Scholarly Publisher
RS Global Sp. z O.O.
ISNI: 0000 0004 8495 2390

Dolna 17, Warsaw, Poland 00-773
Tel: +48 226 0 227 03
Email: editorial_office@rsglobal.pl

JOURNAL	World Science
p-ISSN	2413-1032
e-ISSN	2414-6404
PUBLISHER	RS Global Sp. z O.O., Poland

ARTICLE TITLE	INVESTIGATION OF STRUCTURAL, ELECTRONIC, ELASTIC AND OPTICAL PROPERTIES OF $Cd_{1-x-y}Zn_xHg_yTe$ ALLOYS
AUTHOR(S)	Mehmet Tamer, Zhoomart Moldaliev, Hasan Özdemir
ARTICLE INFO	Mehmet Tamer, Zhoomart Moldaliev, Hasan Özdemir. (2022) Investigation of Structural, Electronic, Elastic and Optical Properties of Cd1-x-yZnxHgyTe Alloys. World Science. 2(74). doi: 10.31435/rsglobal_ws/28022022/7784
DOI	https://doi.org/10.31435/rsglobal_ws/28022022/7784
RECEIVED	16 January 2022
ACCEPTED	21 February 2022
PUBLISHED	24 February 2022
LICENSE	This work is licensed under a **Creative Commons Attribution 4.0 International License.**

INVESTIGATION OF STRUCTURAL, ELECTRONIC, ELASTIC AND OPTICAL PROPERTIES OF $Cd_{1-x-y}Zn_xHg_yTe$ ALLOYS

Mehmet Tamer, *Gazi University, Gaziantep, Turkey*
Zhoomart Moldaliev, *Osh State University, Osh, Kyrgyz Republic*
Hasan Özdemir, *Osh State University, Osh, Kyrgyz Republic*

DOI: https://doi.org/10.31435/rsglobal_ws/28022022/7784

ARTICLE INFO

Received: 16 January 2022
Accepted: 21 February 2022
Published: 24 February 2022

KEYWORDS

$Cd_{1-x-y}Zn_xHg_yTe$, DFT, X-Ray, Vegard law.

ABSTRACT

Structural, optical and electronic properties and elastic constants of $Cd_{1-x-y}Zn_x Hg_yTe$ alloys have been studied by employing the commercial code Castep based on density functional theory. The generalized gradient approximation and local density approximation were utilized as exchange correlation. Using elastic constants for compounds, bulk modulus, band gap, Fermi energy and Kramers–Kronig relations, dielectric constants and the refractive index have been found through calculations. Apart from these, X-ray measurements revealed elastic constants and Vegard's law. It is seen that results obtained from theory and experiments are all in agreement.

Citation: Mehmet Tamer, Zhoomart Moldaliev, Hasan Özdemir. (2022) Investigation of Structural, Electronic, Elastic and Optical Properties of $Cd_{1-x-y}Zn_xHg_yTe$ Alloys. *World Science.* 2(74). doi: 10.31435/rsglobal_ws/28022022/7784

Introduction. Metal chalcogenite are studied intensively because of their big structural varieties super conductivity, optical properties, solar cell transitions and thermo electrical properties [1-4] The alloys which Be, Cd, Cu, Hg, Zn, Ag elements are in II-VI group alloyed with chalcogens of S, Se, Te, are the most important members of $A_xB_{1-x}C$, $A_xB_{1-x,y}C_yD$ type semiconductors because they have a direct band transferring and a wide band gap. Mixed ternary II-VI group semiconductors of them are used to manufacture optoelectronic devices which are coherent to the spectral region closed from blue up to ultraviolet colors and produce X-Ray and γ-ray detectors. They are also used production the device which can be work with the compounds based Cd in short and medium wavelengths [5].

$A_xB_{1-x}C$ type semiconductors obtained by mixing AC and AB compounds, are very important material technologically. Their structural, optical and epitaxial properties is adjusted by x doping. Thus, the properties of material can be expanded for special applications [6-8]. Recent works for getting high class and low priced CdZnTe crystals, continue. Because of their working potential at room temperature, CdZnTe alloys are very important for the nuclear detectors [9-15]. $Zn_xCd_{1-x}Te$ crystals that can be used to develop X-Ray and γ-Ray detectors, to product optoelectronic devices and solar cells which operate in blue-green spectral region, are very important materials [16-18]. Due to the fact that it has energy band gap in 1-30 μm adjustable ranges and its big optical coefficients which maintain high quantum efficiency, HgCdTe ternary alloy is an ideal infrared detector material [19]. x in the $Hg_{1-x}Cd_xTe$ alloys, is the alloy rate of Cd. These type alloys; are important materials for manufacturing defense industry, solar cells and various infrared detectors [20]. II-VI semiconductor alloys which are very significant for the technological appliance, have been found out with binary lattices. Their chemical formulas are generally $A_xB_{1-x-y}C_yD$. Here x and y rates are the atoms of A, B, C, D components. ABCD alloy types are used in photo detectors, fiber optics, the solid laser, light emission diodes and transistors. Although band gap adjusting are so difficult in the binary components, quaternary alloys are very successful in this matter. However some of this type alloys are used for designing of optoelectronic devices, they are also used X-ray, γ-ray detectors [21]. The measurement of all components of semiconductor alloys can be estimated, the very important properties of them like band gaps can be adjusted by changing alloys components and their performances can be adapted. These are the reason for the semiconductor alloys' being studied frequently.

In this article it has been studied on critical properties that are improved and adjusted of semiconductor alloys which have an important place in contemporary technology. In this context, $Cd1_{-x-y}Zn_xHg_yTe$ mixed crystals' parameters like optical and electronic properties, elastic constants, bulk module depending elastic constants, shear module, anisotropic coefficient of obtained by Castep package program based density functional theory (DFT) and X-ray depending on Vegard Law, are compared.

Results and calculations. In our calculations, Castep Program (Cambridge Sequential Total Energy Package) based Density Fuctional Theory, is performed by using plain wave pseudo potential method [22]. Norm conserving pseudo potentials for Cd, Zn, Hg and Te, are obtained by using LDA approaches paramatized by Perdew, Burke, Emzerof and Troullier Simulation [23]. Because of this reason valence electron configuration of Cd, Zn, Hg and Te atoms $4d^{10}5s^2$, $3d^{10}4s^2$, $5d^{10}6s^2$ ve $5s^25p^4$ respectively. Norm conserving pseudo potential is used for explaining the interaction between electron-ion. In this programe plain wave functions of valance electrons are explained by a base constant of plain wave. Using of norm conserving pseudo potentials has to allow a plain wave energy (E_{cut}). Calculations are optimized with kinetic energy values that are less than E_{cut}.

