



Structural and mechanical properties of ZnTe in the zincblende phase

C. Soykan ^{a,*}, S. Ozdemir Kart ^a, T. Cagin ^b

^a Department of Physics, Pamukkale University, Kınıklı Campus, 20017, Denizli, Turkey

^b Department of Chemical Engineering, Texas A&M University, TX 77845-312, USA

* Corresponding author: E-mail address: csoykan08@pau.edu.tr

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ABSTRACT

Purpose: The aim of this work investigate to the structural and mechanical properties of ZnTe in the B3 structure, using the ab initio method based on Density Functional Theory (DFT).

Design/methodology/approach: The Vienna ab initio Simulation Package (VASP) has been used to perform the electronic structure calculations. The projector-augmented wave formalism (PAW) implemented in this package leads to very accurate result comparable to other all-electron methods. The electronic exchange and correlation functions are treated within DFT by using generalized gradient approximation.

Findings: The lattice parameter, bulk modulus, it's pressure derivative and the elastic stiffness coefficients are calculated. Our results for the structural parameters and the elastic constants at the equilibrium phase are in good agreement with the available experimental and other theoretical studies. We have also investigated the pressure dependence of mechanical properties for ZnTe in the structure of B3 to see this effect.

Research limitations/implications: These compounds are convenient for many technological applications because of they have direct energy band gaps and property of light emitters at room temperature.

Practical implications: These compounds used to many technological applications, such as solid state laser devices, photovoltaic devices, solar cells, remote control systems, thin films, transistors, THz emitter, detector and imaging systems etc.

Originality/value: In this work, determination of structural and mechanical properties of ZnTe in the B3 structure at high pressures will lead to new technological applications of these materials.

Keywords: Density Functional Theory (DFT); Ab initio calculation; Lattice parameters; Elastic stiffness coefficients; Bulk modulus

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SHORT PAPER

1. Introduction

The Zinc Telluride is one of the prototype of II-VI semiconductor materials. In last years, this semiconductors have attracted a lot of attention, since they have direct energy band gaps and property of light emitters at room temperature. Besides, the more increase the power of the computers, the easier

computing of material properties, which are structural, electronic and optical of solids with a great accuracy.

These compounds are convenient for many technological applications, such as solid state laser devices, photovoltaic devices, solar cells, remote control systems, thin films, transistors, THz emitter, detector and imaging systems etc. Among the IIB-VIA semiconductors, the high pressure phases of ZnTe have attention due to its technological importance. It is well known that

when the pressure of 9.0 GPa is applied to cubic B3 structure [1], a phase transition from B3 structure to cinnabar (B9) structure take place, resulting in the change in the mechanical properties of material. The most common worth of mechanical properties can be made with the definition of its elastic constants. It is difficult task to get the accurate measurement of these quantities because of experimental conditions at high pressure. However, ab-initio quantum mechanical methods are quite suitable for the elastic properties at high pressure conditions. With the progresses in ab initio methods, it has become possible to compute many properties of materials. Hence, a large number of ab initio studies on the structural and mechanical properties of ZnX (X=O, S, Se, Te) have been carried out. Recently, Yu et al. [2] have investigated the elastic, dielectric and thermodynamic of properties of B3 structure of ZnTe using first-principles ground state and response-function calculations. Walter et al. [3] have studied band structure of ZnTe using pseudo-potential method. Sahraoui et al. [4] have computed the elastic stiffness coefficients and bulk modulus for ZnX under hydrostatic pressure by utilizing DFT within the generalized gradient approximation (GGA) for exchange-correlation energy.

The structural and mechanical properties of B3 structure of ZnTe are scarcity in literature. It is required that the physical properties of B3 structure should be determined in order to define the phase of B3 at high pressures.

The purpose of this work is to obtain structural and mechanical properties of the cubic Zincblende (B3) phase of ZnTe compound under different hydrostatic pressures, using the ab-initio method based on (DFT), within a generalized gradient approximation (GGA). The method of the calculation is given in Section 2. We present and discuss the simulation results for structural and mechanical properties of ZnTe in Section 3.

