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Lattice Thermal Conductivity by using Awad's Model

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Abstract: ***The lattice thermal conductivity of Mg_2Ge has been analyzed on the basis of the Awad's model in the temperature range (4-800)K , In the analysis the phonon scattering from boundary, point defects, four and three-phonon (normal and umklapp) processes has been considered .Good agreement with the experimental results has been obtained.The study broached whipped to the contributions of the transverse and longitudinal phonons in the total lattice thermal conductivity .***

Keywords: thermal conductivity , phonons, Mg_2Ge.

1. Introduction

The lattice thermal conductivities of crystals are of practical and theoretical importance. They are essential for the reliability and performance of energy conversion systems,thermal insulators and conductors, microdevices, and microelectronic systems. For industrial applications, lattice conductivity is often obtained by the measurements of bulk crystals [1].Therefore The lattice thermal conductivities of insulators and semiconductors have been studied by a number of workers [1-4].

Mg_2Ge is a semiconductor with a slightly smaller indirect band gap of (0.57-0.74) eV , K. S. Dubey was used [5] two-mode conduction, has been applied to explain the phonon conductivity data of Mg_2 Ge in the temperature range (4-800) K. while A. H. Awad and K. S. Dubey [6]have been analysed The lattice thermal conductivities of Mg_2Ge and Mg_2Si in the temperature range (2-1000) K.

Recently Awad [7]has been successfully in the calculation lattice thermal conductivity, by using dispersion relation of monatomic and diatomic lattices, he has taken accounts both of dispersion relation for sound phonons and nonequilibrium distribution function consequent at interaction with the nearest and all atoms. A lot of workers have been successfully in using this model [7-9] in the calculation lattice thermal conductivity for many of solids. The aim study present is included by calculation lattice thermal conductivity of Mg_2Ge compound in the the temperatures range (4-800 K),by using awad's relations of diatomic lattices, the effect non equilibrium distribution function , as examination importance The percentage of The contribution of transverse longitudinal phonons in the lattice thermal conductivity . Also we had done by the study Relaxation rates of the phonon scattering as a function for the frequency at constant temperature.

2. Theory

For treatment aberration magnitude on Distribution Function and giving on equation is more accuracy and resilience in calculation conductivity, Awad [7] used relations of diatomic lattice by use Nonequilibrium Distribution Function ,Where the lattice thermal conductivity consists of two parts : the first one KT is attributed to the contribution of transverse phonons, whereas the second part KL is due to the contribution of longitudinal phonons, therefore the lattice thermal conductivity has been written as[11]:

$$K_i = 2K_T + K_L \quad (1)$$

and K [7] is then given by:

$$K_i = c_2 \frac{\theta_i^2}{C_{\upsilon i}} \left[I_1 + I_2 I_3 / I_4 \right] \quad (2)$$

$$c_2 = \frac{MK_B^4}{6\pi^2 a\hbar^2 (M+m)},$$

The specific heat can be written as,

$$C_\upsilon = \frac{V(M+m)\hbar T}{2\pi^2 a^3 M\theta^2} \int_0^{\theta_i/T} \frac{x^3 e^x}{(e^x-1)^2} \frac{(\sin^{-1}\sqrt{J_\circ})^2 (1-2J/M_\circ)}{\sqrt{J_\circ(1-J_\circ)}} dx$$

Where,

$$I_1 = \int_0^{\theta_i/T} \left[\tau_c \frac{x^2 e^x}{(e^x-1)^2} \frac{\sqrt{J_\circ(1-J_\circ)}(\sin^{-1}\sqrt{J_\circ})^2}{(1-2J/M_\circ)} \right] dx \quad ,$$

$$I_2 = \int_0^{\theta_i/T} \left[\frac{\tau_c}{\tau_N} \frac{xe^x}{(e^x-1)^2} (\sin^{-1}\sqrt{J_\circ})^3 \right] dx \quad ,$$

$$I_3 = \int_0^{\theta_i/T} \left[\frac{\tau_c}{\tau_N} \frac{e^x}{(e^x-1)^2} \frac{J_\circ(1-J_\circ)(\sin^{-1}\sqrt{J_\circ})^3}{(1-2J/M_\circ)^2} \right] dx$$

