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Lattice properties, elastic parameters and microhardness of CdTe under hydrostatic compression

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ABSTRACT

Lattice properties and elastic parameters of zinc-blende CdTe are determined from a pseudopotential approach. The pressure dependence of the studied properties is examined and discussed. At zero pressure, the accord between our findings and those of the literature is found to be reasonable. Upon compression, all features of interest have shown a monotonic behavior. A larger cleavage energy in CdTe on (110) plane has been predicted when pressure is applied. Moreover, it is found that CdTe becomes more resistant to the transverse deformations and behaves in a brittle manner at all pressures being considered here. Besides, our results show that the hardness becomes better under compression reducing thus the damaging effect on the dislocations operational performance and degradation behavior induced during the devices fabrication.

1. Introduction

Cadmium telluride (CdTe) is a crystalline direct band-gap semiconductor compound which belongs to the II-VI semiconductor family. It is essentially used in CdTe photovoltaics and as an infrared optical material for optical windows and lenses [1]. It can also be formed in both n-type and p-type conductivity and it is usually sandwiched with CdS in order to form a p-n junction solar photovoltaic cell [2]. Besides, when alloyed with Hg or Zn, CdTe makes HgCdTe which can be used as infrared detector material [3] and CdZnTe that is an excellent solid-state x-and gamma-rays detector [4,5]. In addition, the material of interest was reported to provide good optical performance in a wide range of temperatures and has proven to have adequate mechanical robustness that makes it a good candidate for a use as substrate material [6,7]. Consequently, the properties of CdTe have been intensively studied.

Several investigations have been reported on the fundamental properties of CdTe [8–11], however, a full comprehension of these properties has not been completed yet and still remains a subject of discussion. This has inspired us to investigate the elastic constants and their related properties of CdTe under hydrostatic compression. The aim of this work is to show the effect of hydrostatic pressure on the studied properties, i.e. how these properties behave when hydrostatic pressure is applied on CdTe. As a matter of fact, when pressure is applied on a given material its inter-atomic distances are varied and a change of the fundamental properties of the material under load appears. The rapid development of the diamond anvil cell techniques including x-ray and neutron diffraction and the reliable computational methods for electronic structure calculation makes it possible to realize a wide range of measurements and to run a vast range of programs so as to study the properties of several materials under hydrostatic compression [12–17]. At zero pressure, CdTe crystallizes in the zinc-blende structure and undergoes a first transition pressure to cinnabar phase at pressure of 35.3 kbar as reported in Ref. [18] or at pressure of about 35–41 kbar as recently reported by Brik et al. [10]. In the present contribution the pressure is varied up to 30 kbar and the calculations are performed using a pseudopotential approach where more details are given in section 2 of this paper.

2. Computational details

The present calculations are performed using a pseudopotential approach that is based essentially on the empirical pseudopotential method (EPM). For more details about this method we refer the reader to the books by Cohen and Chelikowsky [19] and by Martin [20]. The major virtue of the pseudopotential approach is that we

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consider only the valence electrons. In the EPM, the potential is a Fourier expanded in plane waves. As a matter of fact, the pseudopotential in momentum space is given by,

$$V(G) = \sum_{\alpha} S_{\alpha}(G) \; V_{\alpha}(G) \tag{1}$$

where $S_{\alpha}(G)$ is the structure factor. G is the reciprocal lattice vector and $V_{\alpha}(G)'s$ are the atomic form factors of the atom α.

For semiconducting compounds $A^{N}B^{8\text{-}N}$ with zinc-blende structure, the expression (1) becomes,

$$V(G) = V^{S}(G)\cos(G\tau) + iV^{A}(G)\sin(G\tau) \tag{2}$$

τ in Eq. (2) is $\tau = \frac{1}{8}(1, 1, 1)$ in units of the lattice constant. $V^{S}(G)$ and $V^{A}(G)$ are the symmetric and antisymmetric form factors, respectively. These symmetric and antisymmetric form factors are the sums and differences of the form factors for the atoms in the primitive cell. Given the fact that the potential is spherically symmetric, we take $V(|G|)$. Usually three $V_{\alpha}(G)'s$ are sufficient for each element comprising a zinc-blende structure.

