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Structural, electronic, elastic and optical properties of $\text{Cd}_x\text{Zn}_{1-x}\text{Te}$ mixed crystals

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Abstract

The structural, electronic, elastic and optical properties of $\text{Cd}_x\text{Zn}_{1-x}\text{Te}$ ternary mixed crystals are investigated by the first-principles plane-wave pseudopotential method within the LDA approximations. Basic physical properties, such as lattice constant, bulk modulus, second-order elastic constants (C_{ij}) and the electronic band structures, are calculated. We also predict the shear modulus, Young's modulus and Poisson's ratio. Moreover, we have calculated the optical properties (dielectric functions, refractive index, extinction coefficient and energy loss function) of these ternary mixed crystals. Our results agree well with the available data in the literature.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Cadmium and zinc chalcogenides (S, Se and Te) which are members of the II–VI semiconductor group, and due to their direct and rather large bandgap, are technologically important materials. Their mixed II–VI ternary semiconductors are used in optoelectronic devices ranging from the blue to near-ultraviolet spectral region [1]. These materials are also used to fabricate x-ray and γ -ray detectors [2–4]. Cd-based compounds can be used as an alternative material for short and medium wavelength infrared focal plane arrays [4, 5].

$\text{Zn}_x\text{Cd}_{1-x}\text{Te}$ mixed crystals have been the subject of several experimental and theoretical studies recently and in the past decades. Polit *et al* [6] have analysed the phonon spectra of the $\text{Zn}_x\text{Cd}_{1-x}\text{Te}$ solid solution. Ammar [7] studied some structural and optical properties of $\text{Cd}_x\text{Zn}_{1-x}\text{Te}$ thin films. de Paiva [8] calculated the effective mass parameters of $\text{Cd}_x\text{Zn}_{1-x}\text{Te}$ alloys by using the *ab initio* method. Park *et al* [9] studied the interface disorder of $\text{Cd}_x\text{Zn}_{1-x}\text{Te}/\text{ZnTe}$ multiple quantum wells grown by using molecular-beam epitaxy.

Hitherto, to the best of our knowledge, no systematic research on the structural elastic, electronic and optical properties of $\text{Cd}_x\text{Zn}_{1-x}\text{Te}$ mixed crystals has been reported. An accurate description of the electronic, elastic and optical properties for the present solids is extremely important because these play significant roles in determining some material properties such as interatomic forces, phase transition, transport coefficients and electron–photon interactions. Also,

the electronic structure and optical properties of semiconductor alloys are important for guiding the successful design and fabrication of optoelectronic devices [6].

In this work, we have aimed to provide some additional information to the existing data on the physical properties of $\text{Cd}_x\text{Zn}_{1-x}\text{Te}$ mixed crystals by using the first-principles plane-wave pseudopotential method, and we have especially focused on the electronic and optical properties. We also present our other results on the structural and elastic properties for $\text{Cd}_x\text{Zn}_{1-x}\text{Te}$ mixed crystals. The obtained results are compared with the previous theoretical calculations and available experimental findings.

2. Method of calculation

The calculations have been performed by using the plane-wave pseudopotential approach to the density functional theory (DFT) by the Cambridge Sequential Total Energy Package (CASTEP) code [10]. The electronic wavefunctions were obtained by using a density-mixing minimization method for the self-consistent field (SCF) calculation, and the structures were relaxed by using the Broyden, Fletcher, Goldfarb and Shannon (BFGS) method [11]. It solves the quantum mechanical equation for the electrons within the density functional approach in the local-density approximation (LDA). For LDA, the exchange–correlation functional of Ceperley and Adler [12], as parametrized by Perdew and Zunger [13], is used.

