



Revealing the structural, elastic and thermodynamic properties of $\text{CdSe}_x\text{Te}_{1-x}$ ($x = 0, 0.25, 0.5, 0.75, 1$)



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ABSTRACT

First-principles calculations are carried out to perform the structural properties using two dimensional search of equation of state (EOS), elastic constants and thermodynamic properties for zinc-blende (ZB) and wurtzite (WZ) phases of $\text{CdSe}_x\text{Te}_{1-x}$ alloys for all compositions x ($x = 0, 0.25, 0.5, 0.75, 1$). We have used the full-potential linearized augmented plane wave (FP-LAPW) method within the density functional theory (DFT), which has been implanted in the WIEN2k code, along with the improved generalized gradient approximation (PBE-GGA) to treat exchange-correlation functional. The mechanical and thermodynamic properties of $\text{CdSe}_x\text{Te}_{1-x}$ alloys are studied using the optimized lattice parameters from two dimensional search of EOS at zero pressure. The ZB and WZ phases of the ternary $\text{CdSe}_x\text{Te}_{1-x}$ alloys are found to be mechanically stable within PBE-GGA exchange-correlation over all the range of the Te concentrations ($x = 0, 0.25, 0.5, 0.75, 1$). We have found that the CdSe is mechanically the strongest material in the ternary $\text{CdSe}_x\text{Te}_{1-x}$ alloys. We concluded that the calculated values of Cauchy pressure and Poisson's ratio predict that the ionic bonds for both ZB and WZ phases of $\text{CdSe}_x\text{Te}_{1-x}$ ternary alloys are more dominant for all compositions of x ($x = 0, 0.25, 0.5, 0.75, 1$) within PBE-GGA exchange-correlation. Our results exhibit a non-linear relationship between elastic constants and Se concentrations. Moreover, the elastic properties of cubic (ZB) and hexagonal (WZ) phases of $\text{CdSe}_x\text{Te}_{1-x}$ alloys, including elastic constants, bulk and shear moduli are calculated and compared with available theoretical and experimental results, good agreement was found.

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1. Introduction

II-VI semiconductors have been studied extensively by researchers because of their unique size-dependent optical and electronic properties, which are technologically important materials and of great fundamental and applied interest. Semiconductor materials such as CdTe, CdSe, and $\text{CdSe}_x\text{Te}_{1-x}$ are essential for modern electronic devices. The pseudobinary compounds $\text{CdSe}_x\text{Te}_{1-x}$ are another group of materials that have been the focus of considerable amounts of attention because they are used in photovoltaic cells [1,2], light-emitting diodes [3,4], production of solar cells [5–8], and fluorescent tags for biological imaging [9,10]. Solid solutions of limited solubility such as $\text{CdSe}_x\text{Te}_{1-x}$ [11,12] have

not been investigated thoroughly in the past. The results published on the physical and photoelectrical properties of $\text{CdSe}_x\text{Te}_{1-x}$ polycrystalline layers depend on the preparation method used [13–15].

In $\text{CdSe}_x\text{Te}_{1-x}$ ternary compounds the band gap and the crystal structure can be modified by changing the content (x) of Se and Te. CdTe and CdSe normally exhibit cubic zinc-blende and hexagonal wurtzite structures, respectively. $\text{CdSe}_x\text{Te}_{1-x}$ films have been prepared using different techniques such as thermal evaporation [16], slurry painting [17], pulse plating [18], electro-deposition [19], brush plating [20,21], hot wall deposition method [22] etc.

$\text{CdSe}_x\text{Te}_{1-x}$ thin films are interesting materials because their band gap lies in the optimal range (1.3–1.7 eV) required for a photovoltaic cell. The ideal band gap for a solar cell is 1.4 eV. Research suggests that the optical properties of $\text{CdSe}_x\text{Te}_{1-x}$ can be tuned between 1.3 and 1.7 eV by altering the value of x , which leads to a reduction in the band gap energy by adding to the Te content [23].

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CdSe_{1-x}Te_x alloys have been used by Das [24] to study the principal requirements of a suitable thin film photoelectrode for high efficiency photoelectrochemical cells. CdSe_{1-x}Te_x thin film is created by Ravichandran et al. [25] using electro-deposition and various doping concentrations of Te, and then looked at the photoconductivity as a function of the applied dc-electric field, wavelength, time, and the strength of incident light at room temperature. Their experiment proved that the energy band gap decreases with increasing Te content for CdSe_{1-x}Te_x ($x = 0.2, 0.3, 0.4$). Muthukumarasamy et al. [22] investigated the structural phase transformation and optical band gap bowing in hot wall deposited CdSe_xTe_{1-x} ($x = 0.0, 0.15, 0.4, 0.6, 0.7, 0.85, 1.0$) thin films. Schenk and Silber [26] studied the lattice constant and microhardness of CdTe_{1-x}Se_x alloys and found the cubic phase exists in the composition range $0 \leq x_{\text{CdSe}} \leq 0.45$, and the hexagonal phase in the range $0.65 \leq x_{\text{CdSe}} \leq 1.0$. Fewer studies have been dedicated to CdSe_{1-x}Te_x [27–29] nanocrystals.

