

ANHARMONIC PROPERTIES OF CADMIUM TELLURIDE (CdTe)

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Abstract

In the present paper, we have investigated the phase transition and elastic properties of CdTe (Cadmium telluride) at high pressure using Three body potential model (TBPM) which include three body interaction (TBI). We predict the B3-B1 phase transition for CdTe. The phase transition pressure (Pt) and associated volume collapse obtained from this approach show a respectably good agreement with experimental and other theoretical (ab-initio method) data. Three body potential model has also been used to derive the correct expressions for third order elastic constants and pressure derivatives of second order elastic constants for CdTe.

Key-words: Pt, TBPM, Elastic constants

Introduction

Over the past few years, study of materials under high pressure has become an extremely important subject displaying explosive growth. Looking many fold advantage of semiconductor, several workers have investigated them both theoretically and experimentally. The semiconductor –ionic and semiconductor –metallic phase transition of III-V and II-VI compound are of current interest under high pressure. The solids, whose conductivity lie between 10^4 and 10^{-10} (ohm cm)⁻¹ are classified as semiconductors. All IVth group semiconductors crystallize in diamond structure III-V compounds like GaAs, InSb, etc. and II-VI compound such as ZnS, CdTe, HgTe, etc. are semiconductor compounds. They crystallize in zinc-blend structure, CdX (X=S, Se, Te) semiconducting compounds have attracted special attention in recent years for their applications in γ -ray detectors, infrared windows, solar cells and other optoelectronic devices [1]. The aim of present investigation is to study lattice mechanical properties and thermodynamic properties of CdTe for which the experimental data are available and their analysis from theoretical model is lacking. Structure of CdTe has been zinc-blend (B3) at ambient pressure and energy gap at 300K is 1.474eV. Melting point of CdTe is very high 1041 °C [2]. With increasing pressure B3 structure undergoes a transition in cinnabar structure, but this structure is stable only in short pressure interval. On further increasing the pressure this structure change in rock salt (B1) [3,4].

Method of calculation

The interatomic potential of the CdTe in the framework of the rigid ion model is expressed as:

$$\Phi = \Phi_C + \Phi_T + \Phi_V + \Phi_R$$

$$\Phi = -\sum_{ij} \frac{Z_i Z_j e^2}{r_{ij}} \left(1 + \frac{2\epsilon}{r} f(r_{ij}) \right) -$$

$$\sum_{ij} C_{ij} r_{ij}^{-12} - \sum_{ij} D_{ij} r_{ij}^{-9} +$$

$$b \left[n \beta_{ij} \exp \left(\frac{-r_{ij} - \rho_{ij}}{\rho} \right) + \right.$$

$$\left. \frac{n}{2} \left(\exp \left(\frac{2r_{ij} + \beta_{ij}}{\rho} \right) + \exp \left(\frac{2r_{ij} - \beta_{ij}}{\rho} \right) \right) \right]$$

This interatomic potential includes first and second term in it are the long-range Coulomb and three body interaction (TBI), the third term and fourth term are the short-range Van der Waals attraction and the remaining terms represent the short range overlap repulsion operative up to the second neighbor ions. Here $f(r)$, b and ρ are TBI parameter, hardness and range (Strength) parameters respectively and can be determined by using equilibrium condition;

$$\left(\frac{d\Phi}{dr} \right)_{r=r_0} = 0$$

(3)

Bulk modulus, given by;

$$\left(\frac{d^2\Phi}{dr^2} \right)_{r=r_0} = 9KrB_T$$

(With $K = V/r^3$ as the structure dependent constant and is well known for structure)

And the equilibrium condition

$$B_1 + B_2 = -1.261 Z(Z + 3f(r))$$

Where B_1 and B_2 force constants

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The electron shell of adjacent ions suffers appreciable overlap during lattice vibrations and consequently gets deformed. This electron shell deformation gives rise to a transfer or exchange of charge between the overlapping ions. These transferred charges, in turn, interact with all other charges of lattice and give rise to long range many body interactions, whose most significant component is the three-body interaction (TBI). The expressions for SOECs are

$$C_{11} = L \left[-0.24777Z (Z + 8f(r_0)) + \frac{1}{3}(A_1 + 2B_1) + \frac{1}{2}(A_2 + B_2) + 5.8243Zaf'(r_0) \right]$$

$$C_{12} = L \left[-2.6458Z (Z + 8f(r_0)) + \frac{1}{3}(A_1 - 4B_1) + \frac{1}{4}(A_2 - 5B_2) + 5.8243Zaf'(r_0) \right]$$

$$C_{44} = L \left[-0.123Z (Z + 8f(r_0)) + \frac{1}{3}(A_1 + 2B_1) + \frac{1}{4}(A_2 + 3B_2) - \frac{1}{3}v(-7.53912Z(Z + 8f(r)) + A_1 - B_1) \right]$$

