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First principles study of structural, elastic and piezoelectric properties of $CdSe_xTe_{1-x}$ ternary alloys in the wurtzite structure

S Saib, S Benyettou, N Bouarissa and S Ferahtia

Laboratory of Materials Physics and its Applications, University of M`sila, 28000 M`sila, Algeria

E-mail: n_bouarissa@yahoo.fr

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Abstract

We performed density functional theory studies of the structural, elastic and piezoelectric properties of $CdSe_xTe_{1-x}$ in the wurtzite structure. The compositional dependence of such properties of interest over the whole composition range was analyzed and discussed using an *ab initio* pseudopotential approach under the virtual crystal approximation within both the local density approximation (LDA) and the generalized gradient approximation (GGA). For parent compounds, i.e. CdTe and CdSe, our findings agree well with the available data in the literature. Our results for piezoelectric properties for the alloy under load in the wurtzite structure are reported for the first time and may serve as a reference for future studies. It is found that the employment of the GGA instead of the LDA has an effect on the structural, elastic and piezoelectric parameters of the material of interest.

Keywords: structural properties, elastic properties, piezoelectric properties

(Some figures may appear in colour only in the online journal)

1. Introduction

Wide band gap II-VI compound semiconductors are expected to be one of the most vital materials for high performance optoelectronic devices such as light-emitting diodes and laser diodes operating in the blue or ultraviolet spectral region. In addition, the high ionicity of these compounds makes them good candidates for high electro-optical and electro-mechanical coupling [1, 2].

CdTe belongs to the II-VI family. It is sandwiched with calcium sulfide to form a p-n junction photovoltaic solar cell. It is suitable for thin film solar cells, infrared optics, detectors and electro-optic modulators. CdSe is also a II-VI compound semiconductor. It is an n-type semiconducting material that is transparent to infra-red light. However, p-type doping of CdSe occurs using nitrogen. It has applications for optoelectronic devices, laser diodes, biomedical imaging, nano-sensing, high-efficiencies solar cells and thin-film transistors. Both compounds of interest exist in zinc-blende and wurtzite structures or in mixed zinc-blende/wurtzite phases. Depending on the growth conditions, one can stabilize one of the two crystal structures either by epitaxial strain on proper substrates or buffer layers or by controlling the growth temperature.

By combining these two compounds that have different physical properties, one can obtain the ternary semiconductor alloy $CdSe_xTe_{1-x}$, which has new properties that are intermediate between those of CdTe and CdSe. $CdSe_xTe_{1-x}$ ternary mixed crystals have semiconducting properties, which are especially suitable for the conversion of solar energy to electrical energy in photovoltaic or photo electro-chemical devices [3, 4]. Due to the technological importance of these materials, the experimental and theoretical studies of fundamental properties of such materials have attracted much attention in recent years [5–10]. Nevertheless, as compared to the zinc-blende structure, only a few studies have been conducted for $CdSe_xTe_{1-x}$ in the wurtzite structure. This has prompted us to take such a study for wurtzite $CdSe_xTe_{1-x}$.

In the present work, we have performed an *ab initio* study based on the density functional theory (DFT) within both the LDA and the GGA under the virtual crystal approximation (VCA) so as to investigate the structural,

elastic and piezoelectric properties of $CdSe_xTe_{1-x}$ in the wurtzite structure. The alloy composition has been varied over the whole range of Se content starting from $x=0$ (CdTe) up to $x=1$ (CdSe). To the best of our knowledge, the piezoelectric properties of $CdSe_xTe_{1-x}$ ternary alloys in the wurtzite structure have been reported for the first time.

The paper is organized as follows: In section 2, a brief description of the method used and details of the calculations are given. In section 3, the results of structural, elastic and piezoelectric properties of the material in question are presented and analyzed. A conclusion is drawn in the last section.