Finally, the conclusion is given in the last Section.

2. Method

The Vienna ab initio Simulation Package (VASP) [5-9] has been used to perform the electronic structure calculations. The projector-augmented wave formalism (PAW) implemented in this package [10] leads to very accurate result comparable to other all-electron methods. The electronic exchange and correlation functions are treated within DFT by using generalized gradient approximation (GGA) [11]. For total energy calculations in cubic B3 structure, shown in Figure 1, we have optimized the kinetic energy cutoff and mesh of k-points by carrying out self-consistent calculations. We have used a kinetic energy cutoff of 450 eV for the plane wave basis set and a Monkhorst-Pack grid of 12x12x12 for Brillouin-zone integrations.

The total energies and pressures calculated as a function of the primitive cell volume for ZnTe are used to define the structural properties, phase behavior, bulk modulus and its pressure derivative of ZnTe by fitting the data to a third order Birch–Murnaghan equation of states (EOS). In the 3rd-order Birch–Murnaghan EOS, the total energy and pressure a function of volume are given as [12]:

$$E(V) = E_0 + (9/16)V_0 B_0 \{[(V_0/V)^{2/3} - 1]^3 B'_0 + [(V_0/V)^{2/3} - 1]^2 [6 - 4(V_0/V)^{2/3}]\} \quad (1)$$

and

$$P(V) = (3/2)B_0[(V_0/V)^{7/3} - (V_0/V)^{5/3}] \{1 + (3/4)(B'_0 - 4)[(V_0/V)^{2/3} - 1]\} \quad (2)$$

respectively, where E_0 is the total energy, V_0 is the equilibrium volume, B_0 is the bulk modulus at zero pressure, and B' is the first derivative of the bulk modulus with respect to pressure.

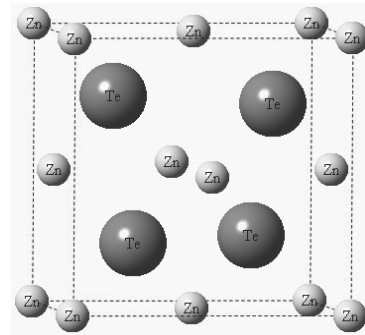


Fig. 1. Crystal structure of the Zincblende (B3) phase of ZnTe. The Zn and Te atoms are located at the origin and (1/4, 1/4, 1/4), respectively. Here, small sphere is Zn, large one is Te

The cubic crystals have just three independent elastic constants, called C_{11} , C_{12} and C_{44} , which have been calculated to find out the mechanical stability of ZnTe in the B3 crystal structures at different pressures. Thus, we need just a set of three equations to calculate these three constants, by applying three types of strain to the crystal structure. The EOS directly gives the behavior under isotropic-volumetric strain and it can be used to compute the bulk modulus B of the crystals. For a cubic crystal, the bulk modulus is defined as $B = (C_{11} + 2C_{12})/3$. Similarly, the relationship between C_{11} and C_{12} , called as tetragonal shear constant of $C_s = (C_{11} - C_{12})/2$, can be obtained by applying the following volume conserving tetragonal strain,

$$\varepsilon = \begin{pmatrix} \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \frac{-\delta^2 - 2\delta}{(1 + \delta)^2} \end{pmatrix} \quad (3)$$

where, δ is the deformation parameter. Hence the tetragonal shear constant is obtained from the deformation energy:

$$E(\delta) = E_0 + 6C_s V_0 \delta^2 + O(\delta^4) \quad (4)$$

where, E_0 is the energy of unstrained state, C_s is the tetragonal shear constant, V_0 is the zero strain volume and $O(\delta^4)$ is negligible term.

