

Correlation between ionic charge and ground-state properties in rocksalt and zinc blende structured solids

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2006 J. Phys.: Condens. Matter 18 8603

(<http://iopscience.iop.org/0953-8984/18/37/018>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 28/05/2010 at 13:45

Please note that [terms and conditions apply](#).

Correlation between ionic charge and ground-state properties in rocksalt and zinc blende structured solids

A S Verma and S R Bhardwaj

Department of Physics, BSA College Mathura, 281004, India

E-mail: ajay_phy@rediffmail.com

Received 18 March 2006, in final form 12 July 2006

Published 1 September 2006

Online at stacks.iop.org/JPhysCM/18/8603

Abstract

In this paper we have evaluated the ground-state properties (i.e., bulk modulus and cohesive energy) of rocksalt and zinc blende structured solids. We have presented two expressions relating the bulk modulus B (GPa) for the alkali halides, alkaline-earth chalcogenides, transition metal nitrides, rare-earth {divalent ($R^{2+}X$) and trivalent ($R^{3+}X$)} monochalcogenides, group IV, III–V and II–VI semiconductors and the cohesive energy E_{coh} (kcal mol^{-1}) for the alkali halides and alkaline-earth chalcogenides with the product of ionic charges ($Z_1 Z_2$) and nearest-neighbour distance d (\AA). The bulk moduli and cohesive energy of rocksalt and zinc blende type structure compounds exhibit a linear relationship when plotted on a log–log scale against the nearest-neighbour distance d (\AA), but fall on different straight lines according to the ionic charge product of the compounds. We have applied the modified relation on rocksalt and zinc blende structured solids and found a better agreement with experimental data as compared to the values evaluated by earlier researchers. The results for bulk modulus differ from experimental values by the following amounts: BaO—0%, LiCl—0%, LaS—0%, SmSe—0%, ZnS—0%, CdS—0%, GaP—0%, InP—0%, MgO—0.61%, CaO—0.89%, SmS—1.7%, YbSe—1.6%, UP—1.9%, EuSe—1.9%; and the results for cohesive energy differ from experimental values by the following amounts: LiCl—0.49%, KF—0.51%, RbF—0.54%, SrO—1.2%, NaCl—1.6%, NaF—1.8%, MgSe—1.9%.

1. Introduction

The extensive research devoted to the physics and chemistry of solids during the end of the last century has led to great advances in the understanding of the properties of solids in general. Alkali halides, alkaline-earth chalcogenides, transition metal nitrides (TMN) and rare-earth monochalcogenides (RX, R = rare-earth metal, X = O, S, Se, Te) have attracted the attention of physicists due to many practical uses, and they have rocksalt crystal structures. Most of the semiconductors that are used in the modern microelectronic industry have the zinc blende

crystallographic structure. The crystals with zinc blende structure range from raw iron and zinc minerals to man-made GaN and BN semiconductors. The particular omnitriangular nature in the atomic structure gives these materials unique physical properties. Alkaline-earth compounds are important in geophysical science and research since they are the link between the highly ionic alkali halides and covalent III–V compounds. Transition metal nitrides (TMN) generally have good properties of large hardness, high melting point and wear resistance. They are widely used for cutting tools and hard coatings. One area of very active research has been mixed oxide systems, which are important to the chemical industry because oxides are widely used as precursors for processing a large variety of materials. Also, rare-earth oxides are receiving attention in industry, because of their potential use as control rods for nuclear reactors, where samarium, gadolinium and europium oxides are used in fuel elements as burnable poisons. Radioactive europium oxide (EuO) is used as heat sources. Rare-earth oxide catalysts may be combined as phosphors for improved cathodoluminophors in colour TV and electro-optic components. In addition they find use in glass making, grinding alloys, composite lasers, phosphor lasers and phosphors [1, 2, 10–13]. The technical development of epitaxial growth in the past few years has provided the possibility for researchers to fabricate man-made materials with expected composition and structure.

In the past 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 require significant effort, the number of publications of empirical calculations has increased exponentially every year. The empirical relations have become widely recognized as the method of choice for computational solid-state studies. In modern high-speed computer techniques, they allow researchers to investigate many structural and physical properties of materials only by computation or simulation instead of by traditional experiments. Optical and other related properties of many metal and semiconductor materials have been studied by empirical calculations [3–6].

