



Structural, Thermodynamic and Mechanical Properties of Zinc Telluride (ZnTe) in the Zincblende Structure

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ABSTRACT: The structural, thermodynamic mechanical properties of Zinc Telluride (ZnTe) in the Zincblende Structure were evaluated by applying the Density Functional Theory (DFT) based on the Pseudopotentials and Planewaves (PP-PW) method and executed with the Quantum Espresso computer code using various standard methods. Results obtained from the Generalized Gradient Approximation (GGA) calculations for elastic constants, lattice parameter, bulk modulus and its derivative. Shear Modulus, Poisson's ratio and Debye temperature were compared with the available theoretical results and experimental data. The comparison displayed slightly overestimated values by GGA when compared with the experimental results, confirming the efficiency of Quantum Espresso computer code in the computation of Structural, Mechanical and Thermodynamic Properties of ZnTe. Results further showed that ZnTe satisfied all cubic stability conditions, hence, it is structurally, mechanically, and thermodynamically stable at room temperature. Hence, these properties, collectively make Zinc Telluride in the zincblende phase a treasured material in the semiconductor industry, particularly for optoelectronic applications, where stability, durability and excellent performance are critical.

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Zinc telluride (ZnTe) is a binary chemical compound composed of Zinc and Tellurium. It is an example of the prototypes of II-VI semiconductor materials (Li *et al.*, 2010). Currently, ZnTe is receiving great attention as a result of its light-emitting properties at room temperature and direct energy band gaps (Schrier *et al.*, 2007; Lee *et al.*, 2013). Zinc telluride is industrially utilized as a back-surface field layer in the solar cells industry. In the PIN diode structures, it serves as a p-type semiconductor. Before now, ZnTe has found several technological applications in

photovoltaic devices, solid-state laser devices, solar cells, transistors, remote control device, THz emitter sensors and imaging systems (Zhang *et al.*, 2018; Kiprotich, 2023; Lee *et al.*, 2013). ZnTe's electronic and optical properties make it suitable for various applications, including solar cells, photovoltaic devices, and optoelectronic applications (Aazi *et al.*, 2019). Recently, research has focused on structural, mechanical, optical and electronic properties of semiconductors especially ZnTe in the wurtzite phase using different methods. However, none of these

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studies have deployed Quantum Espresso computer code for DFT Analysis for Structural, Mechanical, and Thermodynamic Properties of Zinc Telluride (ZnTe) in the Zincblende Structure. In a few cases, the lattice parameters like elastic constants and bulk modulus of ZnTe have been calculated and found to agree well with experimental data (Soykan *et al.*, 2010; Ferahtia *et al.*, 2016; Rowtu *et al.* 2018; Aazi *et al.*, 2019). It is well-known that when the pressure of 9.0 GPa is applied to a cubic B3 structure, it is transformed into the cinnabar (B9) structure by altering the material's mechanical properties. Many mechanical properties of solid materials could be understood and explained by determining their elastic constants (Kim, *et al.*, 2014; Wojnar *et al.*, 2014). Finding accurate measurements of these quantities is challenging due to experimental conditions at high pressure. However, recent advancements in computer programming and computational codes have made it possible to easily calculate material properties—such as structural, electronic, thermodynamic, and optical properties with high precision. Hence, the objective of this paper is to investigate the Structural, Thermodynamic and Mechanical Properties of Zinc Telluride (ZnTe) in the Zincblende Structure

MATERIAL AND METHODS

Zinc telluride in the Zincblende structure is a brownish-red powder but ruby-red crystal when refined through sublimation. It possesses a cubic crystal structure similar to that of sphalerite and diamond. The zincblende structure ZnTe has an experimental lattice of 6.1037Å (Aazi *et al.*, 2019, Kiprotich, 2023) and a direct band gap energy of 2.26 eV at 300K (Adachi *et al.*, 2005).

The ab initio quantum mechanical computational method employed in this study is the Density Functional Theory (DFT) within the Generalized Gradient Approximation (GGA). DFT is a method of finding an approximate solution to the Schrodinger equation for a many-body system.

