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Short Communication,

Linear correlation between Debye temperature and lattice thermal conductivity in II-VI and III-V semiconductors

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Abstract

A simple linear empirical relationship between high intrinsic lattice thermal conductivity K, and Debye temperature θ_a is suggested from data on high intrinsic lattice thermal conductivity K, and Debye temperature θ_a for some selected II-VI and III-V cubic zincblende type, and I-VII and II-VI rock-salt type binary semiconductors. A good linear correlation between Debye temperature and the high intrinsic lattice thermal conductivity was obtained. The minimum average percentage deviations in the present approach reveal that our simple model prove its identity and soundness compared to those of other author relations.

Keywords: *Debye Temperature; Binary Semiconductors; High Lattice Thermal Conductivity.*

1. Introduction

One of a most fundamental and important physical parameter of solid material is thermal conductivity [1]. The manipulation and the control of this physical quantity have impacted a variety of technical applications, including thermal management of mechanical, electrical, chemical, and nuclear systems; thermoelectric materials; thermal barriers and insulation materials; and transducers and sensors [1]. Knowledge of the thermal conductivity, the Debye temperature and other thermal quantities of materials helps in the improvement of the manufacturing of the semiconductor devices by good selecting of the appropriate materials [2]. Due to technological importance of I-VII, II-VI and III-V compounds, several experimental and theoretical works on their electronic, optical, mechanical and thermal properties were published [3-10].
The principal goal of this work is to study the correlation between the high intrinsic lattice thermal conductivity K and Debye temperature θ_a for some selected of I-VII, II-VI and III-V binary semiconductors.

2. Theory, results and discussion

The thermal conductivity of solids results essentially from interactions between phonons and from the scattering of phonons by crystalline imperfections [6]. Knowledge of this physical quantity of materials forms an important part in the design of power-dissipating devices, such as transistors, diodes, and other optoelectronic devices [6]. The lattice thermal conductivity needs careful investigation as it is correlated with several physical quantities such as: cohesivity in solids, nature of covalency between atoms and molecules of materials, bond iconicity, and electronic behavior of the constituent element forming the compounds [3].
Several models between the lattice thermal conductivity and other physical quantities have been established. For example, for zincblende structured solids, the correlation between the lattice thermal conductivity K and the nearest neigh-bour distance (bond length) d (in Å) is given by the following expression [3]

$$K = S\,(Z_1Z_2)^{V}/d^5 \quad (1)$$

Where: Z_1 and Z_2 are the ionic charge of the A and B atoms, respectively, and S and V are two constants, which depends upon crystal structure, they have values of 2 and 1.5, respectively, for zincblende type solids [3].
Another model which is used for various classes of crystalline solids (graphite, silicon nitride and related materials, wide-band-gap Group IV and Group III-V semiconductors,…etc) has been established to write the correlation between the lattice thermal conductivity K and the Debye temperature is given by the following formula [1]:

$$K = AM_a\theta_a^3\delta / \gamma^2 T \quad (2)$$

Where: A is a constant, M_a is the atomic mass of the atom, θ_a is named also Debye temperature. This later quantity is related with the traditional Debye temperature θ_D by: $\theta_a = \theta_D n^{-1/3}$, with n is the number of atoms per unit cell (n = 2 for the rocksalt and zincblende structured compounds), δ^3 is the volume per atom, γ is the Grüneisen constant and T is the temperature.
It can be seen that the Eq. (02) is relatively complicated and contains several parameters; our principal idea is to establish a simple model (empirical formula) to write the correlation between the high intrinsic lattice thermal conductivity K and the Debye temperature for some selected cubic rock-salt and zincblende type semiconductors.
We begin by drawing the evolution of the lattice thermal conductivity K as function of the Debye temperature for some zincblende materials. The experimental values of Debye temperature θ_a and high intrinsic lattice thermal conductivity K of III-V and II-VI type materials reported in Table 1 are taken from the Ref [1].

Table 1: Experimental Value of Debye Temperature θ_a and High Intrinsic Lattice Thermal Conductivity K of III-V and II-VI Zincblende Materials Cited in Ref [1]. Experimental Value of the Thermal Conductivity with * Is Cited In the Ref [4].

Group	Compounds	θ_a (K)	K ($W\,cm^{-1}K^{-1}$)
	BN	1200	7.6
	BP	670	3.5
	AlAs	270	0.98
	AlSb	210	0.56
	GaP	275	1
	GaAs	220	0.45
III-V	GaSb	165	0.4
	InP	220	0.93
	InAs	165	0.3
	InSb	135	0.2
	ZnS	230	0.27
	ZnSe	190	0.19
II-VI	ZnTe	155	0.143*
	CdTe	120	0.075

We can see in table 1 that the boron nitride material has high value of lattice thermal conductivity with numerical value equal to: 7.6 W cm^{-1} K^{-1}; but the boron nitride material hasn't the highest value of lattice thermal conductivity comparatively with the Diamond, this later has a value of thermal conductivity equal to: 20.9 W cm^{-1} K^{-1} (see Table 6.3 of the Ref. [5] page 142). The previous results are plotted in figure 1; from the figure 1, we can see clearly a linear correction between high intrinsic lattice thermal conductivity K and Debye temperature θ_a in III-V and II-VI zinc-blende structured compounds. It's written by the following expression.

