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MECHANICAL AND THERMAL BEHAVIOR OF SEMICONDUCTING CADMIUM OXIDE AT HIGH-PRESSURE

N. Bioud [1, 2], N. Benchiheub [1,3 *]

[1] *Faculty of Sciences and Technology, University Mohamed El Bachir El Ibrahimi of Bordj Bou Arreridj, 34000 Bordj Bou Arreridj, Algeria*

[2] *Laboratoire d'Optoélectronique et Composants (LOEC), Faculté des sciences, Université Ferhat Abbas de Sétif 1, 19000 Sétif, Algérie*

[3] *Laboratory of Materials Physics, Radiation and Nanostructures (LPMRN), University Mohamed El Bachir El Ibrahimi of Bordj Bou Arreridj, 34000 Bordj Bou Arreridj, Algeria*

[*]Corresponding author: nadjat.benchiheub@univ-bba.dz

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Abstract

The effect of high pressures on the mechanical and thermal properties up to phase transition pressure for cubic rock-salt cadmium oxide (CdO) semiconducting compound is presented in this research. The calculations are based on the equation of state (EOS) parameters measured at ambient conditions reported in the literature. The approach used here was previously applied successfully for other materials. Our study shows that the parameters reflect the rigidity of the semiconductor and the melting temperature increases with increasing pressure, while some other parameters decrease gradually for our material of interest. A comparative analysis of some quantities for CdO compound under high pressure was done. Similar behaviors were observed in the literature for particular materials with particular structures. Furthermore, we calculated both the fracture toughness and the fracture surface energy, which are at around 1.23 $MPa.m^{1/2}$ and 5.14 $J.m^{-2}$, respectively.

1. Introduction

Transition-metal oxides, especially group-IIB oxides possess interesting optical and electrical properties that find their applications in various technological areas [1]. Group-IIB oxides semiconducting materials have been used widely in making phototransistors, solar cells, and many other electronic devices [1]. Cadmium oxide (CdO) halite is the most ionic of all the cadmium chalcogenides, having a fractional ionic character (Phillips's ionicity) of bonds of around $f_i = 0.785$ [2] on the Phillips's ionicity scale.

It is noted that under very high pressure, the initial phase was destabilized and a new

phase occurred. For CdO compound, the experience shows that the phase transition from the NaCl-type structure to the CsCl-type appears at a pressure of 90.6 GPa [3].

In recent past years, several theoretical studies on pressure-dependent physical properties and elastic constants of CdO compound have also been published [4-8]. Peng *et al.* [4, 5] have studied the structural stability and the pressure-dependent elastic constants of both NaCl-type and CsCl-type phases using Plane-Wave PseudoPotential (PW-PP) method. They found that the elastic constants C_{11} and C_{12} of NaCl-type phase increase monotonically with increasing pressure, while C_{44} decreases with increasing pressure. The same mechanical behavior was also observed in the theoretical works of JemmyCinthia *et al.* [6] and Feng *et al.* [7].

Using PW-PP method based on density functional theory, Li *et al.* [8] have examined the pressure dependence of the sound velocity and Debye temperature of CdO, while Bahloul and Amirouche [9] have studied the effect of zinc (Zn) concentration on the structural parameters, electronic properties and elastic constants of $Zn_xCd_{1-x}O$ dilute alloys.

In the present work, we propose a simple and accurate method to predict the high-pressure effect on several mechanical and thermal properties of materials using the equation of state (EOS) parameters measured at ambient conditions. We studied the high-pressure effect up to phase transition on the isothermal dilatation, mass density, bulk modulus, microhardness, the first order pressure derivative of the bulk modulus, the Grüneisen parameter, the Debye temperature and the melting temperature of CdO compound in cubic rock-salt phase up to pressure of 90.6 GPa.

2. Theory

Knowledge of the behaviors of solids under high-pressure and high-temperature environments are of great interest and importance for both fundamental research and technological applications [10]. There are different models of the Equation Of State (EOS) that relate the compressed volume V with the pressure p; one of those models is the universal Equation Of State (EOS) of Vinet [11].