Bilateral space coincide on Brillon Zone is resembled Monkhorst-Pack Mesh is used via a sample in finite number [24]. Wave functions are extended in plane waves, until the kinetic cut off energy value becomes 600 eV. Mesh lattice parameter in Brillion Zone is 5x5x4 for the alloys. Charge densities as $1x10^{-5}$ eV /atom are approached to the calculations of the self – consistent. During the optimization, changing of energy, maximum force, stress, displacement and SCF tolerances are taken as $1x10^{-6}$ eV/A, 0.03 eV/A, 0.5 Gpa and 0.001 A respectively. All the alloys are optimized for different cut off values by Castep. Structural properties of BeTe, HgTe and ZnTe binary compounds were calculated in basic cubic structure (F-43M). The structural properties for $Be_{1-x-y}Zn_xHg_ySe$ type alloys are calculated in tetragonal (P-42M) structure. The structural properties of $A1_{-x}B_xC$ type ternary alloys calculated as the parameters dependent the elastic constants. These parameters are obtained for the forces at the equilibrium statues of different concentrations like (x=0.25-y=0.25), (x=0.50-y=0.25), (x= 0.25-y=0.50) in the lights of Castep and Vegards Law by X-ray device quasi-experimentally. A and B are two semiconductors and $A_{1-x}B_xC$ is semiconductor alloy. The lattice parameter of A which is the mole fraction of the alloy or x consistent of the alloy is determined as a^A. The lattice parameter of B is a^B and the parameter of alloy is also a^{AB} $(x)=xa^A+(1-x)a^B$. This is called Vegards Law [25]. We think two semiconductors are A, B and alloy which is $A_{1-x}B_xC$ for the band gap. Baseband gaps for A, B and alloy are E_g^A, Eg^B and $E_g(x) =x\ E_g^A+(1-x)\ Eg^B-x(1-x)\ E_b$ respectively, here E_b is the E_b bowing parameter. And called bowing energy [26].

Electronic and Stuructural properties.

There are eight atoms (4 number Cd and 4 number Te) in unit cell of face centered cubic structure (F-43M) of CdTe compound. When Zn and Hg are added instead of Cd probable crystal structures for $Cd_{0.25}Zn_{0.25}Hg_{0.50}Te$, $Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$ ve $Cd_{0.5}Zn_{0.25}Hg_{0.25}Te$ are in tetragonal (P-4M2) structure depending on increasing x and y of $Cd_{1-x-y}Zn_xHg_yTe$ alloy. Crystal structures and bond lengths of $Cd_{1-x-y}Zn_xHg_yTe$ alloy due to the increasing x and y are shown in Table 1. The largest values of bond lengths are at (x = 0.25, y= 0.50), (x = 0.25, y= 0.50) and (x = 0.25, y= 0.25) for Cd-Te, Te-Zn and Hg-Te respectively.

Table 1. Crystal structures and bond lengths of $Cd_{1-x-y}Zn_xHg_yTe$.

$Cd_{1-x-y}Zn_xHg_yTe$	Cd-Te (Å)	Zn-Te (Å)	Hg-Te(Å)	Hg-Cd(Å)
#1	2.79	2.65	5.20	4.46
#2	2.77	2.64	5.10	4.46
#3	2.77	2.61	5.27	4.46

Lattice constants, cell volume, Bulk module for x and y values of $Cd_{1-x-y}Zn_xHg_yTe$ alloy, are calculated by Castep and X-Ray device. The results with experimental and theoretical values are seen in Table 2. It is seen that the lattice parameters are similar with the lattice parameters calculated by Castep and X-Ray device.

Bulk modules were calculated as 45.84, 52.50 and 57.01GPa by Castep for (x=0.25, y=0.25), (x=0.5, y=0.25) and (x=0.25, y=0.5) respectively. The biggest Bulk Module (57.01 GPa) is for $Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$. The least compressible value is 0.015 1/GPa. Compressibility depends on the x and y values. The alloys can be compared like $Cd_{0.5}Zn_{0.25}Hg_{0.25}Te$ > $Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$ > $Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$ according to compressibility.

Table 2. Calculated equilibrium lattice constants (a_0), bulk modulus (B), cell volume (V) for $Cd_{1-x-y}Zn_xHg_yTe$.

$Cd_{1-x-y}Zn_xHg_yTe$	Space group-structure	Reference	$a_0(A^0)$	$b_0(A^0)$	$c_0(A^0)$	$V(A^0)^3$	B(GPa)
$Cd_{0.25}Zn_{0.25}Hg_{0.50}Te$	P-4M2 Tetrogonal	In this study	6.32	6.32	6.28	251.85	57.01
	P-43M cubic	In this study (X-ray)	6.37	6.37	6.37	258.48	60.79
$Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$	P-4M2 Tetrogonal	In this study	6.32	6.32	6.31	252.04	52.50
	P-43M cubic	In this study (X-ray)	6.38	6.38	6.38	259.69	57.55
$Cd_{0.5}Zn_{0.25}Hg_{0.25}Te$	P-4M2 Tetrogonal	In this study	6.10	6.10	6.10	227,09	45.84
	P-43M cubic	In this study (X-ray)	6.28	6.28	6.28	247.67	54.84

(in this study)

The electronic band sructures at high symetry direction in the first Brillon Zone and the electronic density of state (DOS) at band structuresare obtained by using lattice constants which are calculated for $Cd_{1-x-y}Zn_xHg_yTe$ alloys in equilibrium state and they are shown in Figure 1. It is noticed that band structures and state densities are compatible. As seen in band graphs the energy values show continuity. The curved lines of density of state in bands have sharp peaks. All alloys have direct band transition and show semiconductor property. Calculated results are listed in Table 3.

Table 3. Bandgap energies of $Cd_{1-x-y}Zn_xHg_yTe$.

Cd1-x-yZnxHgyTe	Space group-structure	Reference	Eg(eV)
Cd0.25Zn0.5Hg0.25Te	P-4M2 Tetrogonal	In this study (Castep)	0.82
	P-43M cubic	In this study (X-ray)	0.79
Cd0.25Zn0.5Hg0.25Te	P-4M2 Tetrogonal	In this study (Castep)	1.13
	P-43M cubic	In this study (X-ray)	1.27
Cd0.5Zn0.25Hg0.25Te	P-4M2 Tetrogonal	In this study (Castep)	1.46
	P-43M cubic	In this study (X-ray)	1.42

(in this study)

Band profiles and bad gap values are similar with the values performed previously. The band energies for the x and y values of $Cd_{1-x-y}Zn_xHg_y$Tealloy, are shown in Figure 1.

Bulk modules are calculated as 60.79 - 57.55 - 54.84 GPa by using X-ray data for $Cd_{1-x-y}Zn_xHg_yTe$. The biggest Bulk Module (60.79 GPa) for $Cd_{0.25}Zn_{0.25}Hg_{0.50}Te$. This value shows that $Cd_{0.25}Zn_{0.25}Hg_{0.50}$Tealloy can be less compressed than the others. Compressibility value is 0.016 1/GPa. The alloys can be compared like $Cd_{0.5}Zn_{0.25}Hg_{0.25}Te$ > $Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$ > $Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$ according to compressibility depending the changing values of x and y.