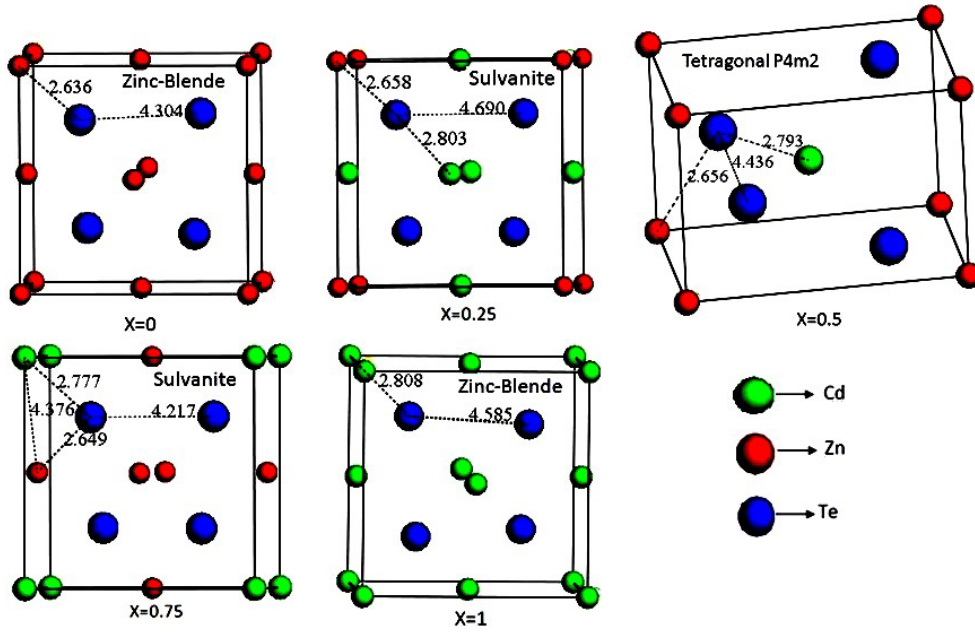


Figure 1. Crystal structures and bond length of $Cd_xZn_{1-x}Te$ ($x = 0, 0.25, 0.5, 0.75, 1.0$).

Table 1. Bond length of $Cd_xZn_{1-x}Te$.

	Structure	Reference	Zn-Te (Å)	Te-Cd (Å)	Te-Te (Å)
CdTe	Zinc-blende	Present		2.808	4.585
		expt. ^a		2.795 ^a	
$Cd_{0.75}Zn_{0.25}Te$	Sulvanite	Present	2.658	2.803	4.217
$Cd_{0.5}Zn_{0.5}Te$	Tetragonal $p4m2$	Present	2.656	2.793	4.436
$Cd_{0.25}Zn_{0.75}Te$	sulvanite	Present	2.649	2.277	4.690
ZnTe	Zinc-blende	Present	2.636		4.304
		expt. ^a	2.655 ^a		

^a Reference [15].

Table 2. Calculated equilibrium lattice constants (a_0), bulk modulus (B), cell volume (V) and other experimental and theoretical works for $Cd_xZn_{1-x}Te$.

	Structure	Reference	a_0 (Å)	b_0 (Å)	c_0 (Å)	V (Å ³)	B (GPa)	
CdTe	Zinc-blende	Present	6.48			272.70	45.52	
		Theory ^a	6.48				48.94	
		Theory ^b	6.48					
		Theory ^c	6.48					41.7
		Theory ^d	6.44					46.6
		Expt. ^e	6.48					44.5
$Cd_{0.75}Zn_{0.25}Te$	Sulvanite	Present	6.38			260.37	47.29	
$Cd_{0.5}Zn_{0.5}Te$	Tetragonal $p4m2$	Present	4.4	4.4	6.31	124.30	49.08	
$Cd_{0.25}Zn_{0.75}Te$	Sulvanite	Present	6.18			236.97	51.18	
ZnTe	Zinc-blende	Present	6.08			225.54	53.68	
		Theory ^f	6.04				55	
		Theory ^g	6.00				55.21	
		Theory ^b	6.08					
		Expt. ^h	6.1					52.8
		Expt. ⁱ	6.06					52.8

^a Reference [16]; ^b reference [17]; ^c reference [18]; ^d reference [19]; ^e reference [20];

^f reference [21]; ^g reference [22]; ^h reference [23]; ⁱ reference [24].

