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Research Paper

Simplified expressions for calculating Debye temperature and melting point of II-VI and III-V semiconductors

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Abstract

Simple empirical expressions between the Debye temperature and the bond length and also between the melting point and the bond length have been proposed. These formulas have been established for two groups of A^NB^{8-N} type binary semiconductors (groups: II-VI and III-V). A good correlation between the Debye temperature and the bond length and also between the melting point and the bond length is obtained. The minimum average percentage deviations in the present approach reveal that our model proves its identity and soundness compared to those of other author relations.

Keywords: *Debye Temperature; Melting Point; A^{II}-B^{VI} and A^{III}-B^{V} Binary Compounds; Bond Length.*

1. Introduction

The Debye temperature θ_D of material is a suitable thermodynamic quantity to describe several phenomena of solid-state physics which are associated with lattice vibrations [1]. It is naturally depends on several other quantities, such as the pressure, elastic constants, and other thermal quantities, such as specific heat and lattice thermal conductivity [2].
At ambient temperature and pressure, several II-VI and III-V binary semiconductors possess the cubic zincblende structure; these binary compounds have potential applications in the fields of electronic and optoelectronic devices [3].
The development of new optoelectronic materials depends mostly on the materials engineering at a practical level, and also on a good understanding of the properties of materials [4]. Knowledge of different thermodynamic properties such as Debye temperature helps engineers in the improvement of the manufacturing of the semiconductor devices by good selecting of the appropriate materials [2].
And due to technological importance of II-VI and III-V semiconductors, several experimental and theoretical works [4-9] on their electronic, optical, mechanical and thermal properties were published.
The present work aims to establish simple empirical expressions between the Debye temperature and the bond length, and between the melting point and the bond length for II-VI and III-V semiconductors.

2. Theory, results and discussion

2.1. Debye temperature

Based on the previous works of Kumar et al. [2, 9] on $A^IB^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ ternary chalcopyrite semiconductors, and on $A^{II}B^{VI}$ and $A^{III}B^{V}$ binary semiconductor compounds, the Debye temperature and some other physical quantities are related by [2], [9].

$$\theta_D = K_1 [(M)^{-1/2} (V)^{1/6} (\hbar\omega_p)^{1.1666}] - K_2 \quad (1)$$

Where, K_1 and K_2 are two empirical parameters, slightly depend on the nature group of material, M is the mean atomic weight, $(\hbar\omega_p)$ is Plasmon energy, and V is the mean atomic volume.

Our principal idea is to write the Debye temperature θ_D as functional of the bond length d; the bond length d in angstroms and the Plasmon energy ($\hbar\omega_p$) in eV can be related by the following formula [10].

$$d = C_1 (\hbar\omega_p)^{-2/3} \quad (2)$$

Where, C_1 is constant, which depends on the nature group of material. The relevant value of the constant C_1 for some binary compounds is: 15.30 [10].
Reciprocally to the formula of Eq. (2), the Plasmon energy ($\hbar\omega_p$) can be written approximately as function of bond length d by the following expression:

$$(\hbar\omega_p) = C_2\, d^{-3/2} \quad (3)$$

Where, C_2 is constant.
In other hand, for cubic zincblende crystals, the mean atomic volume V and the lattice parameter a are related by:

$$V = a^3/8 \quad (4)$$

And the bond length d and the lattice parameter a are related by [4]

$$a = (4/\sqrt{3})d \quad (5)$$

So the mean atomic volume V can be written as function of bond length d by the following expression:

$$V = a^3/8 = (8/3\sqrt{3})d^3 \quad (6\text{-a})$$
$$V = C_3\, d^3 \quad (6\text{-b})$$

For object to simplify the unity of the quantity $[(M)^{-1/2} (V)^{1/6} (\hbar\omega_p)^{1.1666}]$ in the formula of Eq. (1), it's important to write the value: 1.1666 = 7/6.
Replaced in the expression of Eq. (1), the Plasmon energy ($\hbar\omega_p$) with its expression (Eq. (3)), and the mean atomic volume V with its expression (Eq. (6-b)), we obtain the following formula:

$$\theta_D = K_3 [1/(M^{1/2} d^{5/4})] - K_4 \quad (7)$$

Where, K_3 and K_4 are two empirical parameters, slightly depend on the nature group of material.
So a linear regression between the Debye temperature θ_D and the quantity $[1/ (M^{1/2} d^{5/4})]$ has been established.
The values of the mean atomic weight, the experimental lattice parameter a, the bond length d, and the quantity $[1/ (M^{1/2} d^{5/4})]$ (in 10^{12} $Kg^{-1/2}$ $m^{-5/4}$) of III-V and II-VI compounds are listed in Table 1.