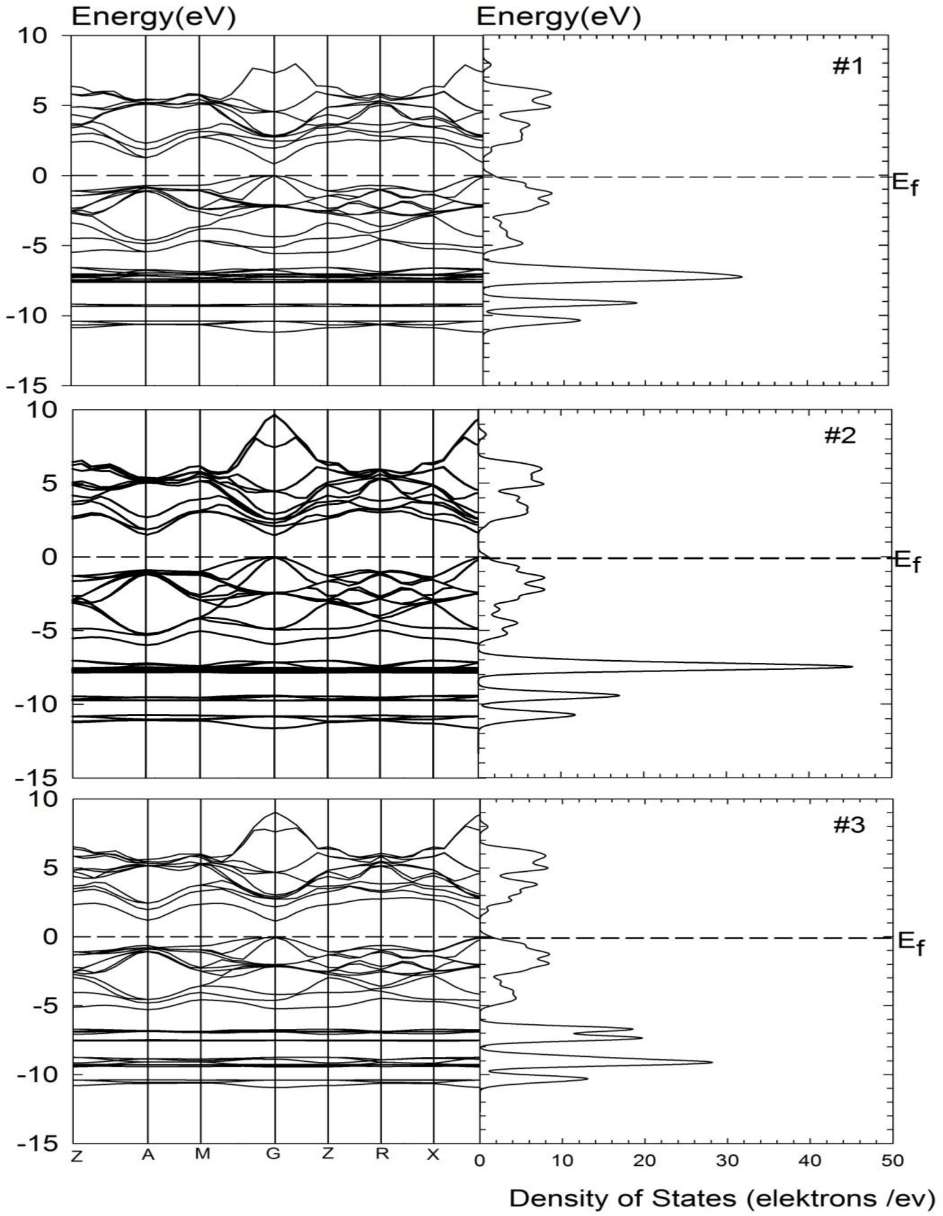

Fig.1. Calculated band structure and DOS of $Cd_{1-x-y}Zn_xHg_yTe$ versus the compositions x and y the position of the Fermi level is at 0 eV.

Elastic Properties. Elastic constants of solids link between mechanical and dynamic properties and give important knowledge about especially hardness and stability. Elastic constants and potentials are the first and the second derivations of the forces. Quadratic elastic constants ($C_{i\,j}$) are calculated by 'Volume Conserving' Technique [27, 28]. Six independent constants for stable cubic crystals must be $C_{i\,j}$ (C_{11}, C_{12}, C_{13}, C_{33}, C_{44} ve C_{66}) and for a stable tetragonal structure and they must supply Born –Huang Criteria for the correction of calculations [29]. $C_{11}>0$, $C_{33}>0$, $C_{44}>0$, $C_{66}>0$, $(C_{11}-C_{12}) >0$, $(C_{11}+ C_{33}- 2C_{13}) >0$, $[2(C_{11}+ C_{12}) + C_{33}+ 4C_{13}] >0$. Three independent constants for stable cubic crystals must be C_{ij} (C_{11}, C_{12} and C44) and for stability and $(C_{11}-C_{12})>0$, $C_{11}>0$, $C_{44}>0$ ve $2(C_{11}+C_{12})>0$ must provide Born- Huang criteria [29, 30]. In this study Elastic constants for $Cd_{1-x-y}Zn_xHg_yTe$ alloys are calculated by using Castep program and X-ray value quasi-experimentally depending on Vegard Law. When Castep Program are used to calculate elastic constant for the $Cd1_{-x-y}Zn_xHg_yTe$ alloys, six number of elastic constants are obtained for tetragonal (P-4M2) structure. After the calculations as cubic (P-43m) by X-ray three elastic constants are obtained. Calculated elastic constants provide all stability conditions and they are shown in Table 4. It is seen that all the results obtained by using both two methods, are compatible.

Table 4. The calculated elastic constants (in GPa) of Cd$_{1-x-y}$Zn$_x$Hg$_y$Te.

Cd$_{1-x-y}$Zn$_x$Hg$_y$Te	Space group-structure	C$_{11}$	C$_{12}$	C$_{13}$	C$_{33}$	C$_{44}$	C$_{66}$
Cd$_{0.25}$Zn$_{0.25}$Hg$_{0.5}$Te	P-4M2 Tetrogonal(Castep)	64.79	43.61	43.42	62.72	24.72	24.63
	P-43M Cubic (X-ray)	64.75	42.05	-	-	26.25	-
Cd$_{0.25}$Zn$_{0.5}$Hg$_{0.25}$Te	P-4M2 Tetrogonal(Castep)	82.02	57.90	59.72	79.76	28.17	27.83
	P-43M Cubic (X-ray)	68.15	41.82	-	-	27.92	-
Cd$_{0.5}$Zn$_{0.25}$Hg$_{0.25}$Te	P-4M2 Tetrogonal(Castep)	66.59	45.34	46.05	67.01	21.63	23.52
	P-43M Cubic(X-ray)	66.75	41.07	-	-	25.42	-

Bulk, Young and Shear (G) Modules, compressibility, B/G and Poisson rate (v) values are calculated by using elastic costants. Calculated results are listed in Table 5 [31].

