IOSR Journal of Applied Physics (IOSR-JAP)
e-ISSN: 2278-4861.Volume 7, Issue 3 Ver. III (May. - Jun. 2015), PP 69-75
www.iosrjournals.org

Role of Three Phonon Scattering in the Thermal Conductivity of KCl and NaCl Compounds

B. H. Mohammed
Department of Physics, College of Sciences, ThiQar University, Nassiriya, Iraq

Abstract: *Using Awad's Model, thermal conductivity of KCl and NaCl in the temperature range between (1-100)K. Specialized present study to the formulas Dubey and Awad of three phonon scattering relaxation rate for the calculation the thermal conductivity lattice.Good agreement with theexperimental data achieved by using the adjustable parameter.*
Keywords: *Thermal conductivity, Three phonon scattering, KCl , NaCl.*

I. INTRODUCTION

Thermal conductivity has been commonly used as fundamental transport property which successfully characterizesthe broad range of crystalline solids and is physically important in understanding the acoustical behavior oflowdimensional systems nowadays[1], therefore many of researchers gave big interest of the property thermal conductivity [2-4].

KCl and NaCl compounds are alkali halides ,Where many workers have studied the thermal conductivity of doped and undoped alkali halides .where Singh and Verma [5] explained the temperature dependence of the thermal conductivity of KC1 and NaCl, found that the transverse phonons make a major contribution towards thermal transport in these alkali halides.WhileDubey [6] separated contributions of longitudinal and transverse phonons for the lattice thermal conductivity of NaF compound in the temperature range (2-100) K. Roth and Anderson [7] has been studied through thermal conductivity of crystals in the range(0.08-5) K ofLiF andNaCl.

For the three phonon scattering relaxation rate is an important role in the calculation lattice thermal conductivity.Guthrie[8] was classifying three phonon scattering relaxation rate to two classes : class I events in which the carrier phonon is annihilated by combination, and class II events in which annihilation takes place by splitting. Guthrie classification leads to the participation of the transverse phonons in class I events only, the longitudinal phonons participate in both class I and class II events.

Awad [9] progressed mathematical model 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. He got more accurate formulas in order to calculate the lattice thermal conductivity. these formulas applied with successfully by many of researchers [9-12].

In the present work, we have introduced how possibly Awad model is applied to calculate the lattice thermal conductivity at a wide range of temperature (1-100 K) of KCl and NaCl, And also study the effect of the three phonon scattering relaxation rate on the calculation of the lattice thermal conductivity by using Dubey's Model and Awad's model of the three phonon scattering relaxation rate.AS the knowledge range communique an agreement with the results experimental and theoretical.

II. THEORY

The three phonon scattering plays an important role in the calculation of lattice thermal conductivity, for this study have used two the Models of The three phonon scattering for study lattice thermal conductivity and as the following:

1. Dubey's Model

Dubey[13] can used formula for both two pragmatism and ,Therefore perishing the total Phonon Scattering Relaxation Rate of transverse phonons take the formula following :

$$\tau_{3ph,T}^{-1} = \left(B_{TN,I} + B_{TU,I}e^{-\theta/\alpha T}\right)\omega T^{m_{T,I}(T)} \qquad for\ 0 < \omega < \omega_4 \quad (1)$$

And for longitudinal phonons is figure the following:

$$\tau_{3ph,L}^{-1} = \left(B_{LN,I} + B_{LU,I}e^{-\theta/\alpha T}\right)\omega^2 T^{m_{L,I}(T)} + \left(B_{LN,II} + B_{LU,II}e^{-\theta/\alpha T}\right)\omega^2 T^{m_{L,II}(T)} \qquad for\ 0 < \omega < \omega_4 \quad (2)$$

As Dubey13] suggested the use of the average value of the upper and lower bounds of *m(T)* reported by Guthrie [8], and *m(T)* is given by

$$[m(T)]_I = x_{max}\,(e^{x_{max}} - 1)^{-1} + 0.5x_{max} \qquad (3)$$

For class processes (I) and for class processes (II) :

$[m(T)]_{II} = 0.5x_{max}\,(e^{x_{max}} - 1)^{-1}e^{0.5x_{max}} + 0.5(4)$

In these expressions, $x_{max} = \hbar\omega_{max}/K_BT$, ω_{max} is the phonon frequency at the boundary of the first Brillouin zone, B's are the scattering strength of the three phonon processes and suffixes*T*, *L*, *U*, I and II refer to transverse phonons, longitudinal phonons, normal process, umklapp process, class I events and class II events respectively.