DFT computational codes are utilized to examine the structural, magnetic, and electronic properties of many molecules. This quantum mechanical modeling approach is broadly applied in material science to explore electronic structures in the ground state of many-body systems. Through this theory, the properties of many-electron systems can be determined by using the function of another function, this study utilized spatially dependent electron density in this study. The computational methods and approximations used to perform the ab initio calculations are briefly presented here. The first-principles calculations were conducted using the Quantum Espresso code (QE), which employs a plane

wave pseudo-potential PWPP method with the generalized gradient approximation GGA. To ensure convergence, a plane wave basis set with a specified kinetic energy cutoff, charge density cutoff, and convergence threshold was utilized. For Brillouin zone sampling, Monkhorst–Pack meshes were applied for ZnTe. During the self-consistent calculations, the energy versus lattice parameter dataset was fitted to the Birch third-order Murnaghan equation of state to determine the equilibrium lattice constant, bulk modulus, and pressure derivative of the bulk modulus.

The Energy version of the 3rd order Birch-Murnaghan equation of states sets the total energy and pressure as a function of the volume is expressed as shown in equation 1:

$$E(V) = E_0 + \frac{9B_0V_0}{16} \left\{ \left[\left(\frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right]^3 B'_0 + \left[\left(\frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right]^2 \left[6 - 4 \left(\frac{V_0}{V} \right)^{\frac{2}{3}} \right] \right\} \quad 1$$

Where E represents Total energy, B_0 is the Bulk modulus at zero pressure, B'_0 is the first derivative of the bulk modulus concerning pressure a fairly constant B'_0 of about 3.5, V represents volume as a function of the pressure P, V_0 is equilibrium volume. If the reduction in volume under compression is low, i.e., for V/V_0 greater than 90%, the Murnaghan equation can model experimental data with satisfactory accuracy (Erum, *et al.* 2023; Bilal *et al.*, 2014).

The first principles are theoretical studies using the pseudopotential method of plane waves to study the elastic and thermodynamic properties of ZnTe in the zinc-blende (ZB) structure at high temperatures and pressures. The calculated lattice parameters of 0.6095 nm are close to the experimental values of 0.6003nm with only 0.1% difference. The elastic constants and bulk modules at 0GPa pressure and 0K temperature also fit well into the experimental data. The transition pressure is estimated at 10 GPa depending on the elastic constant of the high pressure, according to the mechanical stability of the cubic crystal, in line with the available experimental results. Debye temperature (249 K) under normal conditions ($T = 300$ K) and thermal capacity (CV) values under various pressures and temperatures were also derived using the quasi-harmonic Debye model. Our result reduces increasing pressure and approaches the Dulong–Petit limit at high temperatures and pressures

Computational Methods: In this study, approximations based on the Density Functional Theory (DFT) Pseudopotentials and Plane Waves (PP-

PW) method, as implemented in the Quantum ESPRESSO software, were utilized. The Plane Wave Self-Consistent Field (PWSCF) method involves the use of the pw.x code and post-processing tools to plot the band structure of platinum (Pt). The PW code calculates total energy, while the PWSCF method employs techniques within the framework of the plane wave pseudopotential approach to perform self-consistent calculations. The computed results from this work were compared with experimental data obtained from elsewhere (Lalithambika, *et al*, 2019; Horichok, *et al.*, 2016)

The Quantum Espresso computer code used in the computation of the Structural, Mechanical and Thermodynamic Properties of ZnTe proceed as follows:

```
&control
calculation = 'scf'
prefix = 'znte'
pseudo_dir='./',
outdir='./',
/
&system
ibrav=2,
celldm(1)=12.5323,
nat=2, ntyp=2, occupations='smearing',
smearing='mv', degauss=0.02
ecutwfc=45,
/
&electrons
mixing_beta = 0.7
conv_thr = 1.0d-8
/
ATOMIC_SPECIES
Zn 65.409 Cd.pbe-n-van.UPF
Te 127.6 Te.pbe-rrkj.UPF
ATOMIC_POSITIONS
Zn 0.000000000 0.000000000 0.000000000
Te 0.250000000 0.250000000 0.250000000
```

```
K_POINTS (automatic)
8 8 8 0 0 0
```

This input file sets up a basic calculation to optimize the cell parameters and atomic positions of ZnTe using the vc-relax option. After running the calculation, the output files were analyzed to obtain the structural, mechanical, and the thermodynamic properties of ZnTe.