2. Computational details

To perform DFT calculations, we use the norm conserving Troullier and Martins [11] pseudopotentials for the interactions of the electrons and the ion cores, together with the LDA for exchange and correlation in the scheme of Ceperley–Alder [12] as parameterized by Perdew and Zunger [13] and the GGA with the Perdew *et al* [14] form. The electronic wave functions are expanded in a plane wave basis set with the energy cut-off of 140 Ry, which was found to be enough for the convergence of the total energy to an accuracy of about 1 mRy per formula unit. For the Brillouin zone sampling, $10\times10\times8$ Monkhorst and Pack [15] meshes were used for both CdTe and CdSe compound semiconductors. These meshes ensure a convergence of total energy to less than 1 meV/atom.

All the calculations are implemented through the abinit code [16]. The pseudoatom calculations are performed for Cd 4d10 5s2, Se 4s2 4p4 and Te 5s2 5p4. The elastic constants are determined by computing the energy response of the system with respect to the strain perturbation [17]. The piezoelectric tensor components e_{ij} are calculated from the second derivatives of the total energy with respect to strain and the electric field [17], all of which are obtained from the density functional perturbation theory [18]. The treatment of the alloy system of interest is based on the VCA.

3. Results and discussion

3.1. Structural properties

The equilibrium structural parameters, namely a, c, u, B and $B`$, are computed by minimizing the crystal total energy calculated for different values of lattice constants and fitting to the Murnaghan`s equation of state. Our results regarding these parameters for wurtzite $CdSe_xTe_{1-x}$ ternary alloys at various compositions x are listed in table 1. Also shown for comparison are the available experimental and theoretical data reported in the literature. Note that for wurtzite CdTe ($x=0$), our LDA-calculated a and c are slightly underestimated with respect to the experiment [19]. This is not the case when using GGA where our determined values are overestimated with respect to the experiment [19]. The results are consistent with the general trends of the DFT-LDA and DFT-GGA approaches [22]. In terms of theoretical calculations, our LDA results are closer to the experiment [19] than those reported in [9] using an all electron full potential linearized augmented plane wave method. For $x=0.50$, our LDA results are compared to those of [9] and are found to be smaller. However, one can notice that our GGA calculated results agree well with those of [9]. In regard to B, our LDA-obtained value seems to be larger than that of [9]. Nevertheless, our GGA value agrees to within a few percent with that of [9]. For the compositions $x=0.3$ and $x=0.7$, our results are predictions and may serve as a reference for future studies. For wurtzite CdSe ($x=1$), our LDA results regarding a and c agree to within a few percent within the experimental values reported in [20]. Moreover, they show better agreement with the experiment than the theoretical values computed in [9]. However, our GGA results are overestimated with respect to the experiment [20]. The same conclusion can be drawn for the bulk modulus where the deviation between our LDA calculation and the experiment is less than 3%. The deviation seems to be larger when using the GGA approach instead of the LDA one. In the wurtzite configuration, which is not fixed by any symmetry consideration [22] at the ideal values $u_0=\frac{3}{8}$ and $(c/a)_0=\sqrt{\frac{8}{3}}$, all four nearest-neighbor distances are equal, and all bond angles are ideal tetrahedral angles. The computed u in the present work is in very good agreement with the experimental one reported in [21].

The composition dependence of the structural parameters, namely a, c and u for wurtzite $CdSe_xTe_{1-x}$ using the LDA approach, is shown in figure 1. We observe that both parameters a and c decrease monotonically when proceeding from wurtzite CdTe to wurtzite CdSe. This is not the case for u where the variation is non-monotonic. It decreases first when going from $x=0$ up to $x=0.2$, then it increases slightly from $x=0.2$ to $x=0.6$ and rapidly from $x=0.6$ up to $x=1$. The fit of our data regarding a and c parameters by a least-squares procedure has given the following analytical expressions:

$$a(x) = 4.48 - 0.11x - 0.10x^2 \quad (1)$$

$$c(x) = 7.36 - 0.18x - 0.20x^2 \quad (2)$$

where a and c are expressed in angstroms. The quadratic terms in equations (1) and (2) stand for the lattice constant bowing parameters. Their values indicate that these two parameters exhibit a small deviation from Vegard`s law, i.e. from the linearity. The small deviation can be due to the small lattice mismatch between the end binary compounds of the alloy of interest. Such a deviation from Vegard`s rule has also been reported for other II-VI semiconducting ternary alloys [23].