Table 5. The calculated Poisson ratio (ν), Young's modulus (E) and shear modulus (G), Compressibility, Cauchy pressure (P) and Kleinman parameter (ξ)for Cd$_{1-x-y}$Zn$_x$Hg$_y$Te.

Cd$_{1-x-y}$Zn$_x$Hg$_y$Te	v	P(GPa)	E(GPa)	G(GPa)	B/G	Compressibility (1/GPa)	(ξ)
Cd$_{0.25}$Zn$_{0.25}$Hg$_{0.5}$Te (Castep)	0.39	18.89	29.44	17.39	2.89	0.0175	-
Cd$_{0.25}$Zn$_{0.25}$Hg$_{0.5}$Te (X-ray)	0.39	15.8	31.63	18.75	2.43	0.0164	0.75
Cd$_{0.25}$Zn$_{0.5}$Hg$_{0.25}$Te (Castep)	0.35	29.73	32.64	19.28	3.44	0.0190	-
Cd$_{0.25}$Zn$_{0.5}$Hg$_{0.25}$Te (X-ray)	0.38	13.92	36.34	20.64	2.29	0.0173	0.718
Cd$_{0.5}$Zn$_{0.25}$Hg$_{0.25}$Te (Castep)	0.39	23.71	29.58	16.43	3.21	0.0218	-
Cd$_{0.5}$Zn$_{0.25}$Hg$_{0.25}$Te (X-ray)	0.38	15.65	35.46	19.32	2.43	0.0183	0.71

B/G and Poisson (v) rate are important quantity for roughness and durability of the material. If B/G >1.75 alloy is elastic and if B/G <1.75 it is fragile [32]. The alloy which Bulk Module is bigger, has less compressible structure. Cauchy pressure (P=C$_{12}$ - C$_{44}$) for ionic compounds is C12-C$_{44}$> 0 (positive), for covalent compounds is mostly C$_{12}$-C$_{44}$< 0 (negative) [33]. In the event Cauchy Pressure (P) has negative value, directional bond is mentioned. If it has positive values then metallic bond is dominant. Cauchy pressure is generally positive for flexible material and negative for fragile material [34]. Poisson rate is also a measurement of compressibility. While v approaches ½, material shows a tendency to uncompressible property. While Poisson rate v = ½, the material almost cannot be compressed [35]. v value of poisson rate is less than 0.1 for the covolent materials. Typical v value of ionic materials is 0, 25 [36]. Poisson rate can be used for flexibility. Poison rate of the material can behave elastic for V>1⁄3, fragile for V<1⁄3 [37]. Poisson rates (v) = 0, 25 and (v) = 0, 5 are the lower and upper limit of the force which is in the center of solid [38]. Kleinman parameter ξ called internal stress parameter, is an important parameter [39] and related with the maximum stresses. If ξ =0 the atom remains in the center in tetrahedral whose shape is deformed. If ξ =1, only bond twist is observed [39]. Kleinman parameter can be calculated by taking only X-ray data as a reference only for cubic structures [40].

Debye Temperature. Debye temperature is the temperature of the highest vibration mode and shown θ_D symbol. On the other hand it is an important basic physical property related with elastic constants and melting temperature. It is used for classifying the solids according to regions at high and low temperature. If the temperature of solid (T) is bigger than Debye temperature (θ_D), ($T>\theta_D$), all modes have $k_\beta T$ energy. And if $T<\theta_D$, it is seen that the high frequency modes were frozen [40]. From this it is concluded that since wave lengths of phonon vibrations over and under Debye temperature, are small and big respectively. Because of acoustic influences, vibrational excitement occurs at low temperatures, thus at low temperatures Debye temperatures can be obtained from elastic constants. That's why the slope of acoustic vibrations in phonon curve line at low temperatures, gives sound velocity. From this, Debye temperature can be calculated by getting elastic constants. Calculation of Debye Temperature from this relation [41] comes up with the equation. Here h is the Planck constant, k is Boltzmann constant, N_A is Avogadro's number, M Molecular gravity, ρ is density, n atom number in molecule and v_m is average sound velocity. The value of sound is obtained the equation below [42]

$$\theta_D = \frac{h}{k}\left[\frac{3n}{4\pi}\left(\frac{N_A\rho}{M}\right)\right]^{1/3} v_m \tag{1}$$

$$v_m = \left[\frac{1}{3}\left(\frac{2}{v_t^3}+\frac{1}{v_l^3}\right)\right]^{-1/3} \tag{2}$$

v_l and v_t are the horizontal and longitudinal wave lengths and from Navier equation [43]

$$v_l = \sqrt{\frac{3B+4G}{3\rho}} \tag{3}$$

$$v_t = \sqrt{\frac{G}{\rho}} \tag{4}$$

is obtained. Here G is Shear module. The density*(ρ)*, longitudinal (υ_l), transverse (υ_t), average (υ_m), elastic wave velocities and Debye temperature (θ_D) for $Cd_{1-x-y}Zn_xHg_yTe$ are calculated by Castep and X-ray device and they are shown in Table 6.

Table 6. *Density (ρ),* longitudinal (υ_l), transverse (υ_t), average (υ_m) elastic wave velocities and Debye temperature (θ_D) *for* $Cd_{1-x-y}Zn_xHg_yTe$.

Cd1-x-yZnxHgyTe	Referans	ρ(gr/cm3)	$\upsilon_l (10^3\ m/s)$	$\upsilon_t (10^3\ m/s)$	$\upsilon_m (10^3\ m/s)$	$\theta_D (K)$
$Cd_{0.25}Zn_{0.25}Hg_{0.5}Te$(Castep)	In this study	7.18	1.55	3.20	1.75	165
$Cd_{0.25}Zn_{0.25}Hg_{0.5}Te$(X-ray)	In this study	7.1	1.61	3.23	1.82	171
$Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$(Castep)	In this study	6.9	1.66	3.64	1.87	183
$Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$(X-ray)	In this study	6.65	1.76	3.42	1.97	190
$Cd_{0.5}Zn_{0.25}Hg_{0.25}Te$(Castep)	In this study	6.59	1.57	3.36	1.77	168
$Cd_{0.5}Zn_{0.25}Hg_{0.25}Te$(X-ray)	In this study	6.53	1.65	3.26	1.85	179

Optical properties. When electromagnetic phonon is send on the material, optical events occur as a result of interaction between photon and electrons of atom. If energy of sent photon is equal to forbidden energy gap (E_g), the electron of the material is uyarmak to higher energy level. If it is less than forbidden energy gap, photons takes place instead of absorption and material is also called opaque [44]. According to the Quantum Mechanic, the exciting of electron as a result of interaction between a photon and an electron must be depending on the time. Absorption and emission of photons caused to transition between both filled and unfilled statues. In this study, the reaction given against electromagnetic radiation related with interaction of photon and electrons of dielectric function ε(ω) linearly for investigating of optical behavior of $Cd_{1-x-y}Zn_xHg_yTe$, must be described.