2. Awad's Model:

For found formula analytical for equation three phonon scattering relaxation rate , Awad[9] been taken into account all studies earlier and been given two propositions , in the first proposition been assumed the role $\tau_{3ph,N}^{-1}$ in the lattice thermal conductivity process limited on frequencies lower only (ω_1 for transverse phonons ,ω_2 And for longitudinal phonons) , where $\tau_{3ph,U}^{-1}$ been neglected association . while the second proposition had found of expediential use $\tau_{3ph,TU}^{-1} \propto \omega^2$ instead of ω, he proposed equation three phonon scattering relaxation rate,and is for transverse phonons to the following the figure:

$\tau_{3ph,T}^{-1} = B_{TN}\omega T^{m_{T,I}(T)}$ $for\ 0 < \omega < \omega_1$ (5)

$\tau_{3ph,T}^{-1} = B_{TN}\omega T^{m_{T,I}(T)} + B_{TU}\omega^2 T^{m_{T,I(T)}}e^{-\theta_D/\alpha T}$ $for\ \omega_1 < \omega < \omega_2$ (6)

And for longitudinal phonons:

$\tau_{3ph,L}^{-1} = B_{TN,I}\omega^2 T^{m_{L,I}(T)} + B_{LN,II}\omega^2 T^{m_{L,II}(T)}$ $for\ 0 < \omega < \omega_3$ (7)

$\tau_{3ph,L}^{-1} = B_{LN,I}\omega^2 T^{m_{L,I}(T)} + B_{LN,II}\omega^2 T^{m_{L,II}(T)} + B_{LU,I}\omega^2 T^{m_{L,I}(T)}e^{-\theta_D/\alpha T} + B_{LU,II}\omega^2 T^{m_{L,II}(T)}e^{-\theta_D/\alpha T}$ $for\ \omega_3 < \omega < \omega_4$ (8)

In addition to three phonon scattering , must be taken into account the other scattering relaxation rates :the boundary scatteringτ_B^{-1}, point defectsτ_P^{-1} and four phonon scatteringτ_{4Ph}^{-1}.

3.Thermal Conductivity:

While the lattice thermal conductivity relation can wrote with the following formula[14]:

$K = K_L + 2K_T$ (9)

Where, K_L *and* K_T are represents the lattice thermal conductivity for longitudinal andtransverse phonons , for purpose the arriving to results more accuracy in calculation *K* values and for treatment aberration magnitude on Distribution Function , the study has been used Awad's relations of diatomic lattice in one dimension by use Nonequilibrium Distribution Function. The thermal conductivity latticeequation has been become as follows:

$$K_i = c_2\frac{\theta_i^2}{C_{vi}}[I_1 + I_2I_3/I_4] \quad (10)$$

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

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

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

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

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

and

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

As,

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

$J_\circ = J(M+m)(1-J/M_\circ)$, $M_\circ = (M+m)/mM$, $x = \hbar\omega/K_BT$

And where , i refer to longitudinal andtransverse phonons , M is mass of the first atom, m is mass of the second mass , a is lattice constant , x is dimensionless variable, K_B is Boltzmann's constant, T is temperature,ω is The phonon frequency,the τ_c are the relaxation times , given by:

$$(\tau_c^{-1})^i = (\tau_B^{-1})^i + (\tau_P^{-1})^i + (\tau_{4Ph}^{-1})^i + (\tau_{3Ph}^{-1})^i$$
$$= \frac{\upsilon}{L} + A\omega^4 + B_H\omega^2T^2 + \tau_{3ph}^{-1}$$

III. RESULT AND DISCUSSION

By using Awad's[9] relations of diatomic latticeNonequilibrium Distribution Function (eq.10),we can attempt communique role of three phonon scattering relaxation rate in calculation lattice thermal conductivity of KCl and NaCl compounds in the temperature range (1-100 K)as in figures (1,2,3,4) , Therefore the study used two formulas of three phonon scattering relaxation rate, the first of Dubey's Model (eqs.1-4) and the second Awad's Model(eqs.5-8).As the study used the adjustable parameters of the phonon scattering andconstantsappearing in tables (1,2,3).