In the case of hydrostatic compression, the incompressibility of the material could be characterized by the bulk modulus [12-15]. If we consider the Vinet universal equation of state (EOS) model [11], the isothermal bulk modulus B of the material could be given with the following expression [17-19]:

$$B = B_0 x^{-2}\left[1+\left(\eta x+1\right)\left(1-x\right)\right]\exp\left\{\eta\left(1-x\right)\right\} \quad (1)$$

where $x=\left(V/V_0\right)^{1/3}$, $\eta = 3(B_0^{'}-1)/2$, and B_0' is the equilibrium first-order pressure derivative of B.

The Grüneisen parameter γ plays an important role in the study of thermo-elastic properties of materials. It helps on the knowledge of the frequency distribution of the phonon spectrum in solids [18]. There are different methods and approaches usually employed to measure or estimate the Grüneisen parameter γ of materials [15-20]. Under compression, the Grüneisen parameter γ may be calculated for example via the Vashchenko-Zubarev formula as follows [16, 19, 20]:

$$\gamma_{V-Z} = \left(\frac{1}{2}B^{'}+\frac{2}{9}\left(\frac{p}{\mathrm{B}}\right)-\frac{5}{6}\right)\Bigg/\left(1-\frac{4p}{3\mathrm{B}}\right) \quad (2)$$

where B and p denote the bulk modulus and the pressure at the volume V, respectively. B' is the first-order pressure derivative of the isothermal bulk modulus given at the same volume V.

Under compression, the pressure derivative of the isothermal bulk modulus B' could be expressed by the following formula [16-19]:

$$B^{'} = \frac{1}{3}\left[\frac{x\left(1-\eta\right)+2\eta x^2}{1+\left(\eta x+1\right)\left(1-x\right)}+\left(\eta x+2\right)\right] \quad (3)$$

where $x=\left(V/V_0\right)^{1/3}$, and $\eta = 3(B_0^{'}-1)/2$.

Usually, the first-order pressure derivative of the bulk modulus B' decreases monotonically with rising pressure [16, 19].

3. Discussion of results

3.1. Structural parameters

As we have mentioned previously in the introduction section, the CdO compound normally crystallizes in a cubic rock-salt (B1) structure [1, 3]. In order to reproduce the variation of the volume of the unit cell for CdO compound under applied pressure p, we used the experimental EOS parameters reported by Liu *et al.* [3], where B_0 is the bulk modulus, B'_0

is the pressure derivative of B and V_0 is the molar volume, where the subscript 0 indicates a reference state, *i.e.*, all these physical parameters were measured at ambient conditions of pressure and temperature.

Figure 1 discerns the variation of so-called isothermal dilatation ($\Delta V/V_0 = (V_0 - V_p)/V_0$) as a function of pressure p for CdO compound, where V_p is the primitive-cell volume calculated from several values of hydrostatic pressure. The volume V_p is less than the atomic volume V_0. Throughout this manuscript, the pressure varies from 0 up to 90 GPa. At this limit value, phase transition of CdO at ambient temperature from rock-salt type (B1) to CsCl-type (B2) structural is occurred. Figure 1 showed clearly that $\Delta V/V_0$ increases with increasing pressure p. From the curve of this figure, we can obtain an equation of the form: $\Delta V/V_0 = 0.85 \times 10^{-3} + 6.05 \times 10^{-3} p - 0.54 \times 10^{-4} p^2 + 0.23 \times 10^{-6} p^3$, where p is expressed in GPa.

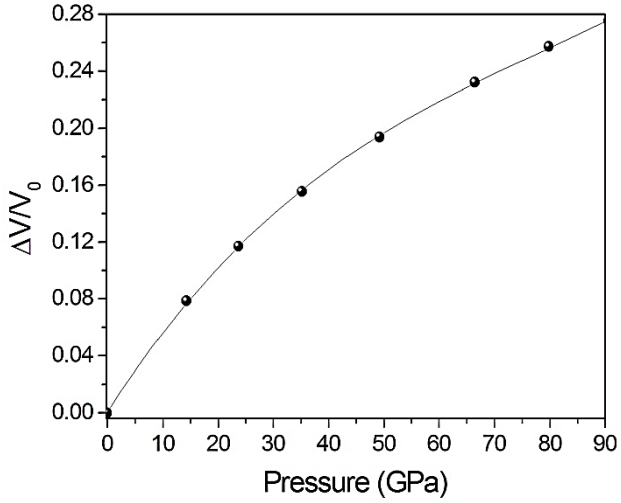

Figure 1. Isothermal dilatation $\Delta V/V_0$ versus pressure p for CdO compound

