High-pressure effect on elastic properties, mechanical stability and microhardness of ZnTe

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Based on a pseudopotential approach, the high-pressure dependence of the elastic properties and microhardness of ZnTe has been investigated. Our results are generally accordant with the available experimental data. Most features of interest are found to vary monotonously with raising pressure. The material in question is found to be mechanically stable for all pressures in the interval 0-80 kbar. Its resistance to deflections or deformations, rigidity, and hardness is augmented upon compression. The calculated Poisson ratio at various pressures implies the brittle manner behavior of ZnTe.

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1. Introduction

II-VI semiconducting materials have demonstrated important properties for technological applications. These include light-emitting diodes, photodetectors, laser diodes, solar cells and magneto-optical devices, to name a few. Information on these materials of interest is continually being reported and consequently a considerable quantity of basic data is actually existing and novel applications are still being proposed [1-9]. The II-VI compound semiconductors crystallize generally either in the zinc-blende structure or the wurtzite structure. In the zinc-blende structure those tetrahedra are arranged in a cubic array. Among II-VI binary compounds, ZnTe is a wide-band-gap which crystallizes in the cubic, zinc-blende structure. It is usually a p-type semiconductor. It is convenient for many technological applications and is one of the more common semiconductors used in optoelectronics [10-13]. It can also be used for solar cells [14].

The investigation of semiconducting materials under high pressure is an extremely useful subject. This is essentially due to the advancements in both theoretical and experimental developments [15-22]. As a matter of fact, a wide range of experimental measurements have been performed at high pressure using the diamond anvil cells. On the theoretical side, the development of algorithms and the quif. ck increase in computers power have made a great impact on high pressure physics. When subjected to high-pressure, the matter undergoes changes in its physical, chemical, and structural characteristics. Several crystalline substances transforms under high-pressure leading thus to a new crystalline forms. As far as ZnTe is concerned, it has been reported that the material in question transforms from the cubic B3 structure to a cinnabar (B9) structure when subjected to high-pressure of 90 kbar [23].

Among fundamental properties of semiconducting materials, the elastic constants and their related mechanical properties are very important in the study of the elasticity and mechanical stability of solid materials [24-27]. On the other hand, the knowledge of the microhardness is an important information for testing the hardness of semiconductors that can usually serve for the characterizing of their mechanical behavior [7]. For that, the present contribution deals with the elastic properties and microhardness of ZnTe at zero and under high-pressure. The aim of this work is to show how the elastic constants and their related mechanical properties including the microhardness behave when the material of interest is subjected to high pressure. The computations are carried out using a pseudopotential approach. Our findings are generally accordant with those available in the literature.

2. Computational details

The calculations in the present contribution are essentially based on the empirical pseudopotential method (EPM) [28,29], in which a certain number of parameters, called the pseudopotential form factors (PPFFs), are required in order to obtain the potential needed for the secular equation. This allows the determination of the energy levels and wavefunctions of electrons. In the EPM, the PPFFs at zero pressure are obtained by the fit of selected band-gap energies of ZnTe at high-symmetry points in the Brillouin zone to experiment. In the present work, the experimental direct (Γ-Γ) and indirect (Γ-X) and

(Γ-L) energy band gaps fixed in the fits for ZnTe at zero pressure are given in Table 1. The parameters of interest have been simultaneously optimized using the non-linear least-squares method as described in Refs. [32,33]. A 136 plane waves have been considered so as to achieve good convergence.

Table 1. Experimental band gap energies for ZnTe fixed in the fits. [a] Ref. [30]; [b] Ref. [31]

$E_{\Gamma-\Gamma}$ (eV)	$E_{\Gamma-X}$ (eV)	$E_{\Gamma-L}$ (eV)
2.263 [a]	3.05 [b]	2.38 [b]

At high-pressures, the first-order pressure coefficients of band-gap energies at Γ, X and L high-symmetry points in the Brillouin zone are fitted to those reported by Tsay et al. [34]. This has allowed the determination of the PPFFs for different pressures in the interval 0-80 kbar. The lattice parameter has been determined at various pressures using the Murnaghan equation of state. The equilibrium bulk modulus is taken to be 5.10×10^{11} dyn/cm^2 [7], whereas its first-pressure derivative is considered to be 4.7 [7]. Table 2 presents the final adjusted PPFFs as well as the calculated lattice parameters for ZnTe in the zinc-blende structure at some pressures in the range 0-80 kbar.