The tolerances for geometry optimization were set as the difference in total energy being within 5×10^{-6} eV/atom, the maximum ionic Hellmann–Feynman force within 0.01 eV \AA^{-1} , the maximum ionic displacement within 5×10^{-4} Å and the maximum stress within 0.02 GPa. The interactions between electrons and core ions are simulated with separable Troullier–Martins [14] norm-conserving pseudopotentials. The wavefunctions are expanded in the plane waves up to a kinetic-energy cutoff of 660 eV. In this paper, the k -points of $6 \times 6 \times 4$ for $x = 0.5$ and $4 \times 4 \times 4$ for the other composition x , which are in the Monkhorst and Pack scheme, are used.

3. Results and discussion

3.1. Structural and electronic properties

The calculated most probable crystal structures and bond lengths for $\text{Cd}_x\text{Zn}_{1-x}\text{Te}$ are given in table 1 and figure 1. Our results for CdTe and ZnTe are completely compatible with the literature [15]. As the composition x increases, it can be seen from table 1 and figure 1 that the bond lengths of Zn–Te and Te–Cd almost remain unchanged except for $x = 0.25$ of Te–Cd, where the bond length (2.277 Å) significantly decreases. The bond lengths between the Te–Te atoms almost linearly increase as the composition x ($x = 0.25, 0.50$ and 0.75) increases.

Table 2 shows the calculated lattice constants, cell volume and bulk modulus for each x of $\text{Cd}_x\text{Zn}_{1-x}\text{Te}$ along with the other experimental and theoretical values [18, 19]. The lattice parameters are found to be 6.48, 6.38, 4.4, 6.18 and 6.08 Å for $\text{Cd}_x\text{Zn}_{1-x}\text{Te}$ compounds ($x = 0, 0.25, 0.5, 0.75$ and 1), respectively. The calculated lattice constants are higher (about 1%) for CdTe and ZnTe compounds than the other theoretical findings in [19, 21, 22]. Our lattice constant for ZnTe is 1% higher than the experimental value of [23] and 1% smaller than the other experimental finding in [24]. These small differences may stem from the different density-functional-based electronic structure methods. The CdTe has the largest lattice constant (6.48 Å) and $\text{Cd}_{0.5}\text{Zn}_{0.5}\text{Te}$ has the smallest (4.4 Å) one for $\text{Cd}_x\text{Zn}_{1-x}\text{Te}$.

In the present case the calculated bulk modulus for $x = 0, 0.25, 0.5, 0.75$ and 1 are 45.52, 47.29, 49.08, 51.18 and 53.68 GPa for $\text{Cd}_x\text{Zn}_{1-x}\text{Te}$, respectively. The largest value of bulk modulus (53.68 GPa) is for ZnTe; consequently, it is a less compressible one. It is seen that the compressibility, according to the decreasing value of x , is changing in the following sequence:

$$\text{CdTe} > \text{Cd}_{0.75}\text{Zn}_{0.25}\text{Te} > \text{Cd}_{0.5}\text{Zn}_{0.5}\text{Te} > \text{Cd}_{0.25}\text{Zn}_{0.75}\text{Te} > \text{ZnTe}.$$

We have predicted the band structure for $\text{Cd}_x\text{Zn}_{1-x}\text{Te}$ along the high symmetry directions in the first Brillouin zone from the calculated equilibrium lattice constant. Figure 2 shows the band structures and corresponding electronic density of state (DOS) for all compositions studied. All these mixed crystals have a direct bandgap along the direction and the obtained results are listed in table 3 along with the other