And for TOECs are

$$C_{111} = L \left[0.51847 (Z + 8f(r_0)) + \frac{1}{9}(C_1 - 6B_1 - 3A_1) + \frac{1}{4}(C_2 - B_2 - 3A_2) - 2(B_1 + B_2) - 9.9326 Zaf'(r_0) + 2.522Za^2f''(r_0) \right]$$

$$C_{112} = L \left[0.3828Z(Z + 8f(r_0)) + \frac{1}{9}(C_1 + 3B_1 - 3A_1) + \frac{1}{8}(C_2 + 3B_2 - 3A_2) - 1106852Zaf''(r_0) + 2.522Za^2f''(r_0) \right]$$

$$C_{123} = L \left[6.1585Z(Z + 8f(r_0)) + \frac{1}{9}(C_1 + 3B_1 - 3A_1) - 12.5060Zaf''(r_0) + 2.522Za^2f''(r_0) \right]$$

$$C_{144} = L \left[6.1585 Z (Z + 8f(r_0)) + \frac{1}{9} (C_1 + 3B_1 - 3A_1) - 4.1681 Zaf'(r_0) + 0.8407Za^2f''(r_0) + v \left[-3.350/Z (Z + 8f(r_0)) - \frac{2}{9}C_1 + 13.5486 Zaf'(r_0) - 1.681Za^2f''(r_0) \right] + v^2 \left[-1.5637Z (Z + 8f(r_0)) + \frac{2}{3}(A_1 - B_1) + \left(\frac{C_1}{9}\right) - 5.3138 Zaf'(r_0) + 2.9350Za^2f''(r_0) \right] \right]$$

TBI parameter $f(r)$ is dependent on the nearest - neighbour distance (r) as

$$f(r) = f_0 \exp(-r/\rho)$$

Using the TBPM given by (2), we have derived the expressions for Second order elastic constant (SOEC), Third order elastic constant and pressure derivative of second order elastic constants (where a is lattice constant)

$$C_{166} = L \left[-2.1392Z (Z + 8f(r_0)) + \frac{1}{9}(C_1 - 6B_1 - 3A_1) - \frac{1}{8}(C_2 - 5B_2 - 3A_2) - (B_1 + B_2) - 4.1681 Zaf'(r_0) + 0.8407 Za^2f'(r_0) + \nabla \left[-8.3768Z (Z + 8f(r_0)) - \frac{2}{3}(A_1 - B_1) - \frac{2}{9}C_1 + 13.5486 Zaf'(r_0) - 1.681 Za^2f''(r_0) \right] + \nabla^2 \left[2.3527Z(Z + 8f(r_0)) + \left(\frac{C_2}{9}\right) - 5.3138 Zaf'(r_0) + 2.9350Za^2f''(r_0) \right] \right]$$

$$C_{456} = L \left[4.897Z(Z + 8f(r_0)) + \frac{1}{9}(C_1 - 6B_1 - 3A_1) - \frac{1}{8}(C_2 - 5B_2 - 3A_2) - B_2 + \nabla \left[-5.0261Z (Z + 8f(r_0)) - \frac{1}{9}C_1 \right] + \nabla^2 \left[-4.8008Z(Z + 8f(r_0)) + \frac{1}{3}(A_1 - B_1) - \left(\frac{C_2}{9}\right) \right] \right]$$