3. Results and discussion

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}. In the present investigation C_{11} and C_{12} for zinc-blende ZnTe have been calculated using the same approach as that described by Bouarissa [27], whereas C_{44} has been obtained from the use of the valence force field model [35]. Our findings regarding C_{11}, C_{12} and C_{44} elastic constants for ZnTe at zero pressure are listed in Table 3. Also shown for comparison are the experimental values reported in Ref. [39] and previous theoretical data published in Refs. [36-38]. Whereas our result concerning C_{11} seems to be larger than the one reported in Ref. [39], the deviations for C_{12} and C_{44} from those measured by Berlincourt et al. [39] are less than 4% and 28%, respectively. On the theoretical side, the authors results concerning C_{12} and C_{44} seem to agree generally with those of Ref. [36] obtained from full-potential augmented plane wave plus local orbitals within the local density approximation, those of Ref. [37] obtained from projector-augmented wave within the conventional generalized gradient approximation, and those of Ref. [38] obtained from full-potential linearized augmented plane wave within the generalized gradient approximation. Nevertheless, C_{11} obtained in this work appears to be overestimated with respect to those of Refs. [36-38].

Fig. 1 illustrates the evolution of the elastic constants C'_{ij}'s as a function of pressure in the interval 0-80 kbar for ZnTe binary semiconductor compound.

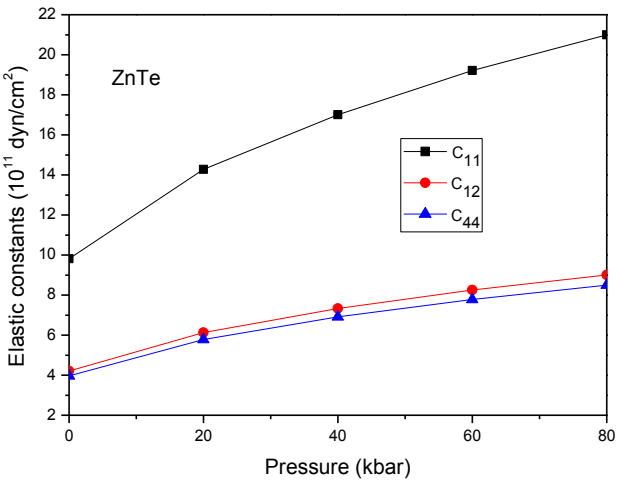

Fig. 1. Elastic constants versus pressure in ZnTe (color online)

Note that all C_{ij}'s increase monotonously with increasing pressure up to 80 kbar. Nevertheless, C_{11} is much higher in magnitude than C_{12} and C_{44}. Also, the rate of change in C_{11} with applied pressure is more important than those of C_{12} and C_{44}. The same trend of C_{ij}'s under compression has been reported for other semiconducting materials [40,41]. However, in their study of ZnTe under pressure, Varshney et al. [42] have reported an increase of C_{11} and C_{12} with increasing pressure, but a decrease of C_{44} with increasing pressure which does not agree with the behavior generally reported in the literature for C_{ij}'s in ZnTe under pressure. The increase of C_{11}, C_{12} and C_{44} under applied pressure indicates that ZnTe becomes more resistant to the applied compression/stretching and shear. The mechanical stability of the material under load can be checked via the C_{ij}'s and pressure using the generalized elastic stability criteria which are,

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

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

$$G' = C_{44} - P > 0 \quad (3)$$

using our obtained C_{ij}'s in the pressure interval 0-80 kbar, we find that all stability criteria are fulfilled suggesting that the zinc-blende ZnTe is mechanically stable for all pressures belonging to the range 0-80 kbar.