RESULTS AND DISCUSSION

Structural Properties: Table 1 gives a comparison of calculated and experimental values for the lattice parameter (a), bulk modulus (B), and pressure derivative of the bulk modulus (B') for the investigated zinc telluride (ZnTe) from the present study and other studies (Ferahtia *et al* 2016; Pellice, 2011; Ma *et al* 2008; Bahloul *et al*, 2015). In this study, the calculated lattice parameter of 6.1999 Å is notably higher than all the reported experimental values, which range from 6.0890 Å to 6.1037 Å. This discrepancy is a pointer to potential overestimation in theoretical calculations. The calculated bulk modulus of 40.8 GPa is substantially lower than the experimental values, which were from 50.50 GPa to 52.80 GPa. This shows that the theoretical model implemented by the computational code slightly underestimates the material's resistance to compression. The calculated pressure derivative of 4.66 GPa is lower than the experimental values which range from 5.00 to 5.04 GPa. This suggests that the theoretical model slightly but less accurately captures how the bulk modulus changes with pressure (Mahmood, 2016; Wu, *et al* 1990). The discrepancies between the calculated and experimental values could arise from several factors in which the theoretical calculations employed approximations or simplifications that were not fully captured in the complex behavior of ZnTe (Zhou *et al.*, 2008).

Table 1: Comparison of computed lattice constant (A), bulk modulus B(GPa), and its pressure-derivative B' for ZnTe with other results obtained experimentally.

MATERIAL (ZnTe)	Lattice parameter Armstrong (A)	Bulk Modulus (Gpa)	Pressure derivative of Bulk Modulus (B')
Present work	6.1999	40.8	4.66
Experimental Others	6.1026	50.50	5.00 (Ferahtia <i>et al</i> 2016)
	6.1010	50.90	5.04 (Pellice, 2011)
	6.1030	51.0-52.8	5.04 (Ma <i>et al</i> 2008)
	6.1037	52.80	(Bahloul <i>et al</i> , 2015)
	6.0890		(Bahloul <i>et al</i> , 2015)

Mechanical Properties: Mechanical properties of zinc telluride (ZnTe) which include Elastic constants C_{11} , C_{12} , and C_{44} (in GPa). Bulk modulus (B), Poisson's ratio (n), Young's modulus (E), and Shear modulus (G) (in GPa) are displayed in Table 2. Comparison of these

properties with other experimental results in the literature are also shown in Table 2. For elastic constants, there are significant discrepancies between the present calculated values of C_{11} , C_{12} , and C_{44} and the values from experimental data. This indicates

potential inaccuracies in the theoretical model or experimental errors (Eickmeier and Steinberg, 2020). The calculated bulk modulus obtained by the average of Reuss and Voigt approximations is lower than the experimental value. This suggests that the theoretical model underestimates ZnTe's resistance to uniform compression. The calculated Poisson's ratio is very close to the experimental values, suggesting a better agreement in this property. Considering Young's Modulus (E) and Shear Modulus (G), Data for E and

G is only provided for the approximations and experimental values. The differences observed in this calculation could be as a result of the theoretical model applied for the calculations which may not have rightly captured all atomic interaction complexities in ZnTe (Isik, *et al.*, 2020). The Reuss and Voigt approximations gave bounds for the elastic properties of polycrystalline materials but might not perfectly represent the actual behavior of ZnTe.

Table 1: Elastic constants (C_{ij} : C_{11} , C_{12} , C_{44}), the Bulk modulus (B), the Poisson's ratio (ν), Young modulus (E), and the shear modulus (G) for ZnTe compared with other experimental and theoretical results.