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

Parameter	Value	
	Dubey's Model	Awad's Model
τ_{BT}^{-1}(s^{-1})	2.7×10^5	2.6×10^5
τ_{BL}^{-1}(s^{-1})	2.3×10^5	1.9×10^5
$A_T s^3$	2×10^{-44}	5×10^{-45}
$A_L s^3$	5×10^{-45}	1×10^{-45}
B_{TN}deg^{-m}	4×10^{-11}	1×10^{-14}
B_{TU}deg^{-m}	1.7×10^{-7}	1×10^{-5}
$B_{LN,I}$s.deg^{-m}	2×10^{-23}	2.5×10^{-21}
$B_{LU,I}$s.deg^{-m}	1×10^{-17}	1×10^{-14}
$B_{LN,II}$s.deg^{-m}	1×10^{-21}	9×10^{-20}
$B_{LU,II}$s.deg^{-m}	1×10^{-16}	5×10^{-14}
B_{HT} s.deg^{-2}	8×10^{-22}	1.5×10^{-21}
B_{HL} s.deg^{-2}	1×10^{-21}	1×10^{-21}

Table 2: The adjustable parameters values calculated and used for theoretical curves of NaCl compound.

Parameter	Value	
	Dubey's Model	Awad's Model
τ_{BT}^{-1}(s^{-1})	3×10^5	3.1×10^5
τ_{BL}^{-1}(s^{-1})	2×10^5	1.5×10^5
$A_T s^3$	1×10^{-44}	1×10^{-46}
$A_L s^3$	1×10^{-45}	1×10^{-46}
B_{TN}deg^{-m}	4×10^{-11}	1×10^{-12}
B_{TU}deg^{-m}	2.3×10^{-6}	4.5×10^{-5}
$B_{LN,I}$s.deg^{-m}	1.7×10^{-23}	1.5×10^{-21}
$B_{LU,I}$s.deg^{-m}	2×10^{-22}	1×10^{-15}
$B_{LN,II}$s.deg^{-m}	8×10^{-21}	8×10^{-20}
$B_{LU,II}$s.deg^{-m}	7.5×10^{-18}	5×10^{-14}
B_{HT} s.deg^{-2}	--------	9×10^{-22}
B_{HL} s.deg^{-2}	--------	22×10^{-22}

Table 3:**Value of constant used to calculate thermal conductivity of KCl and NaCl.**

Parameters	a[15]	θ_D[15]	θ_1[5]	θ_2[5]	θ_3[5]	θ_4[5]	α	M(Cl)kg	M(kg)
KCl	6.162A^0	172^{0}K	63^{0}K	84^{0}K	155^{0}K	190^{0}K	1.5	2.823×10^{-23}	3.155×10^{-23}
NaCl	5.776 A^0	220^{0}K	88^{0}K	126^{0}K	206^{0}K	244^{0}K	1.5	2.823×10^{-23}	1.827×10^{-23}

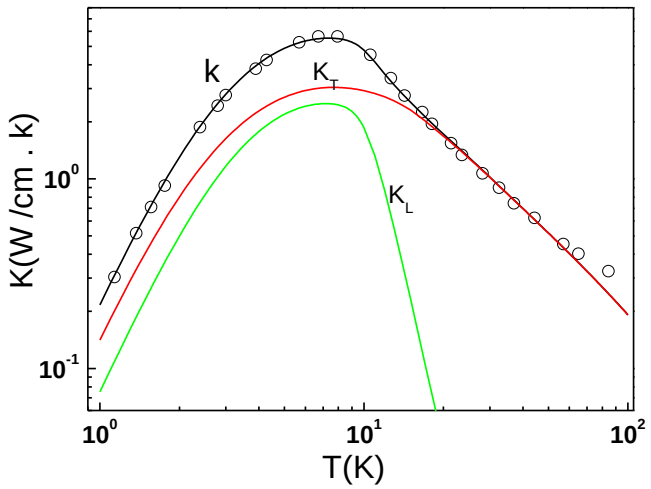

Fig.1:Conductivity curves of KCl ,byused Dubey's model of three phonon scattering relaxation rate.