Based on the obtained C_{ij}'s, the bulk modulus (B) of zinc-blende ZnTe has been calculated using the following expression [43],

$$B = \frac{C_{11}+2C_{12}}{3} \quad (4)$$

At zero pressure, our obtained value is shown in Table 4. Other known data in the literature for B of ZnTe are also given for comparison. The accord between our result and that of Ref. [7] is within 19%, whereas the deviation

of our result from that of Ref. [37] seems to be larger. The variation of B as a function of pressure up to 80 kbar for ZnTe is displayed in Fig. 2. We observe that B increases from 6.08×10^{11} to 13×10^{11} dyn/cm^2 when pressure is increased from 0 to 80 kbar. The behaviour is monotonous and indicates that the stiffness of ZnTe becomes higher when the material in question is subjected to high-pressure.

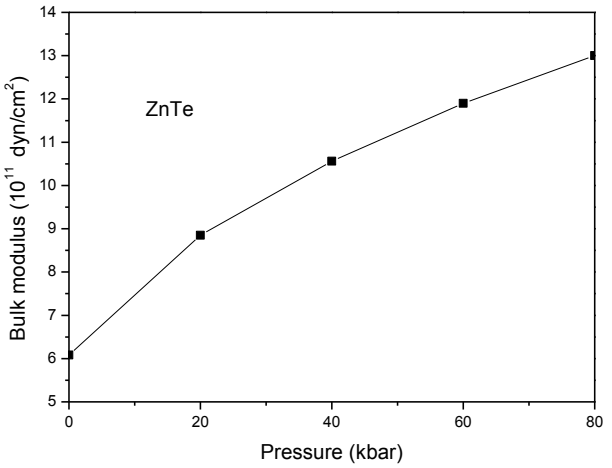

Fig. 2. Bulk modulus versus pressure in ZnTe

The knowledge of C_{ij}'s has also allowed the calculation of the shear modulus (C'). This has been done using the following relation [43],

$$C' = \frac{(C_{11}-C_{12})}{2} \quad (5)$$

At zero pressure, our obtained C' for ZnTe is shown in Table 4. Known data in the literature are also given for comparison. Our calculated C' seems to be overestimated with respect to that quoted by Adachi in Ref. [7]. This is due to the difference between our obtained C_{11} and that of Ref. [7]. The evolution of C' versus applied pressure is plotted in Fig. 3. Note that C' is increased monotonously when pressure is raised

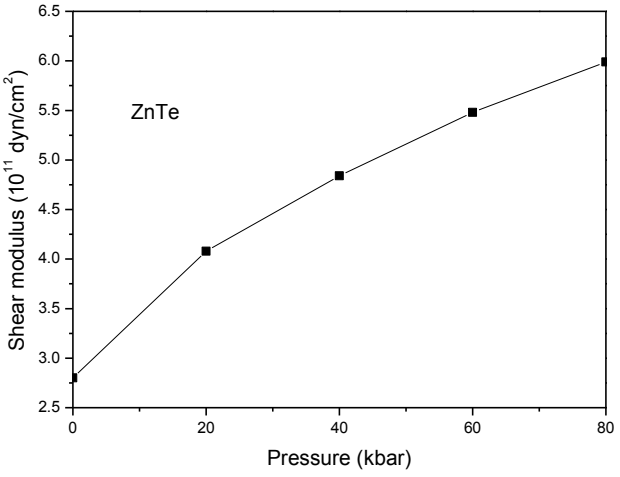

Fig. 3. Shear modulus versus pressure in ZnTe

In the interval 0-80 kbar. This indicates that the response of ZnTe to the shear stress augments with increasing pressure suggesting thus the augmentation of the rigidity of ZnTe under applied pressure.