In previous work we have presented empirical relations for the dielectric constant and heats of formation of rare-earth pnictides and chalcogenides in terms of atomic number of constituent atoms and lattice constants [7, 8]. In many cases empirical relations do not give highly accurate results for each specific material, but they still can be very useful. In particular, the simplicity of empirical relations allows a broader class of researchers to calculate useful properties, and often trends become more evident. In this paper we have presented empirical relations for ground-state properties (i.e., bulk modulus and cohesive energy) of rocksalt and zinc blende structured solids. In the modified proposed empirical relation only the nearest-neighbour distance and ionic charge are required as input; the computation of the bulk modulus (GPa) and cohesive energy (kcal/mol) itself is trivial, and the results reveals are comparable to the experimental values. Our method turns out to be widely applicable.

2. Theoretical background

2.1. Bulk modulus

Anderson and Nafe [9] first proposed an empirical relationship between the bulk modulus B_0 at atmospheric pressure and specific volume V_0 of the form $B_0 \sim V_0^{-x}$. They find it to hold for a particular class of compounds. The value of x depends on the class of compounds. For alkali halides, fluorides, sulfides and tellurides they find x to be 1 and for oxide compounds x is close to 4.

Jayaraman *et al* [19] predicted that the bulk modulus directly depends on the product of the ionic charges. According to them, for rocksalt type crystal structure compounds the bulk

modulus may be expressed as

$$B_0 \sim Z_1 Z_2 (r_0/\rho - 2) r_0^{-4}. \quad (1)$$

Recently [6, 10–17, 41] many theoretical approaches have been reported to determine the value of the bulk modulus of solid-state compounds. Cohen [18] predicted that the zero pressure isothermal bulk modulus B in terms of nearest-neighbour distance d (in Å) for rocksalt type crystal structure compounds might be expressed as

$$B = 550d^{-3}. \quad (2)$$

The relation of bulk moduli and geometrical properties of diamond and zinc blende (ZB) solids has previously been investigated by Cohen [18] and Lam *et al* [42]. Based on the Phillips and Van Vechten scheme [43] and theoretical analysis of bond geometry of covalent ZB solids, Cohen proposed the following empirical relation,

$$B = 1761d^{-3.5} \quad (3)$$

where d is the nearest-neighbour distance in angstroms and B is in GPa. Lam *et al* deduced an analytic relation of bulk moduli to lattice parameters within the local-density formalism and the pseudopotential as approach as [42]

$$B = 1971d^{-3.5} - 408(\Delta Z)^2 d^{-4} \quad (4)$$

where $\Delta Z = 1$ and 2 for III–V and II–VI semiconductors.

Recently Al-Douri *et al* [6] has studied the bulk modulus of IV, III–V and II–VI semiconductors and proposed an empirical relation for the bulk modulus in terms of the transition pressure (P_t). According to them, the bulk modulus of these semiconductors may be expressed as

$$B = [99 - (\lambda + 79)](10P_t)^{1/3} \quad (5)$$

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.

The Krishnan–Roy theory [26], Jayaraman *et al* [19] and Sirdeshmukh *et al* [25] found that substantially reduced ionic charges must be used to get better agreement with experimental values. To obtain better agreement between experimental and theoretical data for rocksalt and zinc blende type crystal structure compounds, Cohen's relation (2) and (3) may be extended to

$$B = (Z_1 Z_2)^A N d^{-3} \quad (6)$$

where Z_1 and Z_2 are the ionic charge of the cation and anion respectively and A and N are constants, which depend upon the crystal structure. For rocksalt crystal structure compounds the values of the constants A and N turn out to be equal to 0.75 and 550, respectively. For zinc blende crystal structure compounds the values of the constants A and N turn out to be equal to 0.2 and 750, respectively.

2.2. Cohesive energy

Recently [17, 27–29, 31, 32], many theoretical approaches have been reported to determine the value of the cohesive energy of solid-state compounds. Schlosser [20, 21] has studied the cohesive energy trends in the rocksalt structure in terms of interatomic distance using the following relation,

$$E_{\text{coh}} d = \text{constant}$$

or

$$E_{\text{coh}} = \text{constant}/d. \quad (7)$$

To obtain better agreement between experimental and theoretical data for rocksalt type crystal structure compounds, we may extend relation (7) in terms of ionic charges in the following form

$$E_{\text{coh}} = Z_1 Z_2 \text{ constant}/d \quad (8)$$

where Z_1 and Z_2 are the ionic charge of the cation and anion respectively. The value of the constant for the rocksalt type crystal structure is 520.