Table 1: Mean Atomic Weight M, Experimental Lattice Parameter *a*, Bond Length d, and the Quantity $[1/ (M^{1/2} d^{5/4})]$ of III-V and II-VI Compounds.

Group	Compounds	M (10^{-3} kg)	a (10^{-10}m) [4]	d (10^{-10} m)	$1/(M^{1/2} d^{5/4})$ (10^{12} $Kg^{-1/2}$ $m^{-5/4}$)
III-V	BN	20.87	4.5383	1.965	9.408
	BP	42.87	4.777	2.069	6.157
	AlP	28.98	5.4635	2.366	6.331
	AlAs	50.95	5.66139	2.451	4.567
	AlSb	74.37	6.1355	2.657	3.419
	GaP	50.35	5.4508	2.360	4.817
	GaAs	72.32	5.6533	2.448	3.840
	GaSb	95.74	6.09593	2.640	3.038
	InP	72.9	5.869	2.541	3.650
	InAs	94.87	6.0583	2.623	3.075
	InSb	118.29	6.47937	2.806	2.532
II-VI	BeS	20.54	4.865	2.107	8.694
	BeSe	43.88	5.137	2.224	5.557
	BeTe	68.31	5.617	2.432	3.983
	ZnS	48.72	5.4102	2.343	4.943
	ZnSe	72.17	5.6692	2.455	3.831
	ZnTe	96.5	6.009	2.602	3.080
	CdS	72.23	5.825	2.522	3.702
	CdSe	95.68	6.077	2.631	3.050
	CdTe	120	6.481	2.806	2.513

Figure 1 show the variation of Debye temperature as function of the quantity [1/ ($M^{1/2}$ $d^{5/4}$)] of III-V and II-VI materials. The empirical parameters obtained for III-V compounds are: K_3 = 112.66 (10^{-12} $Kg^{1/2}$ $m^{5/4}$ K) and K_4 = 90.74 K respectively, and for II-VI compounds are: K_3 = 106.99 (10^{-12} $Kg^{1/2}$ $m^{5/4}$ K) and K_4 = 92.09 K respectively.
Our calculated and known values of Debye temperature θ_D of III-V and II-VI compounds are presented in Table 2.
In the case of III-V materials, the average percentage deviation is calculated and to be found improved in comparison with other result (3.34 %) cited Kumar et al [2], it is only about 2.42 %.
Eq. (7) is used to predict the Debye temperature of BSb material. The experimental lattice parameter of this compound in its zincblende phase is equal to: a = 5.16 Å [11], so the experimental bend length d of BSb compound in its zincblende phase is equal to: 2.2344 Å. The result obtained of the quantity [1/($M^{1/2}$ $d^{5/4}$)] is equal to: 4.496 (10^{12} $Kg^{-1/2}$ $m^{-5/4}$); the predicted value of the Debye temperature of BSb material is equal to 415.81 K; this value is in general in agreement with the value 456.07 K obtained in our previous work [6]. The deviation between our value and this cited in the Ref. [6] is about 8.83 %.