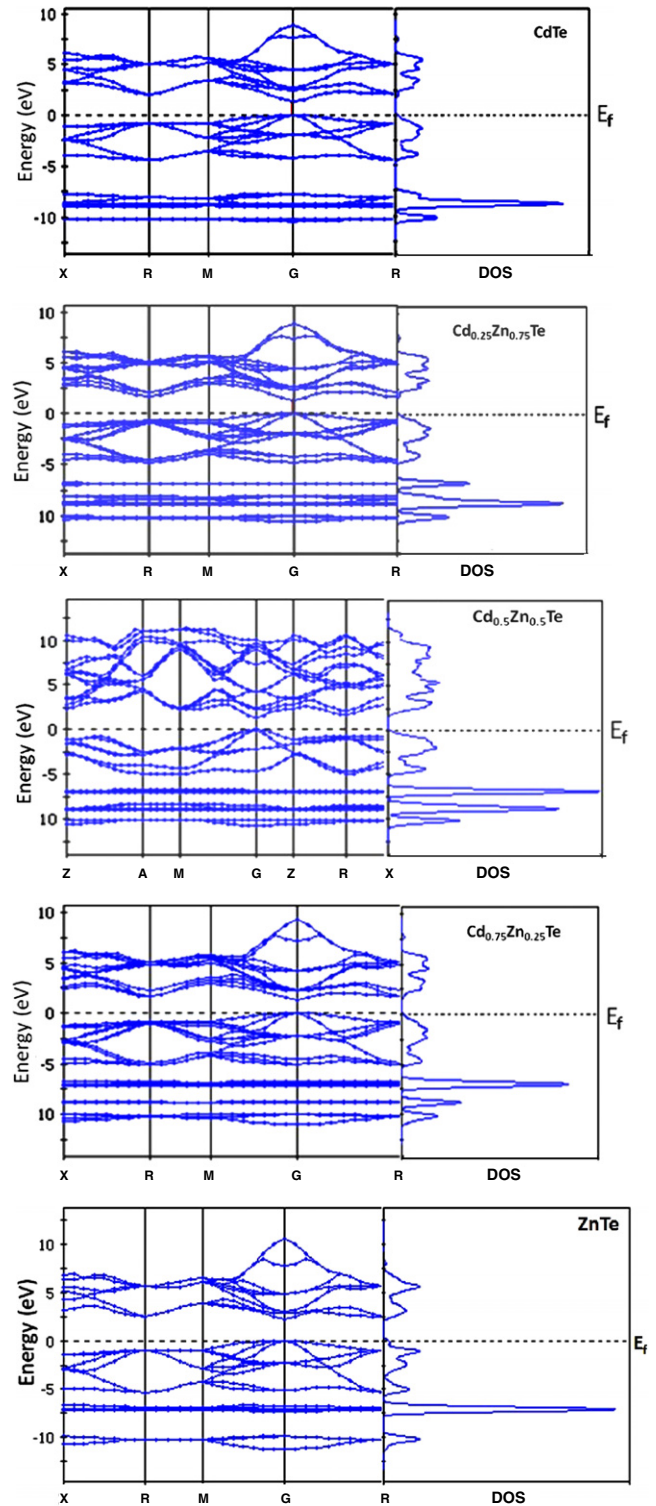


Figure 2. Calculated band structure and DOS of $\text{Cd}_x\text{Zn}_{1-x}\text{Te}$ versus the composition x . The position of the Fermi level is at 0 eV.

theoretical data [16–19, 21, 22]. The band profiles and bandgap values are in good agreement with the earlier works. The energies of the bandgaps versus the composition x (0, 0.25, 0.5, 0.75 and 1) for $\text{Cd}_x\text{Zn}_{1-x}\text{Te}$ are shown in figure 3. It is seen that the energies exhibit a small increasing trend with composition $x = 0.25, 0.5$ and 0.75 .

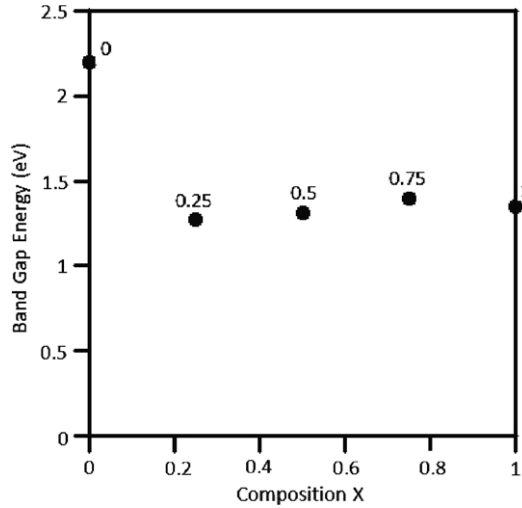


Figure 3. Bandgap energies of $Cd_xZn_{1-x}Te$.

