ELSEVIER

Lattice thermal expansion for normal tetrahedral compound semiconductors

M.S. Omar *

Department of Physics, College of Science, University of Salahaddin, Arbil, Iraqi Kurdistan, Iraq

Abstract

The cubic root of the deviation of the lattice thermal expansion from that of the expected value of diamond for group IV semiconductors, binary compounds of III–V and II–VI, as well as several ternary compounds from groups I–III–VI$_2$, II–IV–V$_2$ and I–IV$_2$V$_3$ semiconductors versus their bonding length are given straight lines. Their slopes were found to be 0.0256, 0.0210, 0.0170, 0.0259, 0.0196, and 0.02840 for the groups above, respectively. Depending on the valence electrons of the elements forming these groups, a formula was found to correlate all the values of the slopes mentioned above to that of group IV. This new formula which depends on the melting point and the bonding length as well as the number of valence electrons for the elements forming the compounds, will gives best calculated values for lattice thermal expansion for all compounds forming the groups mentioned above. An empirical relation is also found between the mean ionicity of the compounds forming the groups and their slopes mentioned above and that gave the mean ionicity for the compound CuGe$_2$P$_3$ in the range of 0.442.
© 2006 Elsevier Ltd. All rights reserved.

Keywords: Lattice thermal expansion; Compound semiconductors; Semiconductor ionicity

1. Intoduction

The ternaries I–III–VI$_2$ and II–IV–V$_2$ (ABC$_2$) have a chalcopyrite type structure and space group $I\bar{4}2d$ with four formula units per cell [1]. Each A and B-atom is tetrahedrally coordinated to four C-atoms while each C-atom is tetrahedrally coordinated to two A and two B-atoms in ordered manner. These compounds are regarded as the ternary analogues of II–VI and III–V binary compounds, respectively, which belong to the diamond structure. There are compounds such as CuGe$_2$P$_3$ and CuSi$_2$P$_3$ belongs to group I–IV$_2$–V$_3$ and regards of the ternary analogue to III–V compounds [2]. These two compounds have Zinc-blend structure with space group $F\bar{4}3m$ and their atoms are distributed in a form that P atoms are occupying cation sites while Cu and Ge or Si are occupying the anion sites randomly [2,3].

The knowledge of thermal expansion is important not only in crystal growth from liquid-vapor epitaxy but also in the formation of hetrojunctions as well as in determining temperature dependence of optical birefringence as it may be necessary in tuning of non-linear optical laser devices [4]. It is also important in determining the band structure of semiconductors [5].

---

* Tel.: +964 662518226; fax: +964 662518226.
  E-mail address: dr_m_s_omar@yahoo.com.

There are several methods in determining lattice thermal expansion in semiconductors, but due to the small changes of the unit cell dimensions, the accuracy of determining this parameter always have been unpredictable. One of the methods of obtaining lattice thermal expansion is from the measurements of the temperature dependence of the unit cell volume [3,6,7], or may be from the crystal dimensions [8]. In this case the results will be dependent on the accuracy of the experimental set-up as well as on the technical information of the researcher. The second method is dependent on the first principles calculations within the quasi-harmonic approximation [9]. The latter method needs a powerful computer and efficient algorithms. There is a simpler method reported as a model depends on an empirical formula build up from the hard sphere model based on diamond [10,11]. In this model, 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 expansion by this method is the bonding length and the melting point. However, due to existence of these parameters with highly accurate values [3,1], the results obtained for thermal expansion will also have high accuracy.

Due to the wide range applications of thermal expansion, as mentioned above, a more accurate value will be important in this regard. However, it has been found that for elementary and binary semiconductors, the cubic root of the deviation of the lattice thermal expansion from that of the expected values for diamond $\Delta^{1/3}$ will be changes linearly with the bonding length for each group [11]. In this work these deviations were investigated for the compound groups mentioned above and the results were compared with those reported earlier. The effects of mean ionicity due to each group on the dependence of $\Delta^{1/3}$ versus mean bonding length d_{mean} were investigated. Depending on the number of valence electrons, which forms the compound semiconductors, investigations were carried out to obtain a general formula for calculating lattice thermal expansion for all such compounds.