3. Results and discussion

The bulk modulus and cohesive energy are important ground-state properties of a material; 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. The solid-state physics of an atom in combination with O, S, Se and Te depends primarily upon its electronic configuration. In the rare-earth series of elements the outer valence electrons (the $5d^1$ and $6s^2$ electrons) are effectively shielded from the increasing nuclear charge as electrons are added to the 4f orbitals. Rare-earth elements are transitional in their chemical properties between the alkaline-earth elements, especially Ba and the 5d transition elements Hf, with certain exceptions they behave like transition elements of the Sc group with additional f electrons in discrete levels. The exceptions are mainly due to the high stability of the empty, half-filled or completely filled 4f shell. Certain compounds formed by Eu and Yb, and in some cases also Sm and Tm, therefore show close similarities with corresponding alkaline-earth compounds (i.e. Eu, Yb, Sm and Tm are divalent) [22, 23]. Rare-earth monochalcogenides are semiconducting if the rare-earth ion is in the divalent state and metallic if trivalent [19]. A divalent rare-earth has the outer electronic structure $4f^{14}5d^06s^2$, and the two s electrons contribute the valence electrons. In the rare-earth monochalcogenides, these two electrons fill the valence band derived from the p state of the anion. In the valence transition towards the trivalent state the outer electronic structure of the rare-earth changes from $4f^{14}5d^06s^2$ to $4f^{(14-x)}5d^x6s^2$, i.e. the fraction x of one 4f electron per formula unit is expected to go into the 5d conduction band state. This should result in a semiconductor to metal transition. Jayaraman *et al* [19] have examined the bulk modulus–volume relationship in rocksalt structured rare-earth compounds. They observe that in the plots of $\log B_0$ and $\log V_0$, the divalent and trivalent chalcogenides lie on lines nearly parallel to the line for the alkali halides. Sirdeshmukh *et al* [25] have examined the bulk modulus of eight divalent oxides. They observe that in the plot of bulk modulus and unit cell volume, the divalent chalcogenides lie on lines nearly parallel to the line for the alkali halide and eight divalent oxides. We have plotted $\log B$ versus $\log d^3$ and $\log E$ versus $\log d$ curves for alkali halides, divalent and trivalent chalcogenides and oxides; these are presented in figures 1 and 2. For zinc blende crystal structures, we have plotted the $\log B$ versus $\log d^3$ curve for group IV, group III–V and group II–VI semiconductors; these are presented in figure 3. We observe that in the plot of bulk modulus and interatomic distance, the divalent chalcogenides and trivalent chalcogenides lie on lines nearly parallel to the line for the alkali halides and in the plot of cohesive energy and interatomic distance, the alkaline-earth chalcogenides lie on lines nearly parallel to the line for the alkali halides. In figure 3, we observe that in the plot of bulk modulus and interatomic distance, the group IV and group III–V semiconductors lie on lines nearly parallel to the line for group II–VI semiconductors. From these figures it is quite obvious that the bulk modulus and cohesive energy trends in these compounds decrease with increasing interatomic distance and fall on straight lines according to the ionic charge product of the compounds.

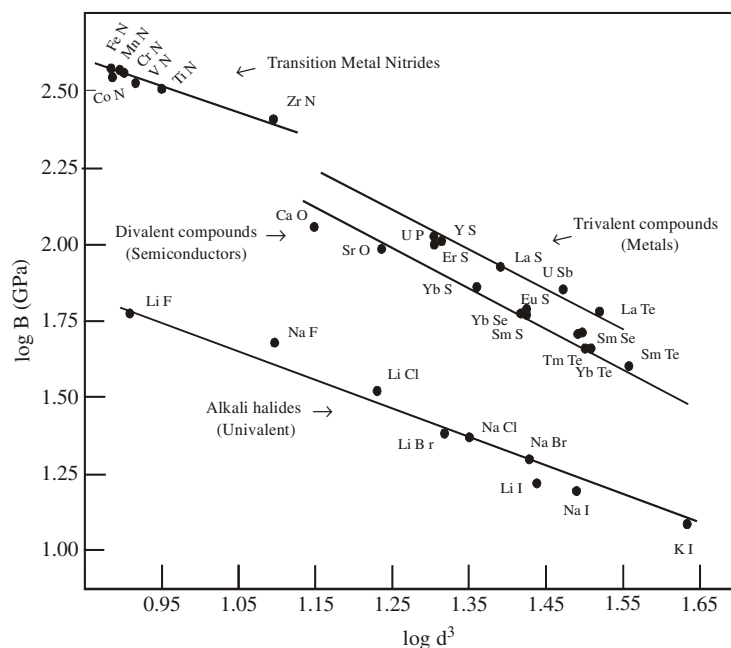


Figure 1. Plot of $\log B$ (bulk modulus) (GPa) against $\log d^3$ (d = interatomic distance) for trivalent and divalent compounds with some transition metal nitrides and alkali halides. In the plots of $\log B$ and $\log d^3$, the divalent and trivalent compounds lie on lines nearly parallel to the line for the alkali halides. In this figure all values are taken from experimental data apart from the TMN values, which are theoretical.

