Journal of Alloys and Compounds 630 (2015) 178–182

Contents lists available at ScienceDirect

Journal of Alloys and Compounds

journal homepage: www.elsevier.com/locate/jalcom

Discussion on the interrelationship between structural, optical, electronic and elastic properties of materials

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ARTICLE INFO

Article history:
Received 20 April 2014
Received in revised form 1 October 2014
Accepted 13 October 2014
Available online 11 December 2014

Keywords:
Bulk modulus
Optical band gap
Optical electronegativity
Electronic polarizability

ABSTRACT

In reference Reddy et al. (2009) the correlations between energy gap, optical electronegativity and electronic polarizability for different materials have been studied. The authors of this paper (Reddy et al., 2009) aimed to make extinction or complete some previous works (Bahadur and Mishra, 2013; Reddy et al., 1999, 2000, 1998, 2005, 2008; Reddy and Nazeer Ahammed, 1996; Oshcherin, 1979; Neumann, 1983, 1987; Deus and Schneider; 1985; Deus et al., 1983; Kumar et al. 1992). However, this paper (Reddy et al., 2009) contains many fundamental errors in the calculation of bulk modulus, especially Tables 4–6. As a result, all the obtained values of the bulk modulus and consequently the electronic polarizability are incorrect. Moreover in Table 4 (Reddy et al., 2009), the bulk modulus of II–VI group semiconductors have been calculated by substituting the values of the band gap, E_g, into Eq. (11) ($B = 14.91\ E_g + 23.3$). The obtained values of B using Eq. (11) are conflicted with that calculated values of B based on the electronegativity and the published previously data. Therefore Eq. (11) in reference Reddy et al. (2009) is not suitable for calculating the values of B for any element or materials. When I recalculated the values of B for all materials in Tables 1 and 4–6 in paper (Reddy et al., 2009) using Eq. (12), I found that, Eq. (12) gives acceptable values of B for all materials except the underlined materials in Table 4 in the present note. The aim of this note is to recalculate both bulk modulus and electronic polarizability for all materials found in Reddy et al. (2009) to introduce the errors present in this paper.

1. Introduction

The chalcogenide glasses and different glass compounds have received a special concern due to their wide range of applications in various solid state devices such as light emitting diodes, switching and memory, image converters and optical mass memories [5,15–18]. Although of their significant importance some of the physical properties of these compounds have not been fully investigated. Many attempts have been made to correlate the bulk modulus (B) of chalcopyrite and different compound semiconductors with many other physical parameters such as optical band gap (E_g), refractive index (n), and electronegativity ($\Delta\chi$) [1–14]. The optical polarizability (α) of many materials has been calculated by Chemla [19] and Kumar et al. [20]. Based on the dielectric theory of Phillips [21–25], Van Vechten [26,27] and the bond charge model of Levine the calculation of the electronic polarizability for different materials have been carried out by many authors [19,20,28–31,6].

The optical electronegativity is very important parameter to understand the nature of the chemical bonding. It was found in the literature many models [29–32] based on the concept of optical electronegativity and some other parameters. These models are very useful in studying the main properties of ionic crystals and semiconductors with the use of only few numerical constants. The present note aims to recalculate the bulk modulus and the electronic polarizability of the chalcopyrite and the compound of semiconductors presented in the Reddy et al. [1]. The calculations were carried out based on different methods in literatures [1–8]. The calculated values will be compared to the corresponding values listed in Reddy et al. [1] to give the reader the correct values of the bulk modulus and the electronic polarizability for different materials found in Tables 1 and 4–6 of the paper [1].

2. Theory

The total optical electronegativity difference, $\Delta\chi$, for ternary and complex systems can be estimated by substituting the value of the band gap, E_g, into Dufy's equation [4]:

$$\Delta\chi = 0.2688E_g, \quad (1)$$

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http://dx.doi.org/10.1016/j.jallcom.2014.10.079
0925-8388/

Reddy et al. [1] suggested two equations to calculate the bulk modulus, B, based on the optical band gap, E_g, for different materials:

$$B = 14.91E_g + 23.3 \quad \text{(Unacceptable for element or material)} \tag{2}$$

$$B = 13.89E_g + 46.9 \quad \text{(Acceptable for all elements and different materials in Table4 except the unlined materials)} \tag{3}$$

Based on the values of the optical electronegativity, the bulk modulus can be estimated using the following relationship [4]

$$B = 168.58 + 30.3\ln(0.102\Delta\chi). \tag{4}$$

Substituting B, $\Delta\chi$ and E_g respectively in Clausius–Mossotti relation gives the value of electronic polarizability (α in A^3) in terms of the bulk modulus as [1,4]:

$$\alpha = 0.395\left(\frac{(5.563 - 0.033B)^2 - 1}{(5.563 - 0.033B)^2 + 2}\right)\left(\frac{M}{\rho}\right), \tag{5}$$

were M and ρ are the molecular weight and density of the material, in terms of the optical electronegativity as [1,3]

$$\alpha = 0.395\left(\frac{4.207 + k}{7.207 + k}\right)\left(\frac{M}{\rho}\right), \tag{6}$$

where $k = (\ln\Delta\chi)(\ln\Delta\chi - 4.564)$ and in terms of the optical bang gap as [5]

$$\alpha = 0.395\left(\frac{12.41 - \sqrt{E_g - 0.365}}{12.41 + 2\sqrt{E_g - 0.365}}\right)\left(\frac{M}{\rho}\right). \tag{7}$$

3. Calculation problems in paper [1]

In paper [1], the authors wrote in the text that the electronic polarizability (α) was calculated using Eq. (7) (Eq. (6) in the present study) while the authors [1] in Table 1, wrote Eq. (10) instead of Eq. (7). Also, there are some errors in the values of electronic polarizability like as $\alpha = 7.14\ A^3$ for AlSb material while, the calculation obtained by different methods especially Eq. (6) confirmed that the value of α is $10.387\ A^3$. Furthermore, all materials found in Table 1 are repeated in Tables 4–6 of Ref. [1] except the element Sn and $ZnSnAs_2$ material in Tables 5 and 6 of Ref. [1]. This helps one to use the values of electronegativity given in Table 1 of Reddy et al. [1] for different materials to calculate both the bulk modulus and the electronic polarizability using Eqs. (4) and (6). After the mathematical calculations one can decide which of these equations (Eq. (2) or (3)) are suitable for calculating the bulk modulus for different materials.

