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Electronegativity estimation of cohesive energy of binary tetrahedral semiconductors

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ABSTRACT

Using electronegativity and principal quantum number a relation has been proposed to quantitatively estimate the cohesive energy of binary tetrahedral semiconductors.The estimated values are in good agreement with the experimental values and also with the reported values. Attempts has been made to give a physical basis of the proposed correlation. It has been shown that the constants appearing in the proposed relation are characteristics of crystal structure.

Keywords : Cohesive energy, Electronegativity, Ionicity, Ionic charge

1.Introduction

During the last few decades a considerable amount of experimental and theoretical work has been done to understand the structural properties such as optical, elastic, electronic and cohesive energy of binary semiconductors. These binary semiconductors have gained considerable importance because of their potential application in the areas of light emitting diodes ,nonlinear optics ,photovoltaic devices and solar cells.

Cohesive energy is an important physical quantity to account for the strength of metallic bonds, which equals to the energy to divide the metallic crystal into individual atoms. The cohesive energy, in other words, is the heat of sublimation, which can be determined by experiments[1] or computed theoretical methods such as cellular methods [2], density functional theory [3], KKR method [4] linear muffin tin orbital methods [5] etc. These methods are developed for calculating the cohesive energy of bulk material. However cohesive energy of nanoparticles is also calculated using the experimental value of cohesive energy of bulkmaterials [6].

Schlosser[12-13] has proposed an empirical inverse relation between cohesive energy and interatomic distance. An empirical relation using ionic charge model was however proposed by Verma and Sharma [20] in determining the cohesive energy of binary tetrahedral semiconductors. Sing et al [21] has proposed an power relation between Plasmon energy and cohesive energy to estimate the cohesive energy of II-VI and III-V semiconductors. Both Plasmon energy and ionic charge depends upon the number valence electrons in outer most orbits. In this study I have tried to give alternative explanation of cohesive energy using electronegativity and principal quantum number of valence electrons.

Theory Results and discussion

The cohesive energy of binary tetrahedral semiconductors is the energy liberated on the formation of a crystal from individual atoms. As the semiconductors are made up of positive and negative ions and valence electrons are transferred from positive ions to negative ions to form a crystal. Therefore valence electrons between two opposite ions play an important role in estimating cohesive energy of binary tetrahedral semiconductors. The cohesive energy of any material depends on attractive potential energy due to coulomb force (being oppositely charged) as well as repulsive potential energy (pauling exclusion principle).This attractive potential energy which is the attractive power of effective charge of valence electrons in outer orbitals which is reflected by electronegativity value. The larger the electronegativity value the more tightly the nuclei hold the valence electrons and larger the cohesive energy .The repulsive potential energy if same charged ions come very close to their electron orbitals begin to overlap and there will be distortion of the outer electronic shell. The larger the principal quantum number, the longer the distance between between nuclei and valence electrons and smaller the cohesive energy. With this consideration for II-VI and III-V semiconductors,cohesive energy is assumed to be correlated

$$E_h = K_1\left(\frac{\eta_a}{\sqrt{\chi_A\chi_B}}\right)+K_2 \qquad (1)$$

where $\eta_a = \left(\eta_A + \eta_B/2\right)$ is the average principal quantum number of valence electrons of atoms A and B, χ_A and χ_B are the electronegativity of atoms A and B respectively. K_1 and K_2 are constants and their values are 29.304,215.51 for II-VI semiconductors and -36.24,259.06 for III-V semiconductors respectively. Using functional empirical relation(1) the cohesive energy of binary tetrahedral semiconductors have been estimated. The estimated values of cohesive energy of binary tetrahedral semiconductors are given in table 1 along with the experimental values and the values reported by earlier researchers.

Table1. Values of cohesive energy (Kcal/mol) for binary semiconductors

		E_{coh} (Kcal/mol)				
Compounds (II-VI)	$\eta_{av}/\left[(\chi_A\chi_B)^{1/2}\right]$	Exp Ref.[20]	Cal.Eq.(1)	Ref.[20]	Ref.[20]	
ZnS	2.45	146.6	148.00	151.3	147.6	
ZnSe	2.93	124.5	128.26	123.7	130.2	

ZnTe	3.55	106.3	110.00	108.6	109.2	
CdS	2.98	131.6	126.54	134.6	122.6	
CdSe	3.51	113.6	111.00	110.3	111.3	
CdTe	4.19	95.8	96.34	95.4	93.4	
HgS	3.35		115.23		121.4	
HgSe	3.9		102.03		110.2	
HgTe	4.61		89.25		94.2	
Avearge % deviation			2.32	2.32	3.1	
III-V						
AlP	1.89	198	197.38	197	199.8	
AlAs	2.29	178.9	175.24	177.2	185.8	
AlSb	2.81	165	154.36	162.4	148.2	
GaP	2.21	173.8	179.14	173.2	199.8	
GaAs	2.62	154.7	161.20	154.6	181.9	
GaSb	3.16	138.6	143.52	140.5	149.6	
InP	2.7	158.6	158.22	159.3	166.3	
InAs	3.15	144.3	143.80	141.7	155.4	
InSb	3.76	128.5	128.86	128.3	129.2	
BAs	1.64		215.53		287.7	
TiP	2.25		177.16		175.8	
TiAs	2.66		159.70		159.9	
TiSb	3.21		142.13		136.3	
Average % deviation			2.25	3.98	5.35	

Results and discussion

The proposed empirical equation estimate cohesive energy of binary tetrahedral semiconductors. Reasonably good agreement has been obtained between the calculated ,experimental and reported values. The percentage deviation (experimental value-calculated value)/experimental value of cohesive energy has been obtained. Average percentage deviation of cohesive energy of binary tetrahedral semiconductors have been found 2.32, 2.32 and 3.1 for equation (1) of II-VI type semiconductors and 2.35, 3.98 and 5.35 for equation(1) of III-V type semiconductors respectively. The empirical proposed equation does not take into account the difference in crystal structure such as cubic and hexagonal for the binaries. The minimum average deviation of 2.32 for II-VI semiconductors and 2.25 for III-V semiconductors respectively. In all cases the average percentage deviation of this model is better than the models proposed by earlier researchers. For comparison average percentage deviation of cohesive energy of earlier researchers have also been estimated.

Conclusion

From the above discussion it is clear that one can calculate the cohesive energy of tetrahedral semiconductors using two parameters, one is the average principal quantum number and another one is the electronegativity of two atoms forming the compounds. The calculated values of cohesive energy are presented in Table 1 and Table 2 respectively. Seeing the percentage deviation it is noted that the proposed relation give better agreement with the experimental data as compared with the values reported by previous researchers. The cohesive energy can serve as a guide in indicating the nature of bonding. The involvement of average principal quantum number and electronegativity of both atoms has direct bearing on the concept of chemical bonding. It is observed that the chemical bond between two atoms in forming the semiconductors delineates the cohesive energy of semiconductors. The present approach in estimating the cohesive energy of binary tetrahedral semiconductors is a step forward in finding a suitable relationship between cohesive energy with the principal quantum number as well as electronegativity of the atoms which constitute the compounds.

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