The Fourier coefficients for a given crystal are determined empirically by fitting the calculated band-gap energies at some selected high-symmetry points in the Brillouin zone to available experimental or known data reported in the literature. Note there, that these coefficients summarizes many of the microscopic electrostatic properties of the crystal. The electronic structure data is specifically used in the fitting procedure rather than available mechanical structural data because the elastic constants and their related mechanical properties calculated in this work depends strongly on the pseudopotential form factors which of course are obtained by a direct fit to the experimental and known data band structures. In this work, the experimental and known data regarding the band-gap energies for zinc-blende CdTe at Γ, X and L high-symmetry points in the Brillouin zone at zero pressure used in the fit are listed in Table 1. The empirical pseudopotential parameters are determined by using the non-linear least-squares method, in which we optimize all the parameters simultaneously. More details about the method are described in Refs. [23–25]. In fact we start first by choosing $V_{\alpha}(G)'s$ for the involved elements. Then, the structure is included via $S(G)$, and we solve the Schrödinger equation for the energy eigenvalues and wavefunctions. We compare our results with experiment (or known data if the experiment is not available), and we alter the $V_{\alpha}(G)'s$ if good accord with experiment is not achieved. The process is repeated until we get satisfactory accord with experiment. 136 plane waves have been considered in the present calculations so as to achieve convergence. Excellent agreement between our results and experiment and known data in the literature is achieved for the direct (Γ-Γ) and indirect (Γ-X) and (Γ-L) band-gaps showing thus the goodness of the fitted potentials.

Upon hydrostatic compression, the pseudopotential form factors have been obtained by fitting the first-order pressure coefficients of energy band-gaps at Γ, X and L high-symmetry points in the Brillouin zone to those quoted in Ref. [26]. The lattice parameter is calculated using the Murnaghan equation of state. The equilibrium bulk modulus (B_0) is taken to be 4.24×10^{11} dyn/cm^2 [18], whereas the first pressure derivative of B_0 (B_0') is taken to be 6.4 [18]. In Table 2 are shown the final adjusted pseudopotential form factors of CdTe at different pressures up to 30 kbar.

Table 1
Band-gap energies for zinc-blende CdTe fixed in the fits at zero pressure.

$E_{\Gamma\text{-}\Gamma}$ (eV)	$E_{\Gamma\text{-}X}$ (eV)	$E_{\Gamma\text{-}L}$ (eV)
1.5045[a]	3.48[b]	2.47[b]

[a] Experimental value reported in Ref. [21].
[b] Theoretical values reported in Ref. [22].

3. Results and discussion

At zero pressure the stable structure of CdTe crystal is zinc-blende. This has been reported experimentally and confirmed by several theoretical studies [18]. The pressure dependence of the lattice parameter for zinc-blende CdTe is illustrated in Fig. 1. We observe that when the hydrostatic pressure is increased from 0 to 30 kbar, the lattice parameter of zinc-blende CdTe is reduced from 12.25 to 11.21 atomic units. As a matter of fact, when pressure is increased more cloud overlap of electrons appears leading to an increase of the amount of charges which migrate from Cd to Te. This reduces the bond length and thus decreases the lattice parameter.

The bond distance in the zinc-blende structure of binary semiconductor compounds $A^{N}B^{8\text{-}N}$ differs significantly in the structure from those of wurtzite structures. There is only one type of first-neighbor distance for the zinc-blende structures which can be expressed as [18],

$$d(A-B)) = \frac{\sqrt{3}}{4} a \; (\mathit{four\ bonds}) \tag{3}$$

In the present work, the near-neighbour distance in zinc-blende CdTe has been calculated at various pressures ranging from 0 to 30 kbar using Eq. (3). The variation in the near-neighbour distance as a function of pressure in CdTe is shown in Fig. 2. Note that as pressure is increased on proceeding from 0 to 30 kbar, the near-neighbour distance decreases from 2.81 to 2.57 Å. The behaviour seems to be monotonic and non-linear. The bond-length and hence the bond strength have an effect on the cleavage energies for the experimentally observed cleavage planes. It has been reported by Berding et al. [27] who calculated the cleavage energies for GaAs and CdTe for the experimentally observed cleavage on (110) plane that both the shorter bond-length and the larger bond-strength of GaAs as compared with CdTe result in a larger cleavage energy in GaAs. Accordingly, one may conclude that upon compression, the weaker CdTe bond-length compared with that at zero pressure predict a larger cleavage energy in CdTe on (110) plane than that at zero pressure.

The elastic constants and their related properties of semiconductors are important parameters that provide useful information about the elasticity and mechanical stability [28–30]. In cubic crystals such as the case here, the number of independent stiffness constants is only three, namely C_{11}, C_{12} and C_{44}. Using a similar approach to that of Bouarissa [31], C_{11}, C_{12} have been obtained in the present work for CdTe in the zinc-blende structure. On the other hand, the use of the model of the valence force field [32] has allowed us to determine C_{44}. Our findings regarding C_{ij}'s for CdTe at zero pressure are given in Table 3. Also shown for comparison are the available experimental and previous theoretical

Table 2
Pseudopotential form factors for zinc-blende CdTe at various pressures up to 30 kbar.