With $L=e^2/4a^4$ and

$$\nabla = \left[\frac{-733912Z(Z+8f(r_0))+(A_1-B_1)}{-3.1416Z(Z+8f(r_0))+(A_1+2B_1)+21.766Zaf'(r_0)} \right] \quad \text{Expression}$$

for pressure derivatives of bulk modulus B_T , Shear moduli and Elastic constant C_{44} using three body potential model are given by

$$\frac{dB_T}{dP} = 104.8433 Zaf'(r_0) + 22.7008Za^2f'(r_0)]$$

$$\frac{dS}{dP} = -(2\Omega)^{-1} \left[-11.5756Z(Z + 8f(r_0)) + 2(A_1 - 2B_1) + \frac{5}{2}A_2 - \frac{7}{2}B_2 + \frac{1}{4}C_2 + 37.5220 Zaf'(r_0) \right]$$

$$\frac{dC_{44}}{dP} = -(\Omega)^{-1} \left[\left\{ 0.4952Z(Z + 8f(r_0)) + \frac{1}{3}(A_1 - 4B_1 + C_1) + \frac{2A_2 - 6B_2 + C_2}{4} + 4.9667 Zaf'(r_0) + 2.522Za^2f''(r_0) \right\} + \nabla \left\{ -17.5913Z(Z + 8f(r_0)) + A_1 - B_1 - \frac{2}{3}C_1 + 40.6461 Zaf'(r_0) - 5.0440Za^2f''(r_0) \right\} + \nabla^2 \left\{ 3.1416Z(Z + 8f(r_0)) + \frac{2}{3}(A_1 - B_1) + \frac{C_2}{3} - 15.9412 Zaf'(r_0) + 8.8052Za^2f''(r_0) \right\} \right]$$

with

$$\Omega = -5.0440Z(Z + 8f(r_0)) + (A_1 + A_2) - 2(B_1 + B_2) + 17.4730 Zaf'(r_0)$$

The stability of a particular structure is decided by the minimum of the Gibb's free energy which is given as $G=U+PV-TS$

(Where U is internal energy)

The Gibb's free energies $G_1(r)$ for one phase and $G_2(r)$ for second phase become equal at the phase transition pressure P and temperature 0K.i.e. $\Delta G=G_1(r) - G_2(r)$ become zero.

Conclusion

The present interaction potential has only three parameters given by equation 2. The value of these parameters has been determined from the knowledge of second order elastic constants Input data and model parameters are give in table 1 and 2. Strategy of calculation of these parameters has already been described.

Table 1: Input data for CdTe

Elastic Constant (10^{11} dyn cm^{-2})			Lattice constant $a(\text{Å})$
C_{11}	C_{12}	C_{44}	
5.3[5]	3.7[5]	1.9[5]	3.238[6]

Table 2: Model parameter of CdTe

$\rho(\text{Å}^0)$	b (10^{-12} erg)	$f(r_0)$	$af'(r_0)$	$a^2 f''(r_0)$
0.372	0.7135	-0.01103	1.096	-0.8387

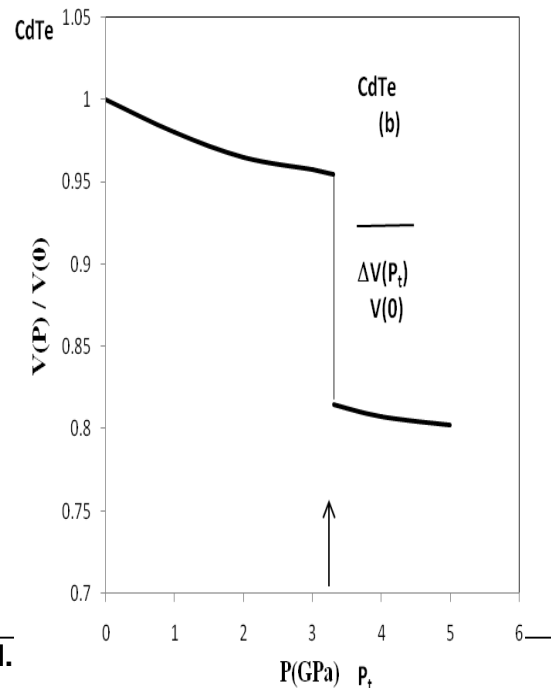
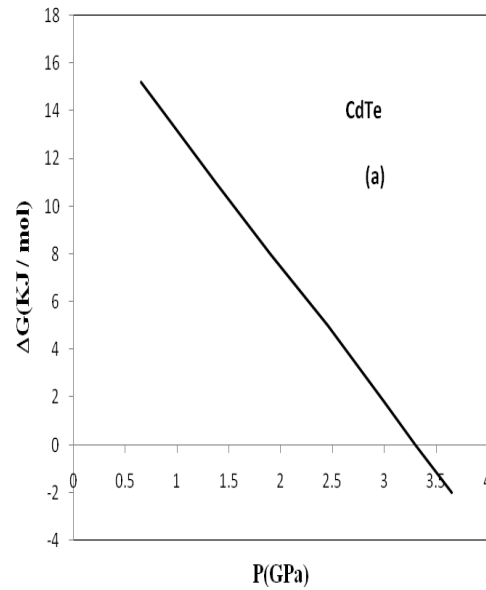
Using the values of these model parameters for CdTe having Zinc blende structure, phase transition pressure has been evaluated by minimizing the cohesive energies given by Eqs. (2) for the equilibrium interionic separations r_1 and r_2 corresponding to B1 and B2 phases. We have reported the value of r_1 and r_2 and corresponding cohesive energies ϕ_1 and ϕ_2 and their differences $\Delta\phi = \phi_1 - \phi_2$ in table 3. With the knowledge of these cohesive energies, we have predicted the relative stability of the competitive structure B1 and B3 by fitting out the energy difference $\Delta\phi = \phi_1 - \phi_2$.