2. Methods of calculation

It has been found for most compound materials, the product of the melting point M_P and their average linear thermal expansion coefficient α_L at near room temperature and above where the value is essentially saturated and tends to be a structure dependent constant [10,11]. The value is $\alpha_L M_P$ (K) = 0.027 for rectilinear structures and 0.016 for close-packed structures [10]. For tetrahedral semiconductors, the saturation value for α_L has to be related to the product $\alpha_L M_P$ (K) = 0.021 derived from data for diamond and the polarization parameter which is proportional to the bond length d is raised to the third power, d^3 [11]. "The product has also been found to be constant for analogous compounds provided that the ionicity and structure do not change". Thermal expansion coefficients used are 1/3 of the volume expansion coefficients in the saturation region. The quotient $0.021/M_P$ (K) is the measure of α_L expected from hard sphere model based on diamond. The term Δ is the difference between the expected α_L calculated for diamond which is equal to $0.021/M_P$ and that obtained by the measurement in the saturation region α_L or α_L is constant at the temperature range near below room temperature and above up to near the melting point of the compound then:

$$\alpha_L = \left(\frac{0.021}{M_P} \right) - [D(d - d_0)]^3 \tag{1}$$

where D is the slope, d_0 is the bond length for diamond and is equal to 1.545 Å and d_{mean} is the mean bond length for the interested semiconductor. In this work, the bond length was calculated using relations applicable to ternary chalcopyrite compounds of the form ABC_2 as [15]:

$$d_{B-C} = \left[a^2 \left(\frac{1}{2} - x \right)^2 + \frac{(4a^2 + c^2)}{64} \right]^{1/2} \tag{2}$$

$$d_{A-C} = \left[a^2 x^2 + \frac{(4a^2 + c^2)}{64} \right]^{1/2} \tag{3}$$

and

$$x = 0.5 - \left[\frac{c^2}{32a^2} - \frac{1}{16} \right]^{1/2} \tag{4}$$

Table 1

Information for melting point, lattice thermal expansion, bonding length and the calculated lattice thermal expansion for some ternary normal tetrahedral compounds

Compounds	M_P (K)	Reference	$\alpha_L \times 10^{-6}$ (Exp.)	Reference	$\Delta^{1/3}$	Bonding length (Å)	$\alpha_L \times 10^{-6}$ (Calc.) Eq. (13)
$ZnSiP_2$	1453	[1]	6.33	[17]	0.0194	2.314	6.82
$ZnSiAs_2$	1389	[1]	5.73	[18]	0.0211	2.406	4.41
$ZnGeP_2$	1298	[1]	6.87	[17]	0.021	2.355	7.26
$ZnGeAs_2$	1123	[1]	5.57	[18]	0.0236	2.443	6.55
$ZnSnP_2$	1223	[1]	5.53	[19]	0.023	2.447	4.86
$ZnSnAs_2$	1048	[1]	2.3	[20]	0.0261	2.538	3.61
$CdSiP_2$	1393	[1]				2.402	4.51
$CdSiAs_2$	1123	[1]	5.4	[19]	0.0237	2.443	6.55
$CdGeP_2$	1063	[1]	6.07	[17]	0.024	2.446	7.48
$CdGeAs_2$	943	[1]	5.68	[21]	0.0255	2.53	6.24
$CdSnP_2$	843	[1]	4	[19]	0.0267	2.535	8.63
$CdSnAs_2$	866	[1]	4.7	[20]	0.0269	2.62	3.41
$CuAlS_2$	1573	[1]	11.17	[22]	0.01296	2.297	10.57
$CuAlSe_2$	1473	[1]	10.47	[22]	0.0175	2.409	10.04
$CuAlTe_2$	1143	[1]			0.0205	2.574	11.24
$CuGaS_2$	1553	[1]				2.299	10.72
$CuGaSe_2$	1343	[1]	10.46	[18]	0.0173	2.417	11.30
$CuGaTe_2$	1143	[1]				2.595	10.80
$CuInS_2$	1300	[1]				2.392	12.18
$CuInSe_2$	1263	[1]	10.27	[18]	0.0183	2.5	10.93
$CuInTe_2$	1053	[1]	9.5	[23]	0.0219	2.676	10.48
$AgAlS_2$	1420	[1]				2.404	10.64
$AgAlSe_2$	1223	[1]				2.515	11.20
$AgAlTe_2$	1000	[1]				2.683	11.36
$AgInTe_2$	953	[1]				2.742	10.81
$AgInS_2$	1120	[1]				2.491	13.21
$AgGaSe_2$	1123	[15]				2.525	12.54
$CuGe_2P_3$	1103	[16]	8.2	[24]	0.0221	2.324	7.81
$CuSi_2P_3$	1451	[3]				2.272	5.35
C (diamond)	3950	[11]	5.3	[11]		1.545	5.3
W–SiC	2970	[11]	6.3	[11]	0.0091	1.887	6.40
Si	1683	[11]	4.3	[11]	0.02	2.35	3.73
Ge	1209	[11]	5.9	[11]	0.0225	2.45	4.93
Sn	505	[11]	5.3	[11]	0.0331	2.81	7.62
AlSb	1353	[11]	4.5	[11]	0.0222	2.656	2.82
GaAs	1513	[11]	7.2	[11]	0.0188	2.45	7.02
GaP	1813	[11]	6.1	[11]	0.0176	2.36	6.57
InSb	806	[11]	5.6	[11]	0.0273	2.805	7.53
InAs	1216	[11]	6.5	[11]	0.0221	2.614	5.95
InP	1333	[11]	5.5	[11]	0.0217	2.541	6.60
ZnS	2103	[11]	6.9	[11]	0.0144	2.342	7.40
ZnSe	1798	[11]	7.7	[11]	0.0159	2.454	7.84
ZnTe	1512	[11]	8	[11]	0.0181	2.636	7.25
CdS	2023	[11]	4.5	[11]	0.018	2.53	5.49
CdSe	1623	[11]	7.3	[11]	0.0178	2.63	6.41
CdTe	1371	[11]	5.1	[11]	0.0218	2.806	5.07
GaSb	985	[11]				2.649	14.44