For determining the pure shear modulus, C_{44} , we have applied the following strain tensor given by

$$\varepsilon = \begin{pmatrix} 0 & \delta & 0 \\ \delta & 0 & 0 \\ 0 & 0 & \frac{\delta^2}{(1-\delta^2)} \end{pmatrix} \quad (5)$$

which gets the total energy as a function of strain for C_{44} as;

$$E(\delta) = E_0 + 2C_{44}V_0\delta^2 + O(\delta^4) \quad (6)$$

Finally, we have used the following isotropic strain tensor induced by hydrostatic stress for the bulk modulus at different pressures:

$$\varepsilon = \begin{pmatrix} \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta \end{pmatrix} \quad (7)$$

The above distortion yields the energy expression for bulk modulus as :

$$E(\delta) = E_0 + (9BV_0/2)\delta^2 + O(\delta^4) \quad (8)$$

3. Results and discussion

In phase of B3, the total energy of ZnTe in the phase of B3 is calculated for different volumes around the equilibrium volume V_0 . The variation of the total energy as a function of volume is given in Figure 2.

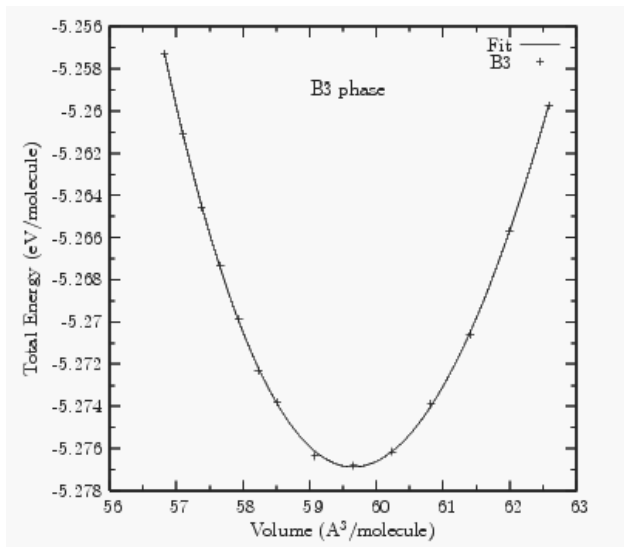


Fig. 2. Energy as a function of primitive cell volume for ZnTe

The data of the total energy versus the volume is fitted to a third-order Birch-Murnaghan EOS to obtain the ground state properties of the equilibrium lattice constant (a_0), bulk modulus (B_0) and pressure derivative of the bulk modulus (B'). These EOS parameter computed for different pressures, are listed in Table 1, along with the available experimental data [18] and previous theoretical calculations [1,2,17].

Table 1.

The hydrostatic pressure P (GPa), the lattice constant a (Å), the bulk modulus B (GPa) from EOS, its pressure derivative B' and the volume V (Å³) of B3 phase structure at different pressure. For comparison and completeness, we tabulated experimental values and results from previous calculations at zero pressure

	P	a	B	B'	V	[Ref.]
Our cal.	0	6.2026	42.00	4.89	59.66	
	3	6.0758			56.07	
	6	5.9790			53.44	
	9	5.9004			51.36	
	12	5.8540			49.64	
Other cal.		6.1580	47.70	4.70	58.39	[1]
		6.2260				[2]
	0	6.0000	55.21	4.60		[13]
		6.0270	55.67	4.90		[14]
		6.1169	51.20	4.18		[15]
		6.0630	50.54			[16]
		6.1700	45.25	4.26	58.73	[17]
Exp.		6.1026	50.50	5.00	56.82	[18]
		6.1010				[19]
	0	6.1030	50.90	5.04		[20]
		6.1037	51.0-52.8	5.04		[21]
		6.0890	52.80			[22]

The equilibrium lattice parameter (a_0) at zero pressure is computed as 6.2025 Å. The deviation from the experimental value of 6.1026 Å [1] is found as 1.6 %.

The bulk modulus at zero pressure and its pressure derivative are comparable with experiments [18] and other calculations [1].