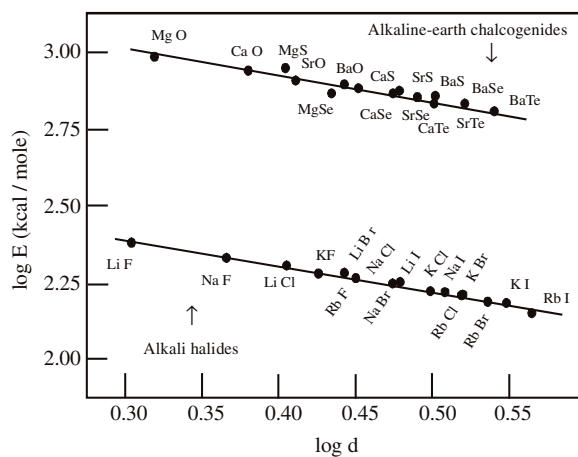


Figure 2. Plot of $\log E$ (cohesive energy) (kcal mol^{-1}) against $\log d$ (d = interatomic distance) for alkaline-earth chalcogenides and alkali halides. In this plot all data are taken from experimental results. In the plots of $\log E$ and $\log d$, the alkaline-earth chalcogenides lie on lines nearly parallel to the line for the alkali halides.

The proposed empirical relations (6) and (8) have been applied to evaluate bulk modulus values for alkali halides, alkaline-earth chalcogenides, transition metal nitrides (TMN), rare-earth monochalcogenides (RX, R = rare-earth metal, X = O, S, Se, Te), group III–V and

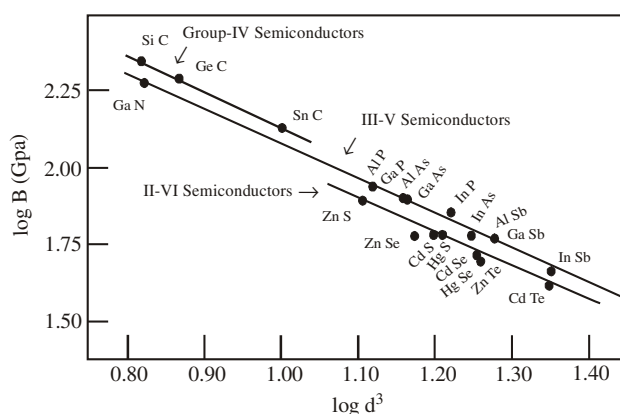


Figure 3. Plot of $\log B$ (bulk modulus) (GPa) against $\log d^3$ (d = interatomic distance) for group IV, group III-V and group II-VI semiconductors. In the plots of $\log B$ and $\log d^3$, the group IV and group III-V semiconductors lie on lines nearly parallel to the line for group II-VI semiconductors. In this figure all data are taken from experimental results apart from GeC, SnC and Hg chalcogenides, whose values are theoretical [11, 44, 45].

group II-VI semiconductors, and the cohesive energy for alkali halides, and alkaline-earth chalcogenides. The values so obtained are presented in tables 1–3 and are compared with the experimental and theoretical data reported so far. We note that the values of bulk modulus and cohesive energy evaluated by our proposed relations are in close agreement with the experimental data as compared to the values reported by previous researchers so far. For example, the results for bulk modulus differ from experimental values by the following amounts: BaO—0%, LiCl—0%, LaS—0%, SmSe—0%, ZnS—0%, CdS—0%, GaP—0%, InP—0%, MgO—0.61%, CaO—0.89%, SmS—1.7%, YbSe—1.6%, UP—1.9%, EuS—1.9%, USb—2.3%, ErS—2.9%, EuS—3.3%, YbTe—4.2%, LaTe—4.7%, NaBr—4.8%; and the results for cohesive energy differ from experimental values by the following amounts: LiCl—0.49%, KF—0.51%, RbF—0.54%, SrO—1.2%, NaCl—1.6%, NaF—1.8%, MgSe—1.9%, LiBr—2.6%, NaBr—2.8%, KCl—2.9%, CaO—3%, KBr—3.1%, CaSe—3.2%, SrSe—3.2%, CaTe—3.4%, NaI—3.6%, RbCl—3.7%, BaS—3.7%, CaS—3.8%, RbBr—3.8%, LiI—3.9%, SrS—4%, BaO—4.2%, LiF—4.3%, BaSe—4.5%, KI—4.5%, RbI—4.7% in the current study.