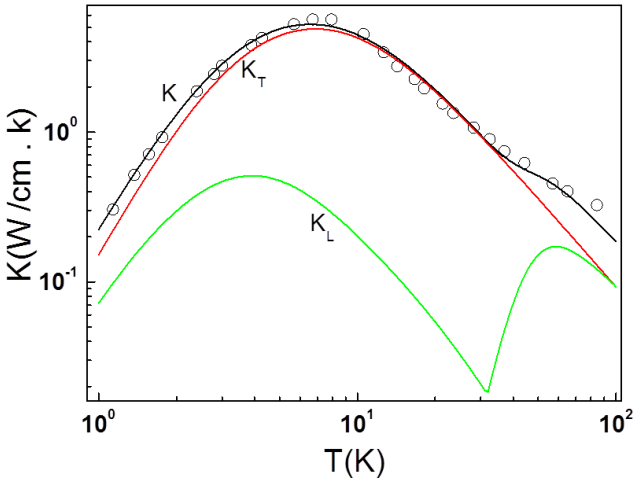

Fig.2:Conductivity curves of KCl by used Awad's model of three phonon scattering relaxation rate.

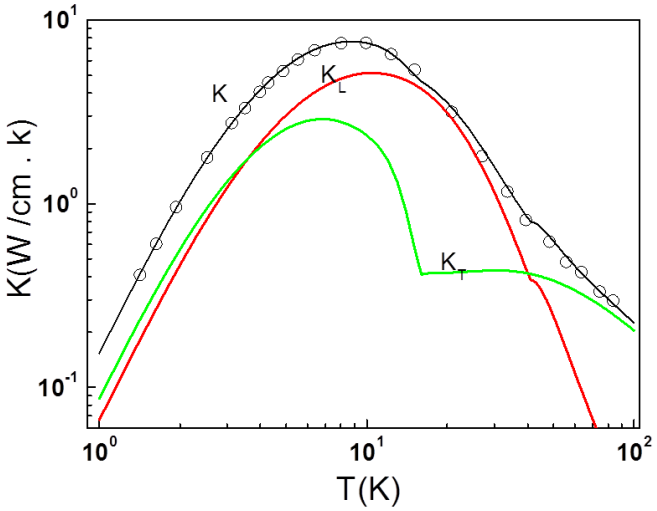

Fig.3:Conductivity curves of NaCl ,byused Dubey's model of three phonon scattering relaxation rate.

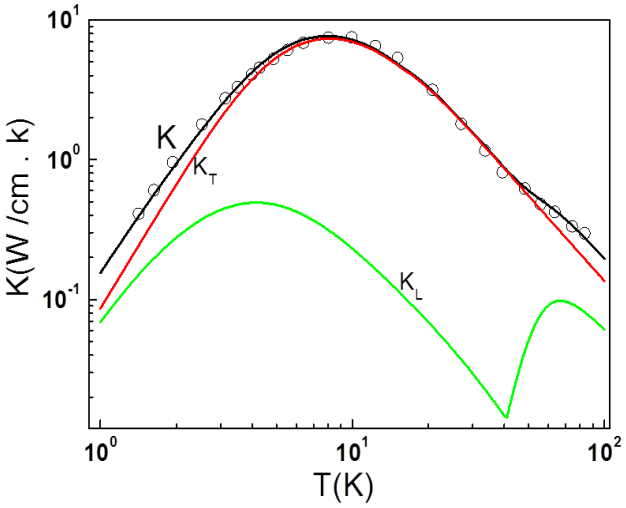

Fig.4:Conductivity curves of NaCl by used Awad's model of three phonon scattering relaxation rate.

As we discriminated between contributions the normal processes and the umklapp processes of three phonon scattering. While we noticed Singh and Verma [5] weren't discriminated between them.Best fitting can be noticed of these results with experimental data[5],especially at the maximum conductivity curve as in figures (1,2,3,4) .

Two figures (1,3) represents the lattice thermal conductivity of KCl and NaCl compounds by usingDubey's Modelof three phonon scattering relaxation rate ,While twofigures (2,4) represents the lattice thermal conductivity of KCl and NaCl compounds by using Awad's Model of three phonon scattering relaxation rate.

For range communique an agreement with the results experimental at use the correction processes different on the thermal conductivity lattice , then for find magnitude the percentage change in the values the thermal conductivity lattice by use equation the following :

$$K = \frac{K_{Theo.} - K_{Exp.}}{K_{Exp.}} \times 100\%$$

Where ,$K_{Theo.}$ and $K_{Exp.}$ represent the thermal conductivity values the theoretical and experimental consecutively.