ε_2 (ω) known as imaginary part of dielectric function, can be calculated by selection rule of filled and unfilled wave functions and matrices components of momentum. ε_1 (ω) is the reel part of Dielectric function, is related with Charmer's croning function. The other optical properties are also derived from the complex part of dielectric function. The statements are used for dielectric function, refraction indices n(ω), decay coefficient $\kappa(\omega)$, absorption coefficient $\alpha(\omega)$ and function of energy lose L(ω), are given as below [45,46].

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi}\int_0^\infty \frac{\varepsilon_2(\omega')\omega' d\omega'}{\omega'^2 - \omega^2} \tag{5}$$

$$\varepsilon_2 = \frac{ve^2}{2\pi\hbar m^2\omega^2}\int d^3k \sum_{nn'} \left|\langle kn|p|kn'\rangle\right|^2 f(kn)x[1-f(kn')]\partial(\mathrm{E}_{kn} - \mathrm{E}_{kn'} - \hbar\omega) \tag{6}$$

Here $\hbar\omega$ is energy of incident photon, p momentum operator, $\frac{\hbar}{i}\frac{\partial}{\partial x}, |kn\rangle$ is eigenvalue of energy with wave function E_{kn} and $f(kn)$ are Fermi dispersion function.

$$n(\omega) = \frac{1}{\sqrt{2}}\left[\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} + \varepsilon_1(\omega)\right]^{1/2} \tag{7}$$

$$\kappa(\omega) = \frac{1}{\sqrt{2}}\left[\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} + \varepsilon_1(\omega)\right]^{1/2} \tag{8}$$

$$L(\omega) = \mathrm{Im}\left[\frac{-1}{\varepsilon(\omega)}\right] = \varepsilon_2(\omega) / \left[\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)\right] \tag{9}$$

$$\alpha(\omega) = \sqrt{2\omega}\left[\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} - \varepsilon_1(\omega)\right]^{1/2} \tag{10}$$

The statements are used for dielectric functions ε1(ω), ε2(ω), refraction indices n(ω), decay coefficient $\kappa(\omega)$, absorption coefficient $\alpha(\omega)$ and function of energy lose L(ω), are calculated. The results are shown in Figures 2, 3, 4, 5.

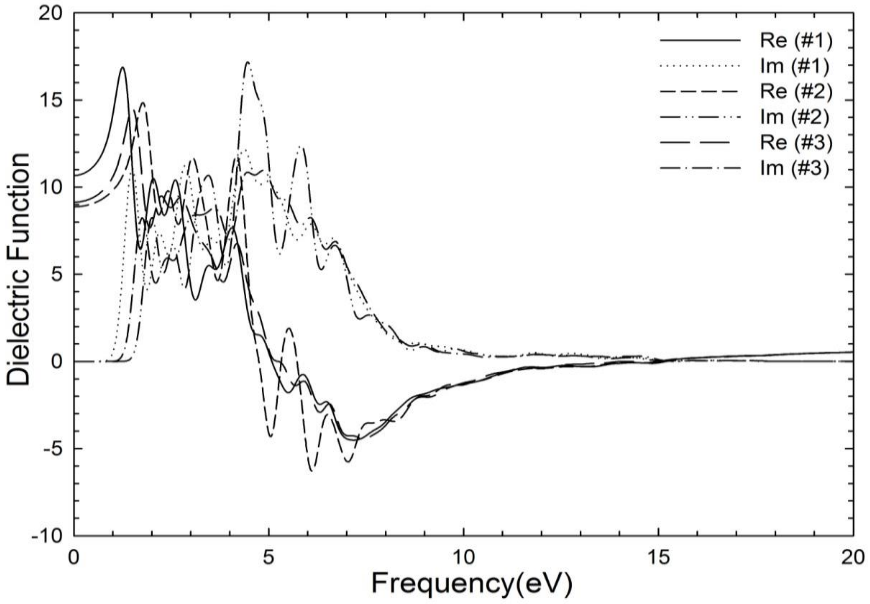

Fig. 2. The real part and the imaginary part of dielectric function for $Cd_{1-x-y}Zn_xHg_yTe$.

Main peaks of the reel part of dielectric function are 1.2 eV, 1.78 eV and 1.44 eV for $Cd_{0.25}Zn_{0.25}Hg_{0.5}Te$, $Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$ and $Cd_{0.5}Zn_{0.5}Hg_{0.25}$ respectively. ε1(0) gives static dielectric constant for frequency values 10.66 eV for $Cd_{0.25}Zn_{0.25}Hg_{0.5}Te$, 8.87 eV for $Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$ and 9.13 eV for $Cd_{0.5}Zn_{0.5}Hg_{0.25}Te$. According to doped values, imaginary part of dielectric coefficient starts to absorb phonon about 0.85 eV, 1.48 eV and 1.17 eV for $Cd_{0.25}Zn_{0.25}Hg_{0.5}Te$, $Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$ and $Cd_{0.5}Zn_{0.25}Hg_{0.25}Te$ respectively. These values are close to the values of band gap energy and they represent optical transmission between conduction band and valence band. Alloy behaves like opaque material up to value which dispersion curve starts to rise and dispersion is low in this region. The values which are maximum of imaginary part of dielectrik coefficient, are 4.65 eV, 4.37 eV and 4.42 eV for $Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$, $Cd_{0.25}Zn_{0.25}Hg_{0.5}Te$ and $Cd0_{.5}Zn_{0.25}Hg_{02.5}Te$ respectively. These values correspond to inter band transitions [47,48].

