Study of Mechanical Properties of ChSC Alloy $Zn_{1-x}Cd_xTe$ Under High Pressure

Dr. Alka Singh[1] and Dr. Navin Kumar[2]

[1]*Assistant Professor, Department of Pure and Applied Physics,*
Guru Ghasi Das Central University, Bilaspur, Chhatisgarh, India
[2]*Centre Coordinator, IGNOU Centre for Engineering, Muzaffarpur, Bihar, India*
E-mail: [1]*singh.alka18@gmail.com,* [2]*ignou.csist@gmail.com*

Abstract—*The Study of the mechanical properties of Chalcogenide Semiconductor compounds (ChSCs) under high pressure is of significant importance from both the view point technology and basic research. The mechanical properties ChSCs are studied through the stress-strain relationship, which is supposed to be linear for small stress(Hooke's law).The knowledge of elastic constants for such specimeans is valuable as these data can be correlated with other physical measurements and thereby provided possible insight into the nature of the atomic forces in solid matter.This strain energy can be interpreted as the atomic vibrations reffered to as the equilibrium. Thus, the elastic constants could be directly related to the atomic interaction potential per unit volume in ChSCs.The three-body potential model is found to be satisfactory to a certain extent in explaining some of the physical properties of ChSCs.The success of this TBP model lies in the fact that it takes into account the forces due to the three-body and van der waals(vdw) interactions along with the long-range Columbic and short-range overlap repulsive interactions.. Analysis of the pressure induced mechanical properties is important for understanding the nature of the inter-atomic forces in the crystals. The second order elastic constants and their pressure derivatives at 0K pressure and, $(dC_{ij}/dP)_0$ have been calculated for all the ChSCs taken into consideration In the present paper, we report the result of our investigations on high pressure and compositional dependence of elastic properties $Zn_{1-x}Cd_xTe$.*

1. INTRODUCTION

In the past few years, many researchers were attracted in knowing the effect of elastic properties of ChSCs at high pressures [1-10]. The quest for the nature of interatomic interactions in solids is of paramount importance as it leads to an understanding of their thermo dynamical, elastic and numerous other physical properties. Pressure is identified as an attractive thermo dynamical variable to reveal the mechanical properties of most of the solids and alloys. In recent years there has been considerable interest in theoretical and experimental studies of $A^N B^{8-N}$ type crystals with zinc blende structure. It is attributed to their high symmetry and simplicity of their ionic bonding (Mujica*et al* 2003). Almost all the A^{II}-B^{VI} compounds crystallize either in the zinc blended or quartzite structures. The common and dominant feature of these structures is the tetrahedral bonding to four atoms of the other elements. In zinc blende 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 cubic (*fcc*) array in the former and a hexagonal closed-packed (*hcp*) array in the latter (Jain 1991). Quite generally at a particular pressure, A^{II}-B^{VI} compounds are known to undergo a first order phase transition from the *B*3 to

*B*1 as observed in diamond cell by optical (polarized light) and IR microscopy measurement(Piermarini and Block 1975). Arora and co-workers (1988) reported the results of a detailed Raman scattering investigation of the zone-centre optical. In the earlier past, there was an extensive theoretical study and understanding of phase-transition and enharmonic properties of solids by means of different forms of cohesion. The major part of cohesion in these potentials is contributed by long-range Coulomb interactions, which are counter balance, by the short-range overlap repulsion owing its origin to the Pauli Exclusion Principle. Born and Mayer (1932) usedoverlap repulsion with a lattice sum to describe the cohesion in most of ionic solids. We refer to an earlier work of Tosi and Fumi (1962) and Tosi (1964) who properly incorporated van der Waals interaction along with d–d (r^{-6}) and d-q (r^{-8}) interactions to reveal the cohesion in several ionic solids. We also quote the work of Singh (1982), who introduced the effects of charge transfer i.e. three-body interactions and followed Hafemeister and Flygare (1965) type overlap repulsion up to second neighbour ions besides short range interactions to discuss the mechanical properties of several solids and alloys. Despite their successes, the basic nature of these interatomic potentials is such that they are inadequate to reveal a consistent picture of the interaction mechanism in ionic solids. The present investigation is organized as follows. We begin with the estimation of van der Waals coefficient from the Slater– Kirkwood variation method with an idea that both the ions are polarizable. elastic constants are deduced

within the framework of the Three body model, that incorporates the long-range Coulomb, van der Waals (vdW) interaction, the short range overlap repulsive interaction up o second neighbour ions within the Hafemeister and Flygare approach and the three-body interaction. After that computed results and numerical analysis are discussed. We aimed at how by minimizing Gibbs free energies of both the phases we trace the results. The results obtained from this method and their comparison is presented

2. EXPERIMENTAL SETUP

The high pressure phase transition for $Zn_{1-x}Cd_xTe$ have been analysed by using three body potential models applied at different Cadmium concentrations. The model parameters ρ, b and f® have been computed through input parameters for host binary (ZnTe and CdTe) and reported in