Table 3. Bandgap energies of $Cd_xZn_{1-x}Te$.

	Structure	Reference	E_g (eV)
CdTe	Zinc-blende	Present	1.35
		Theory ^a	1.35
		Theory ^b	1.88
		Expt. ^c	1.60, 2.55
$Cd_{0.75}Zn_{0.25}Te$	Sulvanite	Present	1.40
$Cd_{0.5}Zn_{0.5}Te$	Tetragonal $p4m2$	Present	1.31
$Cd_{0.25}Zn_{0.75}Te$	Sulvanite	Present	1.27
ZnTe	Zinc-blende	Present	2.2
		Theory ^d	2.27
		Theory ^e	2.06
		Expt. ^f	2.39
		Expt. ^g	2.26
		Expt. ^h	2.2

^a Reference [25]; ^b reference [16]; ^c reference [20];

^d reference [25]; ^e reference [26]; ^f reference [27];

^g reference [28]; ^h reference [29].

3.2. Elastic properties

The elastic constants of solids provide a link between the mechanical and dynamical behaviour of crystals, and give important information concerning the nature of the forces operating in solids. In particular, they provide information on the stability and stiffness of materials, and their *ab initio* calculation requires precise methods. Since the forces and the elastic constants are functions of the first-order and second-order derivatives of the potentials, their calculation will provide a further check on the accuracy of the calculation of forces in solids. The second-order elastic constants (C_{ij}) are calculated by using the ‘volume-conserving’ technique [34, 35] and the findings are given in table 2.

For a stable tetragonal structure, while the six independent elastic constants C_{ij} (C_{11} , C_{12} , C_{13} , C_{33} , C_{44} and C_{66}) should satisfy the well-known Born–Huang criteria for stability [36]:

$$C_{11} > 0, \quad C_{33} > 0, \quad C_{44} > 0, \quad C_{66} > 0,$$

$$(C_{11} - C_{12}) > 0, \quad (C_{11} + C_{33} - 2C_{13}) > 0,$$

$$[2(C_{11} + C_{12}) + C_{33} + 4C_{13}] > 0,$$

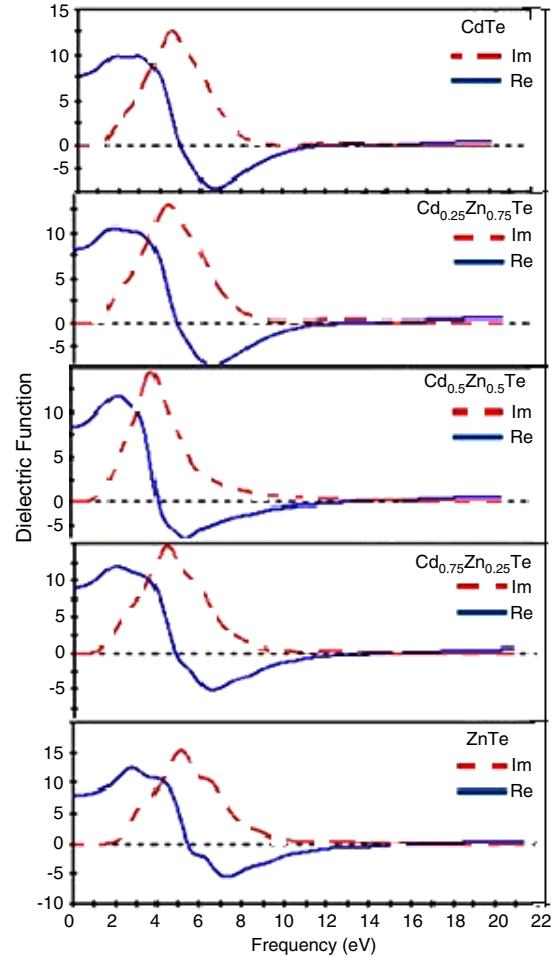


Figure 4. The real and imaginary parts of the dielectric.