4. Summary and conclusions

From the above results obtained using the proposed empirical relations, and the discussion given, it is quite obvious that the parameters such as bulk modulus and cohesive energy reflecting the ground-state properties can be expressed in terms of the product of ionic charges and interatomic distance of these materials. This is definitely a surprising phenomenon and needs further investigations of the reason. The calculated values are presented in tables 1–3. We come to the conclusion that the product of ionic charges of any compound is a key parameter for calculating the ground-state properties. The bulk modulus and cohesive energy of these materials is inversely related to interatomic distance and directly depends on the product of ionic charges. The bulk moduli and cohesive energies of rocksalt type structure compounds exhibit a linear relationship when plotted on a log–log scale against the nearest-neighbour distance d (Å), but fall on distinct straight lines according to the ionic charge product of the compounds. From figure 1 we observe that the data points for the divalent, trivalent and transition metal compounds fall on three straight lines, nearly parallel to the line for the alkali

Table 1. In this table we have presented the values of cohesive energy (E_{coh}) and bulk modulus B (GPa) for alkali halides and alkaline-earth chalcogenides. The value of the product of ionic charge ($Z_1 Z_2$) = 1 for alkali halides and ($Z_1 Z_2$) = 4 for alkaline-earth chalcogenides.

Solids	d (Å)	E_{coh}			B (GPa)		
		Theor.	Exp.	This work	Theor.	Exp.	This work
MgO	2.105 ^e	1002 ^a	932 ^{a,b}	988	162 ^g	165 ^e	166
CaO	2.405 ^b	871 ^a	839 ^{a,b}	865	114 ^c	111 ^g	112
SrO	2.580 ^b	811 ^a	796 ^{a,b}	806	88 ^c	89 ^g	91
BaO	2.761 ^b	756 ^a	786 ^{a,b}	753	61 ^c	75 ^f , 74 ^g	74
MnO	2.222 ^b	911 ^b		936	147 ^c		142
FeO	2.139 ^c	938 ^b		972	163 ^c		159
CoO	2.133 ^b	955 ^b		975	181 ^c		160
NiO	2.084 ^b	976 ^g		998	173 ^c		172
MgS	2.540 ^a	816 ^a	896 ^a	819			95
CaS	2.830 ^a	715 ^a	764 ^a	735			69
SrS	3.010 ^b	652 ^a	720 ^a	691			57
BaS	3.180 ^a	632 ^a	679 ^a	654			48
PbS	2.968 ^c			701	62 ^c		60
MgSe	2.720 ^a	726 ^a	780 ^a	765			77
CaSe	2.960 ^a	664 ^a	726 ^a	703			60
SrSe	3.100 ^a	625 ^a	693 ^a	671			52
BaSe	3.300 ^a	589 ^a	660 ^a	630	40 ⁱ		43
CaTe	3.170 ^a	616 ^a	679 ^a	656			49
PbSe	3.062 ^c			679	54 ^c		54
SrTe	3.330 ^a	587 ^a	667 ^a	625			42
BaTe	3.500 ^a	553 ^a	629 ^a	594	34 ⁱ		36
PbTe	3.227 ^c			645	46 ^c		46
LiF	2.014 ^a	266 ^a	247 ^a	258	63 ^j	63 ^d	67
LiCl	2.570 ^b	205 ^a	203 ^a	202	33 ^j , 30 ^k	32 ^d	32
LiBr	2.750 ^b	191 ^a	194 ^a	189	24 ^h	24 ^d	27
LiI	3.012 ^b	172 ^a	180 ^a	173	17 ^h	17 ^j	20
NaF	2.317 ^b	233 ^a	220 ^a	224	47 ^h , 49 ⁱ	47 ^d	44
NaCl	2.820 ^b	189 ^a	187 ^a	184	25 ⁱ , 24 ^k	23 ^d	25
NaBr	2.987 ^b	180 ^a	179 ^a	174	21 ⁱ , 20 ^k	20 ^d	21
NaI	3.236 ^b	162 ^a	167 ^a	161	16 ⁱ , 15 ^k	15 ^d	16
KF	2.674 ^b	204 ^a	194 ^a	195	30 ^h , 30 ^k	31 ^l	29
KCl	3.146 ^b	172 ^a	170 ^a	165	17 ^h , 17 ^k	18 ^l	18
KBr	3.300 ^b	165 ^a	163 ^a	158	15 ^h , 15 ^k	15 ^l	15
KI	3.533 ^b	152 ^a	154 ^a	147	12 ^h , 12 ^k	12 ^d	13
RbF	2.815 ^a	200 ^a	186 ^a	185	27 ^h , 27 ^k	26 ^l	25
RbCl	3.291 ^b	166 ^a	164 ^a	158	16 ^h , 16 ^k	16 ^l	15
RbBr	3.445 ^b	157 ^a	157 ^a	151	14 ⁱ , 13 ^k	13 ^l	14
RbI	3.671 ^b	149 ^a	149 ^a	142	11 ⁱ , 11 ^k	11 ^l	11