We note in two tables(4,5) , Good agreement between theory and experiment values of the thermal conductivity lattice in temperatures rang (1-100)K of KCl and NaCl compounds , As tables is pear The largest agreement at calculation thermal conductivity lattice by used awad's model of used Dubey's Model .

Table 4: The change percentage between thermal conductivity theoretical and experimental values for KCl compound.

T(K)	%Kδ Dubey's Model	%Kδ Awad's Model
1.1	6.561	4.061
1.5	7.965	7.119
1.7	3.075	2.453
2.3	6.778	5.906
2.7	3.065	1.759
3.0	1.178	2.751
4.2	0.524	1.537
5.6	0.903	2.624
6.7	2.588	7.118
10.0	6.026	1.00
12.0	5.192	11.747
23.0	7.910	13.842
28.0	4.610	1.104
32.0	4.658	5.223
37.0	4.241	7.983
44.0	1.218	9.015
56.0	1.864	1.354
64.0	8.181	3.300
84	23.251	22.00

Table 4:The change percentage between thermal conductivitytheoretical and experimental values for KCl compound.

T(K)	%Kδ Dubey's Model	%Kδ Awad's Model
1.4	2.456	7.166
2.5	2.849	9.798
3.1	1.788	5.361
3.5	1.441	0.391
4.0	2.740	4.567
4.3	1.556	4.684
5.5	0.966	6.256
6.4	1.108	5.677
8.0	1.227	2.403
10.0	0.636	3.906
12.0	3.985	3.018
15.0	5.235	8.298
20.0	12.331	4.823
27.0	11.181	5.184
48.0	7.550	2.891
56.0	6.665	7.273
64.0	1.967	1.645
75.0	0.605	0.506
84.0	4.619	8.099

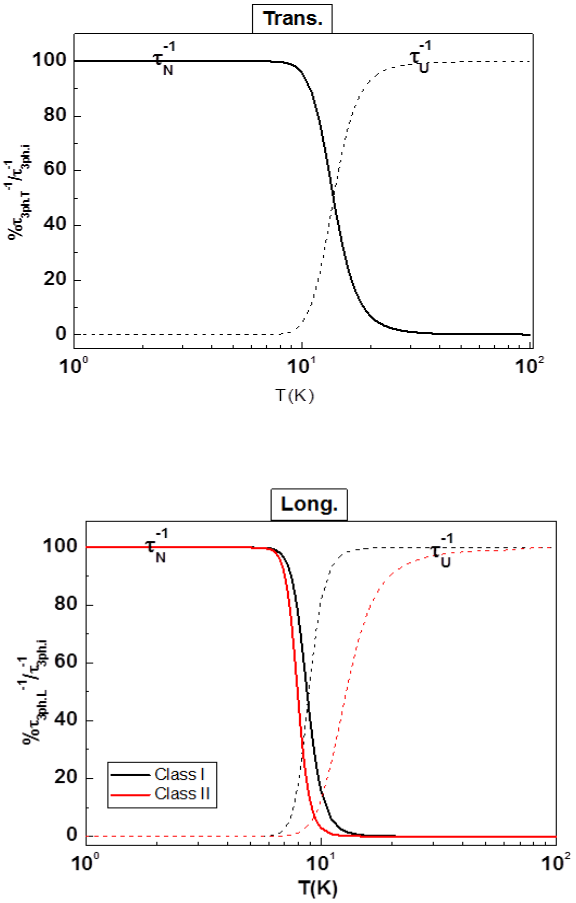

Fig.(5): The percentage contribution for the relaxation rate of normal and umklapp processes towards the relaxation rate of three phonon scattering by used Dubey's model of KCl compound (for Longitudinal and Transverse Phonons).

