



Inherent properties of binary tetrahedral semiconductors

A.S. Verma^{a,*}, B.K. Sarkar^b, V.K. Jindal^a

^a Department of Physics, Panjab University, Chandigarh 160014, India

^b Department of Physics, VIT University, Vallore 632014, India

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ABSTRACT

A new approach utilising the concept of ionic charge theory has been used to explain the inherent properties such as lattice thermal conductivity and bulk modulus of $A^{III}B^V$ and $A^{II}B^{VI}$ semiconductors. The lattice thermal conductivity (K) of these semiconductors exhibit a linear relationship when plotted on a log–log scale against the nearest neighbour distance d (Å), but fall on two straight lines according to the product of the ionic charge of the compounds. On the basis of this result a simple lattice thermal conductivity–bulk modulus relationship is proposed and used to estimate the bulk modulus of these semiconductors. A fairly good agreement has been found between the experimental and calculated values of these parameters for zinc blende structured solids.

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1. Introduction

Most of the physical world around us and a large part of modern technology are based on solid materials. The extensive research devoted to the physics and chemistry of solids during the last quarter of a century has led to great advances in understanding of the properties of solids in general. So it is interesting to study the behaviour and various properties of different solids. In recent years there has been considerable interest in theoretical and experimental studies of $A^{NB}B^{3-N}$ type crystals with zinc blende structure. It is attributed to their high symmetry and simplicity of their ionic bonding [1]. Almost all the $A^{II}B^{VI}$ and $A^{III}B^V$ compounds crystallize either in the zinc blende or wurtzite structures. The common and dominant feature of these structures is the tetrahedral bonding to four atoms of the other elements. In zinc blende these tetrahedral are arranged in a cubic type structure whilst they are in a hexagonal type structure. Indeed, the centres of similar tetrahedral are arranged in a face-centred cubic (*fcc*) array in the former and a hexagonal closed-packed (*hcp*) array in the latter [2]. The particular omnitriangulated nature in atomic structure gives these materials unique physical properties. During the last few years, a number of theoretical calculations based on empirical relations have become an essential part of material research. Because *ab initio* calculations are complex and required significant effort, more empirical calculations [3,4], have been developed to compute properties of zinc blende solids. The empirical relations have become widely recognized as the method of choice for computational solid-state studies. In modern high-

speed computer techniques, it allows researchers to investigate many structural and physical properties of materials only by computation or simulation instead of traditional experiments. Empirical concepts such as valence, empirical radii, electronegativity, ionicity and plasmon energy are then useful [5,6]. These concepts are directly associated with the character of the chemical bond and thus provide means for explaining and classifying many basic properties of molecules and solids.

The valence electrons refer to the electrons that take part in chemical bonding. Recently, Verma and co-authors [7–12] have calculated the electronic, mechanical and optical properties of binary and ternary compounds with the help of ionic charge theory of solids. This is due to the fact that the ionic charge depends on the number of valence electrons, which changes when a metal forms a compound. Therefore, we thought it would be of interest to give an alternative explanation for some inherent properties such as lattice thermal conductivity and bulk modulus of zinc blende solids.

2. Theory, results and discussion

Lattice thermal conductivity and bulk modulus need careful investigation as they are correlated with cohesivity, nature of covalency, bond ionicity and electronic behaviour of the constituent element forming the compound [13,14]. Spitzer [15] and Ioffe [16] experimentally estimated the lattice thermal conductivity (K) of binary and ternary crystals. Different theoretical models, based on bond ionicity and melting temperature, have been proposed by several other researchers [13–16]. The bond ionicity theory of solids has been used by Garbato et al [13] for the calculation of K of the tetrahedral semiconductors and lattice

* Corresponding author. Tel. +91 9412884655.

E-mail address: ajay_phy@rediffmail.com (A.S. Verma).

thermal conductivity (K) of these semiconductors may be expressed as

$$K = K_{\text{cov}}^* (1 - f_i / F_i) (T^* / T) \quad (1)$$

where T^* is the melting temperature, f_i the crystal ionicity and F_i the critical ionicity.