And

$$I_4 = \int_0^{\theta_i/T} \left[\frac{1}{\tau_N} \left(1 - \frac{\tau_c}{\tau_N} \right) \frac{e^x}{x(e^x-1)^2} \frac{\sqrt{J_\circ(1-J_\circ)}(\sin^{-1}\sqrt{J_\circ})^4}{(1-2J/M_\circ)} \right] dx$$

$$J = T^2 x^2 / M\theta^2,\ J_\circ = J(M+m)(1-J/M_\circ)$$

$$M_\circ = (M+m)/mM$$

Where, θ_D is Debye temperature, M is mass of the first atom, m is mass of the second mass , dimensionless variable x ,the τ are the relaxation times is then given by[10]:

$$\tau_i^{-1} = \tau_B^{-1} + \tau_P^{-1} + \tau_{4ph}^{-1} + \tau_{3ph}^{-1}$$
$$= v/L + A\omega^4 + B_H \omega^2 T^2 + \tau_{3ph}^{-1} \quad (3)$$

Where ν is the value of the velocity , L is the characteristic length, *A* is the point defect scattering strength and B_H is the four phonon scattering strength.

While Dubey[12] proposed an expression for the three-phonon scattering relaxation rate τ_{3ph}^{-1} , For the case of transverse phonons, he assumed:

$$\tau_{3ph,T}^{-1} = \left(B_{TN,I} + B_{TU,I} e^{-\theta_D/\alpha T}\right) \omega T^{m_{T,I}(T)} \quad \text{for } 0<\omega<\omega^4 \quad (4)$$

and for longitudinal phonons

$$\tau_{3ph,L}^{-1} = \left(B_{LN,I} + B_{LU,I} e^{-\theta_D/\alpha T}\right) \omega^2 T^{m_{L,I}(T)} +$$
$$\left(B_{LN,II} + B_{LU,II} e^{-\theta_D/\alpha T}\right) \omega^2 T^{m_{L,II}(T)} \quad \text{for } 0<\omega<\omega^4 \quad (5)$$

As Dubey[12] suggested the use of the average value of the upper and lower bounds of *m(T)* reported by Guthrie, and *m(T)* is given by

$$[m(T)]_I = x_{max}\left(e^{m_{max}} - 1\right)^{-1} + 0.5x_{max}$$

$$[m(T)]_{II} = 0.5\, x_{max}\left(e^{x_{max}} - 1\right)^{-1} e^{0.5x_{max}} + 0.5$$

Where $x_{max} = \hbar\omega_{max}/K_B T$

3. Results and Discussion

Awad's model been successfully in analysed The lattice thermal conductivity of Mg_2Ge compound in the temperature range (4-800 K),The study used the study used non equilibrium distribution function in the calculation The lattice thermal conductivity (by used eqs 1,2).while used in the calculation three phonon scattering (eqs4,5).

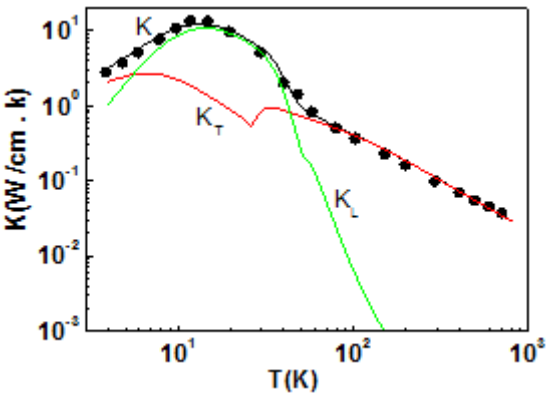

Figure 1: K_T is the contribution of transverse phonons,K_L, is the contribution of longitudinal phonons. K is the total lattice thermal conductivity. Circles represent experimental points[5].