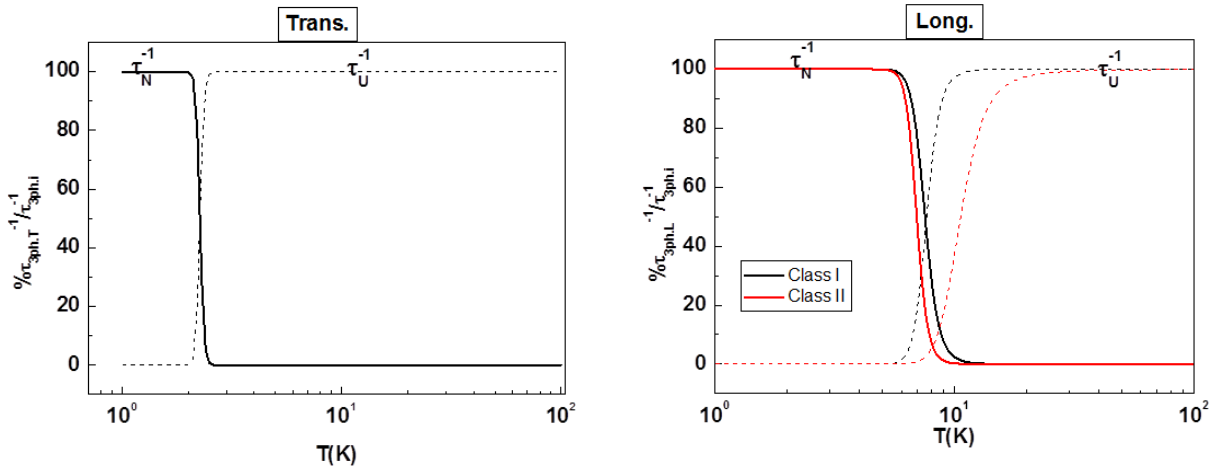

Fig.(6): The percentage contribution for the relaxation rate of normal and umklapp processes towards the relaxation rate of three phonon scattering by used Awad model of KCl compound (for Longitudinal and Transverse Phonons).

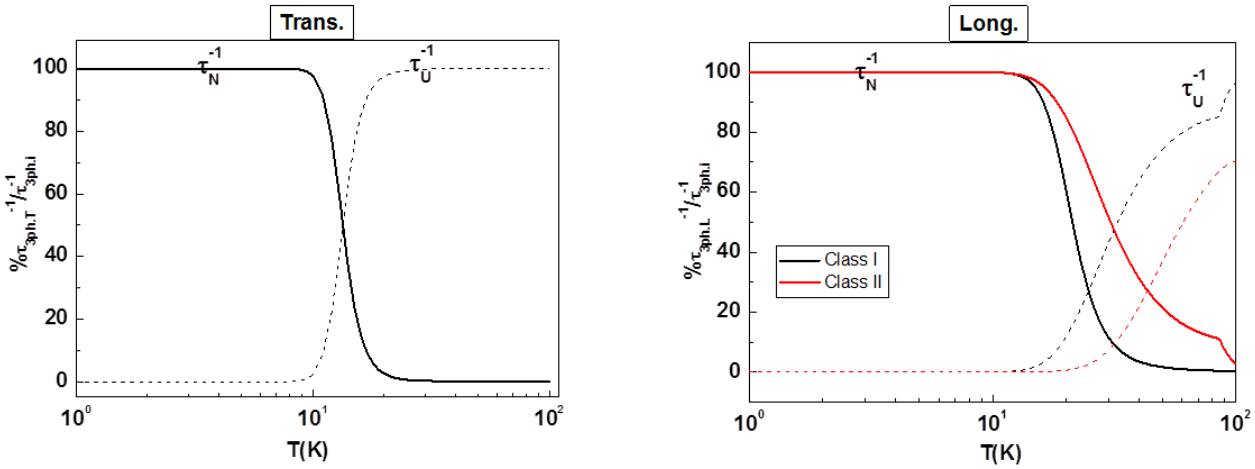

Fig.(7): The percentage contribution for the relaxation rate of normal and umklapp processes towards the relaxation rate of three phonon scattering by used Dubey's model of NaCl compound (for Longitudinal and Transverse Phonons).