We have evaluated phase transition from graphical analysis in which the Gibb's free energy difference $\Delta G = G(B1) - G(B3)$ corresponding to the above cohesive energies have been computed and plotted against the pressure (P) as depicted in Fig.1 for CdTe. The pressure at which ΔG approaches zero corresponds to phase transition pressure (P_t) as indicated by the arrows in these figure. The value of phase transition pressure have been listed in Table 3 and compared with the available experimental [3.7] and theoretical (ab-intio) [8] data. The relative volume changes, $\Delta V(P_t)/V(0)$, associated with the above mentioned compression (or phase transition pressure) have also been computed and plotted against pressure to get the phase diagram as shown in fig 1(b) for CdTe. The value of these relative volume changes along with other results corresponding to the phase transition pressure (P_t) are listed in table. 3. The phase transition predicted in fig.1 (a) has followed a systematic trend similar to those obtained from the experimental observation. The value of the volume collapses $\Delta V(P_t)/V(0)$ at the phase transition

pressure are found to be in good agreement with the experimental observation.

In view of the overall achievements, it may be concluded that the framework of the present three body potential is adequately suitable for the correct prediction of cohesive energy, relative stability, phase transition pressure and volume collapse of the CdTe .

The forces constant A_i , B_i and C_i ($i=1,2,3$) have been evaluated from the knowledge of the model parameters. Their values have been used to compute the TOEC and pressure



derivatives of SOEC of the CdTe. We have described anharmonic properties of CdTe by calculating the TOEC, the pressure derivatives of SOEC and bulk modulus and shear moduli [Table 4].

It is thus obvious from the overall achievements that the present three body potential model is

adequately suitable for describing the relative stability, the phase transition and the anharmonic properties of semiconducting compounds. This model has a promise to predict these properties and phase transition in binary solid of other crystal structure as well.

Table 3: Cohesive properties and High pressure behavior of CdTe

Solid	Equilibrium Separations (Å ⁰)		Cohesive energy (KJ/mole)		ϕ (KJ/mole)	Phase transition pressure (GPa)	Relative change in volume (%)
	$r_0(B_3)$	$r'_0(B_1)$	ϕ_1	ϕ_1			
CdTe Present	2.796	3.055	-	-	19.45	3.35	13.75
Expt.	2.752[6]	2.96[9]	-	-	-	3.3[7],3.8[3]	10[7]
Another theoretical	-	2.96[10],2.91[8]	-	-	-	-	-

Table 4: Value of Second order and third order elastic constant and pressure derivative for CdTe

Elastic constants (10 ¹¹ dyn cm ⁻²)	Present* (10 ¹¹ dyn cm ⁻²)	Pressure derivatives GPa	Present Gpa	Expt. GPa
C ₁₁₁	-1.277	dB _T /dP	4.95	4.30[11]
C ₁₁₂	-0.79			
C ₁₂₃	1.56	dS/dP	-0.21	-0.42[11]
C ₁₆₆	-0.82			
C ₁₄₄	1.96	dC ₄₄ /dP	2.4	-1.25[11]

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