The variation of the bulk modulus as a function of the alloy composition x for wurtzite $CdSe_xTe_{1-x}$ using the LDA approach is displayed in figure 2. Note that the bulk modulus increases monotonically and non-linearly with increasing the alloy composition x, thus exhibiting a large bowing parameter. This suggests that the alloy under load becomes less compressible as far as the composition x becomes larger. Our

Table 1. Equilibrium constants a and c along with their ratio c/a, internal parameter u, bulk modulus B and its pressure derivative B' for wurtzite-$CdSe_xTe_{1-x}$ alloys ($0 \leqslant x \leqslant 1$).

Alloy composition x	$a(A^0)$	$c(A^0)$	(c/a)	(u)	$B(GPa)$	B'
0	4.48[a]	7.360[a]	1.6427[a]	0.3743[a]	46.36[a]	4.89[a]
	4.69[b]	7.70[b]	1.6399[b]	0.3746[b]	38.70[b]	
	4.68[c]	7.65[c]			34.621[c]	
	4.57[d]	7.47[d]				
0.3	4.44[a]		1.6421[a]	0.3741[a]	47.88[a]	4.69[a]
0.5	4.40[a]		1.6413[a]	0.3742[a]	49.42[a]	4.69[a]
	4.43[b]		1.6317 [b]	0.3758[b]	41.98[b]	
	4.437[c]		1.6811[c]		39.135[c]	
0.7	4.36[a]		1.6378[a]	0.3750[a]	51.54[a]	4.69[a]
1	4.27[a]	6.980[a]	1.6349[a]	0.3756[a]	56.45[a]	4.68[a]
	4.56[b]	7.46 [b]	1.6360[b]	0.3752[b]	50.90[b]	
	4.34[c]	7.27[c]		0.3759[f]	43.635[c]	
	4.3[e]	7.01[e]			55[e]	

[a] This work LDA;
[b] This work GGA;
[c] Theor. [9];
[d] Exp. [19];
[e] Exp. [20];
[f] Exp. [21].

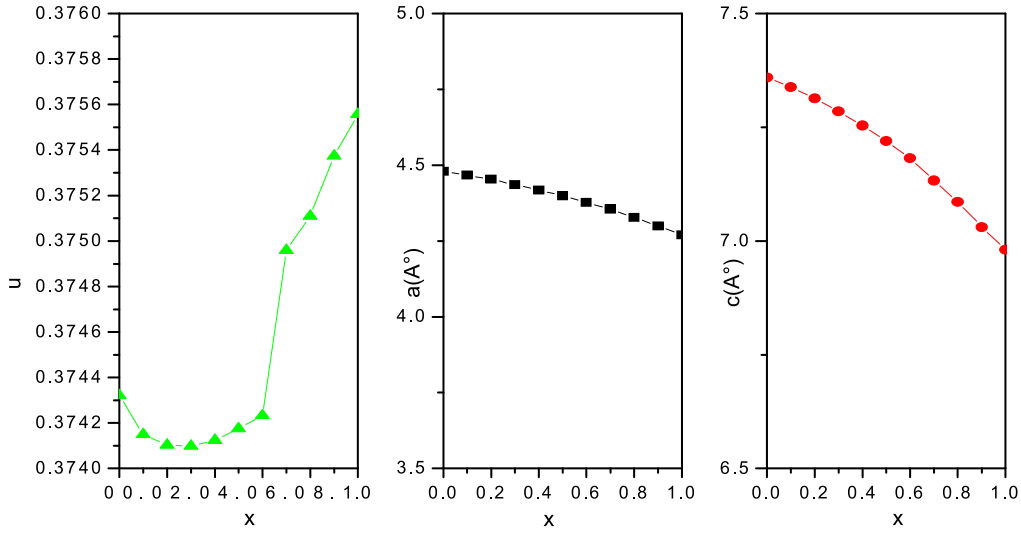

Figure 1. Lattice parameters a and c and internal parameter u versus alloy composition x for wurtzite-$CdSe_xTe_{1-x}$ using the LDA approach.

obtained LDA data for B are fitted by a least-squares procedure, giving the following analytical expression:

$$B(x) = 46.48 + 1.87x + 7.93x^2 \quad (3)$$

where B is expressed in GPa. The large value of the bulk modulus bowing parameter confirms the non-linear behavior of B versus x.