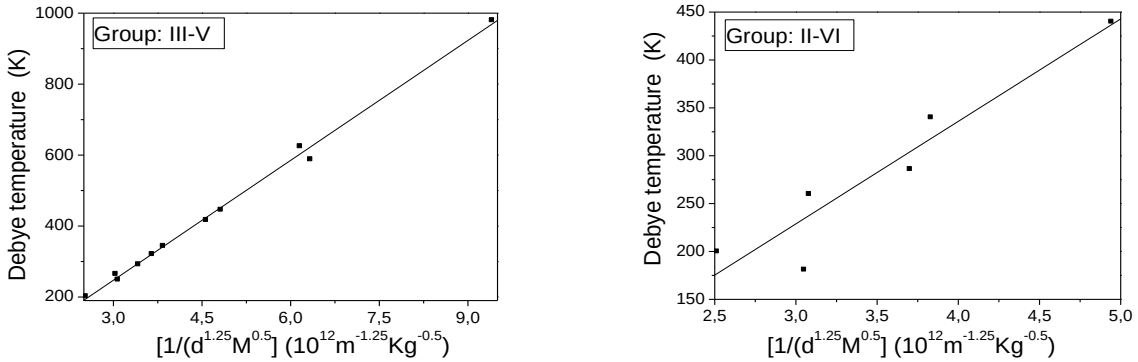

Fig. 1: Plot between Debye Temperature and the Quantity [1/ ($M^{1/2}$ $D^{5/4}$)] Of III-V and II-VI Compounds.

In the case of II-VI materials, the average percentage deviation is also calculated and to be also found improved in comparison with other result (14.01 %) cited by Kumar et al [2], it is about 10.54 %.

Table 2: Debye Temperature Θ_d of III-V and II-VI Compounds. Experimental Values of Debye Temperature Θ_d with * Are Taken From the Ref [4] and References Therein).

Group	Compounds	Experimental Values, cited in Ref [2]	Present Work Eq.(7)	Percentage deviation (%)
III-V	BN	980	969.16	1.11
	BP	625	602.88	3.54
	AlP	588	622.53	5.87
	AlAs	417	423.80	1.63
	AlSb	292	294.41	0.83
	GaP	446	451.97	1.34
	GaAs	344	341.91	0.61
	GaSb	265	251.47	5.10
	InP	321	320.48	0.16
	InAs	249	255.71	2.69
	InSb	202	194.53	3.70
	Average percentage deviation			2.42 %
II-VI	BeS	-	838.08	-
	BeSe	-	502.47	-
	BeTe	-	334.09	-
	ZnS	440*	436.78	0.73
	ZnSe	340*	317.77	6.54
	ZnTe	260*	237.48	8.66
	CdS	286	303.95	6.28
	CdSe	181	234.27	29.43
	CdTe	200	176.80	11.60
	Average percentage deviation			10.54 %

Unfortunately as far as we know, there is no experimental data available in the literature on the Debye temperature of beryllium chalcogenide (BeS, BeSe and BeTe) compounds.

2.2. Melting point

The Debye temperature θ_D and the melting point T_m of some cubic zincblende crystals are related by [2].

$$\theta_D = -K_5 + K_6 T_m \quad (8)$$

Where, K_5 and K_6 are two empirical parameters, slightly depend on the nature group of material.
Reciprocally to the formula of Eq. (8), the melting point T_m can be written approximately as function of Debye temperature θ_D by the following expression:

$$T_m = K_7 \theta_D + K_8 \quad (9)$$

Where, K_7 and K_8 are two constants
Replacing the Debye temperature θ_D in the expression of Eq. (9), with its expression of Eq. (7), we obtain the following formula:

$$T_m = K_9 [1/ (M^{1/2} d^{5/4})] + K_{10} \quad (10)$$

Where, K_9 and K_{10} are two empirical parameters, slightly depend on the nature group of material.
Figure 2 show the variation of the melting point T_m as function of the quantity $[1/ (M^{1/2} d^{5/4})]$ of III-V and II-VI materials.