Knowledge of the P-V data and the structure allows us to predict the theoretical mass density ρ of any crystal, which is calculated as follows: $\rho = ZM/NV$ [12], where M is the molecular weight, Z is the number of molecules per unit cell, N is the Avogadro constant, and V is the unit cell volume.

Likewise, the dependence of the crystal density ρ with the pressure for CdO compound is ported in Table **1**. A monotonic increase of ρ with increasing pressure p was observed. One can find that the variation of the crystal density ρ against pressure reported for the CdO compound is similar to those observed for other materials as per literature [13, 16, 19, 21].

Table 1. Crystal density ρ versus pressure p for CdO semiconducting compound up to 90 GPa.

p (GPa)	0	14.3	23.7	35.2	49.2	66.5	79.8	90.6
ρ (g/cm^3)	8.186	8.885	9.271	9.693	10.154	10.662	11.020	11.294

3.2. Mechanical properties

Fig. 3 discerns the variation of the isothermal bulk modulus B as a function of the pressure for CdO compound, along with the data of Ref [1]. As shown in Fig **3**, monotonic and pseudo-linear behavior of the bulk modulus B has been shown upon compression for CdO compound. The fit of our data regarding the bulk modulus B as a function of p obeys the quadratic form as: $B = 148.06 + 3.91\ p - 0.56 \times 10^{-2} p^2$, where both B and p are expressed in GPa. It can be noted that a similar qualitative behavior of the isothermal bulk modulus B versus pressure has been reported for cubic zinc-blende Gallium antimonide (GaSb) semiconductor [16], for calcium oxide (CaO) compound [17], for cubic rock-salt calcium-based chalcogenides CaX (X = S, Se, Te) materials [19], and for compressed cubic rocksalt CuX (X = Cl, Br) copper halides [21].

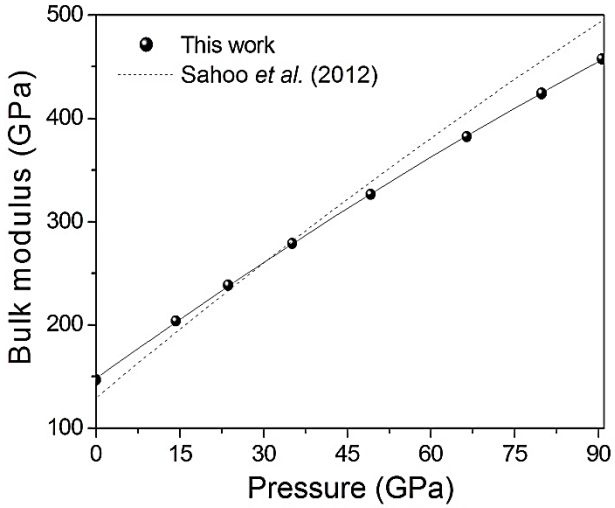

Figure 2. Pressure-dependent bulk modulus for CdO compound, along with the data of Ref [1]

To the best of the author's knowledge, there are very theoretical little works [6, 22-24] that have estimated the microhardness H at equilibrium for CdO compound. Some discrepancies in the obtained results were observed, the values reported are 23.61 GPa [6], 2.11 GPa [22], 6.23 GPa [23], and 6.58 GPa [24], respectively.

It is important to note that the value (23.61 GPa) of H reported previously by Jemmy Cinthia *et al.* [6] for CdO is incorrect. This is because the authors of Ref. [6] estimated the H

of CdO from Young's modulus E and the Poisson's ratio v, using the following empirical expression: $H = (1/6)(1-2v)E/(1+v)$ [6]. So, if we substitute their values (E = 141.67 GPa and v= 0.33 [6]) into the previous equation, we obtain the result of 6.04 GPa. The agreement is satisfactory with the theoretical values (6.23 GPa) [23] and (6.58 GPa) [24].