where a and c are lattice constants, their values for the two groups of II–IV–V_2 and I–III–VI_2 are taken from Ref. [1]. The bond-length used for the calculations are the mean values of the two as in the form:

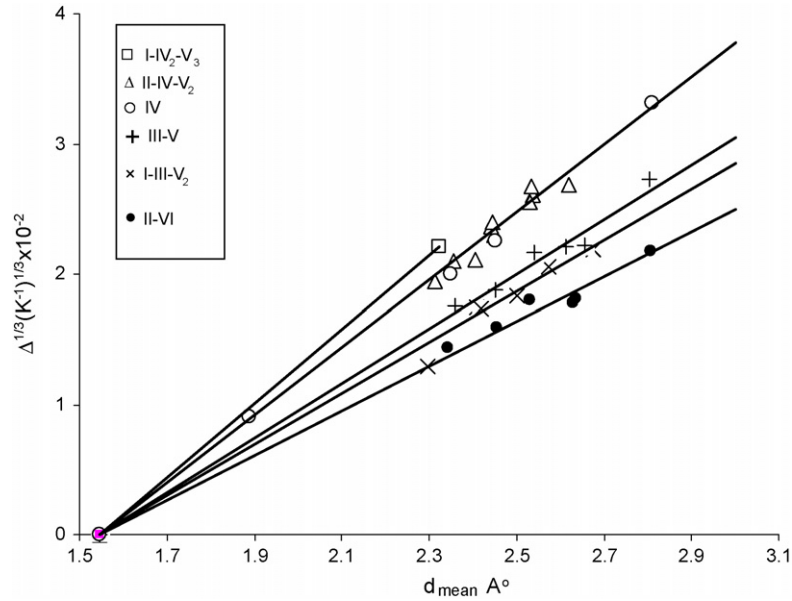$$d_{mean} = \frac{d_{A-C} + d_{B-C}}{2} \tag{5}$$

Fig. 1. The cubic root of the deviation of the lattice thermal expansion of a semiconductor from that of the expected value of diamond $\Delta^{1/3}$ in $K^{-1/3}$ vs. d_{mean} in Å "the mean bonding length" before applying the effects of ionicity.

For compounds of $CuGe_2P_3$ and $CuSi_2P_3$ from the ternary group $I–IV_2–V_3$ having an f.c.c. structure, relations (2)–(5) are reduced to:

$$d_{mean} = \left(\frac{a}{4}\right)\sqrt{3} \qquad (6)$$

Hence d_{mean} is the mean bonding length. Lattice spacing values of 5.3678 Å for $CuGe_2P_3$ and 5.248 Å for $CuSi_2P_3$ are used [3]. The d_{mean} as well as all other information for groups IV, II–VI and III–V compounds are taken from [11]. Values of D, α_L, Δ and M_P for all compounds interested in this work as well as group IV semiconductors are reported in Table 1.