3.2. Elastic constants and related properties

Elastic properties of a solid are important because they are related to various fundamental solid state properties such as interatomic potentials, equation of state and phonon spectra. The elastic properties of a hexagonal crystal are described by five independent elastic constants: C_{11}, C_{12}, C_{13}, C_{33} and C_{44}. In the present work, the elastic constants of the material in question are calculated for various compositions of x ranging from 0 to 1. Our results are given in table 2. Also shown for comparison are the available experimental and previous theoretical data reported in the literature. We observe that for wurtzite CdTe ($x=0$), our LDA results agree reasonably well with the theoretical data reported by Martin [25]. The situation seems to be different for our GGA results, which are underestimated with respect to those of [25]. This is not the case when comparing our LDA results with the theoretical values reported by Yadawa [24], where one can note that except for C_{11} and C_{44}, our Cs are much larger than those of [24]. For wurtzite CdSe ($x=1$), our LDA results seem to agree with the experimental ones reported in [26] to within 8% and deviate from the theoretical calculation reported recently by Sarasamak *et al* [27] by less than 10%. As compared to LDA,

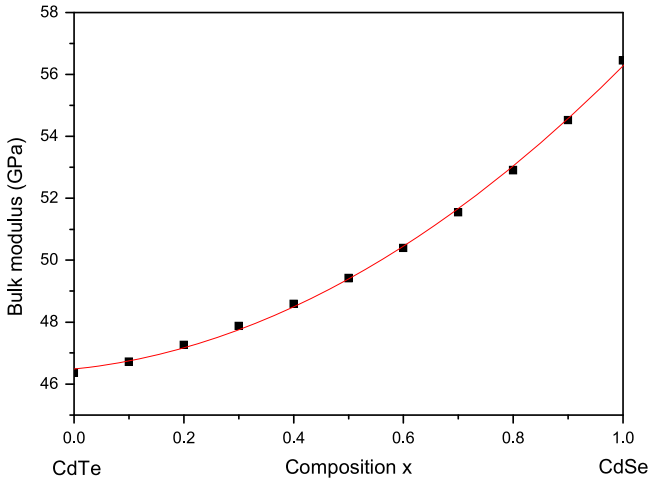

Figure 2. Bulk modulus versus alloy composition x for wurtzite-$CdSe_xTe_{1-x}$ using the LDA approach.

our results obtained by the GGA approach deviate much more from those of [26, 27]. In regard to $CdSe_xTe_{1-x}$ $(0<x<1)$, no data are so far available in the literature for Cs to the best of our knowledge; hence, our results may serve as a reference for future studies.

We define β as the relative change of the c-axis as a function of the deformation of the a-axis. Thus, $\frac{1}{\beta}$ indicates the anisotropy of linear compressibility along the c-axis, with respect to the a-axis, and a value of 1.0 implies the isotropic compressibility. $\frac{1}{\beta}$ can be written as [28]

$$\frac{1}{\beta} = \frac{(C_{33} - C_{13})}{(C_{11} + C_{12} - 2C_{13})} \tag{4}$$

According to our results (see table 2) obtained from both the LDA and GGA approaches, all the anisotropy of linear compressibility are larger than 1. Nevertheless, one can note that $\frac{1}{\beta}$ of wurtzite-CdSe is smaller than that of wurtzite-CdTe. Thus, as one proceeds from wurtzite-CdTe $(x=0)$ to wurtzite-CdSe $(x=1)$, the material of interest tends to have an isotropic compressibility, especially for higher Se concentrations.

