Thermal Conductivity of ZnSe Compound Lattice

Bushra Hussein Mohammed

Department of Physics, College of Sciences, Thi Qar University, Nassiriya, Iraq

Abstract:*The study surveys the ability of applying the dispersion relation of diatomic lattice provided by Awad, to calculate the lattice thermal conductivity for (ZnSe) compound at temperature range between (2-300K) . Where the study reveals a good agreement between the theoretical and experimental values of the lattice thermal conductivity . Taking into account scatterings of phonon by boundary ,point defect and three phonon scattering.As The results showed the possibility of this function to deal with the high temperature lattice thermal conductivity of ZnSe .*

Keywords:lattice thermal conductivity, phonon scattering , ZnSe.

1. Introduction

The thermal conductivity of semiconductors plays an important part in the design of power-dissipating devices. For example, power transistors, solar cells under strong sunlight, diodes, transistors, and semiconductor lasers sustain large internal power dissipation, and a high thermal conductivity of the device material can help transfer this energy to a heat sink. On the other hand, alow thermal conductivity of semiconductor alloys helps increase the figure of merit of thermoelectric devices [1]. Zinc selenide belongs to the most promising wide_gap II–VI materials. This material finds wide use in the development of devices for short_wavelengthsemiconductor electronics and displaying systems and offers promise for electronics of light _ emitting _diodes[2] .

Sood et al. [3] have studied the temperature dependence of phonon conductivity of II-VI semiconductors by considering the relaxation rate due to three phonon scattering for the transverse acoustic phonons , As Bijalwan et al. [4] have studied The lattice thermal conductivity of four 11-VI compounds ZnS , ZnSe , ZnTe and CdTe in the temperature range (2-300 K) taking separate contributions of longitudinal and transverse phonons.

Awad [5] progressed mathematical model exceeding all the approximations used by Callaway[6] or any earlier authors, by using dispersion relation of monatomic and diatomic lattices, he has taken accounts both of dispersion relation for sound phonons and non-equilibrium distribution function consequent at interaction with the nearest and all atoms. He got more accurate formulas in order to calculate the lattice thermal conductivity. He applied these formulas in successfully on Germanium Ge and Gallium Arsenide GaAs in the temperatures range (2-300 K),using this model, a lot of work [7-15] has been done on the lattice thermal conductivity of solids.

2. Theory

Awad [5] ignored Debye approximation of dispersion relation $q = \omega/\upsilon$, which is used by Callaway method [6] , and he used in his the dispersion relation of diatomic lattice in one dimension as [5] :

$$q = \frac{1}{a}\sin^{-1}\sqrt{\frac{M+m}{4}\left(\frac{2\omega^2}{\gamma} - \frac{\omega^4}{\gamma^2 M_0}\right)} \qquad (1)$$

So ,he was getting to the following formula for the lattice thermal conductivity [5] :

$$K_i = \frac{MK_B^3\theta^2}{6\pi^2 a\hbar^2(M+m)}\int_0^{\theta_i/T}\tau\frac{\sqrt{J_O(1-J_O)}\left(\sin^{-1}\sqrt{J_O}\right)^2}{(1-2J/M_O)}\frac{xe^x}{(e^x-1)^2}dx \qquad (2)$$

Where,

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

$J_\circ = J(M+m)(1 - J/M_\circ)$ and $x = \hbar\omega/K_B T$

And where , M is mass of the first atom, m is mass of the second mass , dimensionless variable x ,the τ are the relaxation times.

There are many phonon scattering processes that affect the thermal conductivity in the crystal .According to Casimir [16]the boundary scattering relaxation time is given by:

$$\tau_B^{-1} = v/1.12d = v/L \qquad (3)$$

where d is the width of the sample of square cross section, v is the value of the velocity and L is the characteristic length.

The scattering due to point defects(τ_p^{-1}) is the dominant relaxation processes at temperatures where conductivity is maximum .

$$\tau_p^{-1} = A\omega^4 \qquad (4)$$

Klemens [17] has derived an expression for A:

$A = V_O\Gamma/4\pi v$

Where v₀is the volume per molecule and v is an average velocity given by

$$\frac{1}{v} = \frac{1}{3}\left(\frac{1}{v_L} + \frac{1}{v_T}\right) \text{ and } \Gamma = \Sigma_i f_i\left(1 - m_i/m\right)^2$$

f_i is the relative abundance of isotope i and m is the average mass of the constituents .