Fig. 1 shows the cube root of the deviation $(\Delta)^{1/2}$ versus the mean distance d_{mean} calculated through Eqs. (1)–(6) for semiconductors mentioned in Table 1.

3. Results and analysis

Fig. 1 shows the cub root of the deviation of α_L for the interested sample to that of the calculated from the model of diamond indicated above as $(\Delta)^{1/3} = ((0.021/M_P) - \alpha_L)^{1/3}$ versus the mean distance between the nearest neighbors (mean bond length), calculated through Eqs. (1)–(6). This figure clearly shows the deviation of the slopes for groups having the same configurations of the valence electrons for the elements forming the compound from that of the group IV. The increase of the bonding for compounds in each class mentioned above is subjects to the increase in their metalicity. This means that for a certain group the compounds with a larger bonding length, behaves less like a hard sphere and have a more polarizability. For highly polarizable atoms, such as group IV elements, however, in solids of this group the electron cloud have a spherical non-ionic distribution and that consequently means a high flexibility to the external effect of pressure. From the tetrahedral coordinate of diamond, the displacement of the reference atom presses the electron cloud of the three neighboring atom spheres produces a large orifice sizes with the nucleus remains at their positions and that consequently permits a greater penetration and that in turn produces a less thermal expansion. The information mentioned above could be represented through the ionicities of the compounds. However, lattice thermal expansion dependence on the percentage ionicity has been reported to be linier for many oxide and floride binary compound crystals such as SnO_2, PbO_2, etc. and MgF_2, CoF_2, etc. [12]. The ionicities used in their work were calculated from the relation below:

$$\text{Amount of ionic character} = 1 - e^{-1/4}(X_A - X_B)^2 \qquad (7)$$

Table 2
Values of D in (K$^{-1/3}$ Å^{-1}) "the slope of $\Delta^{1/3}$ vs. mean bonding length" and $\bar{f}_i^2$ "square of mean ionicity" for six groups of normal tetrahedral compound semiconductors

Compound groups	D (K$^{-1/3}$ Å^{-1}) (this work)	D^3 (K$^{-1/3}$ Å^{-3}) $\times 10^{-6}$	D (K$^{-1/3}$ Å^{-1}) [13]	f_i^2
IV	0.0256	16.777	0.0257	0
III–V	0.0210	9.261	0.02154	0.152
II–VI	0.0170	4.913	0.01488	0.422
II–IV–V$_2$	0.0259	17.374	0.02525	0.0784
I–III–VI$_2$	0.0196	7.53	0.01613	0.325
I–IV$_2$–V$_3$	0.0284	22.9		

where X_A and X_B are the electronegativities of the two type atoms. However, attempts for a such dependence regarding compounds in the groups interested in this work was not successful so far.

A similar relation has also been used by Numann to calculate the ionicities f_i of tetrahedral compound semiconductors [13]. He reported an approximate empirical relation between D and f_i as:

$$D^3 = b_0 - b_1 \bar{f}_i^2 \tag{8}$$

where b_0 and b_1 are constants having values of 17.6 and 37.3 $\times 10^{-6}$ K^{-1} Å^{-3}, respectively. Hence $\bar{f}_i$ is the mean ionicities and are arithmetic means of the ionicities of all the compounds of a given family. For binary groups, $\bar{f}_i$ values have been taken from [14], while for ternary chalcopyrite compounds having two types of anions, the average ionicity $\bar{f}_i$ have been used were taken from Ref. [13]. The values of $\bar{f}_i$ are given in Table 2. If the values of D obtained in this work are drawn versus $\bar{f}_i^2$ as shown in Fig. 2, then new values for b_0 and b_1 for this empirical relation obtained as 17.061 and 29.86 $\times 10^{-6}$ K^{-1} Å^{-3}, respectively.

Eq. (8) with its new values of b_0 and b_1 is applicable for all group compounds mentioned in Table 2 except for that of I–IV$_2$–V$_3$. To extend this relation for such a group, it should be written in a new form:

$$D = (b_0 \pm b_1 \bar{f}_i^2)^{1/3} \tag{9}$$

In this relation, the negative sign should be for the group compounds having values of D less than that of the group IV while the positive sign will be for the values of D higher than that. When Eq. (9) was applied the values of ionicity $\bar{f}_i$ for group I–IV$_2$–V$_3$ compounds, namely CuGe$_2$P$_3$ was found to be equal to 0.442.