In the previous work [7–12], we have proposed simple expressions for the electronic, optical and mechanical properties such as heteropolar energy gaps (E_c), average energy gaps (E_g), crystal ionicity (f_i), dielectric constant (ϵ_∞), electronic susceptibility (χ), cohesive energy (E_{coh}), bulk modulus (B) and micro-hardness (H) of rocksalt, zinc blende and complex structured solids in terms of the product of ionic charges of cation and anion by the following relations:

$$f_i = 0.87891 \times d^{0.24} / (Z_1 Z_2)^{0.4} \quad (2)$$

The crystal ionicity (f_i) depends on the product of ionic charges [9]. Thus, there must be a correlation between K and product of ionic charges. The lattice thermal conductivity of zinc blende solids exhibit a linear relationship when plotted against nearest-neighbour distance, but fall on two straight lines according to the ionic charge product of the compounds, this is presented in Fig. 1. We observe that in the plot of lattice thermal conductivity and nearest neighbour distance; the $A^{II}B^{VI}$ semiconductors lie on line nearly parallel to the line for the $A^{III}B^V$ semiconductors. From Fig. 1 it is quite obvious that the lattice thermal conductivity trends in these compounds decreases with increases nearest neighbour distance and fall on different straight lines according to the ionic charge product of the compounds. We are of the view that lattice thermal conductivity (K in W/Kcm) of these semiconductors may be evaluated using their ionic charge by the following relation:

$$K = S(Z_1 Z_2)^V / d^5 \quad (3)$$

where Z_1 and Z_2 are the ionic charge of the A and B, respectively, and d the nearest neighbour distance in Å. S and V are constants, which depends upon crystal structure, they have values of 2 and 1.5, respectively, for zinc blende structured solids.

The bulk modulus defines its resistance to volume change when compressed. Both experimental and theoretical results suggest that the bulk modulus is a critical single material property to indicate hardness. Recently, Al-Douri et al. [1] have studied the bulk modulus of IV, III–V and II–VI semiconductors and proposed an empirical relation for bulk modulus (B in Gpa) in terms of

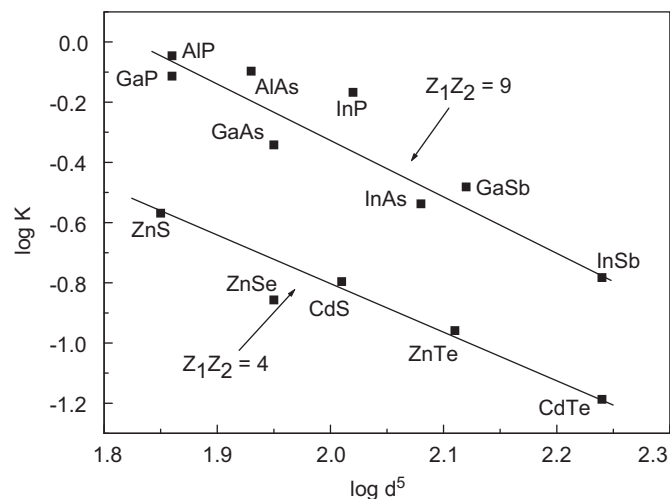


Fig. 1. In the plot of $\log K$ and $\log d^5$, $A^{II}B^{VI}$ semiconductors lie on a line nearly parallel to the line for $A^{III}B^V$ semiconductors, this is depending upon the product of ionic charges. In this figure all experimental values are taken from Ref. [13].

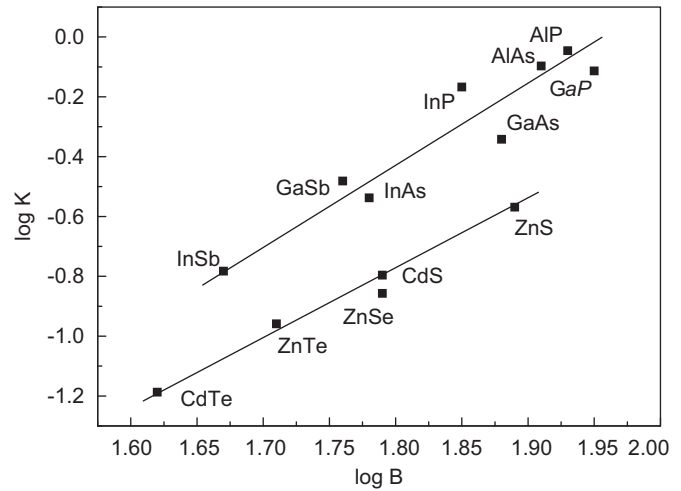


Fig. 2. Plot of $\log K$ against $\log B$ for $A^{II}B^{VI}$ and $A^{III}B^V$ semiconductors. In the plots of $\log B$ and $\log K$, $A^{II}B^{VI}$ semiconductors lie on line nearly parallel to the line for $A^{III}B^V$ semiconductors, this is depending upon the product of ionic charges. In this figure all experimental data are taken from Refs. [13,17,18].