Material ZnTe	$C_{11}(GPa)$	$C_{12}(GPa)$	$C_{44}(GPa)$	$E(GPa)$	$G(GPa)$	ν
Present	58.01282	32.26155	31.16338	-	-	-
Reuss approx.	-	-	-	51.29900	19.87289	0.29068
Voigt approx.	-	-	-	59.88908	23.84828	0.25563
Average	-	-	-	55.59404	23.84828	0.25585
Other experimental	71.70	40.70	31.20			
	71.30	40.70	31.20			

Table 2: Voigt-Reuss-Hill average sound velocity (m/s), sound Velocity =2211.235 m/s

Bulk Vb	2754.784(m/s)
Compressional Vp	3606.143(m/s)
Shear Vg	2015.335(m/s)
Debye temperature	212.411 (Kelvin)
Average Debye sound velocity	2211.235(m/s)

Table 3 gives a set of acoustic parameters for ZnTe, with the VRH average sound velocity being a key calculated value. Bulk Velocity (Vb) of 2754.784 m/s is the ZnTe resistance to volume change. Compressional Velocity (Vp): 3606.143 m/s is the speed of longitudinal waves through the ZnTe. Shear Velocity (Vg): 2015.335 m/s gives the speed of transverse waves through the ZnTe.. Debye Temperature: 212.411 K - An inherent temperature related to the vibrational properties of the ZnTe. The average Debye Sound Velocity: 2211.235 m/s is the average sound speed in the ZnTe. The Voigt-Reuss-Hill (VRH) average is a method used to estimate the elastic properties of polycrystalline materials from their single-crystal counterparts. It provides a mean value by considering both the upper and lower bounds of the elastic moduli (Erum, *et al.* 2023). VRH average sound velocity is 2211.235 m/s. The Average Debye Sound Velocity gives a characteristic sound speed for the material. It is often used in calculations related to thermal properties, specific heat, and lattice dynamics. It gives the basis for computing other material characteristics and acoustic properties (Nemera, 2020).

Thermodynamic Properties: Fig. 1 which displays variations of ZnTe entropy against temperature displays a perfect positive correlation between temperature and entropy. This is consistent with the general thermodynamic principle which proposes that entropy increases with increasing temperature (Isik, *et*

al., 2020). The exponential curve shows that the rate of increasing entropy is not constant with temperature. Initially, at lower temperatures, the entropy increases slowly. However, as the temperature rises, the rate of increase in entropy becomes progressively faster. At higher temperatures, the molecules in ZnTe have more kinetic energy, leading to an increase in vibrational and rotational motion (Isik, *et al.*, 2020). This increase in the motion of molecules results in a higher degree of Chaos that is proportional to the entropy. C_v is the amount of heat needed to raise the temperature of a unit mass of a substance by one degree Kelvin (K) when the volume is kept constant. The relationship between Temperature (T) and specific heat at constant volume (C_v) for a Zinc Telluride (ZnTe) in the Zincblende structure is illustrated in Fig 2. It was observed that as temperature increases, the specific heat (C_v) rapidly increases. This implies that more heat is needed to raise the temperature of Zinc Telluride. At higher temperature values, the curve reached a plateau, indicating that the quantity of heat required to increase the temperature by one degree remains approximately the same notwithstanding the temperature. At low temperatures, the molecules of ZnTe have restricted vibrational energy. As the temperature increases, the molecules vibrate more energetically, requiring more heat to raise their temperature. At higher temperatures, the intermolecular forces among molecules fade. This results in the molecules vibrating more freely and the additional energy needed to increase their temperature becomes less dependent on these forces (Soykan *et al.*,

2010). This behaviour can be attributed to molecular vibrations and intermolecular forces inherent in the ZnTe crystals.

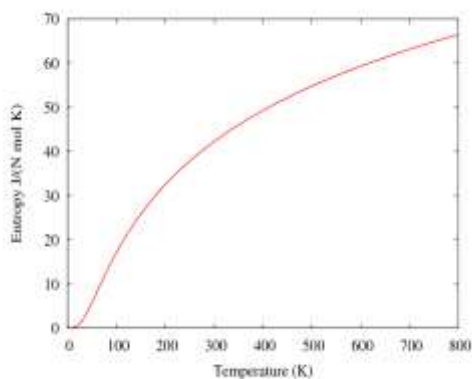


Fig.1: Vibrational entropy S (J/mol)