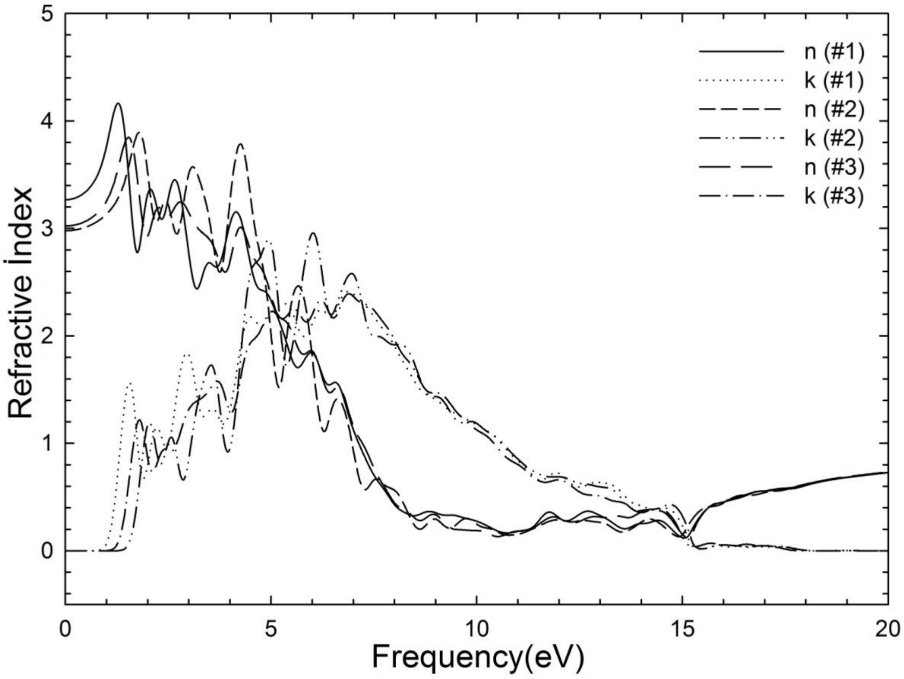

Fig. 3. Refractive index n and extinction coefficient k.

Refraction indices are obtained as 3.25 eV, 3.00 eV and 3.05 eV for $Cd_{0.25}Zn_{0.25}Hg_{0.5}Te$, $Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$ and $Cd_{0.5}Zn_{0.25}Hg_{0.25}Te$ for all x values at n(0) according to the dispersion curves of refraction indices for $Cd_{1-x-y}Zn_xHg_yTe$ and they are shown in Figure 3. When Zn value increases refraction indices increase too. According to the doping values of $Cd_{1-x-y}Zn_xHg_yTe$, the values which decay katsayı values started to increase, are calculated as 0.88 eV, 1.48 eV and 1.14 eV for $Cd_{0.25}Zn_{0.25}Hg_{0.5}Te$, $Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$ and$Cd_{0.5}Zn_{0.25}Hg_{0.25}Te$ respectively. It is seen that the reel part of dielectric coeficient and refraction coefficient are compitable with the imaginary part of dielectric coefficient and decay coefficient.

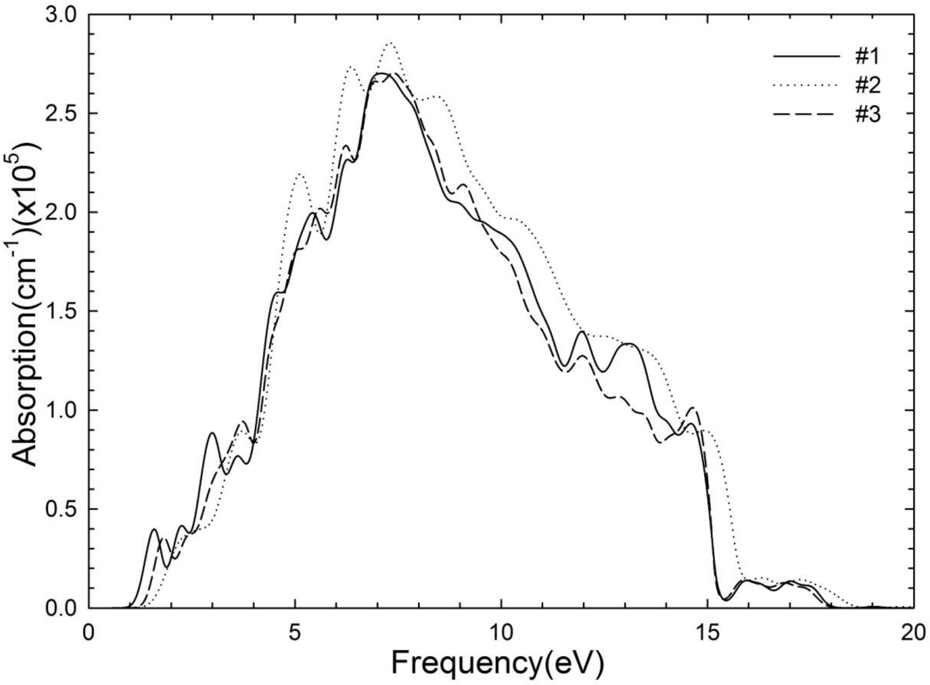

Fig. 4. Absorption coefficient of $Cd1_{-x-y}Zn_xHg_yTe$.

According to the doping values of $Cd_{1-x-y}Zn_xHg_yTe$, the values which absorption coefficient values started to increase, are calculated as 0.87 eV, 1.5 eV and 1.18 eV for $Cd_{0.25}Zn_{0.25}Hg_{0.5}Te$, $Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$ and $Cd_{0.5}Zn_{0.25}Hg_{02.5}Te$ respectively. It is seen that the point which absorption cofficient starts to increase, imaginary part of dielectric function and the values which decay coefficient starts to increase, are very close to each other.

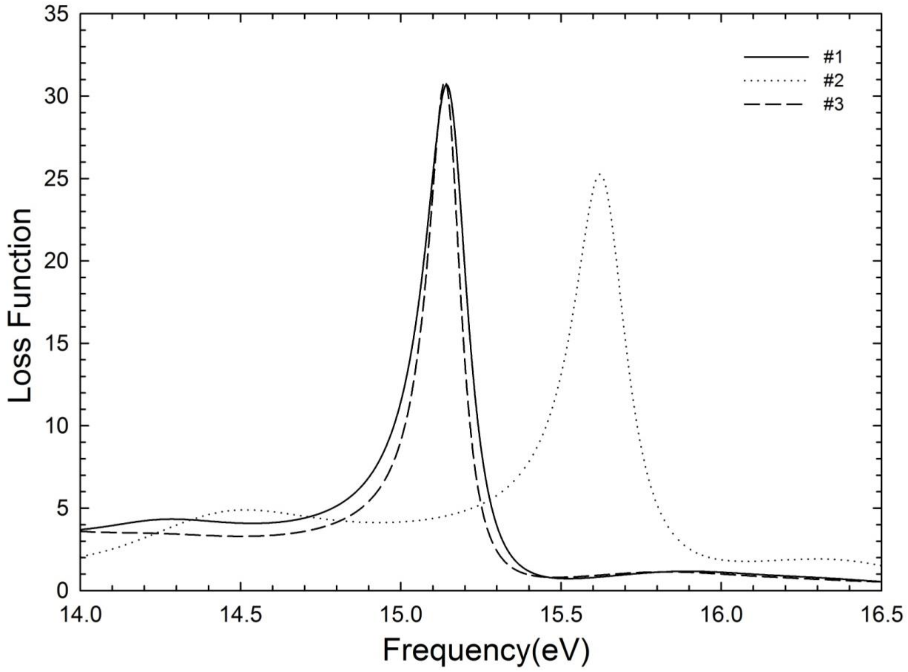

Fig. 5. Loss function L(ω).