transition pressure (P_t). According to them bulk modulus of these semiconductors may be expressed as

$$B = [99 - (\lambda + 79)](10P_t)^{1/3} \quad (4)$$

where P_t is the transition pressure in GPa from ZB to β -Sn and λ is a parameter appropriate for the group-IV ($\lambda=1$), III–V ($\lambda=5$) and II–VI ($\lambda=8$) semiconductors. On the basis of lattice thermal conductivity result a simple lattice thermal conductivity–bulk modulus relationship is proposed and used to estimate the bulk modulus (B in Gpa) of these semiconductors. Therefore, we have plotted a graph between experimental bulk modulus and lattice thermal conductivity values, which is shown in Fig. 2 for the above series of compounds. From Fig. 2 it is quite obvious that the $A^{II}B^{VI}$ and $A^{III}B^V$ semiconductor lies on two straight lines according to the ionic charge product of the compounds. Thus bulk modulus of these compounds may be evaluated by the following relation:

$$B = CK^{0.75} \quad (5)$$

where C is a constant, the numerical value of C is 110 and 235 for $A^{III}B^V$ and $A^{II}B^{VI}$, respectively. A detailed discussion of this parameter for these materials has been given elsewhere [13–19] and will not be presented here. Using Eqs. (3) and (5) lattice thermal conductivity and bulk modulus for $A^{II}B^{VI}$ and $A^{III}B^V$ semiconductors have been calculated. The results are presented in Table 1. The calculated values are in good agreement with the experimental values reported by earlier researchers [13,17–19].

3. Conclusions

In the proposed models, calculations are simple, fast and more accurate; in regards of the applications point of view it can be highly dependent. The only information needed for calculating lattice thermal conductivity and bulk modulus by proposed method is the nearest neighbour distance and ionic charge and evaluated values are in better agreement with experiment data as compared to empirical relations proposed by previous researchers [13–19]. We come to the conclusion that ionic charge of any compound is a key parameter for calculating the electronic, optical and mechanical properties. It is natural to say that this model can easily be extended to complex crystals for which the work is in progress and will be appearing in forthcoming paper.

Table 1

Values of lattice thermal conductivity (K in W/Kcm) and bulk modulus (B in Gpa) for zinc blende ($A^{III}B^V$ and $A^{II}B^{VI}$) semiconductors. The value of product of ionic charge (Z_1Z_2)=4 for $A^{II}B^{VI}$ and (Z_1Z_2)=9 for $A^{III}B^V$ semiconductors.

Solids	d [7]	$K_{exp.}$ [13]	$K_{theor.}$ [13]	$K_{[this\ work]}$	$B_{exp.}$ [17,18]	$B_{theor.}$ [1,3,17–19]	$B_{[this\ work]}$	% error B
ZnS	2.34	0.27	0.29	0.228	77	90	78	1.3
ZnSe	2.46	0.139	0.13	0.178	62	75	64	3.2
ZnTe	2.64	0.11, 0.143	0.15	0.125	51	59	49	3.9
CdS	2.52	0.16, 0.20	0.15	0.157	62	69	59	4.8
CdSe	2.62	0.045	0.07	0.129	53	60	51	3.8
CdTe	2.81	0.055, 0.065	0.07	0.091	42	47	39	7.1
HgS	2.53			0.154		69	58	
HgSe	2.63			0.127		58	50	
HgTe	2.80			0.093		48	40	
AlN	1.87			2.36		186	209	
AlP	2.36	0.9	1.1	0.74	86	89	88	2.3
AlAs	2.43	0.8	0.84	0.64	82	75	79	3.7
AlSb	2.66	0.57, 0.60	0.57	0.41	58	63	56	3.4
GaN	1.88			2.29	190	173	205	7.9
GaP	2.36	0.77	0.73	0.74	89	92	88	1.1
GaAs	2.45	0.455, 0.44	0.46	0.61	75	76	76	1.3
GaSb	2.65	0.33, 0.27	0.29	0.41	57	57	56	1.8
InN	2.08			1.39		137	141	
InP	2.54	0.50, 0.68	0.40	0.51	71	74	66	7.0
InAs	2.61	0.265, 0.29	0.28	0.45	60	70	60	0.0
InSb	2.81	0.165	0.17	0.31	47	40	46	2.1
BN	1.55			6.04	369	321	424	14.9
BP	1.94			1.97	173	173	183	5.8
BAs	2.04			1.53		146	151	
BSb	2.24			0.96		110	107	
TiN	2.11			1.29		141	133	
TiP	2.49			0.56		71	71	
TiAs	2.58			0.47		59	62	
TiSb	2.75			0.34		46	49	

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