Based on the calculated C_{ij}'s in this work, we have also proceeded to the calculation of the [100] Young's modulus (Y_0) using the expression [43],

$$Y_0 = \frac{(C_{11}+2C_{12})(C_{11}-C_{12})}{(C_{11}+C_{12})} \quad (6)$$

At zero pressure, our result is given in Table 4.

Table 2. Final adjusted pseudopotential form factors for ZnTe at various pressures up to 80 kbar

Pressure (kbar)	$V_S(3)$	$V_S(8)$	$V_S(11)$	$V_A(3)$	$V_A(4)$	$V_A(11)$	Lattice Constant (Å)
0	-0.247293	0.021262	0.255724	0.030061	0.116	0.290414	6.1037
20	-0.275102	0.021262	0.275883	0.030061	0.116	0.313968	5.6677
40	-0.286700	0.021262	0.285481	0.030061	0.116	0.322462	5.4704
60	-0.292938	0.021262	0.291598	0.030061	0.116	0.325940	5.3432
80	-0.296466	0.021262	0.295955	0.030061	0.116	0.326856	5.2498

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

Elastic constants	This work	Expt. [39]	Theor.
C_{11}	9.81	7.13	8.2 [36]; 5.136 [37]; 6.295 [38]
C_{12}	4.21	4.07	4.2 [36]; 3.671 [37]; 4.062 [38]
C_{44}	3.97	3.12	5.5 [36]; 3.865 [37]; 4.316 [38]

Table 4. Bulk modulus (B), shear modulus (C'), [100] Young's modulus (Y_0), Poisson ratio (σ_0) and microhardness (H) of zinc-blende ZnTe at zero pressure

Parameter	This work	Known
B (10^{11} dyn/cm^2)	6.08	5.10 [7]; 4.16 [37]
C' (10^{11} dyn/cm^2)	2.8	1.54 [7]
Y_0 (10^{11} dyn/cm^2)	7.28	6.442 [38]
σ_0	0.30	0.276 [38]
H (10^{11} dyn/cm^2)	0.49	0.6-0.9 [7]

Note that our obtained Y_0 for ZnTe is 7.28×10^{11} dyn/cm^2. This value accords to within 13% with that of 6.442×10^{11} dyn/cm^2 reported theoretically in Ref. [38]. The variation of Y_0 as a function of pressure for ZnTe semiconductor binary compound is shown in Fig. 4. Note that the increase of pressure from 0 to 80 kbar leads to the increase of Y_0 from 7.28×10^{11} to 15.58×10^{11} dyn/cm^2. The increase of Y_0 is monotonic. This indicates that when pressure is applied, ZnTe becomes more resistant to deflections or deformations.

Another important parameter to be studied is the Poisson ratio (σ_0) which is defined for a tetragonal distortion of a cubic layer grown on a (001) substrate as [44,45].

