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Bulk Modulus and Cohesive Energy of Zn, Cd, and Hg Monochalcogenides and Oxides

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Abstract – The electronic, bulk, and elastic properties of Zn, Cd and Hg chalcogenides and Oxides have been discussed. The different actual properties like Ionicity, Bulk Modulus, and Cohesive Energy, have been processed and contrasted and the announced information. A conversation dependent on PVV hypothesis has been introduced for the determined homopolar hole (Eh), Ionic hole (EC), Penn hole (Ep), Average hole (Eg), associating iconicity with 'Ec and Eg just as with different hyperfine communications.

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INTRODUCTION

II VI group semiconductor AX (A= Zn, Hg; X = O, S, Se, Te) are currently 3 under intense investigations driven by their unusual properties just as their possible a applications in electronic and opto-electronic devices as ultrasonic transducers, 'surface acoustic wave devices oxygen sensors. There has likewise been a developing interest in the investigation of these materials under high tension conditions, motivated by the need of synthesizing new solids with targeted physical properties (1,2,3). For understanding an assortment of physical phenomena, it is important to know the stretch and bulk E properties of crystals. The studies on structurah phase transition, metallisation, cohesive, elastic and bulk properties under high pressure have attracted quite interest in Zn, Cd, and Hg chalcogenides over the most recent twenty years due to their applications in light emitting diodes (LED) and laser diodes (4). Structural what's more, electronic property of AX compounds have been ii: experimentally and theoretically during the past few years, however, the bonding, elastic and bulk property of these mixtures have been less studied (5). Amlost all the AX compounds crystallize either in zinc blend or wurtzite structures, ZnS, ZnSe, ZnTe, CdS, CdTe, crystallize in both zinc blend, and HgSe, HgTe, crystallize in zinc blend structure only Hgs crystallize in zinc blend and hexagonal Cinnabar Structure, and ZnO, has wurtzite structure, CdC has NaCl structure, HgO has Cinnabar structure (6-7). The common and dominant feather of these structures is that each atom of one kind is tetraheddrally bonded to four atoms of by the other element. In zinc blend these tetrahedral are arranged in a cubic type structure ' whilst they are in a hexagonal type structure. Indeed the centers of similar tetrahedral are arranged in a face-centered hexagonal closed packed (hcp) array in the later (8). Neumann (9) considered the mass modulus of salt halides regarding I spectroscopically defined covalency. We present in this note our examinations a Zn, Cd, and Hg, monochalcoginides and oxides. In this introduction, we assess the honiOpolar hole, ionic hole, normal hole, and henceforth the iconicity of these mixtures utilizing the modified Phillips and Van Vechten hypothesis (10, 11). The assessed estimations of Phillips iconicity, and Neumann scaling law (9) give us the estimations of mass moduli and firm energy for these mixtures.

THEORY AND DISCUSSION:

The term iconicity intrinsically characterizes electronegativity, bond length, electron density (12), flexible constants, bulk molulus, cohesive energy, effective charge etc. The correlationships of iconicity had been arising from the isomer shift. Parameters used in Mossbaur effect. Phillips described the new deprition based on band structure. As indicated by the modified Phillips and Van Vechten hypothesis (P V V theory) (13, 14, 15), the average gap Eg is given by

$$E_g^2 = E_h^2 + E_c^2 \qquad \text{..........} (1)$$

$$E_h = 40.468 / r^{2.5}_{AB} \qquad \text{.........} (2)$$

$$E_c = be^2 \left[\frac{Z_A - Z_B}{r_{AB}/2} \right] \exp(-Ksr_{AB}/2) \ldots \qquad \text{.........} (3)$$

Where Eh and Ec are the contributions of homopolarity and hetropolarity to the AB bond, Z_A, Z_B are the valence states of atoms A & B, respectively Ks the Thomas- ' Fermi screening parameter, and b is an adjustable parameter given by b '4 .089-N_C^2,where Nc is the average coordination number (16) around the cation. Using the above relations Eh, Ec, and Eg, and hence the iconicity fi (fi = Ec2 / Eg^2) is evaluated for these monochalcogenides.

Bulk Modulus:

The evaluated values of iconicity are used in the followmg relation proposed by Neumann for the evaluation of the bulk modulus:

$$B=B_0V^{-n} \qquad \text{--------} \qquad (4)$$

Where n has the value 1.147 and the factor B0 is given by

$$B_o = b_0(1—b_1f_c) \qquad ..... \qquad (5)$$

Here b_0 = 4.134 and b_1 = 2.877, and fc is the covalency fc=(1-fi).