$$K = a + b\,\theta_a \quad (3)$$

Where a and b are two empirical parameters.
The numerical values of the empirical parameters a and b for III-V zincblende compounds are: -0.85 ($W\,cm^{-1}K^{-1}$) and 0.007 ($W\,cm^{-1}K^{-2}$) respectively, and for II-VI zincblende compounds are: -0.132 ($W\,cm^{-1}K^{-1}$) and 0.002 ($W\,cm^{-1}K^{-2}$) respectively. Our calculated values of high intrinsic lattice thermal conductivity K and Debye temperature θ_a of III-V and II-VI zincblende compounds have been presented in Table 2. For object to make comparison, the values obtained in the Ref [1] have been also presented in this Table.
Eq. (03) is used to predict the high intrinsic lattice thermal conductivity of BSb material. The theoretical value (because there is no experimental value) of the traditional Debye temperature θ_D of this compound in its zincblende phase is equal to: 456.07 K [7], so the Debye temperature θ_a of this compound is equal to: 361.98 K. The predicted value of the high intrinsic lattice thermal conductivity K of BSb material is equal to: 1.954 $W\,cm^{-1}K^{-1}$; this value is relatively higher than the theoretical value (0.96 $W\,cm^{-1}K^{-1}$) of the thermal conductivity K obtained by Verma et al [3].

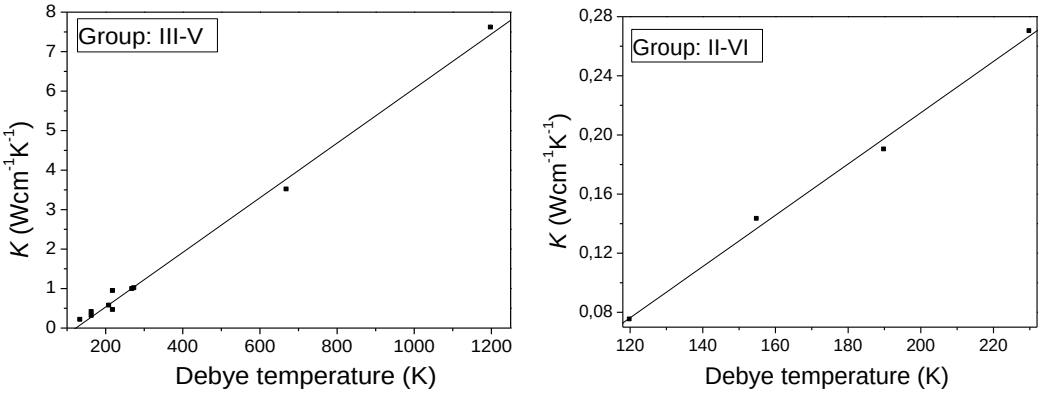

Fig. 1: Plot between the High Intrinsic Lattice Thermal Conductivity K and Debye Temperature θ_a in III-V and II-VI Zincblende Compounds.

Table 2: Our Calculated Values of the Lattice Thermal Conductivity K and the Percentage Deviations of III-V and II-VI Zincblende Materials in Comparison with those Cited in Ref [1].

Compounds	Results of Ref [1] Eq.(02)	Percentage deviation (%)	Present Work Eq.(03)	Percentage deviation (%)
BN	11.05	45.39	7.55	0.66
BP	3.59	2.57	3.84	9.71
AlAs	0.89	9.18	1.04	6.12
AlSb	0.77	37.5	0.62	10.71
GaP	0.72	28	1.08	7.5
GaAs	0.55	22.22	0.69	53.33
GaSb	0.33	17.5	0.31	23.75
InP	0.83	10.75	0.69	25.81
InAs	0.51	70	0.31	1.67
InSb	0.38	90	0.1	52.5
Average percentage deviation		33.31%		19.18%
ZnS	0.4	48.15	0.328	21.48
ZnSe	0.35	84.21	0.248	30.53
ZnTe	0.17	18.88	0.178	24.48
CdTe	0.296	294.67	0.108	44.00
Average percentage deviation		111.47%		30.12%

The average percentage deviation (in the case of III-V zincblende compounds) is calculated, and improved in comparison with the value (33.31 %) obtained with using results reported in Ref [1], it is about 19.18 %. The average percentage deviation (in the case of II-VI zincblende compounds) is also calculated and to be found also improved in comparison with the value (111.47 %) obtained with using the calculated results of Morelli and Slack [1]; our obtained value of the average percentage deviation is about 30.12 %.

Second one; we come to study the relationship between the high intrinsic lattice thermal conductivity K and the Debye temperature for some rock-salt materials. The experimental values of Debye temperature θ_a and high intrinsic lattice thermal conductivity K of I-VII and II-VI rock-salt materials reported in Table 3 are taken also from the Ref [1].

Table 3: Experimental Value of Debye Temperature θ_a and High Intrinsic Lattice Thermal Conductivity K of I-VII and II-VI Rock-Salt Materials Cited in Ref [1].