In semiconductors, ionicities are a function of the configuration of the atomic valence electrons in the compound. However, tetrahedral compounds are formed from the elements of the right and left side of group IV in
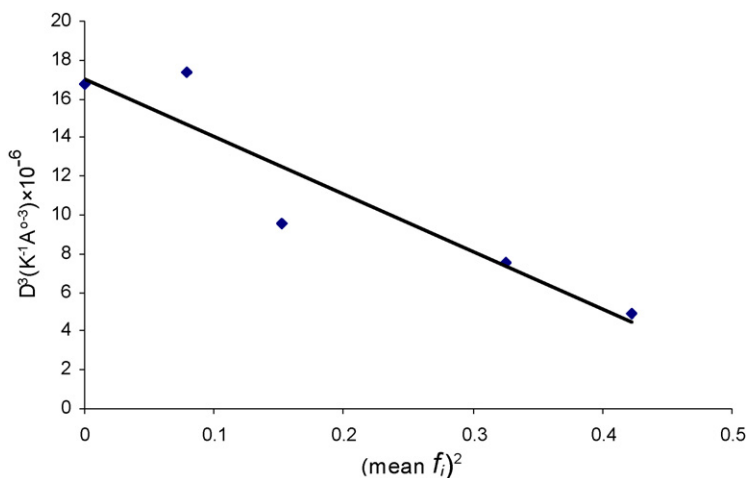

Fig. 2. D^3 in K$^{-1/3}$ Å^{-3} vs. $\bar{f}_i^2$ "square of mean ionicity" for five groups of normal tetrahedral compound semiconductors.

the periodic table, having less and more than four valence electrons, respectively [2]. To form sp^3 hybridization for normal tetrahedral compounds, four electrons per lattice should be available. This consequently is formed through mixing the valence electrons of all the atoms forming the compound, then, the ionic character for both the cation and anion lattices will be produced [15]. However, the latter produces a considerable shrinkage to the atomic shells, and that means a harder sphere and less polarizable. Then the nuclei and electron clouds of the surrounding atoms must shift permanently to allow for penetration, that gives a larger value of thermal expansion. The analysis mentioned above is build from values of D (the slope of $\Delta^{1/3}$ versus bond length) as they are indicated in Table 2.

Values of D for ternary group compounds I–III–V$_2$ and II–IV–V$_2$ indicated in Table 2 are different from that reported in [5]. Although their calculations were build from the diamond model, but the intercepts of the $\Delta^{1/3}$ versus d with the d-axis as the bonding length in their calculation have been left open, which gives different intersection reference points for different compounds. However, due to the hard sphere model based on diamond the curves for all compounds should intercept at the same reference point, which is the value of the bonding length of diamond and that is equal to 1.545 Å [11].

From the information of the dependence of D on the mean ionicity $\bar{f_i}$ for the group compound semiconductors as mentioned earlier, attempts to make a mathematical formula in a long range system for the compounds that belong to the same group was not successful so far.

Since group IV semiconductors have zero ionicity, then the deviation of D for the more complicated compounds mentioned earlier could be related to the number of valence electron difference between the cation and anion atoms, that is, depends on the effect of the electron cloud mentioned earlier. For binary compounds and throughout the process of trial and error the multiplication value to D which makes the slope of the binary to be exactly equal to that of group IV was found to be in the form $(B - A)^{1/3.5}$, where A and B are the number of valence electrons for the anion and cation atoms, respectively. This is the re-correction of the effects of the ionicity on thermal expansion. Results for group II–VI and III–V compounds are shown in Fig. 3. However this parameter makes the equation that belongs to group IV
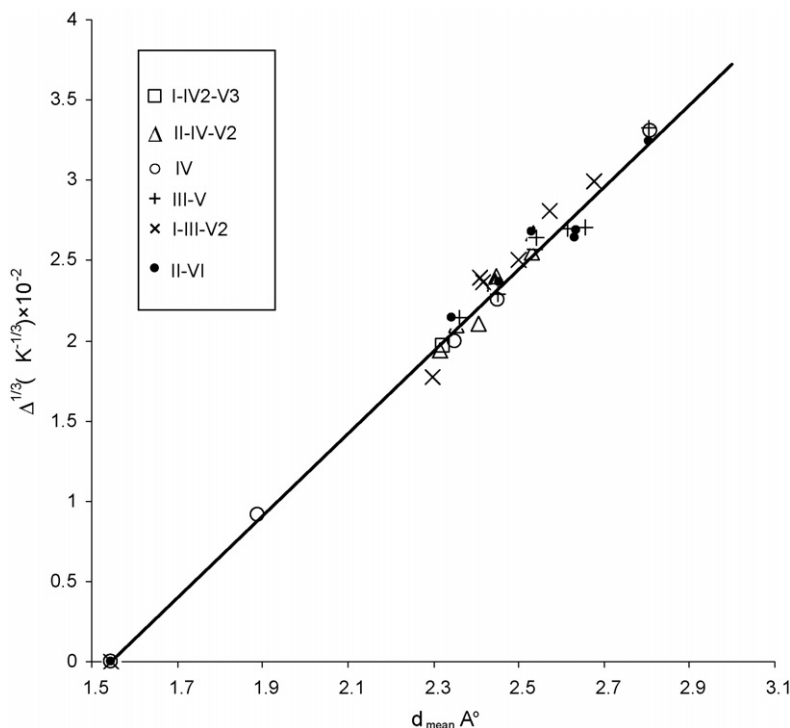