To the best of our knowledge, neither experimental details regarding the elastic constants nor experimental thermodynamic properties are available for CdSe_xTe_{1-x} compounds except for elastic constants of zinc-blende CdTe and wurtzite CdSe. However there are a few theoretical works concentrating on the elastic constants of CdSe and CdTe [30–33]. Recently, Benyettou et al. [32] and Saib et al. [33] studied the elastic constants of CdSe_xTe_{1-x} ternary alloys using the pseudopotential plane wave method for all composition x ($x = 0, 0.3, 0.5, 0.7, 1$) of interest within local density approximation (LDA) [34] for zinc-blende and wurtzite phases, respectively.

Therefore, it is worth performing first-principle calculations of structural properties using a two-dimensional search into equation of state, elastic constants and thermodynamic properties for both phases of CdSe_xTe_{1-x} compounds for all compositions x ($x = 0, 0.25, 0.5, 0.75, 1$) using the full-potential linear muffin tin orbital (FP-LAPW) method [35], based on the density functional theory (DFT) [36] (which has proven to be one of the accurate methods for computation of the structural and elastic properties of solids). The improved generalized gradient approximation (PBE-GGA) [37] has been recommended [38,39] to provide reference data for experimenters.

The organization of this article is as follows: Section 1 describes a brief introduction. Section 2 describes the FP-LAPW computational details and in Section 3 the results are presented followed by a discussion of structural and elastic properties. Finally, a conclusion is given in Section 4.

2. Computational details

The first-principle calculations of a two dimensional search (2D-search) of equation of state (EOS) and mechanical and thermodynamic properties were performed using 2DR-optimize and IRelast packages [40,41] which are compatible with the WIEN2k package [42]. The IRelast package bases its calculations of elastic constants on the second-order derivative ($E''(\delta)$) of the polynomial fit of energy ($E = E(\delta)$) vs. strain at zero strain ($\delta = 0$), and the 2DR-optimize package performs a convenient volume and c/a structure optimization for hexagonal, tetragonal and rhombohedral cases. The details of elastic constants calculations and related properties for hexagonal and cubic compounds, and a two-dimensional search of EOS (2D-search) are available in our previous works [38,43,44].

The program package WIEN2k is an *ab initio* full potential linearized augmented plane wave together with local orbitals (FP-LAPW + lo) technique enabling the electronic ground state of the periodic systems to be calculated based on DFT. The WIEN2k package does this by selecting two areas for the unit cell volume: i) non-overlapping atomic spheres around each atom with a Muffin-

Tin radius (R_{mt}) and ii) the remaining – interstitial – area. Two kinds of basis function are used in these calculations. In the atomic spheres, the wave functions are expanded into atomic orbitals with maximum angular momentum $l_{max} = 9$ and 10 for wurtzite and zinc-blende phases, respectively, and in the second region, a plane-wave basis set is used and the convergence of this basis set is checked by a cutoff parameter $R_{mt}K_{max} = 8$ and 9 for wurtzite and zinc-blende phases, respectively, where R_{mt} is the smallest atomic sphere radius in the unit cell (For finding lattice constants of wurtzite phase $l_{max} = 10$ and $R_{mt}K_{max} = 9$). Numbers of k-points in the full Brillouin zone were 2000 and 3000 k-points for wurtzite and zinc-blende phases, respectively. The positions were updated until forces dropped below $1mRy/bohr$ during the 2D-search and the elastic constants computations. To treat the exchange–correlation potential, we used the improved generalized gradient approximation (PBE-GGA) [37], the recommended exchange–correlation functional [38,39].

3. Results and discussion

3.1. Structural properties

In the first step of these calculations and to increase the precision of the elastic constants calculations, we have optimized the lattice parameters for CdSe_xTe_{1-x} ternary alloys at various compositions ($x = 0, 0.25, 0.5, 0.75, 1$) for both cubic (zinc-blende) and hexagonal (wurtzite) phases and then calculated the elastic constants making use of the optimized lattice constants. Since for hexagonal compounds, there are two degrees of freedom for finding the equation of state (EOS), i.e. volume and c/a changes, we have carried out an appropriate volume and c/a structure optimization (2D-search) using the 2DR-optimize package [40] for the wurtzite phase. Our previous work shows that the 2D-search of EOS is important [43,38] and represents the accuracy of the method used (DFT in this case) better than one-dimensional search of EOS.