Using available crystallogrpahic data (1, 17-23) for these compounds and following the modified PVV theory, the values of iconicity are calculated. The calculate value of iconicity are shown in table 1. The calculated values of iconic1ty and the relations ' (4) and (5) lead us to decide the values of bulk modulus. The determlned values are shown in Table-2. The comparison between our calculated values and known experimental & theoretical values (1, 29-30) shows good agreement.

Cohesive Energy:

Using the Phillips iconicity the cohesive energy (31) is given as

$$E_c' = \frac{\log(1-f_i)Tm}{K} \; ...... \qquad (6)$$

Where fl is the iconicity, Tm is melting temperature, k is adjustable parameter has values -3.63x10^2. The result obtained by equation (6) is found in better agreement. with experiment values (1, 24—26) compared to obtained.

Table 1: The determined estimations of homopolar energy gap(Eh),heteropolar energy gap(Ec),average energy gap(Eg),and precious stone ionicity(Fi) of Zn, Cd and chalcogenidesy.

Compounds	ZA	ZB	Eh	Ec	Eg	Fi
ZnO	2	6	7.400	14.346	16.142	0.789
ZnS	2	6	4.831	9.741	10.873	0.802
ZnSe	2	6	4.307	8.798	9.795	0.806
ZnTe	2	6	3.573	7.416	8.232	0.811
CdO	2	6	4.679	14.520	15.256	0.905
CdS	2	6	4.014	8.236	9.162	0.808
CdSe	2	6	3.642	7.535	8.369	0.810
CdTe	2	6	3.084	6.480	7.177	0.815
HgO	2	6	3.030	12.099	12.473	0.940
HgS	2	6	3.974	8.176	9.091	0.808
HgSe	2	6	3.607	7.487	8.310	0.811
HgTe	2	6	3.084	6.452	7.152	0.813

Table 2: The determined estimations of mass modulus (B) of Zn,Cd and Hg Chalcogenides and correlation with detailed tests, theortical assessed estimations of mass modulus.

Compounds	Fi	Fc=(1-fi)	Bo=bo(1-b₁fc)	Bulk moduus (kbar) calc	Bulk modulus reported experiment	Bulk modulus theoretical estimates
Zno	0.789	0.210	1.633	837	748,750,769	1440
Zns	0.802	0.197	1.785	535	595,647,624	592,613,640,683
ZnSe	0.806	0.193	1.834	468	500,509,528	440,452,472
ZnTe	0.811	0.188	1.893	374		386,402,434
CdO	0.905	0.094	3.014	1472	643,620	
CdS	0.808	0.191	1.851	431	530,550	595,615,694
CdSe	0.810	0.189	1.881	384	424,445	369,439,479
CdTe	0.815	0.184	1.937	312		332,355,356
HgO	0.940	0.059	3.432	517	686	450
HgS	0.808	0.191	1.860	426	486,497,576	649,655,664
HgSe	0.811	0.188	1.892	379	340,423,467	581,588,591
HgTe	0.813	0.186	1.921	313		464,467,478

TABLE 3: The calculated value of cohesive energy of Zn, cd and hg chalcogenides and comparison with reported experiments and theortical estimated values of cohesive energy.

Compounds	Fi	Log (1-fi)	Cohesive energy (Ec)(calc)	Cohesive energy(Ec) (reported experiment)	Cohesive energy(Ec) theortical estimates
Zno	0.789	-0.677	3.685		3.159,3.029
ZnS	0.802	-0.704	3.552	2.851,2.852	2.865,2.903,2.920
Znse	0.806	-0.713	2.988	2.698	2.754,2.756,2.741
ZnTe	0.811	-0.724	2.585	2.396,2.397	2.421,2.426,2.458
CdO	0.905	-1.026	3.469		2.903
CdS	0.808	-0.716	2.912		2.456,2.472,2.473
CdSe	0.810	-0.722	2.466		2.463,2.481,2.481
CdTe	0.815	-0.733	2.206	2.379,2.380	2.207,2.267,2.304
HgO	0.940	-1.229	2.369		2.980
HgS	0.808	-0.718	2.870		
HgSe	0.811	-0.724	1.595		
HgTe	0.813	-0.730	1.348		

CONCLUSION:

The modified PVV hypothesis has been applied to Zn, Cd, and Hg monochalcogenides. The assessed estimations of iconicity and the Neumann connection give us the estimations of mass moduli and durable energy for these monochalcogenide semiconductors. The great understanding between our determined qualities with the detailed exploratory and hypothetical information verifies the legitimacy of the above basic methodology for the assurance of mass moduli and durable energy.

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