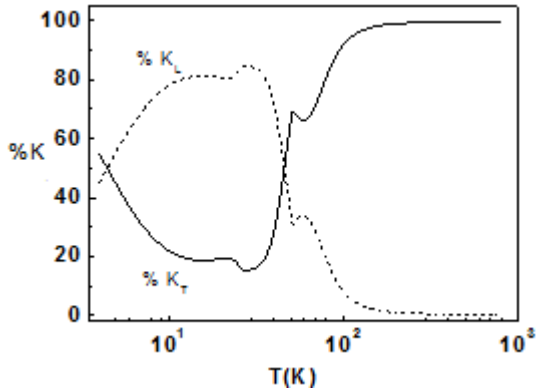

Figure 2: Percentage contribution of longitudinal $\%K_L$ andtransverse phonons $\%K_T$.

In the figure (1) appearing best fitting of the present work by using the adjustable parameters, which it show in table (I,II), with the experimental data[5], especially at the maximum conductivity curve, As showed the lattice thermal conductivity of transverse phonons K_T and the lattice thermal conductivity of longitudinal phonons K_L , As We noticed in the Figure (2) The contribution of transverse phonons towards thermal conductivity is in general greater than that of longitudinal phonons, is approximately 100% of the total conductivity at high temperatures , and come back the cause contribution two mode of transverse phonons and contribution one mode of longitudinal phonons in total thermal conductivity, and this results agreement with [5,10,13].

Table 1: The adjustable parameters values calculated and used for theoretical curves of Mg_2Ge compound .

Parameter	Value
$\tau_{BT}^{-1}(s^{-1})$	$1x10^5$
$\tau_{BL}^{-1}(s^{-1})$	$2x10^5$
$A_T s^3$	$1.5x10^{-44}$
$A_L s^3$	$1x10^{-47}$
B_{TN} deg^{-m}	$1x10^{-14}$
B_{TU} deg^{-m}	$2x10^{-6}$
$B_{LN,I}$ s.deg^{-m}	$2x10^{-24}$
$B_{LU,I}$ s.deg^{-m}	$3.5x10^{-20}$
$B_{LN,II}$ s.deg^{-m}	$1x10^{-21}$
$B_{LU,II}$ s.deg^{-m}	$3.5x10^{-17}$
B_{HT} s.deg^{-2}	$1x10^{-23}$
B_{HL} s.deg^{-2}	$3.5x10^{-23}$

Table 3: Value of constant used to calculate thermal conductivity of Mg_2Ge[5].

a	θ_D	θ_1	θ_2	M(C)kg	M(kg)
6.387°A	570°K	210°K	306°K	$5.314x10^{-23}$	$3.985x10^{-23}$

At constant temperatures (T= 40K ,T=400K)and within low frequencies range ,the figure (3,4) appearing dominance for the boundary phonon scattering over another kinds of scatters for transverse phonons and longitudinal phonons . while at high frequencies with same temperatures (T= 40K

,T=400K) appearing dominance for umklapp processes of three phonon scattering on other scatters ,and for transverse and longitudinal phonons as in the figure (3,4) ,this is an agreement with the results of the authors[8,10,14].

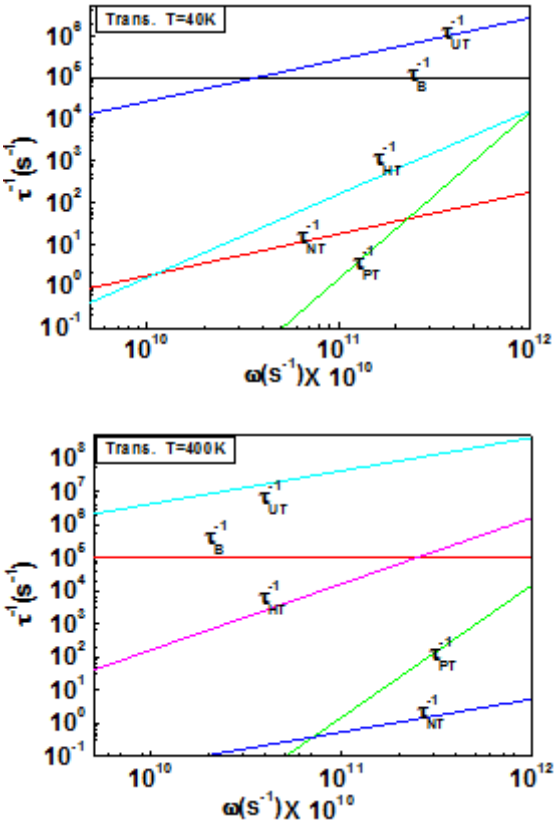

Figure 3: Relaxation rates of the deferent phonon scattering for transverse phonons as a function to the Frequency at constant temperature(T=40,400K).