To make a meaningful comparison, these results and earlier theoretical results as well as the experimental data are listed in Table 1. For zinc-blende CdSe ($x = 1$) and CdTe ($x = 0$), our calculated a -lattice parameter within PBE-GGA is overestimated with respect to the experimental reports [45–49] and previous DFT-LDA calculations [30]. However, it is clear that our outcomes come to the same conclusions as the previous DFT-(PBE-GGA) calculations [23,50]. For $x = 0.75$, our PBE-GGA a -lattice parameter is smaller than that reported by Reshak et al. [23] while for $x = 0.5$ and $x = 0.25$ it is bigger. Although we used the same method (FP-LAPW), we added more k-points (2000 k-points) in the full Brillouin zone and selected $l_{max} = 10$, whilst in previous calculations [23] they have used 1400 k-points and $l_{max} = 6$. This could be the main reason for the disagreement.

Table 1 shows that the structural parameters, namely a -lattice parameter and bulk modulus for zinc-blende CdSe_xTe_{1-x} within PBE-GGA exchange-correlation, increase and decrease monotonically when moving from zinc-blende-CdSe to zinc-blende-CdTe, respectively.

This is not the case for derivatives of bulk modulus where the variation is non-monotonic. For wurtzite CdSe ($x = 1$) and CdTe ($x = 0$), our calculated a and c lattice parameters within PBE-GGA are overestimated with respect to the experimental reports [26,49,51] and previous [33] DFT-LDA calculations. However one can see that our findings match the previous [23,49] DFT-PBE-GGA or DFT-GGA calculations. For $x = 0.75$ and $x = 0.5$, our PBE-GGA a -lattice (c -lattice) parameters are bigger (smaller) than that reported by Reshak et al. [23], while for $x = 0.25$ we obtained bigger a -lattice (c -lattice) parameters than that reported previously [23]. However the disagreement is attributed to the difference in the k-points and

Table 1The structural parameters of the zincblende and wurtzite phases of CdSe_xTe_{1-x} (x = 0.0, 0.25, 0.5, 0.75, 1.0) alloys compared with theoretical and experimental data.

Compounds	a(Å)	c(Å)	B(GPa)	B'
CdSe _{cubic}	6.208		44.52	4.56
Theor	6.207 ^a , 6.210 ^b , 6.050 ^c , 6.216 ^d		45.60 ^a , 65.12 ^c , 45.16 ^d	
Exp	6.052 ^f , 6.084 ^{g-h} , 6.050 ⁱ		53.00 ⁱ	
CdSe _{wurtzite(2D)}	4.39	7.17	44.83	4.36
Theor	4.34 ^a , 4.27 ^j	7.27 ^a , 6.98 ^j	43.64 ^a	
Exp	4.30 ^k , 4.30 ^l	7.02 ^k , 7.01 ^l		
CdSe _{0.75} Te _{0.25} cubic	6.312		42.23	4.55
Theor	6.526 ^a		43.08 ^a	
CdSe _{0.75} Te _{0.25} wurtzite(2D)	4.463	14.579	41.21	4.59
Theor	4.429 ^a	14.891 ^a	42.32 ^a	
CdSe _{0.5} Te _{0.5} cubic	6.418		39.17	4.72
Theor	6.407 ^a		42.21 ^a	
CdSe _{0.5} Te _{0.5} wurtzite(2D)	4.536	7.421	39.06	4.35
Theor	4.437 ^a	7.459 ^a	39.14 ^a	
CdSe _{0.25} Te _{0.75} cubic	6.522		37.62	4.50
Theor	6.322 ^a		40.14 ^a	
CdSe _{0.25} Te _{0.75} wurtzite(2D)	4.610	15.088	36.59	4.42
Theor	4.563 ^a	14.653 ^a	36.31 ^a	
CdTe _{cubic}	6.625		34.96	4.76
Theor	6.620 ^a , 6.626 ^b , 6.480 ^c , 6.631 ^d , 6.540 ^m		36.24 ^a , 48.94 ^c , 33.78 ^d	
Exp	6.480 ^g , 6.540 ^h , 6.477 ^m		44.50	
CdTe _{wurtzite(2D)}	4.680	7.675	35.25	4.36
Theor	4.680 ^a , 4.560 ^m , 4.48 ^j	7.650 ^a , 7.540 ^m , 7.36 ^j	34.62 ^a	
Exp	4.570 ^m	7.470 ^m		

^a Ref. [23].^b Ref. [45].^c Ref. [30].^d Ref. [50].^f Ref. [45].^g Ref. [46].^h Ref. [47].ⁱ Ref. [48].^j Ref. [33].^k Ref. [26].^l Ref. [51].^m Ref. [49].

the value of l_{max} used in previous and present calculations.

Table 1 shows that the structural parameters, namely the **a**-lattice parameter and bulk modulus for wurtzite CdSe_xTe_{1-x} (x = 0, 0.25, 0.5, 0.75, 1), increase and decrease monotonically within PBE-GGA exchange-correlation when we move from wurtzite-CdSe to wurtzite-CdTe, respectively.