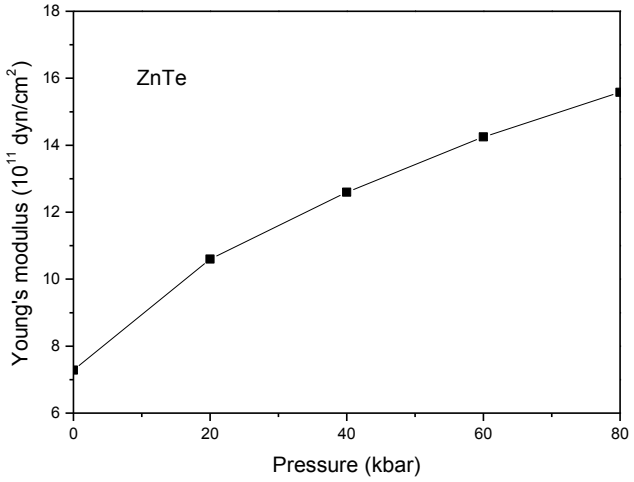

Fig. 4. [100] Young's modulus versus pressure in ZnTe

$$\sigma_0 = \frac{C_{12}}{C_{12}+C_{11}} \tag{7}$$

using Eq. (7), σ_0 has been determined for ZnTe at various pressures ranging from 0 up to 80 kbar. At zero pressure, our result is given in Table 4. From Table 4, one can note that our value of σ_0 for ZnTe is σ_0= 0.30. This value accords well with that of 0.276 reported in Ref. [38]. Frantsevich et al. [46] have used σ_0 so as to distinguish between the ductile and brittle nature of materials. According to their description, if σ_0 is less than 0.33, the material in question is considered to have a brittle nature. Nevertheless, if σ_0 is superior to 0.33, this material has a ductile nature. Based on the value of σ_0 obtained in our case at zero pressure and Frantsevich et al. criteria, one can conclude that ZnTe can be considered as a brittle. The pressure dependence of σ_0 shows that the latter remains almost constant (the effect of pressure on σ_0 in zinc-blende ZnTe is negligible). Accordingly, we suggest a pressure independent value of 0.30 for σ_0 of ZnTe material (i.e. for pressures up to 80 kbar, the material under load is still have a brittle nature).

In order to characterize the mechanical behaviour of materials, people generally are using a hardness test [47,48]. In this context, the microhardness (H) of semiconductors can be measured using different methods. The most commonly used are those of Knoop and Vickers indentations [7]. For that, in this work the Knoop microhardness has been calculated using the relation [7],

$$H = 0.139\, G_V \tag{8}$$

The parameter G_V in Eq. (8) represents the Voight averaged shear modulus. The latter is given by the expression [7],

$$G_V = \frac{(3C_{44}+C_{11}-C_{12})}{3} \tag{9}$$

At zero pressure, our calculated H for ZnTe is found to be 0.49×10^{11} dyn/cm^2 (see Table 4). This value accords to within 18% with that of 0.6 quoted by Adachi in Ref. [7]. The variation of H as a function of pressure up to 80 kbar is displayed in Fig. 5.

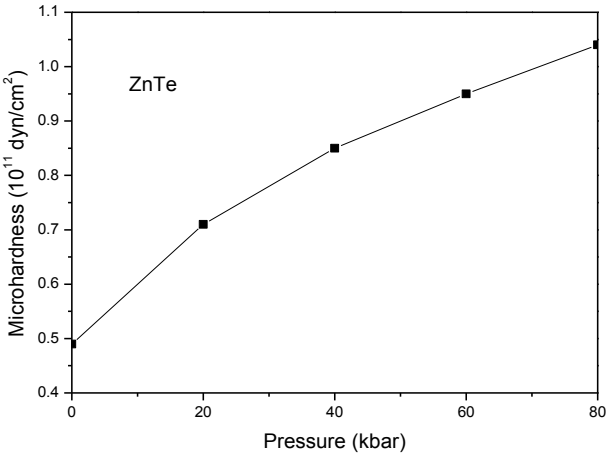

Fig. 5. Microhardness versus pressure in ZnTe.

We observe that H augments monotonously with increasing pressure in the interval 0-80 kbar. This indicates that the hardness of the material under load becomes better when the material is subjected to high-pressure. This can be beneficial for the fabrication of the devices based on the material of interest.

4. Conclusions

The effect of high-pressure up to 80 kbar on elastic constants and their related mechanical properties such as bulk modulus, shear modulus, [100] Young's modulus, Poisson ratio, and microhardness were studied for zinc-

blende ZnTe using a pseudopotential approach. At zero pressure, our findings were found to be generally in reasonable accord with those reported in the literature. The behavior of all physical quantities being studied here with pressure was found to be monotonic. All mechanical stability criteria were checked via the elastic constants and pressure and suggested that ZnTe semiconducting material is mechanically stable for all pressures belonging to the interval 0-80 kbar. Our results showed that upon compression ZnTe becomes more resistant to deflections or deformations, more rigid and its stiffness becomes higher. Moreover, its hardness becomes better. The obtained values of the Poisson ratio at various pressures up to 80 kbar indicated the brittle behavior of ZnTe in the pressure interval of 0-80 kbar.

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