for cubic crystals, the three independent elastic constants C_{ij} (C_{11} , C_{12} and C_{44}) satisfy the inequalities [37]:

$$(C_{11} - C_{12}) > 0, \quad C_{11} > 0, \quad C_{44} > 0, \quad (C_{11} + 2C_{12}) > 0.$$

Our results for elastic constants in table 4 satisfy all these stability conditions for $Cd_xZn_{1-x}Te$ compounds.

The shear modulus (C'), Poisson’s ratio (ν) and Young’s modulus (E), which are the most interesting elastic properties for applications, are often measured for polycrystalline materials when investigating their hardness. In table 5, we list the calculated Poisson’s ratio and Young’s modulus along with the other theoretical values. These quantities are calculated based on the relations given in [38]. The $\nu = 0.25$ and 0.5 are the lower limit and upper limit for central force solids, respectively [39]. Our ν value is about 0.38, which indicates that the interatomic forces in the $Cd_xZn_{1-x}Te$ are predominantly central forces. It can be seen from this table that the calculated shear modulus and Young’s modulus decrease with the increasing value of the composition x , but the Poisson’s ratio shows a small increase for the same value of x .

Table 4. The calculated elastic constants (in GPa) of Cd_xZn_{1-x}Te.

	Structure	Reference	C ₁₁	C ₁₂	C ₁₃	C ₃₃	C ₄₄	C ₆₆
CdTe	Zinc-blende	Present	57.30	39.63			19.04	
		Theory ^a	68.1	39.3			22.1	
		Theory ^b	50.3	37.6			12.1	
		Theory ^c	53.2	36.0			31.8	
		Theory ^d	56.5	32.1			19.2	
		Expt. ^e	53.5	36.81			19.9	
Cd _{0.75} Zn _{0.25} Te	Sulvanite	Present	60.92	40.47			22.69	
Cd _{0.5} Zn _{0.5} Te	Tetragonal <i>p4m2</i>	Present	64.10	40.34	41.75	66.21	35.09	35.24
Cd _{0.25} Zn _{0.75} Te	Sulvanite	Present	69.42	42.07			30.39	
ZnTe	Zinc-blende	Present	75.17	42.94			38.86	
		Theory ^f	82	42			55	
		Expt. ^g	71.7	40.7			31.2	

^a Reference [16]; ^b reference [18]; ^c reference [30]; ^d reference [31]; ^e reference [32]; ^f reference [22]; ^g reference [33].

Table 5. The calculated Poisson ratio (ν), Young's modulus (E) and shear modulus (C') for Cd_xZn_{1-x}Te.

	Structure	Reference	C' (GPa)	E (GPa)	ν
CdTe	Zinc-blende	Present	13.68	24.88	0.40
		Theory ^a	—	49.55	0.33
Cd _{0.75} Zn _{0.25} Te	Sulvanite	Present	16.47	28.60	0.39
Cd _{0.5} Zn _{0.5} Te	Tetragonal <i>p4m2</i>	Present	17.91	32.57	0.37
Cd _{0.25} Zn _{0.75} Te	Sulvanite	Present	20.41	37.66	0.37
ZnTe	Zinc-blende	Present	27.29	43.94	0.36

^a Reference [16].