The pressure dependence of the hardness of materials can be determined using Mukhanov's *et al* model: $H(p) = C$ x $B(p)$ [16, 17, 25], where $C = H(0)/B(0)$ [16, 17], we take the highest value of $H(0)$ *i.e.*, $H(0)$ = 6.58 GPa [24]. Replacing the value of H(0) = 6.58 GPa [24] into the previous equation, the pressure dependence of the Knoop microhardness H for CdO compound is listed in Table **2**. This revealed that H of CdO increases gradually with increasing pressure.

Table 2. Knoop microhardness H versus pressure p for CdO compound up to 90 GPa.

p (GPa)	0	14.3	23.7	35.2	49.2	66.5	79.8	90.6
H (GPa)	6.58	9.12	10.67	12.48	14.61	17.12	18.98	20.47

Acounting the effect of pressure on B', the data of the first-order pressure derivative of the bulk modulus B' versus pressure for CdO material is listed in Table **3**. Such as the volume, B' also decreases monotonically with rising pressure for our material of interest. The behavior of B' versus pressure for CdO compound is similar to those reported, for cubic zinc-blende GaSb semiconducting compound [16], for calcium oxide (CaO) material [17], for calcium-based chalcogenides (CaS, CaSe, and CaTe) compounds [19], and for several metal materials (Cu, Au, Ag, Zn, Cd, In, and Pb) [26].

Table 3. Pressure derivative of the bulk modulus B′ versus pressure p for CdO up to 90 GPa.

p (GPa)	0	14.3	23.7	35.2	49.2	66.5	79.8	90.6
B′	4.20	3.78	3.61	3.45	3.31	3.18	3.10	3.04

3. 3. Thermal properties

Using the Vashchenko-Zubarev expression at zero pressure for the Grüneisen parameter $\gamma_{v\text{-}z}$, our obtained value of $\gamma_{v\text{-}z}$ for the CdO compound was found at around 1.27, which is lower than the theoretical one (1.79) reported by Sahoo *et al.*[1], and slightly higher than the theoretical result (1.042) reported by Bhardwaj [27]. Our value of $\gamma_{v\text{-}z}$ for CdO material is also slightly higher than the value (1.20) reported for the calcium oxide compound [17] obtained from MacDonald's approach. Fig. **3** depicts the Grüneisen parameter $\gamma_{v\text{-}z}$ variation versus pressure p for the CdO compound, along with the results reported for the

calcium oxide (CaO) compound [17]. As appears in Fig **3**, the Grüneisen parameter γ decreases gradually with pressure p for CdO material.

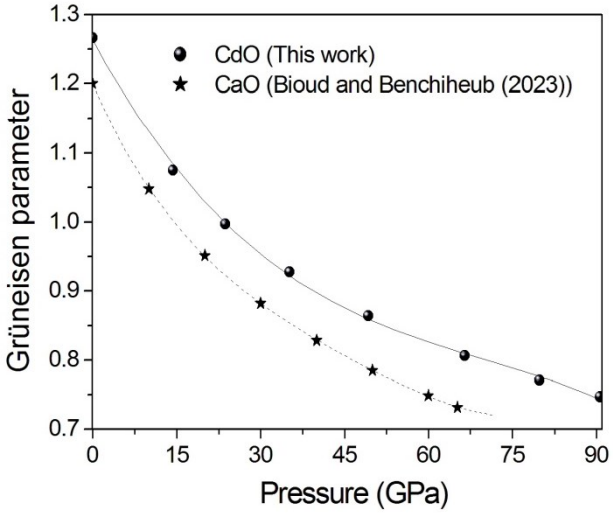

Figure 3. Grüneisen parameter $\gamma_{v\text{-}z}$ versus pressure p for CdO compound, along with the results reported for CaO compound [17]

The best fit of our data on the Grüneisen parameter $\gamma_{v\text{-}z}$ as a function of pressure obeys the following expression: $\gamma_{v\text{-}z} = 1.262 - 1.50 \times 10^{-2} p + 1.78 \times 10^{-4} p^2 - 0.84 \times 10^{-6} p^3$, where $\gamma_{v\text{-}z}$ is dimensionless and p is expressed in GPa. Similar qualitative behavior of γ versus pressure has been reported for calcium oxide (CaO) compound [17], for bulk and nano ZnO materials [18], and for cubic rock-salt calcium-based chalcogenides materials [19].