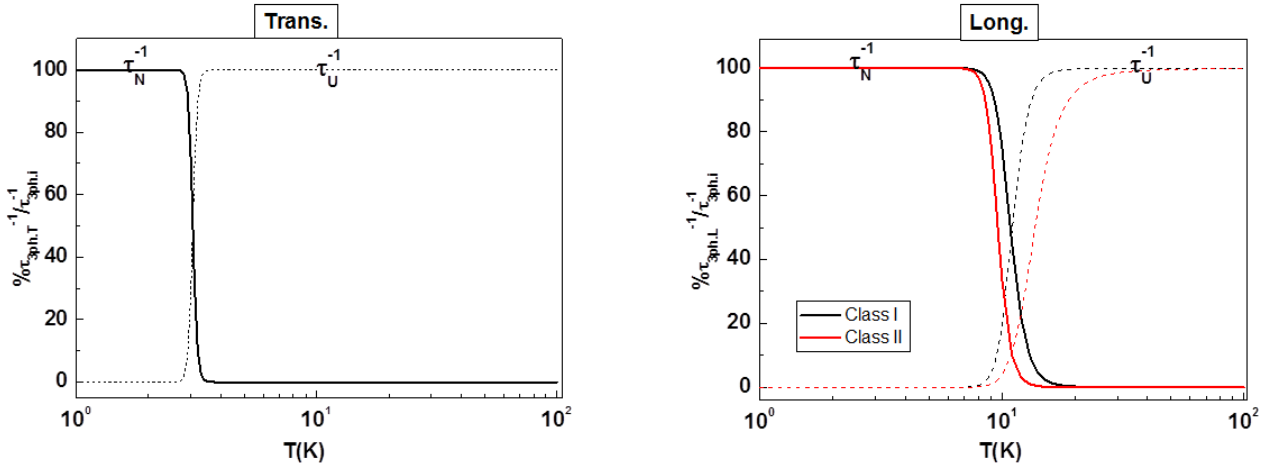

Fig.(8): The percentage contribution for the relaxation rate of normal and umklapp processes towards the relaxation rate of three phonon scattering by used Awad's model of NaCl compound (for Longitudinal and Transverse Phonons).

Figures (5,6,7,8),they are cleared the contributions due to three-phonon N and U-processes are included in the wide temperature range (1 - 100) K for transverse and longitudinal phonons ,the normal processes of three phonon scattering were dominant at temperatures low, while the umklapp processes were dominant at high temperatures , this is an agreement with the results of authors [10,12,16].

IV. CONCLUSION

The lattice thermal conductivity of KCl and NaCl compounds has been measured over the temperature range (1-100 K). Awad method has been applied to analyze the obtained data. Results shows that the three phonon scattering is played an important role in calculation total thermal conductivity.So it is necessary to take this scattering into account to find thermal conductivity.

Results shows good agreement between theory and experiment values of the thermal conductivity lattice, as study is pear the largest agreement at calculation thermal conductivity lattice by used awad's model of used Dubey's Model of the three phonon scattering.

Acknowledgements

I am grateful to Mr.FouadNimrAjeel from College of Sciences, ThiQar University, Iraq for helpful .

REFERENCES

[1]. M. AtaullahAnsaria, V. Ashokanb, B.D. Indub,and R. Kumarc,ACTA PHYSICA POLONICA A,Vol. 121,No. 3,2012.
[2]. Nico de Koker, PHYSICAL REVIEW LETTERS, 103, 125902 (2009).
[3]. S. M. Mamand , M. S. Omar, Advanced Materials Research, 832 (2014) (33-38).
[4]. H. Kim, M. H. Kim, and M. Kaviany, J. Appl. Phys. 115, 123510 (2014).
[5]. D. P. Singh and G. S. Verma , PH YSICA L REVIEW B, 6, 10, 1972.
[6]. K. S. Dubey, PHYSICAL REVIEW B,7,6,1973.
[7]. E. P. Roth and A. C. Anderson, PHYSICAL REVIEW B , 17, 8 , 1978.
[8]. G.L. Guthrie, Phys. Rev. B3, 3373 (1971).
[9]. A.H. Awad,"New Theoretical Analysis to the Lattice Thermal Conductivity of Semiconductors: Application to Ge and GaAs" Ph.D. Thesis, Basrah University, Basrah (Iraq) (2003).
[10]. D. B. Habesh, Journal of Basrah Researches ((Sciences))Vol. 36, No. 3, 15 June ((2010)).
[11]. Isra'aM.Ali, Journal of Basrah Researches ((Sciences)),37,5,(1817-2695),2011.
[12]. B. H. Muhamad,"Role of Debye Temperature in the Lattice Thermal Conductivity of(ZnS,ZnTe and ZnSe)Semiconductors", M. Sc. Thesis, Basrah, University, Basrah, Iraq(2012).
[13]. K.S. Dubey, J. of Thermal Analysis 19, 263 (1980).
[14]. S. M. Mamand, M. S. Omar and A. J. Muhammed, Adv. Mat. Lett., 3,6, (449-458), 2012.
[15]. S. L. Shinde and J. S. Goela," High Thermal Conductivity Materials", Springer Science and Business Media (2006).
[16]. A. H. Awad and Q. H. A. Hussain,Engineering and Technology,13, 7 (1994).