In conclusion, lose function of electron is obtained from the reel and imaginary part of dielectric function and the results are shown in Figure 5. Lose function has variable peaks at between 9.8-18.3 eV values. The main peak of lose function is called as Plasmon Frequency. The imaginary part of dielectric coefficient is minimum at the value that the peak is maximum. Depending on the doping values of x and y, Plasmon frequency has the values 15.60 eV, 15.14 eV and 15.13 eV for $Cd_{0.25}Zn_{0.5}Hg_{025}Te$, $Cd_{0.25}Zn_{02.5}Hg_{05}Te$ and $Cd_{0.25}Zn_{02.5}Hg_{05}Te$ respectively. The values that is bigger than peak, behave like insulator, the values that lower than it, behave like metal. As seen in the graphs that absorption is very low at between 0-9.8 eV values. The reason of this that imaginary part of dielectric coefficient absorbs between this frequencies [49].

Results. In this study, the structural, electronic, optical properties and elastic constants for $Cd_{1-x-y}Zn_xHg_yTe$ have been investigated by using Castep program which is based Density Function Theory (DFT). GGA and LDA are withdrawn as swap correlation. Elastic constants for zero pressure, depending on elastic constants; Bulk module (B), Young module (E), Shear module (G), compressibility, B/G rate, Cauchy Pressure, Poisson rate (v), density (ρ), longitudinal (υ_l), horizontal (υ_t), average (υ_m) sound volumes and Debye temperature (θ_D) are calculated by using Castep Program and x-ray values.

The results obtained for alloys by using two methods.

1. Because B/G rate of results obtained from Vegart by using the data of Castep and HRXRD device, this type of alloys have elastic property.
2. Because Poisson rate (v) values are bigger than 0.25 alloys have ionic structures.
3. The forces between atoms are mainly central forces for this type alloys because Poisson rate (v) values are at between 0.25 and 0.5.
4. The biggest Bulk Module value that measured by Castep for $Cd_{1-x-y}Zn_xHg_yTe$, is (57,55 GPa) and it has the least compressibility. Its value is 0.0173 /GPa.
5. The biggest Bulk Module value that measured by X-ray for $Cd_{1-x-y}Zn_xHg_yTe$, is (60.79GPa) and it has the least compressibility. Its value is 0.0164 1/GPa.
6. Kleinman parameters (ξ) measured by Castep, are 0.76, 0.79 and 0.77 for $Cd_{0.25}Zn_{0.25}Hg_{0.50}Te$, $Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$and $Cd_{0.5}Zn_{0.25}Hg_{0.25}Te$ respectively.

7. Kleinman parameters (ξ) measured by using Vegard with the data of X-ray, are 0.75, 0.718 and 0.71 for $Cd_{0.25}Zn_{0.25}Hg_{0.50}Te$, $Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$ and $Cd_{0.5}Zn_{0.25}Hg_{0.25}Te$ respectively.
8. Cauchy Pressure which is calculated by the two methods of $Be_{1-x-y}Zn_xHg_ySe$ for $Be_{0.5}Zn_{0.25}Hg_{0.25}Se$ alloy, comes about positive. This situation shows that all alloys have ionic character. Furthermore Cauchy Pressure is generally positive on the elastic material.
9. According to the measurements performed by Castep, Debye Temperatures are found as 165 K, 183 K and 168 K for $Cd_{0.25}Zn_{0.25}Hg_{0.50}Te$, $Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$ and $Cd_{0.5}Zn_{0.25}Hg_{0.25}Te$ respectively.
10. Reportedly the measurements performed by the data of X-ray, Debye Temperatures are found as 171 K, 190 K and 179 K for $Cd_{0.25}Zn_{0.25}Hg_{0.50}Te$, $Cd_{0.25}Zn_{0.5}Hg_{0.25}Te$ and $Cd_{0.5}Zn_{0.25}Hg_{0.25}Te$ respectively.

Forbidden band gap obtained by using Castep program, dielectric constants, kırılma indices, absorption coefficient and energy lose function obtained by utilizing Chromer -Croning equations, are calculated. These alloys show semiconductor property that has direct band transmission. It is seen that the values which imaginary part and decay coefficient of dielectric function start to increase, are very close to the forbidden band gap. Reel parts of refraction indices and dielectric constant show similar properties. The main peak of lose function reached 15.60 eV value that is the highest Plasmon frequency for $Cd_{0.5}Zn_{0.25}Hg_{0.25}Te$. Finally every two theoretical and experimental results for $Cd_{1-x-y}Zn_xHg_yTe$ alloys are consistent.

