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 compounds have attracted special attention in recent years for their applications in X-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].

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 respectively 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

Method of calculation

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

\[ \Phi = \Phi_c - \sum_1^4 \frac{K}{r_i} - \frac{1}{2} \sum_1^4 \frac{f_{ij}}{r_{ij}} \]

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;

\[ 0 = \frac{d\Phi}{dr} = \frac{f(r)}{r} \quad \text{at} \quad r = r_0 \]

(3)

Bulk modulus, given by:

\[ \frac{1}{B_0} = \frac{1}{K_r B_r} \]

(With K =V/ρ³ as the structure dependent constant and is well known for structure)

And the equilibrium condition

\[ B_1 + B_2 = -1.261Z(Z + 3f(r)) \]

Where B1 and B2 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 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)

\[
 C_{11} = L \left[ -0.2477Z \left( Z + 8f(r_0) \right) + \frac{1}{6} (A_1 + 2E_2) + \frac{1}{4} (A_2 + B_2) + 5.8243Zaf'(r_0) \right]
\]
\[
 C_{12} = L \left[ -2.5458Z \left( Z + 8f(r_0) \right) + \frac{1}{6} (A_1 - 4E_1) + \frac{1}{4} (A_2 - 5B_2) + 5.8243Zaf'(r_0) \right]
\]
\[
 C_{44} = L \left[ -0.123Z \left( Z + 8f(r_0) \right) + \frac{1}{6} (A_1 + 2B_1) + \frac{1}{4} (A_2 + 3B_2) + \frac{1}{9} \sqrt{-7.53912Z(Z + 8f(r_0))} + 0 \right]
\]

And for TOECs are

\[
 C_{111} = 10.5147 \left( Z + 8f(r_0) \right) + \frac{1}{6} (C_1 - 6B_1 - 3A_1) + \frac{1}{4} (C_2 - 2B_2 - 3A_2) - 7.9326 \text{Zaf}'(r_0) + 2.5222Za^2f''(r_0)
\]

\[
 C_{112} = L \left[ 0.3828Z \left( Z + 8f(r_0) \right) + \frac{1}{6} (C_1 + 3B_1 - 3A_1) + \frac{1}{4} (C_2 + 3B_2 - 3A_2) - 1106052Zaf''(r_0) + 2.5222Za^2f''(r_0) \right]
\]

\[
 C_{123} = L \left[ 6.1585Z \left( Z + 8f(r_0) \right) + \frac{1}{6} (C_1 + 3B_1 - 3A_1) - 12.5069Zaf''(r_0) + 2.5222Za^2f''(r_0) \right]
\]

