I_3/I_1 - (LA/2v)(k_B T/\hbar)^4 I_2/I_1] \qquad (4)$$

where

$$K_0 = (3k_B/2\pi^2 v)(k_B T/\hbar)^3 (L/v) I_1 \qquad (5)$$

$$I_1 = \int_0^\infty x^3 (e^x - 1)^{-1} dx = 6\cdot 5 \qquad (6)$$

$$I_2 = \int_0^\infty x^7 (e^x - 1)^{-1} dx = 5\cdot 06\ 10^3 \qquad (7)$$

$$I_3 = \int_0^\infty x^6 (e^x - 1)^{-1} dx = 7\cdot 26\ 10^2 \qquad (8)$$

k_B is the Boltzmann constant, $\hbar$ is the Planck constant divided by 2π, L is the Casimir[10] length of the crystal under sthdy, v is the average phonon velocity, T is the temperature and $x = (\hbar w/k_B T)$. Substituting the numerical value of the integrals, eqn. (5) reduces to

$$K = 3\cdot 060\ 10^{10} (L/v^2) T^3 (1 - 1\cdot 253\ 10^{35} \times (Lc/v) T^3 - 1\cdot 143\ 10^{47} (LA/v) T)^4 \qquad (9)$$

where K, L, v, c, A and T are expressed in watt/deg/cm, cm, cm/sec, sec^2, sec^3 and °K respectively.

It should be noted that to avoid the complications, the scattering relaxation rates due to other defects have been ignored in eqn. (4) and only dislocation core has been considered together with isotopic scattering. However, if one considers dislocation strain field scattering also together with core scattering, the expression for the lattice thermal conductivity stated in eqn. (9) can be expressed as

$$K = 3\cdot060\ 10^{10}\ (L/v^2)\ T^3\ [1 - 1\cdot253\ 10^{35}\ (Lc/v)\ T^3 - 1\cdot143\ 20^{47}\ (LA/v)\ T^4 - 2\cdot507\ 10^{11}\ T\ (La/v)] \qquad (10)$$

where a is the strain field scattering strength and other terms have the same meaning as defined earlier.

Substituting core scattering strength $c = 0$, *i.e.*, in the absence of core, eqn. (4) reduces to

$$K = K_0\,(1 - (LA/2v)\,(k_B T/\hbar)^4\, I_2/I_1) \qquad (11)$$

which is similar to the expression reported by KN for a sample having isotopic impurities alone.

Due to lack of experimental data, a comparative study is made between results obtained in the frame of the expression reported and in the frame of the Callaway[11] theory. The lattice thermal conductivity has been calculated in the temperature range 0·2–10° K using eqn. (9) as well as using the Callaway integral[11], and results obtained are reported in Table I. The

TABLE I

The values of the lattice thermal conductivity obtained in the frame of the expression reported and in the frame of the Callaway theory in the temperature range 0·2–10° *K. K (present) is the lattice thermal conductivity obtained in the frame of eqn.* (9) *and K (Callaway) is the same obtained using the Callaway integral*

T (° K^3)	K (present)*	K (Callaway)*	% Difference**
0·2	4·08 10^{-4}	4·08 10^{-4}	0
0·4	3·26 10^{-3}	3·26 10^{-3}	0
0·6	1·10 10^{-2}	1·10 10^{-2}	0
0·8	2·61 10^{-2}	2·61 10^{-2}	0
2·0	5·09 10^{-2}	5·09 10^{-2}	0
2·0	4·07 10^{-1}	4·07 10^{-1}	0
3·0	1·37	1·37	0
4·0	3·24	3·20	1·25
5·0	6·27	6·14	2·12
6·0	10·70	10·34	3·48
7·0	16·65	15·88	4·88
8·0	24·15	22·77	6·06
9·0	33·02	30·16	6·65
10·0	42·81	40·35	6·10

* The values are expressed in watt/deg/cm.

** % Difference = K (present) − K (Callaway)/ K (Callaway).

percentage difference between these two results is also listed in this table. From this table, it is clear that below 4° K, the results obtained in the frame of the expression reported in the present work is exactly the same as in the frame of the Callaway theory. However, there are some descrepancies above 4° K, and the values obtained using eqn. (9) are larger than that based on the Callaway integral. This is because of the phonon-phonon scattering processes which have not been included in the present expression. At the same time, it should also be noted that the KN theory is valid only at low temperatures where the boundary scattering plays a dominating role over other scattering processes.

From eqns. (4) and (9), it is clear that the expression obtained for the lattice thermal conductivity of a sample having core together with the point-defect, in the frame of the nonlinear heat transfer theory, is very simple and one can estimate the lattice thermal conductivity of such samples without going through any complication. In the absence of core scattering, the expression obtained also reduces to the expression obtained by KN for a lattice having isotopic impurities alone. At the same time, it is interesting to note that the expression reported in the present note is much simpler than the expression proposed by Callaway. With the help of Table I, it is also clear that it gives good results at low temperatures.

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