The variation of the elastic constants as a function of the alloy composition x for wurtzite $CdSe_xTe_{1-x}$ using the LDA approach is plotted in figure 3. Note that except for C_{44}, all the remaining C_{ij} `s increase with increasing the composition x. The increase is monotonic and non-linear. The elastic constant C_{44} decreases with increasing x. The behavior of C_{44} is also monotonic. Furthermore, one can note that the elastic constants of wurtzite CdSe are larger than those of wurtzite CdTe. This suggests that wurtzite CdSe is mechanically stronger than wurtzite CdTe. For all compositions x of interest, the values of C_{44} are smaller than those of C_{11} and C_{33}. This reflects the weak resistance to shear deformation compared to the compressional deformations. Our data concerning Cs are fitted by a least-squares procedure, giving the following analytical expressions:

$$C_{11}(x) = 69.14 - 2.31x + 11.79x^2 \tag{5a}$$

$$C_{12}(x) = 38.19 + 3.62x + 6.86x^2 \tag{5b}$$

$$C_{13}(x) = 30.93 + 4.21x + 6.19x^2 \tag{5c}$$

$$C_{33}(x) = 81.41 - 0.84x + 8.46x^2 \tag{5d}$$

$$C_{44}(x) = 13.21 - 1.75x + 2.00x^2 \tag{5e}$$

The determination of elastic constants makes it possible to proceed with the bulk sound speeds, as follows [29]:

The shear wave speed (v_s) and compressional wave speed (v_p) are determined as

$$v_s = \left(\frac{G}{\rho}\right)^{\frac{1}{2}} \tag{6}$$

where

$$G = \left(G_V + G_R\right)/2 \tag{7}$$

with

$$\begin{cases} G_V = \dfrac{C_{11} - C_{12} + 3C_{44}}{5} \\ G_R = \dfrac{5C_{44}\left(C_{11} - C_{12}\right)}{4C_{44} + 3\left(C_{11} - C_{12}\right)} \end{cases} \tag{8}$$

and ρ is the density.

$$v_p = \left(\frac{3B + 4G}{3\rho}\right)^{\frac{1}{2}} \tag{9}$$

where B represents the bulk modulus, which can be obtained as

$$B = \frac{\left(C_{11} + C_{12}\right)C_{33} - 2\,C_{13}^2}{C_{11} + C_{12} + 2C_{33} - 4C_{13}} \tag{10}$$

The knowledge of v_s and v_p may allow one to calculate the average sound speed v_m through the relation

$$v_m = \left[\frac{1}{3}\left(\frac{2}{v_s^3} + \frac{1}{v_p^3}\right)\right]^{-\frac{1}{3}} \tag{11}$$

The sound velocities as calculated from these relations for wurtzite-$CdSe_xTe_{1-x}$ $(0 \leqslant x \leqslant 1)$ using the LDA approach are given in table 3. Due to the lack of both experimental and theoretical data in the literature regarding these parameters for wurtzite-$CdSe_xTe_{1-x}$, to the best of the authors knowledge, our results are only for a reference which would be beneficial to verify experimentally. In figure 4, we display the dependence of the sound velocities, namely v_s, v_p and v_m on the alloy composition x of wurtzite-$CdSe_xTe_{1-x}$ using the LDA approach. Note that all the parameters of interest increase monotonically with increasing the alloy composition x upon going from CdTe $(x=0)$ to CdSe $(x=1)$. Since the sound velocities are directly derived from the elastic constants, one would expect a similar qualitative behavior. However, this behavior is slightly different because of the mass density involved in the sound velocity, which changes as a function of the alloy composition x.

Table 2. Elastic constants (C_{11}, C_{12}, C_{13}, C_{33} and C_{44}) and anisotropy of linear compressibility ($1/\beta$) for wurtzite-$CdSe_xTe_{1-x}$ alloys ($0 \leqslant x \leqslant 1$).