This is not the case for derivatives of bulk modulus where the variation is non-monotonic. Since the bulk modulus is related to the resistance against the volume changes, we can conclude that increasing the Te content in ternary CdSe_xTe_{1-x} alloys led to the decrease in resistance against the volume changes (hardness) for both phases.

The polynomial fit (*order of fit 2*) of our calculated data regarding the **a**-lattice parameter and the bulk modulus of ternary CdSe_xTe_{1-x} alloys within PBE-GGA exchange-correlation for both phases have exhibited the following analytical expressions:

$$a_C(x) = -0.005x^2 - 0.413x + 6.625$$

$$a_W(x) = -0.006x^2 - 0.285x + 4.680$$

$$B_C(x) = -0.880x^2 + 8.612x + 35.064$$

$$B_W(x) = 1.589x^2 + 8.151x + 35.091$$

Where **a** represents the **a**-lattice parameter for cubic (C) and wurtzite (W) phases in units of angstrom and **B** displays bulk modulus in units of GPa.

The above equations indicate that the **a**-lattice parameter for the cubic phase has deviates a little from the linearity as a function of x composition, but deviation from linearity for the wurtzite phase is larger than for the cubic phase. While the bulk modulus has large bowing parameters which emphasize the non-linear behavior of B against x changes as bowing parameter of the cubic phase from linearity is smaller than for the wurtzite phase.

3.2. Elastic constants

The complete sets of zero-pressure and zero-temperature single crystal's elastic constants of cubic and wurtzite phases of ternary CdSe_xTe_{1-x} alloys at various compositions (x = 0, 0.25, 0.5, 0.75, 1) are calculated by using IRelast package [41] at their optimized lattice constants, as displayed in Tables 2 and 3 where they are compared with available experiments [52,53] and previous theoretical calculations [31–33]. First-principle calculations of the elastic constants lead us to estimate the main technological properties— stiffness, brittleness/ductility, hardness, and types of bonds— for the material in question.

If the B/S ratio is less(more) than 1.75 [43], a material acts as brittle (ductile). The sign of Cauchy pressure ($C_{12} - C_{44}$) is useful in predicting the types of bonds (for wurtzite phase $C_{44} = C_{55}$). Normally, the Cauchy pressure of compounds with more dominant covalent (ionic) bonds is negative (positive) [43]. The sorts of bonds can be forecast using the value of Poisson's ratio. For a typical covalent compound, the value is a much less than 0.25 (around 0.1), while it is nearly 0.25 or more for a typical ionic compound [54]. However, in earlier research [43] we propose the typical value of

Table 2

The calculated elastic constant (C_{ij} in GPa), Bulk modulus (B), Shear modulus (S) and Young's modulus (Y) in Voigt (V)–Reuss (R)–Hill (H) approximations (in GPa), Poisson's ratio (ν), transverse elastic wave velocity (V_t in m/s), longitudinal elastic wave velocity (V_l in m/s), average wave velocity (V_m in m/s), Debye temperature (Θ_D in K) and Vickers hardness (H_V) for zinc-blende $CdSe_xTe_{1-x}$ ($x = 0.0, 0.25, 0.5, 0.75, 1.0$) alloys in comparison with available experimental and theoretical data.

Cubic	CdSe	CdSe _{0.75} Te _{0.25}	CdSe _{0.5} Te _{0.5}	CdSe _{0.25} Te _{0.75}	CdTe
C_{11}	54.24, 67.81^a,88.4^b	53.44	51.22, 59.17^a	49.86	46.81, 57.38^a ,(53.51) ^c
C_{12}	39.70, 50.12^a,38.3^b	36.53	34.24, 42.04^a	32.08	29.93, 39.19^a ,(36.81) ^c
C_{44}	19.88, 22.89^a,35.7^b	18.69	19.40, 20.95^a	18.35	17.95, 21.31^a ,(19.94) ^c
B_V	44.55	42.17	39.90	38.00	35.49
B_R	44.55	42.17	39.90	38.00	35.49
B_H	44.55	42.17	39.90	38.00	35.49
S_V	14.84	14.60	15.03	14.56	14.11
S_R	11.74	12.59	12.82	12.87	12.29
S_H	13.29	13.60	13.93	13.72	13.20
Y_V	40.06	39.26	40.07	38.74	37.37
Y_R	32.36	34.36	34.73	34.69	33.04
Y_H	36.25	36.83	37.42	36.73	35.22
ν_V	0.350	0.344	0.332	0.330	0.324
ν_R	0.378	0.364	0.354	0.347	0.344
ν_H	0.364	0.354	0.343	0.338	0.334
V_t	10581.35	10590.44	10602.85	10585.55	10551.58
V_l	3423.33	3349.35	3284.29	3212.22	3111.99
V_m	1781.40	1789.23	1800.58	1780.02	1740.88
Θ_D	170.86	168.77	167.06	162.51	156.46
H_V	-0.79	-0.55	-0.27	-0.19	-0.16

Theoretical results are bold while Experimental results are given in parenthesis.