3.3. Optical properties

We now consider the optical properties for Cd_xZn_{1-x}Te. The dielectric function $\varepsilon(\omega)$ can be used to describe the linear response of the system to electromagnetic radiation, which relates to the interaction of photons with electrons [40]. It is well known that the imaginary part $\varepsilon_2(\omega)$ of the dielectric function can be calculated with the momentum matrix elements between the occupied and unoccupied wavefunctions within the selection rules, and the real part $\varepsilon_1(\omega)$ of the dielectric function follows from the Kramer–Kronig relations. Other optical properties can be derived from the complex dielectric function. Expressions used for the dielectric functions, refractive index $n(\omega)$, the extinction coefficient $k(\omega)$ and energy loss function $L(\omega)$ are given as follows [41–43]:

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} \int_0^\infty \frac{\varepsilon_2(\omega')\omega' d\omega'}{\omega'^2 - \omega^2} \quad (1)$$

$$\varepsilon_2(\omega) = \frac{Ve^2}{2\pi\hbar m^2 \omega^2} \int d^3k \sum_{nn'} |\langle kn|p|kn' \rangle|^2 f(kn) \times [1 - f(kn')] \partial(E_{kn} - E_{kn'} - \hbar\omega) \quad (2)$$

where $\hbar\omega$ is the energy of the incident photon, p is the momentum operator, $\frac{\hbar}{i} \frac{\partial}{\partial x}$, $|kn\rangle$ is the eigenfunction with eigenvalue E_{kn} and $f(kn)$ is the Fermi distribution function:

$$n(\omega) = \frac{1}{\sqrt{2}} \left[\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega) + \varepsilon_1} \right]^{1/2} \quad (3)$$

$$k(\omega) = \frac{1}{\sqrt{2}} \left[\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega) + \varepsilon_1} \right]^{1/2} \quad (4)$$

$$L(\omega) = -\text{Im}(1/\varepsilon) = \varepsilon_2(\omega)/[\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)]. \quad (5)$$

By using these relations (equations (1)–(5)), dielectric functions ($\varepsilon_1(\omega)$, $\varepsilon_2(\omega)$), refractive index $n(\omega)$, extinction coefficient $k(\omega)$ and energy loss function $L(\omega)$ are calculated. The present results for Cd_xZn_{1-x}Te are displayed in figure 4 in the range 0–22 eV, where the blue solid lines and red dashed lines represent the real part $\varepsilon_1(\omega)$ and imaginary part $\varepsilon_2(\omega)$, respectively. The main peaks of the real part of Cd_xZn_{1-x}Te arise at 2.9, 1.90, 2.65, 1.97 and 2.78 eV, respectively. The same peaks reduce due to the interband transition and approach the minimum at about 5 eV for each composition x . For each composition x ($x = 0, 0.25, 0.50, 0.75$ and 1.0) of Cd_xZn_{1-x}Te, the dielectric constant $\varepsilon_1(0)$ is found to be 6.75, 8.1, 8.4, 9.1 and 8.0, respectively. For the imaginary part of the dielectric function for the same Cd_xZn_{1-x}Te, the absorption starts at about 1.03, 1.0, 1.1, 1.06 and 1.91 eV, respectively. The prominent peaks which are mainly related to the interband transition occur at about 4.5, 4.4, 4.5, 4.4 and 5.1 eV, respectively, for Cd_xZn_{1-x}Te. Our peak values are consistent with the values of [22, 44] for CdTe and ZnTe.

The dispersion curves of refractive indices are plotted in figure 5 for each composition x , and the refractive indices $n(0)$ for Cd_xZn_{1-x}Te are found to be 2.5, 2.8, 2.9, 3.0 and 2.8, respectively. The extinction coefficient ($k(\omega)$) for each x is estimated as 1.3, 0.7, 0.8, 0.6 and 1.5, respectively.

Finally, from the real and imaginary parts of the complex dielectric response function, the electron energy loss function can easily be obtained. It is the imaginary part of the reciprocal of the complex dielectric function, and our results are displayed in figure 6. This function has a main peak so-called plasmon