Alloy composition x	$C_{11}(GPa)$	$C_{12}(GPa)$	$C_{13}(GPa)$	$C_{33}(GPa)$	$C_{44}(GPa)$	$1/\beta$
0	68.93[a]	38.09[a]	30.82[a]	81.10[a]	13.17[a]	1.11[a]
	51.99[b]	27.99[b]	22.17[b]	60.34[b]	10.61[b]	1.07[b]
	63.96[c]	15.71[c]	13.66[c]	65.70[c]	16.38[c]	
	62.2[d]	35.9[d]	29.1[d]	68.9[d]	13.1[d]	
0.3	69.72[a]	40.01[a]	32.87[a]	82.14[a]	12.91[a]	1.12[a]
0.5	70.94[a]	41.72[a]	34.60[a]	83.21[a]	12.83[a]	1.12[a]
	53.88[b]	30.37[b]	24.53[b]	61.84[b]	10.56[b]	1.06[b]
0.7	73.15[a]	44.00[a]	36.79[a]	84.49[a]	12.95[a]	1.09[a]
1	78.88[a]	48.81[a]	41.48[a]	89.48[a]	13.51[a]	1.07[a]
	62.76[b]	36.39[b]	30.17[b]	70.36[b]	11.93[b]	1.04[b]
	74.1[e]	45.2[e]	39.3[e]	83.6[e]	13.17[e]	
	80[f]	47[f]	40[f]	92[f]	15[f]	

[a] This work LDA;
[b] This work GGA;
[c] Theor. [24];
[d] Theor. [25];
[e] Exp. [26];
[f] Theor. [27].

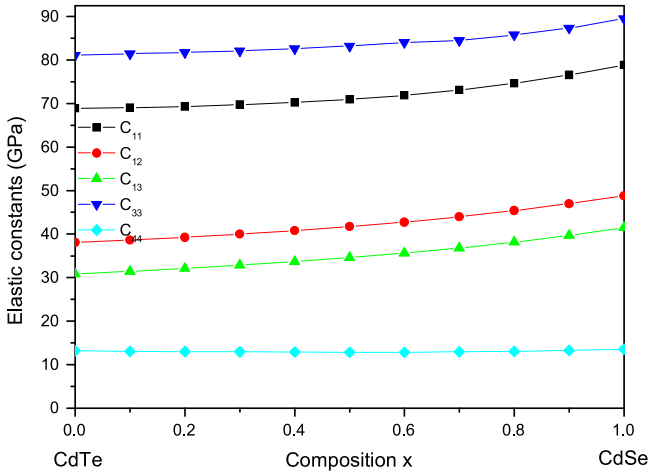

Figure 3. Elastic constants versus alloy composition x for wurtzite-$CdSe_xTe_{1-x}$ using the LDA approach.

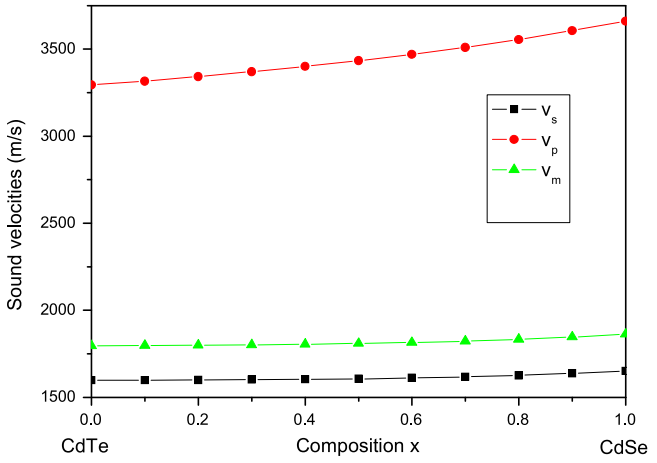

Figure 4. Shear wave speed (v_s), compressional wave speed (v_p) and average sound speed (v_m) versus alloy composition x for wurtzite-$CdSe_xTe_{1-x}$ using the LDA approach.