Table 4 in Reddy et al. [1] the calculation of the values of bulk modulus according to Eq. (2) ($B = 14.91\ E_g + 23.3$) is false. For example the first compound in Table 4 ZnS has an optical gap of 3.7 eV, according to Eq. (2) ($B = (14.9 \times 3.7) + 23.3 = 78.467$ GN m^{-2}) while the authors of paper [1] wrote it as 7.85 GN m^{-2}. This error is repeated with all semiconductor materials of groups II–VI consequently the calculated value of the polarizabilities in the same table also incorrect. The bulk modulus for all II–VI group semiconductor materials found in Table 4 of Reddy et al. [1] has been recalculated by substituting the values of E_g into Eqs. (2) and (3) and substituting the value of the electronegativity into Eq. (4). Comparing the results of the three Eqs. (2)–(4) one can find that Eq. (11) in Reddy et al. [1] (Eq. (2) in this study) gives values of B smaller than (by at least 20%) that given by Eqs. (3) and (4) which means that Eq. (2) failed to calculate B for II–VI group semiconductor materials.

Reddy et al. [1] comparing his data with the experimental data that published by Neumann [33] while Neumann's paper concerned with the microhardness parameter, H, not bulk modulus (B). It is illogic to compare bulk modulus results with microhardness one. This error was also repeated in Tables 5 and 6 of Reddy et al. [1]. While, the bulk modulus (B) is correlated to the microhardness (H) through the following relationship [33]:

$$B = \frac{C_o a^{-n}}{T_m c_1(f_1)}H, \tag{8}$$

where c_o, a, n, T_m and $c_1(f_1)n$ are constants with the same meaning found in Ref. [33].

The values of the electronic polarizability can be calculated by three different methods. The first method by substituting values of, B, (calculated by Eqs. (2)–(4)) into Eq. (5) that listed in Table 1 as α_1, α_2 and α_3 respectively. The second method by substituting the values of electronic polarizability (α) into Eq. (6) that was denoted in Table 1 as α_4. The third method by substituting the optical band gap into Eq. (7) that observed in Table 1 as α_5. Table 1 in the present study represents the calculated values of B and α for II–VI group semiconductors. The comparison between my results and the results of Reddy et al. [1] showed that, the values of α_2, α_3, α_4 and α_5 are closed to each other while the obtained values of the electronic polarizability, α_1, based on Eqs. (2) and (5) is larger than α_2–α_5. Although the values of α_1 were calculated using the same values and equation used by Reddy et al. [1]. But also there are some errors in the calculated values in Ref. [1]. Therefore Eq. (2) is not suitable for calculating B for II–VI group semiconductor materials while the obtained values of B based on Eq. (3) confirmed that Eq. (3) gives acceptable values of B for II–VI group semiconductors. The values of the electronic polarizability based on B values (calculated by Eqs. (3) and (4)) are found in good agreement with the previously published data [34].

In Tables 5 and 6 of Ref. [1], the calculation of the values of bulk modulus according to Eq. (12) (Eq. (3) in the present study) ($B = 13.89\ E_g + 46.90$) is incorrect. For example the last compound in Table 5 of Ref. [1] ($ZnGeAs_2$ with optical gap 1.15 eV) according to Eq. (3) ($B = (13.89 \times 1.15) + 46.90 = 78.467$ GN m^{-2}) while the authors of Ref. [1] calculate it as 7.85 GN m^{-2}. This mistake was

Table 1
Optical electronegativity, bulk modulus and electronic polarizability of II–VI group semiconductors materials.

Comp.	E_g (eV) Ref. [1]	$\Delta\chi$	M (gm mol^{-1})	ρ (gm cm^{-3})	Bulk modulus B (GN m^{-2})				Electronic polarizability, α (A^3)						
					Eq. (2)	Eq. (3)	Eq. (4)	Incorrect Ref. [1]	Incorrect Ref. [1]	Eq. (5)			Eq. (6)	Eq. (7)	Ref. [34]
										α_1	α_2	α_3	α_4	α_5	
ZnS	3.70	0.948	97.44	4.079	78.47	98.29	97.79	7.85	–	6.825	5.600	5.639	5.638	6.217	5.49
ZnSe	2.58	0.800	144.34	5.420	61.77	82.74	92.65	6.17	–	8.331	7.371	6.707	6.706	7.467	6.61
ZnTe	2.10	0.605	192.98	6.340	54.61	76.07	84.19	5.46	8.48	9.789	8.837	8.326	8.325	8.865	7.77
CdS	2.40	0.700	144.46	4.820	59.08	80.24	88.60	5.91	9.26	9.480	8.456	7.877	7.876	8.519	7.57
CdSe	1.70	0.455	191.36	5.660	48.65	70.51	75.55	4.86	–	11.086	10.14	9.848	9.847	10.210	9.13
CdTe	1.50	0.385	240.00	6.200	45.67	67.74	70.49	4.56	–	12.804	11.78	11.61	11.61	11.929	11.41