Pressure (kbar)	Form factors (Ry)					
	$V_S(3)$	$V_S(8)$	$V_S(11)$	$V_A(3)$	$V_A(4)$	$V_A(11)$
0	−0.396388	0.198275	0.459548	0.1311	0.28	0.708145
5	−0.396388	0.196840	0.463735	0.1311	0.28	0.709870
10	−0.396388	0.196538	0.467002	0.1311	0.28	0.711524
15	−0.396388	0.196773	0.469829	0.1311	0.28	0.713181
20	−0.396388	0.197330	0.472401	0.1311	0.28	0.714861
25	−0.396388	0.198098	0.474800	0.1311	0.28	0.716564
30	−0.396388	0.199018	0.477076	0.1311	0.28	0.718290

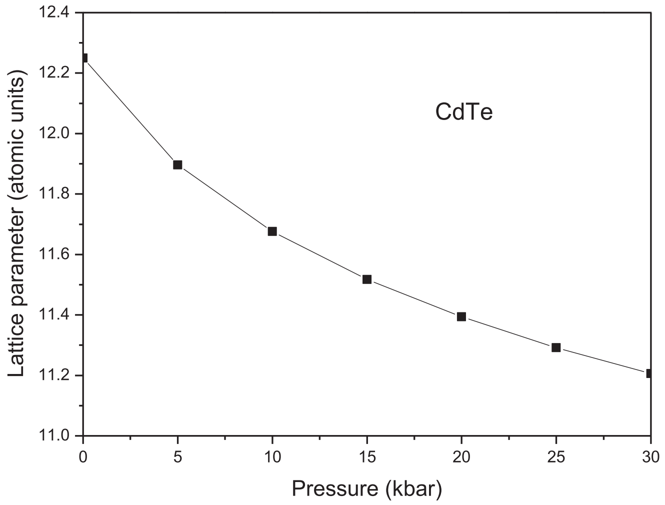

Fig. 1. Lattice parameter versus pressure in CdTe.

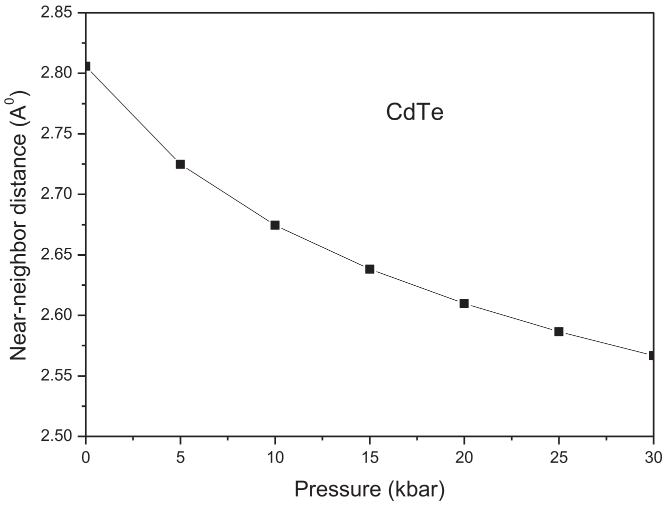

Fig. 2. Near-neighbor distance versus pressure in CdTe.

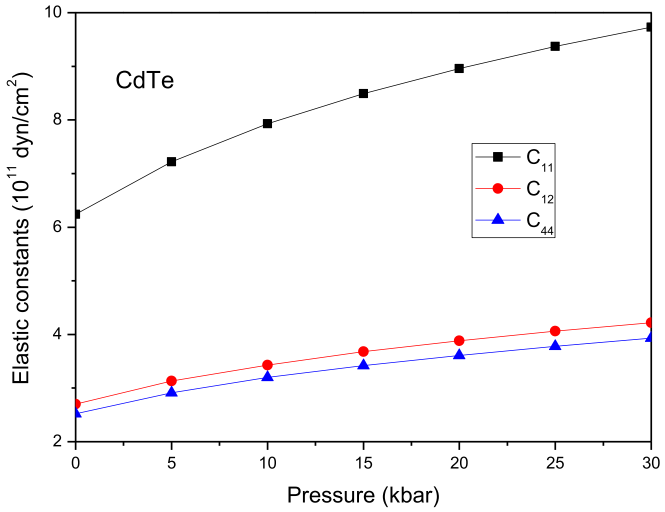

Fig. 3. Elastic constants versus pressure in CdTe.