The Debye temperature θ_D is a critical thermodynamic quantity, which is employed for delineating high-temperature regions from low-temperature regions in solids [17]. The Debye temperature calculated from elastic constants at low temperature is near to that obtained from specific heat measurements [28]. Several expressions and formulas have been used to determine the Debye temperature θ_D of crystals [17, 28]. One of these formulas is a function of pressure, and is given as follows [16, 17, 29]:

$$\theta_D \approx \theta_D(0)(\rho/\rho_0)^{\gamma} \tag{4}$$

where ρ is the mass density, γ is the Grüneisen parameter, and $\theta_D(0)$ and ρ_0 are the normal conditions of the Debye temperature and the mass density, respectively.

It is seen from the literature that the previous formula is remarkably successful in giving the pressure dependence of the Debye temperature θ_D for semiconducting and ionic materials [16, 17]. Using the experimental value θ_{D0} = 255 K reported in Refs. [2, 30], our

obtained values of θ_D for CdO are illustrated in Fig.**4**, along with other theoretical data [4, 31, 32]. The Debye temperature of CdO increases monotonously and non-linearly with increasing pressure from 0 to 90 GPa. The pressure dependence of θ_D is represented by a quadratic equation as follows: $\theta_D = 257.48 + 1.42p - 7.72 \times 10^{-3}p^2$, where θ_D is expressed in K and p is in GPa.

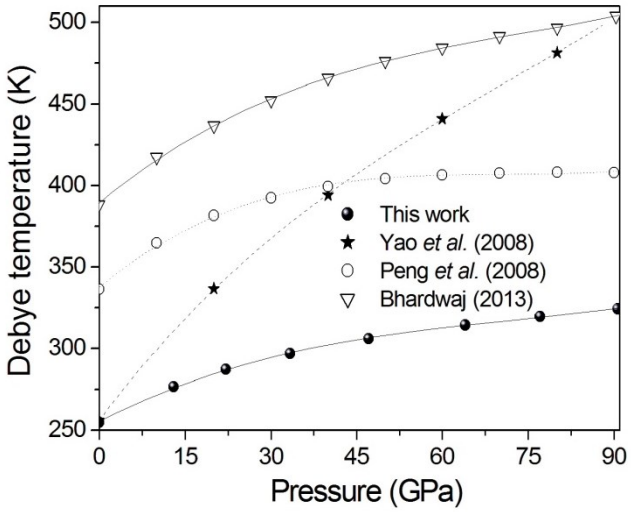

Figure 4. Debye temperature θ_D of CdO compound versus pressure up to 90.6 GPa, along with other theoretical data [4, 31, 32]

We note that the same behavior of the Debye temperature θ_D against pressure was reported for a wide range of materials such as for CaO up to 65.2 GPa in the theoretical work of Bioud and Benchiheub [17], for Na_2He in cubic fluorite-type (CaF_2) structure [33], for MgO and SrO compounds [34], for boron-arsenide (BAs) [35], and for boron antimonide compound [36].

Another way to present the obtained data on θ_D is by utilizing the normalized Debye temperature $\Delta\theta_D/\theta_{D0} = (\theta_D(p) - \theta_D(0))/\theta_D(0)$ curves; the results obtained for the CdO are presented in Fig. **5**. We can see that the effect of high pressure on the magnitude of $\Delta\theta_D/\theta_{D0}$ evaluated from this model is the same and agree quite well with those reported in the works of Peng *et al.*[4] using the Plane Wave PseudoPotential (PW-PP) method, and Bhardwaj [32] using the Three-Body Potential (TBP) model, which in turn demonstrates the soundness of the present semi-empirical approach.