^a Ref. [32] (LDA).

^b Ref. [31].

^c Ref. [52] (at 25 °C).

Table 3

The calculated elastic constant (C_{ij} in GPa), Bulk modulus (B), Shear modulus (S) and Young's modulus (Y) in Voigt (V)–Reuss (R)–Hill (H) approximations (in GPa), Poisson's ratio (ν), transverse elastic wave velocity (V_t in m/s), longitudinal elastic wave velocity (V_l in m/s), average wave velocity (V_m in m/s), Debye temperature (Θ_D in K) and Vickers hardness (H_V) for wurtzite $CdSe_xTe_{1-x}$ ($x = 0.0, 0.25, 0.5, 0.75, 1.0$) alloys in comparison with available experimental and theoretical data.

HEX	CdSe	CdSe _{0.75} Te _{0.25}	CdSe _{0.5} Te _{0.5}	CdSe _{0.25} Te _{0.75}	CdTe
C_{11}	73.49, 78.88^a,62.76^b ,(74.6) ^c	62.28	61.14, 70.94^a,53.88^b	57.68	55.98, 68.93^a,51.99^b
C_{12}	35.27, 48.81^a,36.39^b ,(46.1) ^c	30.76	28.15, 41.72^a,30.37^b	28.69	24.77, 38.09^a,27.99^b
C_{13}	31.83, 41.48^a,30.17^b ,(39.4) ^c	27.25	21.14, 34.60^a,24.53^b	28.17	20.77, 30.82^a,22.17^b
C_{33}	71.63, 89.48^a,70.36^b ,(81.7) ^c	70.08	69.54, 83.21^a,61.84^b	62.54	62.01, 81.10^a,60.34^b
C_{55}	16.50, 13.51^a,11.93^b ,(13.0) ^c	13.98	14.63, 12.83^a,10.56^b	12.44	12.69, 13.17^a,10.61^b
B_V	46.273, 56.45^a,50.90^b ,(53.4) ^c	40.569	36.963, 49.42^a,41.98^b	38.663	34.066, 46.36^a,38.70^b
B_R	46.224, 56.45^a,50.90^b ,(53.4) ^c	40.536	36.960, 49.42^a,41.98^b	38.621	34.058, 46.36^a,38.70^b
B_H	46.248, 56.45^a,50.90^b ,(53.4) ^c	40.552	36.961, 49.42^a,41.98^b	38.642	34.062, 46.36^a,38.70^b
S_V	18.402	16.036	17.242	14.066	15.372
S_R	18.248	15.708	16.683	13.906	14.919
S_H	18.325	15.872	16.962	13.986	15.145
Y_V	48.74	42.51	44.76	37.63	40.09
Y_R	48.38	41.73	43.50	37.25	39.05
Y_H	48.56	42.12	44.14	37.44	39.57
ν_V	0.324	0.325	0.298	0.337	0.303
ν_R	0.325	0.328	0.303	0.339	0.308
ν_H	0.325	0.326	0.300	0.338	0.306
V_t	1856.53, 1598.05^a	1718.45	1769.68, 1606.77^a	1602.15	1663.15, 1651.97^a
V_l	3646.14, 3661.09^a	3388.56	3316.62, 3433.46^a	3242.61	3147.87, 3294.34^a
V_m	2080.40, 1862.93^a	1926.14	1976.94, 1808.91^a	1798.55	1859.21, 1795.78^a
Θ_D	199.59, 183.82^a	181.69	183.38, 172.87^a	164.14	167.03, 168.42^a
H_V	0.709	0.359	1.213	-0.149	0.802

Theoretical results are bold while Experimental results are given in parenthesis.

^a Ref. [33] (LDA).

^b Ref. [33] (PBE-GGA).

^c Ref. [48] (at 300 K).

$\nu = 0.236$ for Poisson's ratio as a limit for defining types of bonds.

Stiffness is characterized by resistance to forces of distortion. Young's modulus—the ratio of stress to strain — is used to ascertain the level of stiffness. Using this formula, the greater the value of Young's modulus (Y), the stiffer the material is. Hardness is characterized by how much the material is resistant to changes of shape. There are three ways of exemplifying it; (i) bulk modulus, i.e. the resistance to volume changes, (ii) shear modulus, i.e. resistance against reversible deformations and (iii) Vickers hardness as

$H_V = 2(k^2S)^{0.585} - 3 \left(k = \frac{S}{B}, S - \text{shear and } B - \text{bulk modulus} \right)$ [55]. It is clear that between shear modulus and bulk modulus, shear modulus predicts hardness better [43], whilst Chen et al's recent research [55] shows that Vickers hardness represents hardness better than shear modulus. As the Voigt and Reuss equations (VRe) signify the upper and lower limits of mechanical properties [43], thermodynamic characteristics such as average sound velocity (V_m) — which consists of the longitudinal (V_l) and transversal (V_t) sound velocities — and Debye temperature (Θ_D) are

computed by using the Hill scheme which is an average of VRE.