Fig. 3. The cubic root of the deviation of the lattice thermal expansion of a semiconductor from that of the expected value of diamond $\Delta^{1/3}$ in K$^{-1/3}$ vs. d_{mean} in Å "the mean bonding length" after applying the effects of ionicity.

(Eq. (1)) be extended to that including the binary normal tetrahedral compounds as:

$$\alpha_L = \frac{0.021}{M_P} - \left[D(B-A)^{-1/3.5}(d-d_0)\right]^3 \tag{10}$$

where D in units of $K^{-1/3}$ $Å^{-1}$ and is the value of the slope for diamond as reported in Table 2.

To have values of D that belong to ternary normal tetrahedral compounds having two anion type lattices be exactly equal to the value of D for diamond, it was found that the difference between the anion lattice atom valence electrons in these groups has a significant effect on the relation. For chalcopyrite ternary semiconductors such as II–IV–V$_2$ and I–III–VI$_2$ groups, when the number of the two different anion lattices are equal, their difference of the valence electrons will be add to the factor found for the binary and become $[\{(C-A)+(C-B)-(B-A)\}1/q]^{1/3.5}$. Then values of D belong to these ternaries, changes exactly to that of diamond as shown in Fig. 3. For making Eq. (10) applicable to ternary compounds of this type, this factor should be multiplied by the values of D in Eq. (1), which is applicable to group IV, then a general equation will be formed:

$$\alpha_L = \frac{0.021}{M_P} - \left[D\left[\{(C-A)+(C-B)-(B-A)\}\frac{1}{q}\right]^{-1/3.5}(d-d_0)\right]^3 \tag{11}$$

where A and B are the number of the first and second cation valence electron in the compound and q is the number of cation or anion lattices and is equal to 2 in this case. For a more complicated ternary group compounds such as I–IV$_2$–V$_3$, where anion lattices are occupied by different number of different type of bases, additional information should be considered. Through the process of trial and error, new correction parameters were found to bring values of D for group I–IV$_2$V$_3$ exactly to that for diamond .The factor is: $[[\{(C-A)+2(C-B)\}-\{(B-A)+[B-(B-A)]\}]1/q]^{1/3.5}$ and the results are shown in Fig. 3. When this factor is added to Eq. (11), the equation will be extended to include the above group compounds and becomes:

$$\alpha_L = \frac{0.021}{M_P} - \left[D\left[[\{(C-A)+2(C-B)\}-\{(B-A)+[B-(B-A)]\}]\frac{1}{q}\right]^{-1/3.5}(d-d_0)\right]^3 \tag{12}$$

where 2 is regarded as a two of a one type bases in the cation lattice and q for this case is equal to 3 which is the number of cation or anion lattices. In this equation, if the value of D is belongs to group IV compounds and its value is given in Table 2, d_0 is the mean bonding length for diamond, then Eq. (12) for α_L can be rewritten in a new form:

$$\alpha_L = \frac{0.021}{M_P} - \left[0.0256\left[[\{m(C-A)+n(C-B)\}-\{(B-A)+[B-(B-A)]\}]\frac{1}{q}\right]^{-1/3.5}(d-1.545)\right]^3 \tag{13}$$

where m and n are the number of the first and second cation lattices, respectively. They are equal to 1 and 2, respectively, for the ternary group I–IV$_2$–V$_3$, while both of them are equal to 1 for both of the compound groups II–IV–V$_2$ and I–III–VI$_2$.