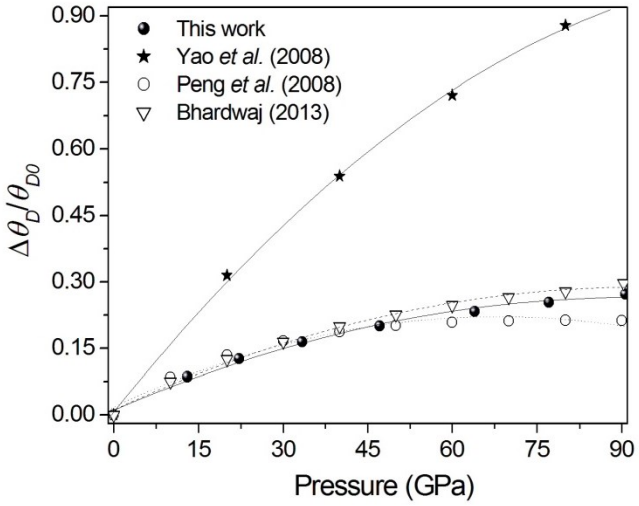

Figure 5. Normalized Debye temperature $\Delta\theta_D/\theta_{D0}$ of CdO compound versus pressure up to 90.6 GPa, along with other theoretical data [4, 31, 32]

The melting temperature T_m is correlated with the structural parameters, and it is frequently determined from the elastic constants [37]. We determined the variation of the melting temperature T_m of the CdO compound under compression using the following equation [38]:

$$T_m = T_m^0\left[1+2\left(\gamma-\frac{1}{3}\right)\frac{\Delta V}{V_0}\right] \tag{5}$$

where $\Delta V/V_0$ is the isothermal dilatation, $\Delta V/V_0 > 0$, $T_m{}^0$ is the normal conditions melting point.

The normal conditions melting point's $T_m{}^0$ of several solids crystallized in a cubic structure depends on the bulk modulus B by this empirical formula: $T_m{}^0 = 9.3B_0 + 607$ [39], where $T_m{}^0$ is expressed in K, while B_0 is in GPa. By substituting the experimental value (147 GPa) [3] of B_0 into this equation, the value of $T_m{}^0$ for CdO was found to be 1974.1 K. It is important to note that the Ref. [7] has mentioned that the value of $T_m{}^0$ for CdO compound is > 1773 K.

Using the value $T_m{}^0$ = 1700 K mentioned in Ref. [2], the obtained values of the melting temperature T_m for CdO compound are illustrated in Fig. **6**. As we can see, the T_m of CdO increases monotonously and non-linearly with increasing pressure from 0 to 90.6 GPa. Similar qualitative behavior of T_m versus pressure has been reported for Na_2He binary compound in cubic fluorite-type (CaF_2) structure [33], for Gabbro up to 0.6 GPa [40], for several metals [41], for CdO semiconductor [42] using Gilvarry approach, for periclase

(MgO) up to 150 GPa [43], and for calcium oxide compound [44]. To our knowledge, this is the first theoretical prediction of the melting point T_m under compression for CdO material and still awaits experimental confirmations.

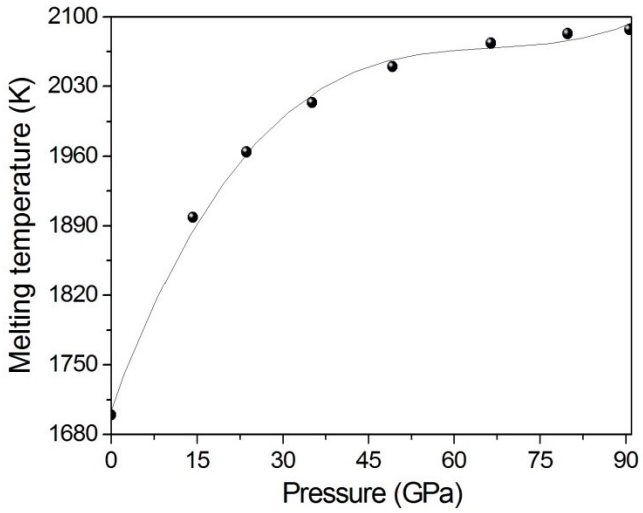

Figure 6. Melting temperature of CdO semiconductor versus pressure up to 90.6 GPa