Paper ID: SUB153351

684

The three – phonon processes(τ^{-1}_{3ph}) are dominant at high temperature and also give a substantial contribution near the conductivity maximum . As a result, the combined scattering relaxation rates for transverse phonons take the forms [18]:

$$\tau^{-1}_{3ph,T} = \left(B_{TN,I} + B_{TU,I} e^{-\theta_D / \alpha T} \right) \omega T^{m_{T,I}(T)} \quad \text{for } 0 < \omega < \omega^4 \qquad (5)$$

and for longitudinal phonons

$$\tau^{-1}_{3ph,L} = \left(B_{LN,I} + B_{LU,I} e^{-\theta_D / \alpha T} \right) \omega^2 \, T^{m_{L,I}(T)} +$$

$$\left(B_{LN,II} + B_{LU,II} e^{-\theta_D / \alpha T} \right) \omega^2 \, T^{m_{L,II}(T)} \quad \text{for } 0 < \omega < \omega^4 \qquad (6)$$

Dubey suggested the use of the average value of the upper and lower bounds of m(T) reported by Guthrie [19], and m(T) is given by:

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

for class I events, and

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

for class II events. In these expressions,

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

Become,

$$\tau^{-1} = \tau^{-1}_B + \tau^{-1}_P + \tau^{-1}_{3ph}$$

3. Results and Discussion

The lattice thermal conductivity of ZnSe compoundcalculated for dispersion relation on by using the adjustable parameters of the phonon scattering appearing in tables (II) the results represented in figures (1). Best fitting can be noticed of these results with experimental data [7, 9-15] . especially at the maximum conductivity curve , where The obtainedresultsshow a goodagreement with the experimental data .as 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 , these results are shown in figure (2) ,and is agreement with[15,20].

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

Parameter	Value
τ^{-1}_{BT} (s^{-1})	1.2x10^6
τ^{-1}_{BL} (s^{-1})	3.5x10^5
A_Ts^3	2.7x10^{-44}
A_Ls^3	1x10^{-46}
B$_{TN}$ deg^{-m}	2.5x10^{-10}
B$_{TU}$ deg^{-m}	2x10^{-6}
B$_{LN,I}$ s.deg^{-m}	3.8x10^{-24}
B$_{LU,I}$ s.deg^{-m}	1.5x10^{-19}
B$_{LN,II}$ s.deg^{-m}	3x10^{-21}
B$_{LU,II}$ s.deg^{-m}	1.8x10^{-16}

Table 2: Value of constant used to calculate thermal conductivity ofZnSe compound.

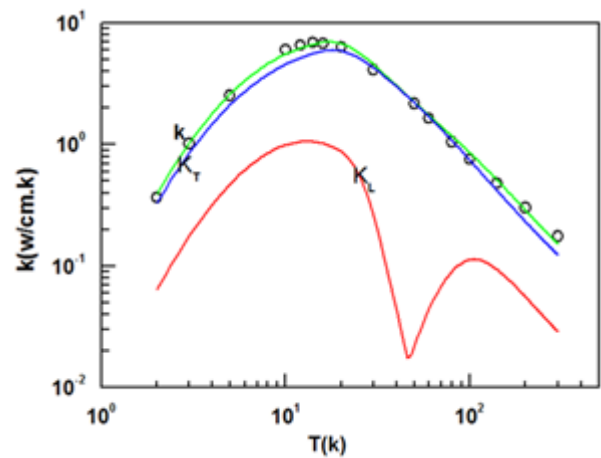| a(A^0)	θ_D	θ_T	θ_L	M$_1$(mkg)	M$_2$(mkg)
5.67	315 ^{0}K	104 ^{0}K	278 ^{0}K	5.65x10^{-23}	4.98 x10^{-23}

Figure 1: Conductivity curves of ZnSe compound. Solid line is the present work.
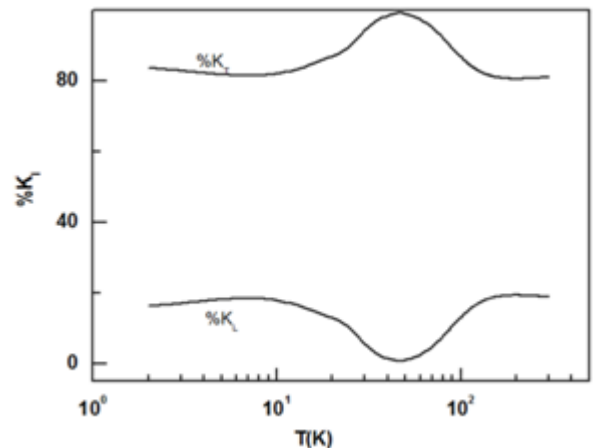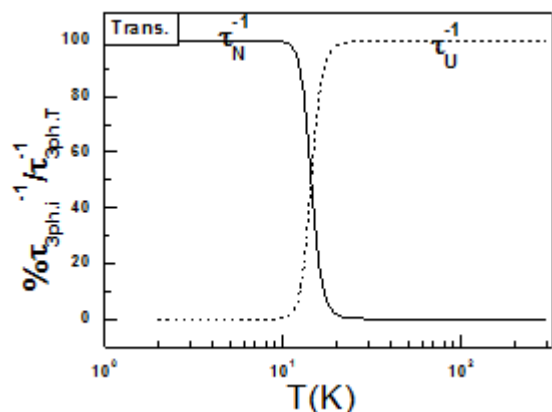