^a Reference [27]. ^b Reference [21]. ^c Reference [25]. ^d Reference [40]. ^e Reference [30]. ^f Reference [31]. ^g Reference [32]. ^h Reference [20]. ⁱ Reference [19]. ^j Reference [33]. ^k Reference [47]. ^l Reference [48].

halides, and from figure 2 we observe that the data points for the divalent compounds fall on a straight line, nearly parallel to the line for the alkali halides. The bulk moduli of zinc blende type structure compounds exhibit a linear relationship when plotted on a log–log scale against the nearest-neighbour distance d (Å), but fall on three distinct straight lines according to the ionic charge product of the compounds. From figure 3 we observe that the data points for the

Table 2. In this table we have presented the values of bulk modulus B (GPa) for divalent and trivalent rare-earth monochalcogenides and group II–VI semiconductors. The value of the product of ionic charge ($Z_1 Z_2$) = 6 for trivalent rare-earth monochalcogenides and ($Z_1 Z_2$) = 4 for divalent rare-earth monochalcogenides and group II–VI semiconductors (T = trivalent, D = divalent).

Solids	d (Å)	B (GPa)			Valent system
		Theor.	Exp.	This work	
LaS	2.925 ^a		84 ^a	84	T
LaSe	3.030			76	T
LaTe	3.210 ^a		61 ± 2 ^a	64	T
SmS	2.985 ^b	51 ^c	60 ^b	59	D
SmSe	3.110 ^b	45 ^c	52 ^b	52	D
SmTe	3.300 ^b	36 ^c	40 ^b	43	D
EuO	2.570 ^a	90 ± 10 ^a	110 ± 5 ^a	92	D
EuS	2.985 ^a	51 ^c	61 ± 5 ^a	59	D
EuSe	3.095 ^a	46 ^c	52 ± 5 ^a	53	D
EuTe	3.300 ^a	37 ^c	40 ± 5 ^a	43	D
ErS	2.715 ^a		102 ± 1 ^a	105	T
TmS	2.710			78	D
TmSe	2.920			63	D
TmTe	3.170 ^b		46 ± 5 ^b	49	D
YbS	2.840 ^a	63 ^c	72 ± 5 ^a	68	D
YbSe	2.965 ^b	54 ^c	61 ± 5 ^b	60	D
YbTe	3.180 ^b	41 ^c	46 ± 5 ^b	48	D
YS	2.745 ^a	100 ^a		102	T
US	2.735	110 ^d		103	T
USe	2.870	94 ^d		89	T
UTe	3.100	63 ^d		71	T
UP	2.730	107 ^e	102 ± 3 ^e	104	T
UAs	2.850	75 ^f	101 ^f	91	T
USb	3.095	68 ^e	72.7 ± 5 ^e	71	T
ZnS	2.340 ^g	90 ^g	77 ^g	77	D
ZnSe	2.460 ^g	75 ^g	62 ^g	67	D
ZnTe	2.640 ^g	59 ^g	51 ^g	54	D
CdS	2.520 ^g	69 ^g	62 ^g	62	D
CdSe	2.620 ^g	60 ^g	53 ^g	55	D
CdTe	2.810 ^g	47 ^g	42 ^g	45	D
HgS	2.530 ^h	69 ^h		61	D
HgSe	2.630 ^h	58 ^h		54	D
HgTe	2.800 ^h	48 ^h		45	D

^a Reference [19]. ^b Reference [24]. ^c Reference [39]. ^d Reference [38]. ^e Reference [36].
^f Reference [37]. ^g Reference [18]. ^h Reference [45].