Table 2 shows that our calculated PBE-GGA elastic constants for zinc-blende CdSe and CdTe are smaller than previous theoretical LDA calculations reported by Benyettou et al. [32]. This discrepancy between PBE-GGA and LDA calculations roots from the fact that LDA uses uniform electron gas approximations for predictions of exchange-correlation potential, while PBE-GGA improves it by adding the gradient terms of the electron density to the exchange-correlation energy of LDA [38].

For zinc-blende CdSe, our PBE-GGA elastic constants calculations compared to the theoretical calculations of Hannachi and Bouarissa [31], show a large difference for C_{11} and C_{44} while for C_{12} they are almost the same. We should emphasize that we have used FP-LAPW while Hannachi et al. have used the empirical pseudo-potential method. For zinc-blende CdTe, our calculated PBE-GGA elastic constants are in good agreement with experimental data [52] but the results of Benyettou et al. [32] within LDA are in better agreement than our PBE-GGA calculations. It is important to mention that our results and Benyettou et al. [32] results are in zero-temperature conditions whilst the experiment was conducted at 298 K. For zinc-blende CdSe_{0.5}Te_{0.5}, our PBE-GGA elastic constants are smaller than/correlating to the previous LDA calculations [32].

Our research shows us that no theoretical value for the elastic constants of zinc-blende CdSe_xTe_{1-x} ($x = 0.25$ and 0.75) is available in literature, and we thus believe that our results can serve as an important point of reference for future research.

Our Cauchy pressure ($C_{12} - C_{44} > 0$) within PBE-GGA predicts that for zinc-blende CdSe and CdTe, ionic bonds have greater dominance, which is a result consistent with the prediction of Cauchy pressure using experimental elastic constants and theoretical data. Our calculations show that $\nu = 0.364$ and $\nu = 0.334$ for zinc-blende CdSe and CdTe, respectively (see Table 2). Therefore, based on our obtained values for the Poisson's ratio, we again predict that zinc-blende CdSe and CdTe are materials with ionic bonds, consistent with our last prediction using the sign of the Cauchy pressure. Our results show that the $\left(\frac{B_H}{S_H}\right)$ ratio for zinc-blende CdSe and CdTe are 3.35 and 2.69, respectively. This means that zinc-blende CdSe is more ductile than zinc-blende CdTe.

The higher value of bulk modulus and Hill's shear modulus for zinc-blende CdSe indicates that it is harder than zinc-blende CdTe while Vickers hardness (Hill's shear modulus was used) shows that zinc-blende CdTe is harder than zinc-blende CdSe.

Hill's Young's modulus predicts that zinc-blende CdSe is stiffer than zinc-blende CdTe. Since elastic constants of zinc-blende CdSe are larger than zinc-blende CdTe, therefore CdSe is mechanically stronger than CdTe.

Our results (see Table 2) show that the mechanical and thermodynamic properties, namely C_{11} , C_{12} , Bulk modulus, Poisson's ratio, Debye temperature and longitudinal elastic wave velocity for zinc-blende CdSe_xTe_{1-x} within PBE-GGA exchange-correlation decrease monotonically but Vickers hardness increases monotonically with increasing the Te concentration. However it is not the case for C_{44} . As can be seen C_{44} is less sensitive when the Te concentration is increased.

Our Cauchy pressure ($C_{12} - C_{44} > 0$) and Poisson's ratio indicate that with increasing Te concentration the effect of ionic bonds decreases.

Bulk modulus results predict that zinc-blende CdSe is the hardest material while shear modulus calculations predict that zinc-blende CdSe_{0.5}Te_{0.5} is the hardest material for all compositions x ($x = 0, 0.25, 0.5, 0.75, 1$) of interest. But Vickers hardness (Hill's shear modulus was used) offers zinc-blende CdTe as the hardest material. Moreover our calculated Young's modulus indicates that zinc-blende CdSe_{0.5}Te_{0.5} can be considered as the stiffest material

for all values of x ($x = 0, 0.25, 0.5, 0.75, 1$). Elastic constants of zinc-blende CdSe have the largest values for all changes of x ($x = 0, 0.25, 0.5, 0.75, 1$). This means that zinc-blende CdSe is mechanically the strongest material in the zinc-blende ternary CdSe_xTe_{1-x} alloys ($x = 0, 0.25, 0.5, 0.75, 1$).