Table 5.7 (a). These model parameters have been used to computed the lattice energies (Φ) of two competitive structures at T=O K. Further the study has been made to observe the effect of pressure on interatomic spacing (r_0), lattice energy (Φ), relative volume $[-\Delta V(P_T)/V_0]$ and morphology of the system. The relative volume factors $[-\Delta V(P_T)/V_0]$ were determined from the equilibrium inter nuclear separations in the crystals at P, evaluated by minimizing the Gibbs free energy. The computed values of variations in Gibbs free energy as a function of pressure for the various Cd compositions in the host ZnTe have been tabulated in Tables 5.7 (b). The lattice parameter (r_0), Cohesive energies (Φ) of two competitive structures, difference in Free energy (ΔG), volume collapse $[-\Delta V(P_T)/V_0]$ and Transition Pressure (P_T) for $Zn_{1-x}Cd_xTe$ solid solution in B_3 and B_1 type structures have been reported in table 5.7 (b). The positive lattice energy difference ΔG as observed in the host binary as well as solid solutions are explains the Sangster criterion of structural stability. It is observed the transition from B3 to B1 type phase in the host binary ZnTe(CdTe) and their solid solutions $Zn_{1-x}Cd_xTe$ are given in Fig. 1 explains the understanding of phase transition, when change in Gibbs free energy ΔG reaches zero or negative. Another observation is the variation of transition pressure as a function of Zn composition in ZnS binary, it is found that increase in Cd composition decreases the transition pressure for $Zn_{1-x}Cd_xTe$ System in fig. 5.7. The plot of difference in Gibbs free energy as a function of pressure clearly confirms the phase transition phenomenon as and when it crosses the zero line. Looking at table 1 and 2 it can easily be observed that the lattice parameter and transition pressure follows the Vegard's law

3. SUMMARY AND CONCLUSION

Analysis of the pressure induced mechanical properties is important for understanding the nature of the interatomic forces in the crystals. The second order elastic constants and their pressure derivatives at 0K pressure and, $(dC_{ij}/dP)_0$ have been calculated for all the ChSCs taken into consideration.

The calculated values of C_{11}, C_{12}, C_{44}, Bulk modulus at P = 0 Gpa reported in tables .As results obtained from TBI model are predicted for Zinc Chalcogenide (ZnS, ZnSe, ZnTe), Cadmium Chalcoginde (Cds, CdSe, CdTe), MurcuryChalcoginde (HgS, HgSe, HgTe),and their solid solutions. We find that the magnitudes of SOEC systematically decrease as the cation radius increase i.e. in the order ZnX<CdX<HgX (X = S, Se, Te).

This shows that the size of the caption and inter-atomic distance provide a dominant effect on elastic constants.

Table 1. The input (van der Waals coefficient (in units10^{-60}ergcm^6)) and D (inunits10^{-60} ergcm^6) interatomic separation r_0(10^{-1}Nm) second order elastic constantC_{44}(Mbar), and Bulk modulus B_0(Mbar), and model parameters (range {b}, hardness{ρ} and TBI{f®}) for $Zn_{1-x}Cd_xTe$

$Zn_{1-x}Cd_xTe$	C	D	r_o	C_{44}	B_o	b	ρ	f(r)
0	5612.82	45247.70	2.64	0.31	0.51	0.32	0.22	-0.05
0.25	7958.04	66556.71	2.68	0.28	0.49	0.48	0.28	-0.06
0.5	10303.27	87865.72	2.72	0.26	0.47	0.63	0.34	-0.08
0.75	2648.49	109174.73	2.77	0.23	0.44	0.79	0.39	-0.09
1	1499.71	130483.74	2.81	0.20	0.42	0.94	0.45	-0.10

Table 2. The lattice parameter (r_0), Cohesive energies (Φ) of two competitive structures, difference in Free energy (ΔG), volume collapse $[-\Delta V(P_T)/V_0]$and Transition Pressure (P_T) for $Zn_{1-x}Cd_xTe$.

$Zn_{1-x}Cd_xTe$	r (10^{-1}Nm)$_0$		Φ (KJmole^{-1})		ΔG	-$\Delta V(P_T)/V_0$	P (GPa)$_T$
	B_1	B_3	B_1	B_3			
0	2.64	2.87	-2697.00	-3426.	57.00	0.03	11.85

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0.25	2.68	2.91	-2627.00	-3161.75	52.73	0.06	10.09
0.5	2.72	2.96	-2557.00	-2897.50	48.45	0.09	8.33
0.75	2.77	3.00	-2487.00	-2633.25	44.18	0.12	6.56
1	2.81	3.05	-2417.00	-2369.00	39.90	0.16	4.80

Figure 1. Phase Transitions in Zn$_{1-X}$Cd$_X$Te at different Cd composition (x)

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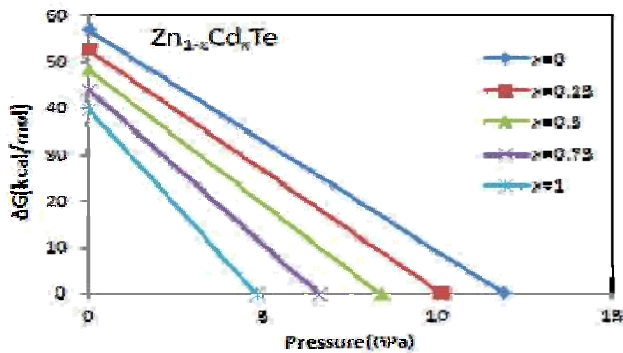15. M.Born and K.Haung, "Dynamical theory of crysal lattices " Oxford Univ. Press (1954)