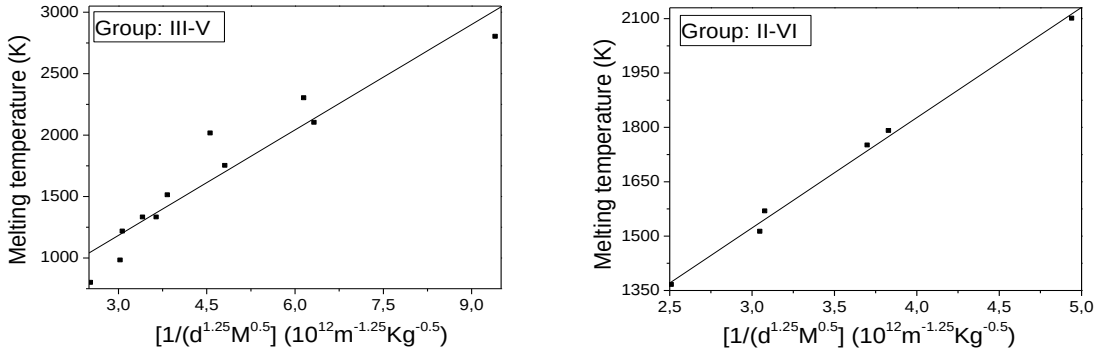

Fig. 2: Plot between Melting Point T_m and the Quantity $[1/ (M^{1/2} D^{5/4})]$ of III-V and II-VI Materials.

The empirical parameters obtained for III-V compounds are: K_9 = 286.21 (10^{-12} $Kg^{1/2}$ $m^{5/4}$ K), and K_{10} = 325.17 K respectively, and those obtained for II-VI type compounds are: K_9 = 304.24 (10^{-12} $Kg^{1/2}$ $m^{5/4}$ K), and K_{10} = 609.93 K respectively.
The present calculated and known values of melting point T_m of III-V and II-VI compounds are presented in Table 3. Unfortunately as far as we know, there is no experimental data available in the literature on the melting point of beryllium chalcogenide (BeS, BeSe and BeTe) compounds.
In the case of III-V materials, the average percentage deviation is calculated and to be found improved in comparison with other results (from 9.99 % to 10.45 %) cited Kumar et al [2], it is about 9.57 %; and in the case of II-VI materials, the average percentage deviation is also calculated and also to be found improved in comparison with other results (from 2.37 % to 3.11 %) cited Kumar et al [2], it is only about 1.0 %.
Eq. (9) is used to predict the meting point of BeS material. The experimental lattice parameter of this compound in its zincblende phase is equal to: a = 4.865 Å [4], so the experimental bend length d of BeS compound in its zincblende phase is equal to: 2.107 Å. The result obtained of the quantity $[1/ (M^{1/2} d^{5/4})]$ is equal to: 8.694 (10^{12} $Kg^{-1/2}$ $m^{-5/4}$); the predicted value of the melting point of BeS material is equal to 3255 K; this value is very higher than the value 2293 K cited in the previous work of Verma et al. [12].

3. Conclusion

A simple model has been established for calculating the Debye temperature and the melting point of II-VI and III-V semiconductors. The average percentage deviations were estimated for different materials. The maximum average deviation of 10.54 % was obtained in the case of II-VI compounds, and about 2.42 % in the case of III-V materials for the Debye temperature. For melting point, the maximum average deviation of 9.57 % was obtained in the case of III-V compounds, and exactly 1 % in the case of II-VI materials respectively. So the correlation between the Debye temperature θ_D and the quantity $[1/ (M^{1/2} d^{5/4})]$, and also between the melting point and the quantity $[1/ (M^{1/2} d^{5/4})]$ gives a good agreement with the experimental values.

Table 3: Melting Point T_m and Percentage Deviation of III-V and II-VI Compounds Using a Linear Fit.

Group	Compounds	Experimental Values, cited in Ref [2]	Present Work Eq.(10)	Percentage deviation (%)
III-V	BN	2800	3017.83	7.78
	BP	2300	2087.30	9.25
	AlP	2100	2137.22	1.77
	AlAs	2013	1632.34	18.91
	AlSb	1330	1303.64	1.98
	GaP	1750	1703.92	2.63
	GaAs	1510	1424.31	5.67
	GaSb	980	1194.56	21.89
	InP	1330	1369.87	3.00
	InAs	1215	1205.32	0.80
	InSb	798	1049.89	31.56
	Average percentage deviation			9.57 %
II-VI	BeS	-	3255.00	-
	BeSe	-	2300.64	-
	BeTe	-	1821.83	-
	ZnS	2100	2113.83	0.66
	ZnSe	1790	1775.42	0.81
	ZnTe	1568	1547.11	1.33
	CdS	1750	1736.12	0.79
	CdSe	1512	1537.97	1.72
	CdTe	1365	1374.55	0.70
	Average percentage deviation			1.00 %

References

[1] H. Siethoff, "Debye temperature, self-diffusion and elastic constants of intermetallic compounds", *Intermetallics*, Vol. 5, No. 8, (1997), pp. 625-632. http://www.sciencedirect.com/science/article/pii/S096697959700037X. http://dx.doi.org/10.1016/S0966-9795(97)00037-X.