The polynomial fit (order of fit 2) of our calculated elastic constants of zinc-blende ternary CdSe_xTe_{1-x} alloys within PBE-GGA exchange-correlation as a function of x composition (see the following equations) shows that for C_{11} and C_{12} , the bowing parameters are larger than C_{44} . They suggest a non-linear relationship between elastic constants and Se concentration.

$$C_{11}(x) = -4.16x^2 + 11.536x + 46.906$$

$$C_{12}(x) = 2.48x^2 + 7.116x + 30.008$$

$$C_{44}(x) = -0.21x^2 + 1.885x + 17.988$$

As can be seen from Table 2, the Born elastic stability conditions [56] for the cubic systems [56,57] given as following are obviously satisfied by our results. From the first two conditions, we can conclude that $C_{11} > 0$. Thus, this is an extra condition which is sometimes used.

$$C_{11} - C_{12} > 0, C_{11} + 2C_{12} > 0, C_{11} > 0, C_{44} > 0$$

This means that zinc-blende ternary CdSe_xTe_{1-x} alloys within PBE-GGA exchange-correlation are mechanically stable over all the range of the Te concentration ($x = 0, 0.25, 0.5, 0.75, 1$).

Our calculated elastic constants for wurtzite CdSe_xTe_{1-x} ternary alloys within PBE-GGA exchange-correlation are collected in summary in Table 3, compared with available experimental [53] and theoretical data [33]. As far as we are aware, there are no theoretical and experimental data for the elastic constants of wurtzite CdSe_xTe_{1-x} ($x = 0.25$ and 0.75) available in the literature, thus our results are adding useful data to the field which we hope will prove useful reference material.

One can see that our results within PBE-GGA exchange-correlation agree well with the previous PBE-GGA calculation [33] for $x = 0, 0.5, 1$ and the experimental data [53]. We would like to mention that our calculated elastic constants within PBE-GGA are smaller than previous LDA calculations reported by Saib et al. [33] except for C_{55} . This inconsistency between our calculations and the experimental data of wurtzite CdSe could be attributed to our calculations being done at zero temperature, while the other experiments are done at 300K or the lack of a correct selection of exchange-correlation functional. Moreover, Table 3 shows that the results of CdSe calculated by Saib et al. [33] within LDA are in better agreement with the experimental data at 300 K.

Our Cauchy pressure ($C_{12} - C_{55} > 0$, for hexagonal compounds $C_{44} = C_{55}$) and Poisson's ratio within PBE-GGA foretell that for wurtzite CdSe and CdTe ionic bonds are more dominant which is in keeping with the expectation of Cauchy pressure using experimental elastic constants and theoretical data. As can be seen from Table 3, Bulk modulus and shear modulus of wurtzite CdSe are larger than wurtzite CdTe which predicts that CdSe is harder than CdTe, while our calculated Vickers hardness using Hill's data predicts that CdTe is harder than CdSe. Since Young's modulus of wurtzite CdSe is larger than wurtzite CdTe we can predict that wurtzite CdSe is stiffer than wurtzite CdTe. Our $\left(\frac{B_H}{S_H}\right)$ ratio for wurtzite CdSe and CdTe (2.52 and 2.25, respectively) suggest that wurtzite CdSe is more ductile than wurtzite CdTe.

It can be seen that the elastic constants of wurtzite CdSe are larger than wurtzite CdTe. This means that CdSe is mechanically stronger than CdTe which is consistent with the previous

theoretical prediction [33].

As can be seen from Table 3, it is clear that the mechanical and thermodynamic properties, namely C_{11} , approximately C_{12} , C_{33} and longitudinal elastic wave velocity for wurtzite $\text{CdSe}_x\text{Te}_{1-x}$ within PBE-GGA exchange-correlation decrease monotonically with increasing Te concentration. However C_{13} , C_{55} , Bulk modulus, shear modulus, Young's modulus and Debye temperature behave as non-monotonic.

Comparing the value of Cauchy pressure ($C_{12}-C_{55}>0$) and the value of Poisson's ratio, we can deduce that for wurtzite $\text{CdSe}_x\text{Te}_{1-x}$ ternary alloys within PBE-GGA exchange-correlation, the ionic bonds are more dominant for all compositions x ($x = 0, 0.25, 0.5, 0.75, 1$) of interest.

Our calculated Bulk modulus, shear modulus and Vickers hardness (Hill's shear modulus and bulk modulus were used) suggest that the wurtzite $\text{CdSe}_{0.75}\text{Te}_{0.25}$, CdSe and $\text{CdSe}_{0.5}\text{Te}_{0.5}$ should be the hardest material for all compositions x ($x = 0, 0.25, 0.5, 0.75, 1$), respectively.