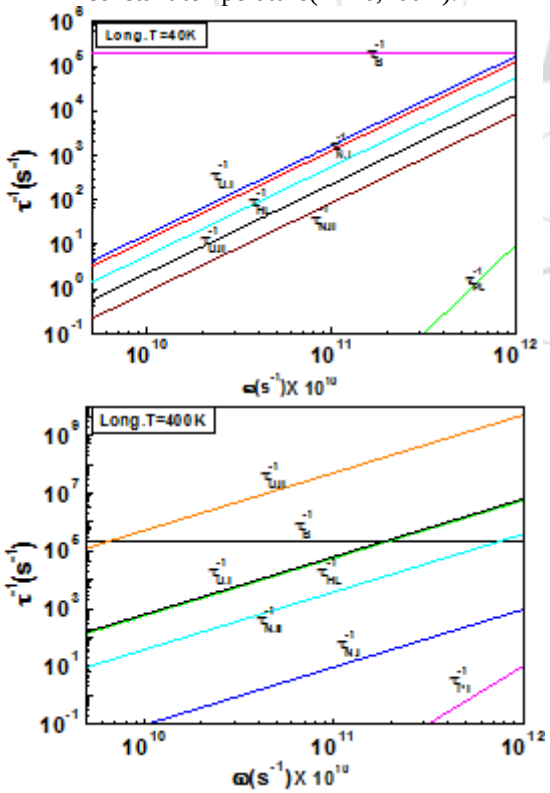

Figure 4 : Relaxation rates of the deferent phonon scattering for longitudinal phonons as a function to the Frequency at constant temperature(T=40,400K).

4. Conclusion

The lattice thermal conductivity of Mg2Ge compound has been measured over the temperature range (4 - 800K). Awad method has been applied to analyze the obtained data. Where it can be seen from a results a good fitting between experimental and theoretical thermal conductivity resulted.

As it has been found the transverse phonons in general make have the major contribution to the lattice thermal conductivity.
Aslo The boundary and umklapp processes of three phonon scattering play important roles in the lower and higher frequencies consecutively.

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References

[1] B. L. Huang and M. Kaviany , JOURNAL OF APPLIED PHYSICS, 100, 123507 (2006).
[2] Mei-Jiau Huang, Wen-Yen Chong, and Tai-Ming Chang, JOURNAL OF APPLIED PHYSICS , 99, 114318 (2006).
[3] B. J. Abdullah, Phys. Rev, B75, (2007) .
[4] Zhao Wang and Natalio Mingo , APPLIED PHYSICS LETTERS 97, 101903 (2010).
[5] K. S. Dubey, P HYSI CAL RE VIE W B 13, 4 , 1976.
[6] A. H. Awad and K. S. Dubey, Journal of Thermal Analysis, 24 (1982) (233-260).
[7] A.H. Awad , Ph.D. Thesis , Basrah University, Basrah (Iraq) (2003).
[8] A. J. Mohammed , M. Sc. Thesis , Basrah University,_Basrah , Iraq(2007).
[9] H.A.Hasan, M.Sc. Thesis, Basrah University, Basrah, Iraq(2011).
[10] B. H. Mohammed, Journal of Collger of Education, B3, 38 , 2012.
[11] S. M. Mamand, M. S. Omar and A. J. Muhammed, Adv. Mat. Lett., 3(6), 2012,(449-458).
[12] K.S. Dubey , J. Thermal Analysis 19, 263 (1980).
[13] Isra'a M . Ali , Journal of Collger of Education, No. 6 ,(554-571) , (2011).
[14] D. B. Habesh, Journal of Basrah Researches (Sciences) Vol . 36, No. 3, 15 June (2010).