Group	Compounds	$\theta_a(K)$	K ($W\,cm^{-1}K^{-1}$)
I-VII	NaF	395	0.184
	KCl	172	0.071
	KI	87	0.026
	RbBr	105	0.038
	RbI	84	0.023
II-VI	CaO	450	0.27
	SrO	270	0.12
	PbS	115	0.029
	PbSe	100	0.02
	PbTe	105	0.025

The later results are plotted in figure 2; from this figure, we can see clearly also a linear correction between the high intrinsic lattice thermal conductivity K and Debye temperature θ_a in I-VII and II-VI rock-salt compounds. The

numerical values of the empirical parameters a and b for I-VII compounds are: -0.018 ($W\,cm^{-1}K^{-1}$) and 5.15 x 10^{-4} ($W\,cm^{-1}K^{-2}$) respectively, and for II-VI rock-salt compounds are: -0.053 ($W\,cm^{-1}K^{-1}$) and 7 x 10^{-4} ($W\,cm^{-1}K^{-2}$) respectively.

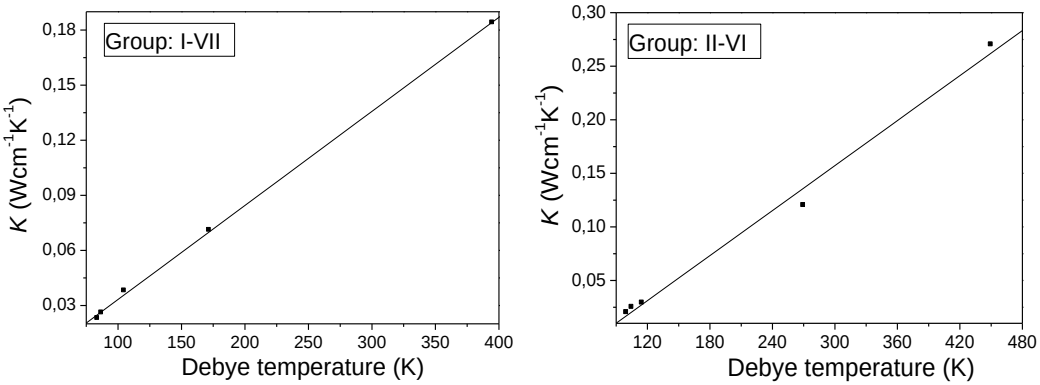

Fig. 2: Plot between the High Intrinsic Lattice Thermal Conductivity K and Debye Temperature θ_a in I-VII and II-VI Rock-Salt Compounds.

Our calculated values of the high intrinsic lattice thermal conductivity K and Debye temperature θ_a of I-VII and II-VI rock-salt compounds have been presented in Table 4 and compared with those of the Ref [1].

Table 4: Our Calculated Values of the Lattice Thermal Conductivity K and the Percentage Deviations of I-VII and II-VI Rock-Salt Materials in Comparison with those Cited in Ref [1].

Compounds	Results of Ref [1] Eq.(02)	Percentage deviation (%)	Present Work Eq.(03)	Percentage deviation (%)
NaF	0.179	2.72	0.185	0.77
KCl	0.038	46.48	0.071	0.59
KI	0.010	61.54	0.027	3.10
RbBr	0.021	44.74	0.036	5.07
RbI	0.015	34.78	0.025	9.83
Average percentage deviation		38.05%		3.87%
CaO	0.332	22.96	0.262	2.96
SrO	0.152	26.67	0.136	13.33
PbS	0.017	41.38	0.028	5.17
PbSe	0.035	75.00	0.017	15.00
PbTe	0.040	60.00	0.020	18.00
Average percentage deviation		45.20 %		10.89 %

The average percentage deviation (in the case of I-VII rock-salt compounds) is calculated and to be found improved in comparison with the value (38.05 %) obtained with using the results reported in Ref [1], it is only about 3.87 %. The average percentage deviation (in the case of II-VI rock-salt compounds) is also calculated and to be found also improved in comparison with the value (45.20 %) obtained with using the calculated results of Morelli and Slack [1]; our obtained value of the average percentage deviation is about 10.89 %.

3. Conclusion

A simple linear model has been found between the high intrinsic lattice thermal conductivity K and the Debye temperature θ_a for some selected II-VI and III-V zincblende and I-VII and II-VI rock-salt binary semiconductors. The average percentage deviations were estimated for different types of materials. The values: 30.12 % and 19.18 % of the average percentage deviations were obtained in the case of II-VI and III-V zincblende materials respectively; and the values: 3.87 % and 10.89 % of the average percentage deviations were obtained in the case of I-VII and II-VI rock-salt compounds respectively.

In comparison of ours results with these estimated from the formula proposed by Morelli and Slack [1], the linear correlation between the high intrinsic lattice thermal conductivity K and the Debye temperature θ_a of some selected II-VI and III-V zincblende and I-VII and II-VI rock-salt semiconductors gives better agreement with the experimental values than the model proposed by earlier worker, which is demonstrate the soundness of the present model.

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