The present values of Young's modulus (see Table 3) suggest that wurtzite CdSe can be considered the stiffest material for all changes of x ($x = 0, 0.25, 0.5, 0.75, 1$). Elastic constants of wurtzite CdSe have the largest values for all compositions x ($x = 0, 0.25, 0.5, 0.75, 1$). Thus the wurtzite CdSe is mechanically the strongest material in the wurtzite ternary $\text{CdSe}_x\text{Te}_{1-x}$ alloys ($x = 0, 0.25, 0.5, 0.75, 1$).

In the process of finding bowing parameter behaviors and linear/non-linear relationships, we have fitted our calculated elastic constants of wurtzite ternary $\text{CdSe}_x\text{Te}_{1-x}$ alloys within PBE-GGA exchange-correlation with a polynomial of degree 2 for all compositions x ($x = 0, 0.25, 0.5, 0.75, 1$). As can be seen (see the following equations) C_{11} has the largest bowing parameter from linearity and they offer a non-linear relationship between elastic constants and Se concentration.

$$C_{11}(x) = 19.08x^2 - 3.238x + 56.576$$

$$C_{12}(x) = 4.95x^2 + 4.279x + 25.532$$

$$C_{13}(x) = 8.57x^2 - 0.091x + 22.663$$

$$C_{33}(x) = -5.05x^2 + 15.763x + 61.172$$

$$C_{55}(x) = 3.09x^2 + 0.578x + 12.602$$

For hexagonal compounds, three necessary and sufficient conditions [58] for elastic stability (given as follows) are suggested which is obviously satisfied by our calculations.

$$C_{11} > |C_{12}|, \quad 2C_{13}^2 < C_{33}(C_{11} + C_{12}), \quad C_{55} > 0$$

The above three conditions means that wurtzite ternary $\text{CdSe}_x\text{Te}_{1-x}$ alloys within PBE-GGA exchange-correlation are mechanically stable for all changes of x ($x = 0, 0.25, 0.5, 0.75, 1$).

4. Conclusion

We have optimized the lattice parameters for $\text{CdSe}_x\text{Te}_{1-x}$ ternary alloys at various compositions ($x = 0, 0.25, 0.5, 0.75, 1$) for both cubic and hexagonal phases. For the wurtzite phase, we performed a two dimensional search of EOS to find the optimal lattice parameters. The zero-pressure and zero temperature mechanical and thermodynamic properties of the $\text{CdSe}_x\text{Te}_{1-x}$ ternary alloys were calculated using these parameters. Our results show that the structural parameters, namely the **a**-lattice parameter and the bulk modulus for both phases of $\text{CdSe}_x\text{Te}_{1-x}$ within the PBE-GGA

exchange-correlation increase and decrease monotonically when moving from CdSe to CdTe, respectively. Our calculations indicate that the **a**-lattice parameter for the cubic phase has minimal deviation from the linearity as a function of x composition but deviation from linearity for the wurtzite phase is larger than for the cubic phase. However the bulk modulus has large bowing parameters, which emphasize the non-linear behavior of B against x changes. For zinc-blende CdTe and wurtzite CdSe, our calculated PBE-GGA elastic constants are in good agreement with experimental data which are not at zero-temperature. Vickers hardness (Hill's shear and bulk modulus were used) suggests that zinc-blende CdTe and wurtzite $\text{CdSe}_{0.5}\text{Te}_{0.5}$ as the hardness materials for all compositions x ($x = 0, 0.25, 0.5, 0.75, 1$). Elastic constants of zinc-blende and wurtzite CdSe have the largest values for all changes of x ($x = 0, 0.25, 0.5, 0.75, 1$). This means that CdSe is mechanically the strongest material in the ternary $\text{CdSe}_x\text{Te}_{1-x}$ alloys ($x = 0, 0.25, 0.5, 0.75, 1$). The Born elastic stability conditions for both phases are obviously satisfied by our results. Thus the zinc-blende and wurtzite ternary $\text{CdSe}_x\text{Te}_{1-x}$ alloys within PBE-GGA exchange-correlation are mechanically stable over all the range of the Te concentration ($x = 0, 0.25, 0.5, 0.75, 1$). Our calculated Young's modulus indicates that zinc-blende $\text{CdSe}_{0.5}\text{Te}_{0.5}$ and wurtzite CdSe can be considered as the stiffest materials for all changes of x ($x = 0, 0.25, 0.5, 0.75, 1$). If we compare the value of Cauchy pressure ($C_{12}-C_{44}>0$) and the value of Poisson's ratio, it can be said that for both phases of $\text{CdSe}_x\text{Te}_{1-x}$ ternary alloys (in the PBE-GGA exchange-correlation), the ionic bonds are more dominant for all compositions x ($x = 0, 0.25, 0.5, 0.75, 1$) of interest. Our results exhibit a non-linear relationship between elastic constants and Se concentration.

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