Table 3. Calculated (this work) shear wave speed (v_s), compressional wave speed (v_p), average sound speed (v_m) and Debye temperature (θ_D) for wurtzite-$CdSe_xTe_{1-x}$ alloys ($0 \leqslant x \leqslant 1$) using the LDA approach.

Alloy composition x	v_s (m s^{-1})	v_p (m s^{-1})	v_m (m s^{-1})	$\theta_D(K)$
0	1598.05	3294.34	1795.78	168.42
0.3	1601.65	3370.82	1801.78	170.71
0.5	1606.77	3433.46	1808.91	172.87
0.7	1617.89	3509.63	1822.74	176.09
1	1651.97	3661.09	1862.93	183.82

We have also determined the Debye temperature (θ_D) using the expression [29]

$$\theta_D = \frac{h}{k_B}\left(\frac{3n}{4\pi\ V}\right)^{\frac{1}{3}} v_m \tag{12}$$

where h, k_B, n and V are the Planck`s constant, the Boltzmann`s constant, the number of atoms in the unit cell and the volume of the unit cell.

Our LDA results concerning θ_D for wurtzite-$CdSe_xTe_{1-x}$ ternary alloys at various compositions x are listed in table 3.

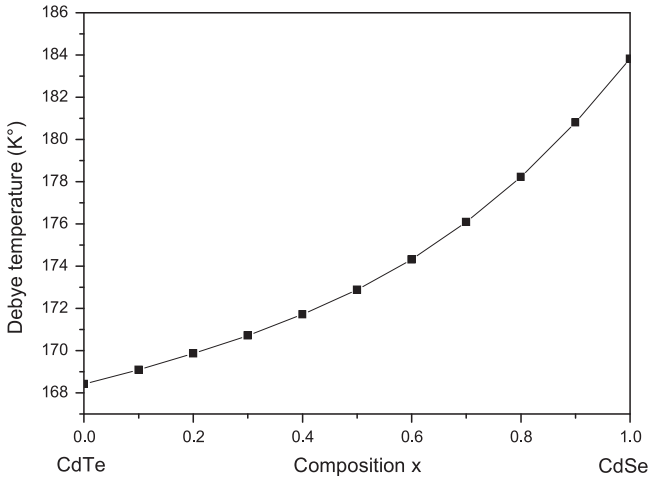

Figure 5. Debye temperature versus alloy composition x for wurtzite-$CdSe_xTe_{1-x}$ using the LDA approach.

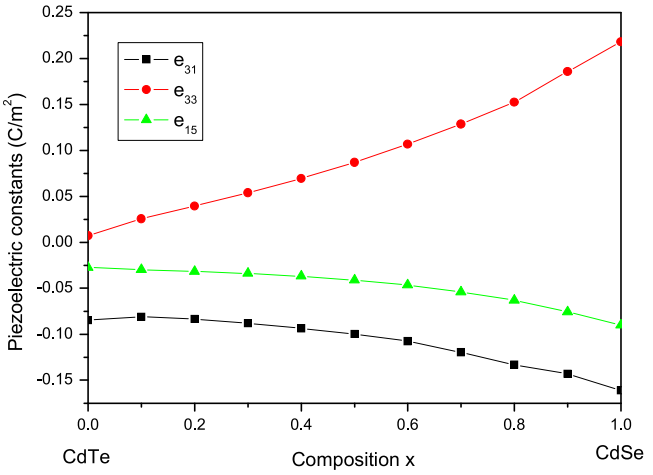

Figure 6. Piezoelectric constants versus alloy composition x for wurtzite-$CdSe_xTe_{1-x}$ using the LDA approach.

Table 4. Piezoelectric constants for wurtzite-$CdSe_xTe_{1-x}$ alloys ($0 \leqslant x \leqslant 1$).