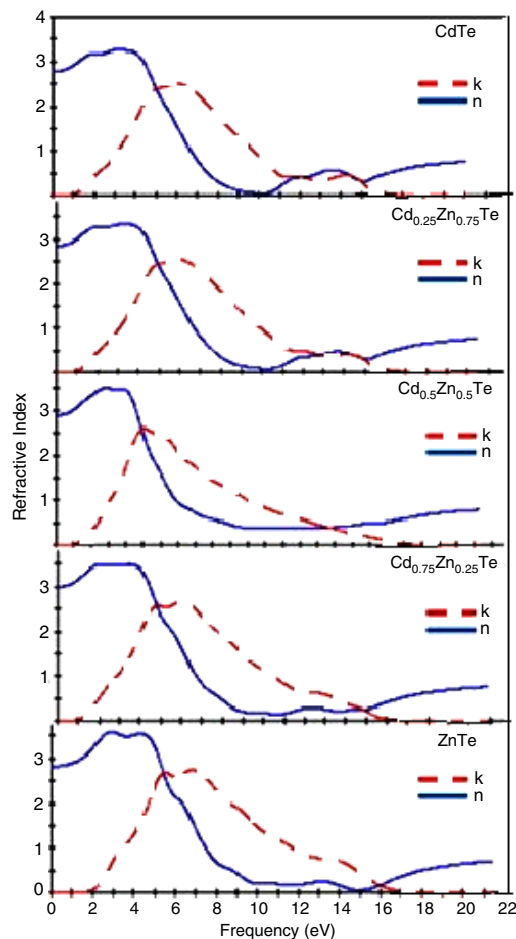


Figure 5. Refractive index n and extinction coefficient k .

frequency for each composition x at 15.1, 15.1, 16.6, 15.0 and 15.9 eV, respectively. The composition dependence of the plasmon frequency does not show a regular change. However, it is seen that the highest value is found for $x = 0.5$ (tetragonal $P4m2$ structure) of the $Cd_xZn_{1-x}Te$ compound.

4. Summary and conclusion

In this work, we have presented structural, electronic, elastic and optical properties of the $Cd_xZn_{1-x}Te$ ternary mixed crystals, using the first-principles calculations based on the plane-wave pseudopotential method within the LDA approximation. Specifically, the lattice constants, bulk modulus, pressure derivative of the bulk modulus, energy bandgap, zero-pressure elastic constants and their related quantities, such as Young's modulus, shear modulus and Poisson's ratio, have been calculated. The elastic constants satisfy the traditional mechanical stability conditions for these ternary mixed crystals. For all compositions these compounds are characterized by direct bandgap materials along the direction. The considered optical properties are consistent with the available experimental and theoretical findings. The plasmon frequency occurs at the highest energy (16.6 eV) for the composition $x = 0.5$. We hope that some of our results

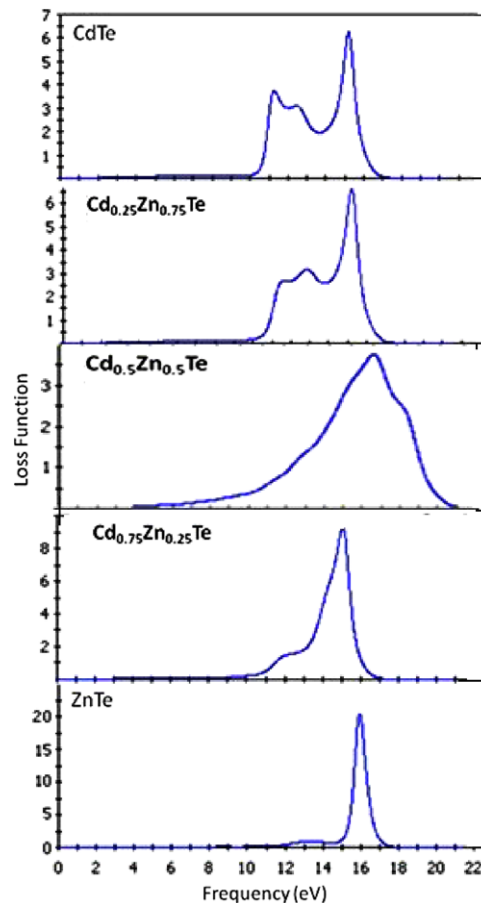


Figure 6. Loss function $L(\omega)$.

will be tested, to confirm their reliability, in future experiments and theoretically with different methods.

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