[2] V. Kumar, V. Jha & A. K. Shrivastava, "Debye temperature and melting point of II-VI and III-V semiconductors", *Crystal Research and Technology*, Vol. 45, No. 9, (2010), pp. 920-924. http://www. onlinelibrary.wiley.com/doi/10.1002/crat.201000268/pdf. http://dx.doi.org/10.1002/crat.201000268.

[3] A. Bahadur & M. Mishra, "Correlation between refractive index and electronegativity difference for A^NB^{8-N} type binary semiconductors", Acta Physica Polonica A, Vol. 123, No. 4, (2013), pp. 737-740. http://przyrbwn.icm.edu.pl/APP/PDF/123/a123z4p18.pdf. http://dx.doi.org/10.12693/APhysPolA.123.737.

[4] S. Adachi, "*Properties of Group-IV, III-V and II-VI Semiconductors*", John Wiley & Sons, England, (2005). Print ISBN: 9780470090329. Online ISBN: 9780470090343. http://dx.doi.org/10.1002/0470090340.

[5] A. S. Verma, B. K. Sarkar & V. K. Jindal "Inherent properties of binary tetrahedral semiconductors", *Physica B*, Vol. 405, (2010), pp. 1737-1739. http://www.sciencedirect.com/science/article/pii/S0921452610000396. http://dx.doi.org/10.1016/j.physb.2010.01.029.

[6] S. Daoud, "Sound velocities and thermal properties of BX (X=As, Sb) compounds", *International journal of scientific world*, Vol. 3, No. 1, (2015), pp. 43-48. http://www.sciencepubco.com/index.php/IJSW/article/view/4039. http://dx.doi.org/10.14419/ijsw.v3i1.4039.

[7] S. Daoud, N. Bioud, N. Lebgaa & R. Mezouar "Optoelectronic and thermal properties of boron- bismuth compound", *International Journal of Physical Research*", Vol. 2, No. 2, (2014), pp. 27-31. http://www.sciencepubco.com/index.php/IJPR/article/view/2760. http://dx.doi.org/10.14419/ijpr.v2i2.2760.

[8] M. Ustundag, M. Aslan, & Battal G. Yalcin, "The first-principles study on physical properties and phase stability of Boron-V (BN, BP, BAs, BSb and BBi) compounds", *Computational Materials Science*, Vol. 81, (2014) pp. 471- 477.

[9] V. Kumar, A. K. Shrivastava, R. Banerji, & D. Dhirhe, "Debye temperature and melting point of ternary chalcopyrite semiconductors", Solid State Communications, Vol. 146, No. 25-26, (2009), pp. 1008-1011. http://www.sciencedirect.com/science/article/pii/S0038109809002026. http://dx.doi.org/10.1016/j.ssc.2009.04.003.

[10] S. K. Gorai & P. Mahto, "Plasmon energy and lattice energy of binary tetrahedral semiconductors and I-VII ionic compounds", Indian Journal of Physics, Vol.86, No.4, (2012), pp. 273-277. http://www.link.springer.com/content/pdf/10.1007%2Fs12648-012-0053-y.pdf. http://dx.doi.org/10.1007/s12648-012-0053-y.

[11] E. V. Clougherty & L. Kaufman, "Thermodynamic study of synthesis of new compound phases under high pressure", Scientific Report N.1, Cambridge, Massachusetts, 1967. www.dtic.mil/cgi-bin/GetTRDoc?AD=AD0670561.

[12] A. S. Verma, R. K. Singh & S. K. RathiV, "Thermal property of binary tetrahedral semiconductors", Physica B, Vol. 404, No. 21, (2009), pp. 4051-4053. http://www.sciencedirect.com/science/article/pii/S0921452609006681. http://dx.doi.org/10.1016/j.physb.2009.07.157.