Using the Birch-Murnaghan EOS of pressure definition (Eq. 2) for a selected value of the pressure corresponding volume, we first determine the lattice parameter for the reference structure describing this pressure. Then three different strain tensors given in Eqs. 3, 5, 7 are applied to this reference structure to obtain the pressure dependence of the bulk modulus and two shear module of C_s and C_{44} . We strained the lattice by varying δ from -0.03 to 0.03 in steps of 0.01 to obtain the total minimum energies at these strains. Total energy as a function of distortion parameter δ are fitted to the third-order polynomial fit to identify the elastic constants as a proportional to the second-order coefficient of this fit. The results for the elastic constants of ZnTe in the B3 structure are presented in Table 2. The elastic constants of C_{12} and C_{44} and bulk modulus are in good agreement with the experiments [23], while the elastic constants of C_{11} is less than those of experiments [23] and other calculations [13].

Table 2.

The elastic constants C_{ij} (GPa) and bulk modulus B (GPa) from (Eqs. 8) of B3 phase structure at zero pressure, along with the available experimental [23] and other calculations [13]

	P	B	C_{11}	C_{12}	C_{44}	[Ref.]
Our cal.	0	41.59	51.36	36.71	38.65	
	3	55.76	68.80	49.24	44.35	
	6	69.29	85.50	61.09	62.49	
	9	82.24	100.96	72.88	73.33	
	12	94.92	116.17	84.30	78.71	
Other cal.			82.00	42.00	55.00	[13]
	0		64.00	44.30	18.10	[15]
Exp.			71.70	40.70	31.20	[23]
	0		71.30	40.70	31.20	[23,24]

The mechanical stability conditions in the cubic structures can be expressed in terms of the elastic constants: $C_{11} - C_{12} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$. The elastic constants of ZnTe given in Table 1 satisfy these stability conditions. We are also interested in investigating the pressure dependence of elastic constants of ZnTe to see this effect. The variation of elastic constants and bulk modulus of ZnTe in the B3 structure as a function of pressure are shown in the Figure 3. They increases linearly with applying pressure.

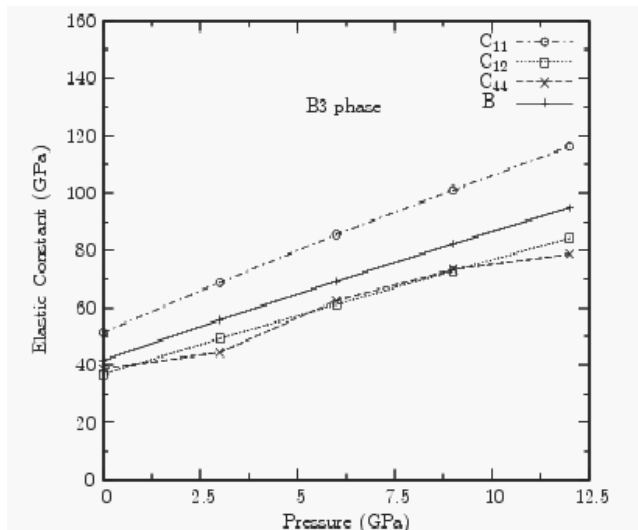


Fig. 3. Elastic constants C_{11} , C_{12} , C_{44} and the bulk modulus B of ZnTe in the B3 structure as a function of the pressure

4. Conclusions

We have presented first-principle calculations of the structural and mechanical properties for ZnTe in the B3 phase, in this study. The lattice constant, bulk modulus and the pressure derivative of

the bulk modulus are predicted as a structural properties, and the elastic constants are determined as a mechanical properties for ZnTe. We report that cubic phase take place at $a = 6.2025 \text{ \AA}$ which is in good agreement with the experimental value of 6.2025 \AA , as are the calculated Bulk modulus and its pressure derivative. Three elastic constants of the cubic B3 structure as a function of pressure are also calculated on the basis of the results on the total energies of the distortions. To the best of our knowledge, the pressure dependence of the this structure are calculated for the first time, in this study.

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