group IV and group III–V semiconductors fall on two lines, nearly parallel to the line for II–VI semiconductors, which means that ionic binding dominates all these compounds. It is also noteworthy that the proposed empirical relations are simpler, widely applicable, and values obtained are in better agreement with experiment data as compared to the empirical relations proposed by previous researchers. We have been reasonably successful in calculating these parameters using the product of ionic charges and interatomic distance of the materials for rocksalt and zinc blende crystals. It is natural to say that this model can easily be extended to chalcopyrite crystals, for which the work is in progress and will be appearing in forthcoming paper. Hence it is possible to predict the order of ground-state properties of semiconducting

Table 3. In this table we have presented the values of bulk modulus B (GPa) for TMN, group IV and group III–V semiconductors. The value of the product of ionic charge ($Z_1 Z_2$) = 9 for TMN and group III–V semiconductors and ($Z_1 Z_2$) = 16 for group IV semiconductors.

Compounds	d (Å)	B (Exp.)	B (Theor.)	B (This work)
TiN	2.125 ^a		288 ^a , 304–331 ^b	298
VN	2.019 ^c		346 ^c , 338–383 ^b	347
CrN	1.990 ^c		364 ^c	363
MnN	1.972 ^c		374 ^c	373
FeN	1.965 ^c		368 ^c	377
CoN	1.965 ^c		358 ^c	377
NiN	1.991 ^c		311 ^c	362
ZrN	2.310 ^b		251 ^b	232
AlN	1.87 ^d		186 ^e	178
AlP	2.36 ^f	86 ^d	89 ^d	89
AlAs	2.43 ^f	82 ^d	75 ^d	81
AlSb	2.66 ^f	58 ^d	63 ^g	62
GaN	1.88 ^d	190 ^e	173 ^h	175
GaP	2.36 ^f	89 ^f	92 ^d	89
GaAs	2.45 ^f	77 ^d	76 ^d	79
GaSb	2.65 ^f	57 ^f	57 ^d	63
InN	2.08 ^d		137 ^h	129
InP	2.54 ^f	71 ^f	74 ^d	71
InAs	2.61 ^f	60 ^f	70 ^g	66
InSb	2.81 ^f	47 ^f	40 ^g	53
BN	1.55 ^d	369 ^e	321 ^e	313
BP	1.94 ^d	173 ^d	173 ^d	159
BAAs	2.04 ^d		146 ^d	137
BSb	2.24 ^d		110 ^d	104
TiN	2.11 ^d		141 ^d	124
TiP	2.49 ^d		71 ^d	75
TiAs	2.58 ^d		59 ^d	68
TiSb	2.75 ^d		46 ^d	56
SiC	1.87 ^d	224 ^d	212 ^f	200
GeC	1.95 ^d		188 ^d	176
SnC	2.15 ^d		133 ⁱ	131

^a Reference [35]. ^b Reference [34]. ^c Reference [13]. ^d Reference [11]. ^e Reference [16].
^f Reference [18]. ^g Reference [6]. ^h Reference [46]. ⁱ Reference [44].

and metallic compounds from their ionic charges. The method presented in this work will be helpful to material scientists for finding new materials with desired bulk modulus and cohesive energy among a series of structurally similar materials.

Acknowledgments

We are sincerely thankful to the University Grant Commission, New Delhi, India, for providing financial assistance under the research project entitled ‘Study of electronic and magnetic properties of rare-earth semiconducting materials’.

References

- [1] Eyring L 1979 *Hand Book on the Physics and Chemistry of Rare Earths* vol 3, ed K A Gschneidner Jr and L Eyring, pp 337–99