Eq. (13) is found to be applicable to calculate lattice thermal expansion for all group semiconductors mentioned in this work except group IV compounds where Eq. (1) is applicable. As mentioned for Eq. (1), this equation is applicable at temperatures near below room temperature and above up to near the compound melting point. However calculated values of thermal expansion α_L by using this equation for all the compounds interested in this work are given in Table 1.

4. Conclusions

A suitable empirical relation was found to calculate lattice thermal expansion at near room temperature and above for normal tetrahedral semiconductors based on six groups of compound semiconductors, namely IV, III–V, II–VI, II–IV–V$_2$, I–III–VI$_2$ and I–IV$_2$–V$_3$. The slope D, of the graph of the cubic root of the deviation of the lattice thermal expansion of the interested compound from that of the expected value of diamond $\Delta^{1/3}$ versus their bonding length, was found to be strongly dependent on the mean ionicity $\bar{f_i}$ of the compounds in a group and a general empirical

relation between the two was formed. The valence electrons for the elements forming these compound groups were found to be controlling the values of *D* mentioned above.

Acknowledgment

References

[1] J.L. Shay, J.H. Wernick, in: B.R. Pamplin (Ed.), Ternary Chalcopyrite Semiconductors; Growth, Electronic Properties, and Applications, Pergaman Press, 1975.
[2] N.A. Goryunova, The Chemistry of Diamond-like Semiconductors, Chapman & Hall Ltd., London, England, 1965.
[3] M.S. Omar, Ph.D. Thesis, Bath Uni, England, 1985.
[4] L.K. Somanata, Phys. Stat. Solidi A 57 (1980) 735.
[5] H. Neumann, P. Deus, R.D. Tomlinson, G. Kunn, B. Hintze, Phys. Stat. Solidi A 84 (1984) 87.
[6] G. Bhikshamaiah, M.V. Sabrahmanya Sarma, S.V. Suryanarayana, M.S. Omar, J. Less-Common Met. 113 (1985) L5.
[7] G. Bhikshamaiah, S.V. Suryanarayana, M.S. Omar, J. Mater. Sci. Lett. 5 (1986) 121.
[8] R. Feder, T.B. Light, J. Appl. Phys. 43 (7) (1972) 3115.
[9] A.A. Quong, A.Y. Liu, Phys. Rev. B 56 (13) (1997) 7767.
[10] L.G.O. Van Uitert, H.M. Bryan, M.E. Lines, H.G. Guggenheim, G.M. Zydzik, Mater. Res. Bull. 12 (1977) 261.
[11] L.G. Van Uitert, Mater. Res. Bull. 12 (1977) 315.
[12] K.V. Krishna Rao, in: M. Balakrishna, B. Krishnamurahi, B. Ramachandra Raw (Eds.), ''Thermal Expansion of Solids'' in Physics of the Solid State, Academic Press, London, 1969.
[13] H. Neumann, Krist. Tech. 15 (7) (1980) 849.
[14] J.A. Van Vechten, Phys. Rev. 187 (1969) 1007.
[15] J.A. Van Vechten, J.C. Phyllips, Phys. Rev. 2B (1970) 2160.
[16] B.R. Pamplin, M.S. Omar, Prog. Cryst. Growth Ch. 10 (1985) 183.
[17] A. Miller, R.G. Humphreys, B. Chapman, J. Phys. (Paris) Colloq. C-3 (1975) 31.
[18] G.C. Bhar, L.K. Samanta, Phys. Rev. B 26 (4) (1982) 2275.
[19] American Inistituete of Physics Handbook, 3rd ed., McGraw Hill, New York, 1972.
[20] L.I. Berger, V.D. Prochukhan, Ternary Diamond-Like Semiconductors, Consultants Bureau, New York, 1969.
[21] H. Kildal, Ph.D. Thesis, Stanford University, California, 1972.
[22] N. Yamamoto, Ph.D. Thesis, University of Osaka Prefecture, Japan, 1976.
[23] S.I. Novicova, Thermal Expansion of Solids, Moscow, 1974.
[24] T.V. Hailing, G.A. Saunders, M.S. Omar, B.R. Pamplin, Phys. Chem. Solids 43 (2) (1984) 163.