\[
 C_{144} = L \left[ 6.1585Z \left( Z + 8f(r_0) \right) + \frac{1}{6} (C_1 + 3B_1 - 3A_1) - 4.1681 \text{Zaf}'(r_0) + 0.8407Za^2f''(r_0) + \sqrt{-3.35U/2 \left( Z + 8f(r_0) \right) - \frac{2}{9} C_1 + 13.5486 \text{Zaf}'(r_0) - 1.0612Za^2f''(r_0)} \right]
\]
$C_{256} - L \left[ -2.1392Z \left( Z + 8f(r_0) \right) + \frac{1}{9} \left( c_1 - 6B_1 - 3A_2 \right) - \frac{1}{9} \left( c_2 - 5B_2 - 3A_2 \right) - (B_1 + B_2) - 4.1681 Z \psi(f(r_0)) + 0.8407 Z a^2 f''(r_0) + \sqrt{9.3768Z \left( Z + 8f(r_0) \right) - \frac{2}{3} (A_1 - B_2) - \frac{2}{3} c_1 + 13.5486 Z \psi(f(r_0)) - 1.681Z a^2 f''(r_0)} \right] + \sqrt{2.357Z(Z + 8f(r_0)) + \frac{(c_2)}{3}} - 5.3138 Z \psi(f(r_0)) + 2.9356 Z a^2 f''(r_0) \right] \right] \\
C_{456} = L \left[ 4.897Z \left( Z + 8f(r_0) \right) + \frac{1}{9} \left( c_1 - 6B_1 - 3A_2 \right) - \frac{1}{9} \left( c_2 - 5B_2 - 3A_2 \right) - B_2 + \sqrt{-5.0261Z \left( Z + 8f(r_0) \right) - \frac{1}{4} c_1} \right] + \sqrt{2.43008Z(Z + 8f(r_0)) + \frac{1}{9} (A_1 - B_2) - \frac{(c_2)}{3}} \right] \\
With \ L = e^{3/4a^4} \ and \ V = \frac{-75.912Z \left( Z + 8f(r_0) \right) + (A_1 - B_2)}{-2.43008Z(Z + 8f(r_0)) + (A_1 - B_2) - 27.009Z a^2 f''(r_0)} \\
Expression \ for \ pressure \ derivatives \ of \ bulk \ modulus \ B_1, \ Shear \ modulii \ and \ Elastic \ constant \ C_{14} \ using \ three \ body \ potential \ model \ are \ given \ by \\
\frac{\partial P}{\partial f} = \frac{104.8433 Z \psi(f(r_0)) + 22.7008Z a^2 f''(r_0)}{104.8433 Z \psi(f(r_0)) + 22.7008Z a^2 f''(r_0)} \\
\frac{\partial P}{\partial f} = -(2Q)^{-1} \left( -11.5756Z \left( Z + 8f(r_0) \right) + 2(A_1 - 2B_1) + \frac{2}{9} A_2 - \frac{2}{3} B_2 + \frac{1}{3} C_2 + 37.5220 Z \psi(f(r_0)) \right) \\
\frac{\partial P}{\partial f} = -(Q)^{-1} \left[ 0.4952Z \left( Z + 8f(r_0) \right) + \frac{1}{3} (A_1 - 4B_1 + C_4) + \frac{2}{9} A_2 + \frac{2}{9} a^2 f''(r_0) + 4.9667 Z \psi(f(r_0)) + 2.522Z a^2 f''(r_0) \right] + \sqrt{17.5913Z \left( Z + 8f(r_0) \right) + A_1 - B_2 - \frac{2}{3} C_2 + 40.4461 Z \psi(f(r_0)) - 5.0440Z a^2 f''(r_0)} \right] + \sqrt{3.1416Z \left( Z + 8f(r_0) \right) + \frac{2}{3} (A_1 - B_2) + \frac{2}{3} - 15.9412 Z \psi(f(r_0)) + 6.8052Z a^2 f''(r_0)} \right] \right] \\
with \ \Omega = -5.0440Z \left( Z + 8f(r_0) \right) + (A_1 + A_2) - 2(B_2 + B_2) + 17.4730 Z \psi(f(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 given in table 1 and 2. Strategy of calculation of these parameters has already been described.

<table>
<thead>
<tr>
<th>Elastc Constant ($10^4 \text{dyn cm}^{-2}$)</th>
<th>Lattice constant ($\text{a(A}_0^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{11}$</td>
<td>$C_{12}$</td>
</tr>
</tbody>
</table>

Table 2:  Model parameter of CdTe

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 $\phi_1$ and $\phi_2$ 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 $\Delta G$ 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**

<table>
<thead>
<tr>
<th>Solid</th>
<th>Equilibrium Separations (Å)</th>
<th>Cohesive energy (KJ/mole)</th>
<th>$\phi_1$</th>
<th>$\phi_1$</th>
<th>Phase transition pressure (GPa)</th>
<th>Relative change in volume (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$r_0(B_1)$</td>
<td>$r'_0(B_1)$</td>
<td></td>
<td></td>
<td>2917.32</td>
<td>2897.87</td>
</tr>
<tr>
<td>CdTe Present</td>
<td>2.796</td>
<td>3.055</td>
<td>-</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Another theoretical</td>
<td>-</td>
<td>2.96[10], 2.91[8]</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Elastc constants $(10^{11}\text{dyn cm}^{-2})$</th>
<th>Present* $(10^{11}\text{dyn cm}^{-2})$</th>
<th>Pressure derivatives GPa</th>
<th>Present Gpa</th>
<th>Expt. Gpa</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{111}$</td>
<td>-1.277</td>
<td>dB/dP</td>
<td>4.95</td>
<td>4.30[11]</td>
</tr>
<tr>
<td>$C_{112}$</td>
<td>-0.79</td>
<td>dS/dP</td>
<td>-0.21</td>
<td>-0.42[11]</td>
</tr>
<tr>
<td>$C_{123}$</td>
<td>1.56</td>
<td>dC/dP</td>
<td>2.4</td>
<td>-1.25[11]</td>
</tr>
<tr>
<td>$C_{166}$</td>
<td>-0.82</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_{144}$</td>
<td>1.96</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**References**