- [2] Marsella L and Fiorentini V 2004 *Phys. Rev. B* **69** 172103
- [3] Nag B R 1994 *Appl. Phys. Lett.* **65** 1938
- [4] Xue D, Betzler K and Hesse H 2000 *J. Phys.: Condens. Matter* **12** 3113
- [5] Marquez R and Rincon C 1995 *Phys. Status Solidi b* **191** 115
- [6] Al-Douri Y, Abid H and Aourag H 2005 *Mater. Lett.* **59** 2032
- [7] Verma A S, Sharma D and Bhardwaj S R 2004 *Proc. Ferro Electrics and Dielectrics (NSFD XIII) (Delhi University, Delhi, India, Nov. 2004)* pp 309–12
- [8] Verma A S, Rathi S K, Sharma D and Bhardwaj S R 2006 *Acta Ciencia Indica* vol xxxii p 65
- [9] Anderson O L and Nafe J E 1965 *J. Geophys. Res.* **70** 3951
- [10] Cheng D Y, Wang S Q and Ye H Q 2001 *Phys. Rev. B* **64** 024107
- [11] Wang S Q and Ye H Q 2002 *Phys. Rev. B* **66** 235111
- [12] Kanoun M B, Goumri-Said S, Merad A E, Merad G, Cibert J and Aourag H 2004 *Semicond. Sci. Technol.* **19** 1220
- [13] Li C-B, Li M-K, Liu F-Q and Fan X-J 2004 *Mod. Phys. Lett. B* **18** 281
- [14] Jha P K, Aynyas M and Sanyal S P 2004 *Indian J. Pure Appl. Phys.* **42** 112
- [15] Merad A E, Kanoun M B, Merad G, Cibert J and Aourag H 2005 *Mater. Chem. Phys.* **92** 333
- [16] Tutuncu H M, Bagci S, Srivastava G P, Albudak A T and Ugur G 2005 *Phys. Rev. B* **71** 195309
- [17] Liu L M, Wang S Q and Ye H Q 2005 *J. Phys.: Condens. Matter* **17** 5335
- [18] Cohen M L 1985 *Phys. Rev. B* **32** 7988
- [19] Jayaraman A, Batlogg B, Maines R G and Bach H 1982 *Phys. Rev. B* **26** 3347
- [20] Schlosser H 1992 *J. Phys. Chem. Solids* **53** 855
- [21] Schlosser H 1993 *Phys. Status Solidi b* **179** k1
- [22] Vogt O and Mattenberger K 1995 *J. Alloys Compounds* **223** 226
- [23] Gschneidner K G 1961 *Rare Earth Alloys* (Princeton, NJ: Van Nostrand)
- [24] Jayaraman A, Singh A K, Chatterjee A K and Ushadevi S 1974 *Phys. Rev. B* **9** 2513
- [25] Sirdeshmukh D B and Subhadra K G 1986 *J. Appl. Phys.* **59** 276
- [26] Krishnan K S and Roy S K 1952 *Proc. R. Soc.* **210** 481
- [27] Gupta V P and Sipani S K 1982 *Phys. Status Solidi b* **111** 295
- [28] Haglund J, Grimvall G, Jarlborg T and Guillermet A F 1991 *Phys. Rev. B* **43** 14400
- [29] Guillermet A F, Haglund J and Grimvall G 1993 *Phys. Rev. B* **48** 11673
- [30] Alfe D 2005 *Phys. Rev. Lett.* **94** 235701
- [31] Mota R C, Costa S C, Pizani P S and Rino J P 2005 *Phys. Rev. B* **71** 224114
- [32] Gupta B R K and Goyal R P 1984 *Solid State Commun.* **49** 559
- [33] Kumari M and Dass N 1990 *J. Phys.: Condens. Matter* **2** 7891
- [34] Simunck A and Vackar J 2001 *Phys. Rev. B* **64** 235115
- [35] Liu L M, Wang S Q and Ye H Q 2003 *J. Phys.: Condens. Matter* **15** 8103
- [36] Leger J M, Oki K, Redon A M, Vedel I, Mignod J R and Vogt O 1986 *Phys. Rev. B* **33** 7205
- [37] Leger J M, Vedel I, Redon A M, Mignod J R and Vogt O 1988 *Solid State Commun.* **66** 1173
- [38] Brooks M S S 1984 *J. Phys. F: Met. Phys.* **14** 653
- [39] Singh D V and Gupta V P 1992 *Phys. Status Solidi b* **171** k71
- [40] Fang Z H and Chen L R 1993 *Phys. Status Solidi b* **180** k5
- [41] Wang S Q and Ye H Q 2005 *J. Phys.: Condens. Matter* **17** 4475
- [42] Lam P K, Cohen M L and Martinez G 1987 *Phys. Rev. B* **35** 9190
- [43] Phillips J C 1973 *Bonds and Bands in Semiconductors* (New York: Academic)
- [44] Rucker H and Methfessel M 1995 *Phys. Rev. B* **52** 11059
- [45] Wei S H and Zunger A 1988 *Phys. Rev. B* **37** 8958
- [46] Kim K, Lambrecht W R L and Segall B 1996 *Phys. Rev. B* **53** 16310
- [47] Bosi L 1993 *Phys. Status Solidi b* **175** k47
- [48] Neumann H 1988 *Cryst. Res. Technol.* **23** 531