REFERENCES

1. K. Mitchell, J.A. Ibers, Chem. Rev. 102, 1929, (2002).
2. X.-Y. Huang, J. Li, Y. Zhang, A. Mascarenhas, J. Am. Chem. Soc. 125, 7049, (2003).
3. J.M. Steward, W.S. Chen, W.E. Deveny, R.A. Mickelson, S.K. Deb, A. Zunger, in: Proceedings of the 7th Conference on Ternary and Multinary Compounds, Materials Research Society, Pittsburgh, PA, p. 59, (1987)
4. D.-Y. Chung, T. Hogan, P. Brazis, M. Rocci-Lane, C. Kannewurf, M. Bastea, C. Uher, M.G. Kanatzidis, Science, 287(5455), 1024-1027 (2000).
5. B.V. Robouchа, A. Kisiel, A. Marcelli, M. Cestelli Guidi, M. Piccinini, E. Burattini, A. Mycielski, Statistical model of sphalerite structured quaternary $A_{1-x}B_xY_yZ_{1-y}$ systems, Journal of Alloys and Compounds, 426(1–2), 31–42 (2006).
6. N.N. Berchenko, V.E. Krevs, and V.G. Sredin, Poluprovodnikovye tverdye rastvory $A^{II}B^{VI}$ i ikh primenenie (Solid Solutions between II–VI Semiconductors and Their Applications), Moscow: Voenizdat, (1982).
7. R.K. Ahrenkiel, B.M. Keyes, D.L. Levi, Keith A. Emery, T. L. Chu, S. S. Chu, Spatial Uniformity of Minority-Carrier Lifetime in Polycrystalline CdTe Solar Cells, Appl. Phys. Lett., 64(21), 2879-2881, (1994).
8. A. Parich, S.D. Pearson, T.K. Tran, et al., Growth and Characterization of HgCdTe Heterostructures by Metalorganic Molecular Beam Epitaxy, J. Cryst. Growth, 159, (1-4), 1152-1156, (1996).
9. Cs. Szeles, M.C. Driver, Proc. of Proc. SPIE Int. Soc. Opt. Eng., 3446(1), 2-9, SPIE, San Diego, CA, USA, (1998).
10. M. Schieber, T.E. Schlesinger, R.B. James, H. Hermon, H.Yoon, M. Goorsky, J. Crystal Growth 237–239(3), 2082-2090 (2002).
11. T.E. Schlesinger, J.E. Toney, H. Yoon, E.Y. Lee, B.A. Brunett, L. Franks, R.B. James, Mater. Sci. Eng.32, 103-189, (2001).
12. T.E. Schlesinger, B. Brunett, H. Yao, J. Van Scyoc, R.B.James, S. Egarievwe, K. Chattopadhyay, X. Ma, A.Burger, N. Giles, U. El-Hanany, A. Shahar, A. Tsigelman, J. Electron. Mater. 28(6), 864, (1999).
13. F.P. Doty, in: Proceedings of the Presentation at the 1998US Workshopon the Physics and Chemistry of II–VI Semiconductors, Charleston, SC, 21–22 October (1998).
14. L. Chibani, M. Hage-Ali, P. Siffert, J. Crystal Growth 161(1-4),153-158, (1996).
15. M. Fiederle, A. Fauler, J. Konrath, V. Babentsov, J. Franc, R.B. James, IEEE Trans. Nucl. Sci. 51(4), 1864-1868, (2004).
16. T.E. Schlesinger, R.B. James (Eds.), Semiconductors and Semimetals, 43, Academic Press, San Diego, (1995).
17. T. Asahi, O. Oda, Y. Taniguchi, A. Koyama, J. Crystal Growth 161(1-4) 20-27, (1996).
18. F. Bassani, S. Tatarenko, K. Saminadayar, J. Bleuse, N. Magnea, J.L. Pautrat, Appl. Phys. Lett., 58(23), 2651-2653, (1991).
19. M. B. Reine, Fundamental properties of mercury cadmium telluride Encyclopedia of Modern Optics, Academic Press, London, (2004).
20. D. G. Seiler, S. Mayo and J. R. Lowney, Semicond. Sci. Technol. 8 753-776, (1993).
21. K. Hacini, H. Meradji, S. Ghemid, and F. El Haj Hassan, Chin. Phys. B, 21(3), 036102 (2012).
22. M. D. Segall, P. J. D. Lindan, M. J. Probert, C. J. Pickard, P. J. Hasnip, S. J. Clark, M. C. Payne, J. Phys.: Condens. Matter 14 (11), 2717–2744 (2002).
23. T. H. Fischer, J. Almlöf, J. Phys. Chem. 96, 9768–9774, (1992).
24. H.J. Monkhorst, J.D. Pack, Special points for Brillouin-zone integrations, Phys. Rev. B, 13 (12) 5188–5192, (1976)

25. M. Androulidaki, N. T. Pelekanos, K. Tsagaraki, E. Dimakis, E. Iliopoulos, Phys. Status Solidi C, 3(6) 1866–1869, (2006).
26. J. Wu, W. Walukiewicz, K.M. Yu, J.W. Ager III, S.X. Li, E.E. Haller, Hai Lu, William J. Schaff Solid State Communications, 127, 411–414, (2003).
27. N. W. Ashcroft and N. D. Mermin, Solid State Physics, Philadelphia, PA: Saunders College, (1976).
28. J. F. Nye, Physical Properties of Crystals, Oxford: Clarendon, (1957).
29. M. Born and K. Huang, Dynamical Theory of Crystal Lattices, Oxford: Clarendon, (1956).
30. Z. J. Wu, E.J. Zhao, H. P. Xiang, X. F. Hao, X. J. Liu, and J. Meng, Phys. Rev. B, 76, 054115, (2007).
31. H. Zhai, X. Li, J. Du, Materials Transactions, 53(7), 1247-1251, (2012).
32. K. A. Matori, M. H. M. Zaid, H. A. A. Sidek, M. K. Halimah, Z. A. Wahab and M. G. M. Sabri, Int., J.Physical Sciences, 5, 2212-2216, (2010).
33. A. V. Ponomareva, E. I. Isaev, Yu. Kh. Vekilov, and I. A. Abrikosov Phys. Review B, 85, 144117, (2012).
34. D.P. Rai, M.P. Ghimire, R.K. Thapa, A DFT study of BeX (X = S, Se, Te) semiconductor: modified Becke Johnson (mBJ) potential, Semiconductor Physics and Technology, 48(11), 1447-1457, (2014).
35. P.H. Mott, J.R. Dorgan, C.M. Roland. J. Sound and Vibrations, 312(4), 572-575, (2008).
36. V. V. Bannikov, I. R. Shein, A. L. Ivanovskii, Phys. Status Solidi, Rapid Res. Lett. 3 89–91, (2007)
37. I. N. Frantsevich, F. F. Voronov, S. A. Bokuta, Elastic Constants and Elastic Moduli of Metals and Insulators Handbook, in: I.N. Frantsevich (Ed.), Naukova Dumka Kiev, 60, (1983).
38. Y. Shena, Z. Zhou, J. Appl. Phys., 103, 074113–074118, (2008).
39. L. Kleinman, Deformation potentials in silicon, 1. uniaxial strain. Phys. Rev., 128(6), 2614-2621, (1962).
40. X. Zhang, P. Kung, A. Saxler, D. Walker, T. Wang and M. Razeghi, Acta Physica Polonica A, 88(4), (1995).
41. J.R. Chrisman, “Fundamentals of Solid State Physics”, John Wiley & Sons, New York, 217-218, (1988).
42. I. Johnston, G. Keeler, R. Rollins, S. Spicklemire, Solid State Physics Simulations, The Consortium for Upper-Level Physics Software, John Wiley, New York, 45-59, (1996).
43. E. Schreiber, O.L. Anderson, N. Soga, Elastic Constants and their Measurements, New York: McGraw-Hill, 102-105, (1973).
44. M. Fox, Optical Properties of Solids, Oxford Master Series in Con-densed Matter Physics, Oxford University Press, Oxford, New York, (2001).
45. M. Dadsetani, A. Pourghazi, Phys. Rev. B, 73, 195102–195108, (2006).
46. F. Wooten, “Optical Properties of Solids”, Academic, New York, (1972).
47. S. M. Hosseini, Physica B, 403 1907–1915, (2008).
48. R. Khenata, A. Bouhemadou, M. Sahnoun, A.H. Reshak, H. Baltache, M. Rabah, Comput. Mater. Sci. 38 (1) 29-38, (2006).
49. Z. Hongsheng, Y. Tao, W. Deqi, First Principles Calculations of the Electronic and Optical Properties in $Cd_xZn_{l-x}Se$ Ternary Alloys, Journal of Ningxia University (Natural Science Edition), 33(1), 43-49, (2012).