Table 3
Elastic constants (C_{ij}) (in 10^{11} dyn/cm^2) of zinc-blende CdTe at zero pressure.

Elastic constants	This work	Expt. [18]	Theor. [8]
C_{11}	6.24	5.35	6.81
C_{12}	2.70	3.69	3.93
C_{44}	2.52	2.02	2.21

data quoted in Refs. [8,18]. The agreement between our results and those reported in Refs. [8,18] seems to be reasonable. Fig. 3 The shows the variation in C_{ij}'s as a function of pressure up to 30 kbar for zinc-blende CdTe. Note that when pressure is increased from 0 to 30 kbar, the values of all C_{ij}'s increase gradually. The behaviour of all C_{ij}'s versus pressure is monotonic. Nevertheless, the rate of change with pressure in C_{11} seems to be more important than those of C_{12} and C_{44}. This is generally consistent with the pressure behaviour of C_{ij}'s reported for tetrahedral compound semiconductors [33–35]. The knowledge of C_{ij}'s has allowed the check of the mechanical stability of CdTe in the pressure range 0–30 kbar using the generalized elastic stability criteria [35],

$$K = \frac{1}{3}(C_{11} + 2C_{12} + P) > 0 \tag{4}$$

$$G = \frac{1}{2}(C_{11} - C_{12} - 2P) > 0 \tag{5}$$

$$G' = (C_{44} - P) > 0 \tag{6}$$

According to our results, all these criteria are satisfied for all pressures of interest. This suggests that CdTe is mechanically stable for all pressures in the range 0–30 kbar.

The elastic anisotropy is the mechanical property of being directionally dependent. The anisotropy factor (A) is a useful mechanical parameter that is related to the elastic constants in cubic crystals as [36],

$$A = \frac{C_{11} - C_{12}}{2C_{44}} \tag{7}$$

Using Eq. (7), A has been calculated for zinc-blende at various pressures up to 30 kbar. At zero pressure, our calculation yielded a value of $A \approx 0.70$. As a matter of fact, an isotropic semiconductor material must have $A = 1$. Hence, the degree of elastic anisotropy depends on the deviation of A from 1. Accordingly, the material of interest is characterized by a shear anisotropy at zero pressure. Upon hydrostatic compression up to 30 kbar, the variation of A is found to be very weak (negligible). This suggests that the degree of anisotropy in the material in question remains almost the same when pressure is applied.

The response of the semiconductor material to the shear stress is described by what is called the shear modulus and referred to as C' in the present paper. The latter can be obtained from the knowledge of elastic constants C_{11} and C_{12} using the following relation [36],

$$C' = \frac{(C_{11} - C_{12})}{2} \tag{8}$$

The calculated C' at zero pressure that is obtained using Eq. (8) for zinc-blende CdTe is found to be 1.77×10^{11} dyn/cm^2. The variation of C' versus hydrostatic pressure up to 30 kbar is plotted in Fig. 4. Note that C' increases monotonically with raising pressure from 0 to 30 kbar. This indicates that upon compression CdTe becomes more resistant to the transverse deformations.

The effect of mechanical stresses that results from device

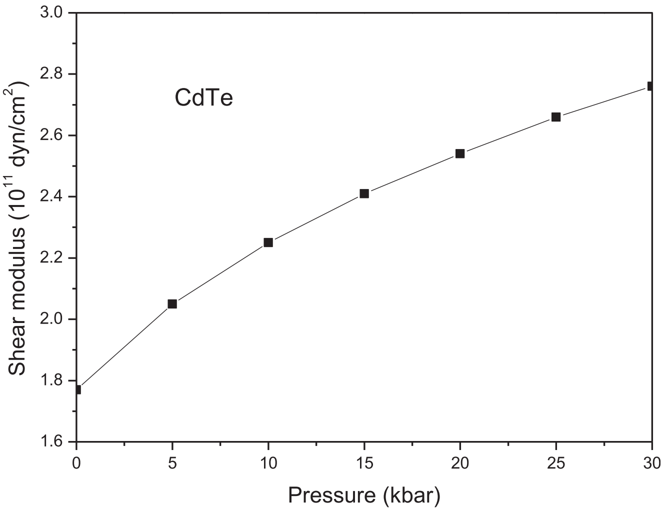

Fig. 4. Shear modulus versus pressure in CdTe.

