Three-Body Interaction Effects on Cohesive Properties of $CdS_{1-x}Se_x$

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Abstract— In the present work, we investigated salient experimental result in $CdS_{1-x}Se_x$ ($0 \le x \le 1$) at different concentration (x) and discuss theoretical frame work, in order to understand the effect of three body interaction on cohesive properties. The Structure response of zinc blende structure of $CdS_{1-x}Se_x$ is analyzed using three-body Potential Model and experimental data for $CdS_{1-x}Se_x$ ($0 \le x \le 1$) has been generated by the application of Vegard's law. Evaluated properties are intermediate between pure end point members except some properties. We are good compared with the availably results of experimental and other theoretical data. Present model reproducing the cohesive properties, which exhibit important aspects and are directly related to the thermal, optical, elastic dielectric and dynamical behaviour of these compounds.

Key words: TBI; Mixed Ionic Crystal; Vegard's Law; Cohesive Properties

I. Introduction

Last several decay the alloy have been popular for both industry and laboratory applications. The several physical and chemical properties of alloy can be improved and controlled by composition of another material into a pure material [1-5].In the present study on cadmium Sulfide selenium alloy have hexagonal wurtzite (WZ) or zinc blende (ZB) at ambient pressure. At phase transition pressure found to crystallize in the rock salt structure. Cadmium chalcogenides and their alloy have unique Structural [5-8], electronic [9-11], thermodynamic [12-15], luminescence and optical properties [16-17]. Because it's have high melting Point, large bulk modulus, wide band gap, and low thermal conductivity. It is found wide range of technological applications. The present work is intended to investigate three body interaction Effects on cohesive energy, Debye Temperature, Molecular force Constant, Gruneisen Parameter, and Moelwyn- Hughes constant of $CdS_{1-x}Te_x$ ($0 \le x \le 1$) using by three-body potential model (TBIM) and experimental data generated by using Vegard's law.

II. Methodology

In the present work we have applied three body interaction potential under the framework of rigid ion modal for mixed crystal. These potential consists long-range and short range interaction. Inter-ionic potential theory is a reasonable assumption, where we have consider the ion a core and shell charge and but not consisting a point charge. The ions during lattice vibrations suffer an appreciable overlap and consequently their electron shells undergo deformation. This electron shell deformation gives rise to a transfer or exchange of charge between the overlapping ions. These transferred charges interact via Coulomb law with all other charges and give rise to the long range many body interactions whose most significant component is the three body interactions (TBI). The existence of these three-body interactions has been explained both by quantum concepts by Lowdin [18] Lundqvist [19] and classical theory by Singh and Verma [20]. Extensive studies, carried out by Verma and Singh and their coworkers [21] have shown that these interactions have significance influence on the mechanical properties of ionic solids. According, the binding energy of solid from the proposed inter-ionic potential can be expressed as

$$\emptyset = (\emptyset_C + \emptyset_T)_{\text{long range}} + (\emptyset_{VdW} + \emptyset_R)_{\text{short range}} \quad (2.1)$$

$$\emptyset = \sum_{ij} \frac{z_i z_j e^2}{r_{ij}} \left(1 + \frac{2n}{Z} f(r_{ij})\right) - \sum_{ij} C_{ij} r_{ij}^{-6} - \sum_{ij} D_{ij} r_{ij}^{-8} + b\left[n\beta_{+-} \exp\left(\frac{r_+ + r_- + r_0}{\rho}\right) + \left[\frac{n'}{2}\left\{\beta_{++} \exp\left(\frac{2r_+ + kr_0}{\rho}\right) + \beta_{--} \exp\left(\frac{2r_- + kr_0}{\rho}\right)\right\}\right]\right] \quad (2.2)$$

III. Result and Discussion

The present result obtained using the present theoretical model. The values of input data at different concentration x (x=0, 0.25, 0.50, 0.75, 1) have been determined by three body interaction effect and Vegard's law, that values listed in Table (3.1). Using values of these model parameters calculated cohesive properties of $CdS_{1-x}Se_x$ having Zinc blende structure together with allied properties listed them in table (3.2) and computed results intermediate between end point members. In this paper we are calculated silent experimental result such as Gruneisen Parameter, Compressibility, and ratio of volume expansion to specific heat and Moelwyn- Hughes constant. Present result Listed in the table have followed a systematic trend approximately similar to those obtained from the experimental observation as well as and theoretical. It is thus obvious from the overall achievements that the present three body potential model (TBPM) is adequately suitable for describing the relatively stable in B_3 structure with minimum energy of $CdS_{1-x}Se_x$ with all concentrations.

Solid	Lattice constant a (Å)	Hardness parameter b (10^{-11}erg)	Range parameter ρ (Å)	Three-body interaction parameter f(r)
CdS	5.82[22]	1.5	0.412	-0.012
CdSe	6.05[22]	1.04	0.399	-0.025

Table 1: Input Parameters

Solid		CdS	$CdS_{0.75}Se_{0.25}$	$CdS_{0.50}Se_{0.50}$	$CdS_{0.25}Se_{0.75}$	CdSe
Lattice Constant r_0	Present	2.669	2.679	2.689	2.699	2.709
	Expt.	2.52[22]				2.62[22]

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	Other	2.54[23],2.55[24], 2.57[25,5]				2.68[23], 2.62[26],2.7[5]
Cohesive Energy ϕ_0 (KJ/Mole)	Present	-2774.62	-2754.04	-2737.12	-2724.11	-2698.38
	Other	-3104.105[27]				-3099.117[27]
Molecular force Constant f (10^{-2} $N^{-1}m^2$)	Present	2.7458	2.7782	2.7992	2.8069	2.867
Compressibility β (10^{-11} $N^{-1}m^2$)	Present	8.412	8.397	8.417	8.476	8.377
Infrared absorption frequency ν (THz)	Present	4.097	3.667	3.389	3.189	3.07
Debye Temperature θ_D(K)	Present	196.638	175.995	162.671	153.095	147.379
	Expt.	219.32[29]				181[29]
	Other	230[5],280[28]				231[5],300[28], 197-200[30]
Gruneisen Parameter γ	Present	1.146	1.139	1.131	1.122	1.116
	Other					1.94[41]
α_v/C_v(10	Present	5.502	5.361	5.211	5.08	8.125
Moelwyn- Hughes constant C_1	Present	7.911	7.964	8.017	8.071	0.087

Table 2: Cohesive Properties of $Cds_{1-X}se_x$

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