Alloy composition x	e_{31} (C m^{-2})	e_{33} (C m^{-2})	e_{15} (C m^{-2})
0	−0.085[a]	0.007[a]	−0.027[a]
	−0.026[b]	−0.036[b]	0.007[b]
0.3	−0.088[a]	0.054[a]	−0.034[a]
0.5	−0.010[a]	0.087[a]	−0.041[a]
	−0.042[b]	0.007[b]	0.005[b]
0.7	−0.120[a]	0.129[a]	−0.054[a]
1	−0.161[a]	0.218[a]	−0.090[a]
	−0.090[b]	0.127[b]	−0.047[b]
	−0.160[c]	0.347[c]	−0.138[c]

[a] This work LDA;
[b] This work GGA;
[c] Known data from [31].

Once again our results are only for a reference for future studies. In figure 5, the Debye temperature for the wurtzite-$CdSe_xTe_{1-x}$ is plotted against the alloy composition x using the LDA approach. Note that as one goes from wurtzite-CdTe to wurtzite–CdSe, θ_D increases monotonically and non-linearly, thus giving more diverse opportunities for obtaining θ_D by varying the alloy composition x.

3.3. Piezoelectric properties

Tetrahedral semiconductors of the II-VI type are within the piezoelectric materials which have attracted interest for computational studies [30]. Three independent non-zero piezoelectric constants, namely e_{31}, e_{33} and e_{15} in the hexagonal wurtzite phase, characterize the full piezoelectric tensors of such crystals. The calculated e_{ij} are listed in table 4 and compared to previous data, which are only available for wurtzite CdSe [31]. Note that for wurtzite CdSe, our calculated e_{31} using the LDA approach is in excellent agreement with that reported in [31]. In addition, the agreement between our LDA computed e_{15} and that reported in [31] is reasonable. However, a somewhat larger discrepancy between our LDA calculated e_{33} and that of [31] can be noticed. On the other hand, our GGA results are largely different from those of [31]. Considering the well-known experimental uncertainties in the measurement of piezoelectric constants, one can conclude that our LDA findings are in reasonable agreement with the experiment [31].

The variation of the piezoelectric constants as a function of the alloy composition x in the wurtzite-$CdSe_xTe_{1-x}$ using the LDA approach is shown in figure 6. We observe that as x increases upon going from 0 to 1, both piezoelectric constants e_{31} and e_{15} decrease. This can be traced back to the ionic contribution that tends to prevail over the electronic 'clamped-ion' term as the anion becomes lighter. A similar trend has been reported by Barnardini *et al* [32] for III-V nitrides. The situation is quite different for e_{33}, which increases with increasing x. The behaviour exhibited by all piezoelectric constants is monotonic and non-linear. Interestingly, one can note that e_{33} of wurtzite-CdSe is larger than that of wurtzite-CdTe. This is closely related to the difference of the electric polarizability between Se and Te atoms. Another interesting trend is the connection between the chemical nature of the anion and the piezoelectric constant. The fit of our LDA data by a least-squares procedure gives the following analytical expressions:

$$e_{31}(x) = -0.083 + 0.011x - 0.089x^2 \quad (13a)$$

$$e_{33}(x) = 0.013 + 0.096x + 0.106x^2 \quad (13b)$$

$$e_{15}(x) = -0.030 + 0.013x - 0.071x^2 \quad (13c)$$

4. Conclusion

In conclusion, we have presented *ab initio* plane-wave pseudopotential calculations of structural, elastic and piezoelectric properties of the wurtzite-$CdSe_xTe_{1-x}$ ternary alloys. Our calculations were mainly based on the DFT within the LDA and GGA approaches under the VCA. The compositional dependence of the properties of interest over the whole compositional range from wurtzite-CdTe to wurtzite-CdSe

has been examined and discussed. Generally, the agreement between our LDA results and the available experimental and previous theoretical data reported in the literature was found to be reasonably good. Our GGA results differ from those of the LDA ones, thus suggesting that the use of the GGA approach affects our findings of structural, elastic and piezoelectric parameters of the material of interest. For most concentrations of the alloy under load, our findings are predictions and may serve for a reference for future studies. In most cases, the studied features exhibited a monotonic behavior with the alloy composition x. All the investigated parameters were expressed by a quadratic function of the alloy composition x considering the bowing parameter.

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