Fracture toughness K_{IC} plays a pivotal role in the design and selection of materials [45-47]. This parameter is one of the most important mechanical properties of materials; it reflects the resistance of a material against crack propagation [47]. Experimentally, K_{IC} values could be determined from crack length measurements near Vickers indentations for example [48]. The fracture toughness K_{IC} of CdO has been calculated using the following empirical model: $K_{IC} = V_0^{1/6}(B/G)^{1/2}G$ [16, 45-47], where V_0 is the atomic volume (given in m^3), B is the bulk modulus, and G is the shear modulus (both B and G are given in MPa). The substitution of the theoretical values of B = 130.8 GPa and G = 49.43 GPa [32] into the last equation gives K_{IC} = 1.23 MPa.$m^{1/2}$. Since there is a correlation between the fracture toughness K_{IC} and the hardness H in several covalent and ionic materials [16, 17, 45-47], it is remarkable that the value (1.23 MPa.$m^{1/2}$) of K_{IC} for CdO (H = 6.58 GPa) is higher than the theoretical value 0.77 MPa.$m^{1/2}$ reported for the GaSb (H = 4.68 GPa) [16]. In the other hand, it is lower than the theoretical value of 1.46 MPa.$m^{1/2}$ reported for CaO (H =14.8 GPa) [17], the value 1.39 MPa.$m^{1/2}$ reported for the scandium phosphide (ScP) semiconducting compound (H =12.9 GPa) [44], and the value 1.33 MPa.$m^{1/2}$ reported for the Silicium (H = 11.7 GPa) [47]. Generally, the compounds with covalent bonding exhibit a relatively high hardness [48]. It is important to note that both the hardness H and the fracture toughness K_{IC} values exhibit strong load dependence as shown in boron phosphides superhard materials [49].

For some covalent tetragonal materials, Ericson *et al.* [50] established a simple expression between the fracture surface energy Γ_{IC} and the fracture toughness K_{IC}, given as follows: $\Gamma_{IC} = (1/2)K_{IC}^2(1- \nu^2)/E$ [16, 50], where ν is the Poisson's ratio and E is the linear elasticity modulus (Young's modulus). The values of ν are in the range -1 and 0.5 [51]. The critical value of ν for covalent bonding is about 0.1, for ionic crystals is 0.25 [52], for elastomeric polymers are ~ 0.5, for metals 0.25–0.35, and for cork is near zero [53].

For ideally brittle fracture, Γ_{IC} is equal to the reversible surface energy γ [50]. Although the CdO compound is an ionic octahedral material, we evaluate approximately its fracture surface energy Γ_{IC}. Replacing the theoretical values of $\nu = 0.332$ and $E = 131.7$ GPa [32] into the previous formula, the fracture surface energy Γ_{IC} of the CdO compound (H= 6.58 GPa) has been estimated at around 5.14 J.m^{-2}, which is Higher than the value 3.23 J·m^{-2} reported for GaSb (H = 4.68 GPa) [16].

4. Conclusions

We determined the effect of high-pressure on the structural parameters, mechanical properties, and some other thermal properties for CdO compound. Consequently, several analytical expressions have been established.

The parameters reflect the rigidity of CdO compound increases gradually with increasing pressure, while both the pressure derivative of the bulk modulus and the Grüneisen parameter decreased by raising the pressure. In comparison with other previous works, similar qualitative behaviors versus pressure have been also reported for several materials in different structures.

Due to the absence of the experimental and theoretical values of the microhardness for CdO compound at high pressures, the achieved results are a theoretical predictions and still waiting for confirmation using experimental techniques or other theoretical approaches.

Here, we report on the melting curve of CdO material up to 90.6 GPa as obtained by using a *Kraut–Kennedy's* approach. The present results can be used as reference data for future high-pressure experiments and theoretical works.

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