Figure 2: The percentage contributionfor transverse phonons and longitudinalphonons .
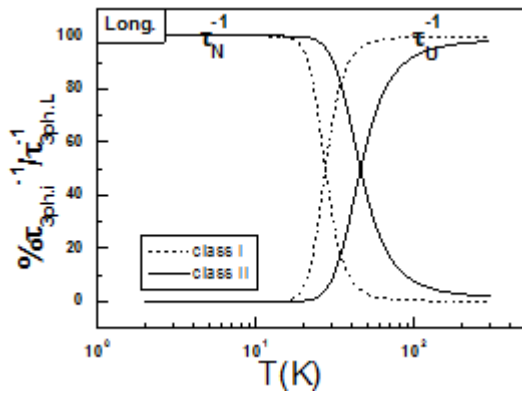
Figure 3: The percentage contribution for the relaxation rate of normal and umklapp processes towards the relaxation rate of three phonon scattering for transverse phonons and longitudinal phonons.

In figure (3), the normal processes of three phonon scattering were dominant at temperatures low less than (T<50K), but at high temperatures the umklapp processes were dominant, this is an agreement with the results of authors [7,9-11,15] .

In figures (4,5), The phonon scattering processes of the point defects and boundary show the domination at low frequencies, but three phonon scattering of two kinds (normal and umklapp processes) dominate at high frequencies. Atconstanttemperature (T= 20K, T=100K)for transverse phonons and longitudinal phonons and within low frequencies range, the figure (4) appearing dominance for the boundary and phonon scattering over another kinds of scatters , this is an agreement with the results of the authors [5,7,10]. on the umklapp processes other hand the scattering dominion at high frequencies and at temperature (T= 20K,T=100K) for transverse phonons, (T=100K) for longitudinal phonons as the figure (5),while at temperature (T=20K) for longitudinal phonons and within same frequencies range appearing dominance for normal processes of three phonon scattering and phonon scattering over another kinds of scatters as the figure (5) , this is an agreement with the results of the authors [5,7,10,15].
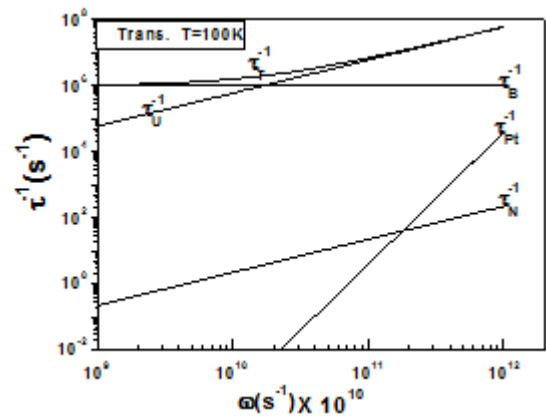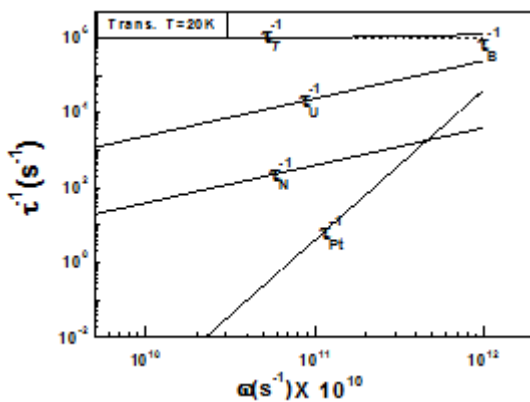