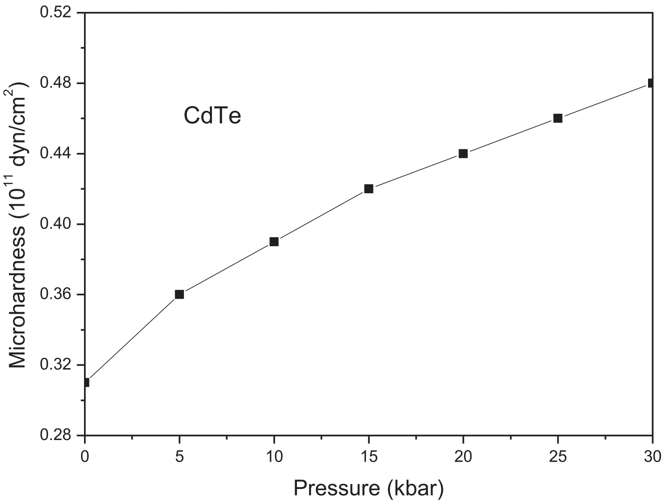

Fig. 5. Microhardness versus pressure in CdTe.

processing and crystal growth on the reliability and behaviour of semiconductor devices has received a considerable importance [18]. Thus, an accurate knowledge of such stresses needs knowledge of the Poisson ratio (σ_0). The latter for a tetragonal distortion of a cubic layer grown on a (001) substrate is given by Ref. [36],

$$\sigma_0 = \frac{C_{12}}{C_{12} + C_{11}} \tag{9}$$

Our results at zero pressure yielded an σ_0 of 0.30 for zinc-blende CdTe. The Poisson ratio has been used by Frantsevich et al. [37] in order to distinguish between the ductile and brittle nature of materials. The rule used by Frantsevich et al. [37] consists in separating the ductile and brittle nature of materials in such a way that the value of 0.33 represents the critical limit value between ductile and brittle. If the value of σ_0 is less than 0.33, the material of interest is considered to behave in a brittle manner. However, if σ_0 is larger than 0.33, the material in question behaves in a ductile manner. Following the rule of Frantsevich et al., one can conclude that at zero pressure the material of interest behaves in a brittle manner. The pressure dependence of σ_0 up to 30 kbar showed that σ_0 remains almost constant. This suggests that zinc-blende CdTe still behaves in a brittle manner under hydrostatic pressure up to 30 kbar.

The hardness test has been used to characterize the mechanical behavior of materials for a long time [38]. The interest in the hardness of semiconductors stems essentially from their use in several device applications [38,39]. Many methods have been used so as to measure the microhardness (H) of semiconductor materials. Nevertheless, Knoop and Vickers indentations are reported to be the most commonly used [18]. The Knoop microhardness has been calculated in this work using the relation [18],

$$H = 0.139\ G_V \tag{10}$$

G_V in Eq. (10) is the Voigt averaged shear modulus which is expressed as [18],

$$G_V = \left(\frac{3C_{44} + C_{11} - C_{12}}{5}\right) \tag{11}$$

Our findings at zero pressure regarding H yielded a value of 0.31×10^{11} dyn/cm^2 for zinc-blende CdTe. The variation in H as a function of pressure up to 30 kbar is plotted in Fig. 5. We observe that H increases gradually with increasing pressure up to 30 kbar. The behaviour seems to be monotonic. This indicates that upon compression the hardness of CdTe semiconductor compound becomes better reducing thus the damaging effect on the dislocations operational performance and degradation behaviour induced during the devices fabrication.

4. Conclusion

In summary, based on a pseudopotential approach, the effect of hydrostatic pressure on lattice parameters and elastic properties in zinc-blende CdTe was investigated. At zero pressure, our results were found to be in reasonable accord with the available experimental and previous theoretical data reported in the literature. The variation in the studied physical quantities as a function of pressure in the range 0—30 kbar was found to be monotonic. As expected, the lattice parameter was found to decrease with raising pressure exhibiting a non-linear behavior. The variation in near-neighbor distance versus pressure showed that the CdTe bond-length becomes weaker compared with that at zero pressure predicting thus a larger cleavage energy in CdTe on (110) plane under pressure. The mechanical stability of CdTe was checked in terms of the elastic constants and pressure showing that CdTe is mechanically stable at all pressures of interest. The anisotropy factor was found to be almost independent of pressure. The trend in the shear modulus showed that CdTe becomes more resistant to the transverse deformation. Based on the Poisson ratio, we predicted that CdTe behaves in a brittle manner for all pressures of interest. Upon hydrostatic compression, the hardness was found to become better which improves the quality of the devices fabrication.

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