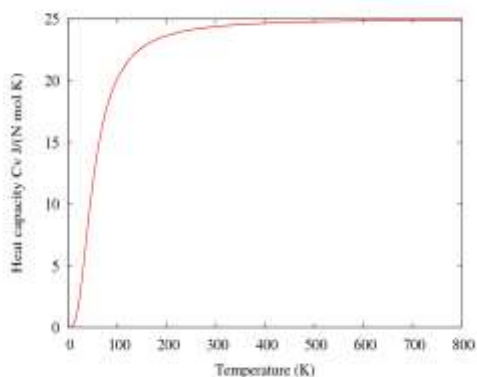


Fig.2: Specific heat at constant volume C_v

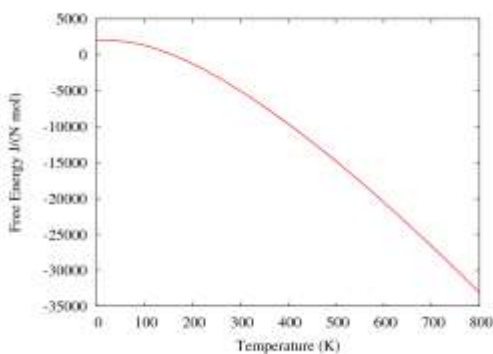


Fig. 3: Free energy ΔF

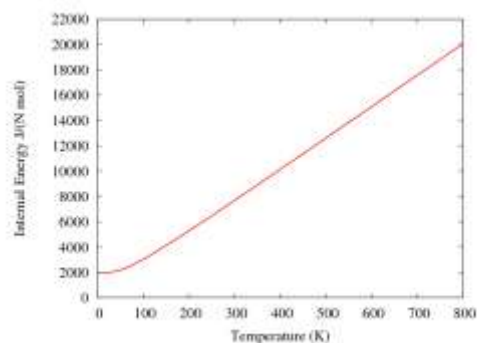


Fig.4: Internal energy ΔE

Fig. 3. illustrates the variation of free energy (G) with temperature (T) for zinc telluride (ZnTe) in the zincblende structure. The graph shows a negative slope, indicating that the free energy decreases as temperature increases. This is a characteristic behaviour of most materials (Li *et al* 2010). The curve is not linear but rather exhibits a slight curvature. This suggests that the rate of decrease in free energy with temperature is not constant. The minimum point is a temperature around 500 K. This represents the temperature at which the system is in its most stable state. The free energy is significantly influenced by temperature. This implies that the stability and properties of ZnTe in the zincblende structure are temperature-dependent. The temperature dependence of free energy can influence the occurrence of phase transitions. For example, if the free energy of a different crystal structure becomes lower at a certain temperature, the system may undergo a phase transformation. The free energy can be used to calculate other thermodynamic properties, such as enthalpy, entropy, and Gibbs free energy. These properties are important for understanding the behaviour and stability of materials. Fig. 4 displays the variation of internal energy (U) with temperature (T) for zinc telluride (ZnTe) in the zincblende structure. it shows that the internal energy of ZnTe in the zincblende structure increases linearly with temperature. This suggests that the specific heat capacity of the material is relatively constant. The temperature dependence of internal energy is a fundamental property that affects various thermodynamic properties of ZnTe.

Conclusion: The lattice parameter is slightly overestimated by the GGA when compared with the experimental results. Also, the band structure, shows that the ZnTe compound has a direct energy band gap from GGA calculations. Employing the PW-PP approach based on density functional theory, within GGA, the study of the structural, mechanical, and

thermodynamic properties of ZnTe was determined. Results show that the calculated equilibrium lattice constant, the bulk, and its pressure derivative agree with the available theoretical and experimental results. The comparison displayed slightly overestimated values by GGA when compared with the experimental results, confirming the efficiency of Quantum Espresso computer code in the computation of Structural, Mechanical and Thermodynamic Properties of ZnTe. The zinc-blende phase is more stable than the wurtzite phase at room temperature. Hence, Zinc Telluride in the zinc blend phase is a valuable material in the semiconductor industry, especially for optoelectronic applications, where stability, durability and excellent performance are critical.

Declaration of Conflict of Interest: The authors declare no conflict of interest

Data Availability Statement: Data are available upon request from the corresponding author

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