Figure 4: Relaxation rates of the deferent phonon scattering for for transverse phonons as a function to the Frequency at constant temperature(T=20,100K) .
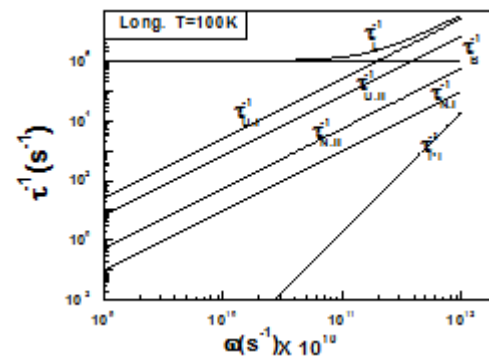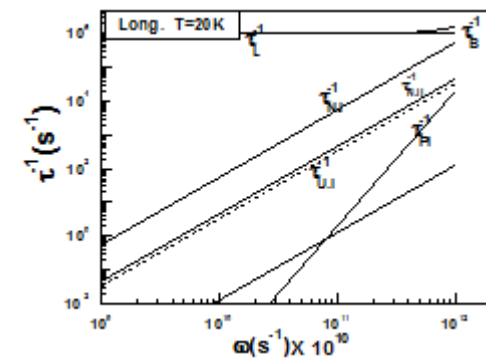

Figure 5: Relaxation rates of the deferent phonon scattering for for longitudinal phonons as a function to the frequency at constant temperature(T=20,100K) .

4. Conclusion

In this paper, is showed that the Awad model can be successfully applied to explain the thermal conductivity of ZnSe compound at temperature range between (2-300K) ,where The obtained results show a good agreement between the theoretical and experimental values of the lattice thermal conductivity for this compound ,As It is also found that the transverse phonons give a major contribution towards the thermal conductivity of semiconductors. We have used the phonon scattering rates boundary ,point defect and three phonon scattering in the calculation lattice thermal conductivity, noted at constant temperature and within low frequencies the boundary show the domination over another kinds of scatters , but three phonon scattering of two kinds (normal and umklapp processes) dominate at high low frequencies for transverse phonons and longitudinal phonons . and at temperatures low appeared the normal processes of

three phonon scattering were dominant , but at high temperatures the umklapp processes were dominant.

5. Acknowledgements

References

[1] S. L. Shinde and J. S. Goela," High Thermal Conductivity Materials", Springer Science and Business Media (2006) .

[2] V. Ya. Degoda and A. O. Sofienko ,"Specific Features of the Luminescence and Conductivity of Zinc Selenide on Exposure to X_Ray and Optical Excitation", published in Fizika i Tekhnika Poluprovodnikov, Vol. 44, No. 5, pp. 594–599, 2010.

[3] 3 . K.C. Sood, M.A. Singh and G.S. Verma, Phys. Rev. B3, 385 (1971) .

[4] R.D. Bijalwan, P.N. Rami and M.D. Tiwarii,"Lattice thermal conductivity of 11-VI compounds", J. Phys. C: Solid State Phys., 16, 2537(1983).

[5] A.H. Awad, Ph.D. Thesis,"New Theoretical Analysis to the Lattice Thermal Conductivity of Semiconductors: Application to Ge and GaAs", Basrah University, Basrah (Iraq) (2003).

[6] J. Callaway, Phys. Rev. 113, 1046 (1959) .

[7] A.J. Mohammed, M. Sc. Thesis,"Lattice thermal conductivity of Silicon at a wide range of temperature

[8] ",Basrah University,_Basrah , Iraq(2007).

[9] A. S. Mahdi, M. Sc. Thesis, Basrah University, Basrah, Iraq(2007).

[10] D. B. Habesh, M. Sc. Thesis, Basrah University, Basrah, Iraq(2008).

[11] A. Lifta, M.Sc. Thesis, Basrah University, Basrah, Iraq(2010).

[12] D. B. Habesh, "Lattice Thermal Conductivity of Solid Neon", Journal of Basrah Researches (Sciences)Vol. 36, No. 3, 15 June (2010).

[13] H.A.Hasan, M.Sc. Thesis, Basrah University, Basrah, Iraq(2011).

[14] Isra'a M .Ali , Journal of Collger of Education, No. 6,(554-571), (2011).

[15] Isra'a M .Ali, Journal of Basrah Researches (Sciences),B5, No37, (2011).

[16] B. H. Mohammed , Journal of Basrah Researches (Sciences) , B3, No38,(2012).

[17] H.B.G. Casimir, Physica 5, 595 (1938) .

[18] 46. P.G. Klemens, Solid State Physics 7, edited by F. Seitz and D. Turnbull, Academic Press, New York, 1 (1958).

[19] K.S. Dubey, J. Thermal Analysis 19, 263 (1980) .

[20] G.L. Guthrie , Phys. Rev. B3, 3373 (1971) .

[21] K. S. Dubey and G. S. Verma, Physical Review B , Vol. 4, No12,1971.

[22] C.Kittel, (1986),"Introduction to Solid State Physics", 6th, ed.John Wiley and Sons, Inc, New York.