Gazi University Journal of Science
GU J Sci
28(4):577-586 (2015)

The Study of Structural, Electronic, Elastic and Optical Properties of Be1-XZnxSe Alloys

Ali GÜLTEKIN[1,2], Mustafa Kemal ÖZTÜRK[1,2,♠] , Mehmet TAMER [3], Yunus BAŞ[4], Süleyman ÖZÇELIK[2]

[1] *GaziUniversity, Photonics Application and Research Center, Ankara, Turkey*
[2] *GaziUniversity, Science Faculty Physics Department, Ankara, Turkey,*
[3] *ZirveUniversity, Gaziantep, Turkey*
[4] *National Boron Research Institute, Ankara, Turkey*

Received: 09/06/2015 Revised:21/09/2015 Accepted: 16/10/2015

ABSTRACT

The structural, electronic, optical properties and elastic constants of Be1-xZnxSe alloys were studied thoroughly using a program called CASTEP that grounds on the density function theory (DFT). The exchange correlation, GGA (Generalized Gradients Approximation) was also used. The elastic constants, mechanical properties, forbidden band gap, Kleinman parameter, dielectric constants, refractive index, absorption coefficient, and loss coefficient calculations have been calculated for these compounds. In addition to this, elastic constants, and bulk modulus were obtained via an X-Ray values depending on Vegard's law. As an important result, the bulk module and forbidden band gap decreases with Zn doping to the structure. The obtained results are consistent with the available experimental and theoretical values.

Keywords: *DFT, CASTEP, BeZnSe, Vegards*

1. INTRODUCTION

There is a growing demand to various semiconductor electric and optical devices. Alloys of II-VI and III-V compounds were widely studied [1]. The use of the compounds composed of beryllium and chalcogen upon optoelectronics devices attracted a great deal of attention [2]. Within the leds and laser diodes (LDs); it is crucial to use in the technology, the height of which is a green and blue wave in the visible region. Beryllium and chalcogen compounds draw attention on account of BeSe and BeTe strong lattice, hard and high covalent connexion. The

doping of Be upon ZnSe (that is BexZn1-XSe ternary alloys) was brought forward by Waag and his companions. As a result of this, work was done to improve the life span and hardness of the equipment [2,3]. Studies were carried out that would shed light upon the luminous transmission nature of the doped ZnBeSe equipment to a certain degree [4]. The limited use of ZnSe upon the production of LED and laser diodes was researched [5]. Generally samples such as InGaN and InGaS were used in the manufacturing of LED [6-8]. Crystal ZnBeSe Epilayers of high quality were obtained [9]. The definition of elastic, optical and electronic properties for solids is important for atom interior forces and electron-photon interactions [10]. Electronic structures and optical properties are crucial in order to design semiconductor alloys and to manufacture optoelectronic devices. Beryllium chalcogens BeX (X=S, Se, Te) have recently become the center of interest in that

---

[♠] Corresponding author, e-mail: *ozturkm@gazi.edu.tr* they seem to display a unique covalent connection among II-VI compounds and to possess massive band gaps [4]. Therefore, the usage of Be is significant in order to increase the hardness of ternary alloys (Zn1-xBexSe) equipment based on ZnX, and to decrease the degradation level and finally to contribute to the life span of a more developed device [11,12]. The other extraordinary property of Beryllium chalcogens is the possible lattice adaptation in the circumstance of a Zn1-xBexSe ternary alloy [13,14]. Zn1-xBexSe alloys, via composition modification, lead to substantial modifications on physical characteristics such as ionic bond, electronic band structures and lattice parameter. In order to improve hetero structures that base on these recent equipment systems, it is necessary to carry out an elaborate research upon alloys. The AP-LAPW method (Linear Augmented Plane-Wave) was used to design blue-green laser diodes and to study the structural and electronic properties of (Zn1-xBexSe) alloys composed of beryllium and chalcogens [15].

The objective of this study is to obtain Be1-xZnxSe mixed crystals through the CASTEP packet program that focuses on optical, electronic properties and elastic constants, bulk and shear modulus, Poisson ratio, compressibility and B/G Density Functional Theory (DFT). In addition to that, this study aims to compare the results of second rank elastic constants, bulk and shear modulus, poisson ratio, compressibility and B/G that were obtained by means of X-Ray values depending on Vegard's law.

2. CALCULATIONS

In this study, through using the CASTEP program code [16], which is based on the density functional theory Be, Zn and Se norm-conserving pseudo potentials were obtained via the GGA(Generalized Gradient Approximations) approach parameterized by Perdew, Burke, Emzerkof scientists and through Troullier simulation. Electronic wave functions, and self-constituent field calculation (SCF), were calculated by means of density-mixing minimization method. The structures were softened using Broyden, Fletcher, Goldfarb and Shannon (BFGS) methods [17].

For geometric optimation, the tolerances total energy difference 5x10-6 eV/atom was adjusted to be the assumed difference. The maximum ionic Hellman-Feynman force and the maximum stress are 0.01 eVA-1 and 0.02 GPa respectively. The interaction between electrons and core ions were stimulated through detachable Troullier- Marteinsnorm–conserving pseudopotentials [18]. Upon the plane of wave functions, kinetics – energy cut off values for x =0.25 and 0.75, as 600 eV and for x=0.5, as 540 eV were adjusted. For the lattice parameters within the Brillion region, by means of monkhorst and Pack packet, values were taken to be k=6x6x5 for x=0.25-0.75, k=5x5x4 for x=0.5

The structural properties of BeSe and ZnSe binary compounds were calculated upon faced-centered cubic(F-43m). A1-x BxC types of ternary alloys, depending on CASTEP and Vegards law, through X-ray values as semi experimental for different x=0.25, 0.50, 0.75 values were calculated for the forces upon balance states of concentrations. For various cut - off values of CASTEP, Binary and alloys, optimization was practiced.

Vegard's law elastic constants were calculated by an X–ray values semi-experimentally for various x=0.25, 0.50, 0.75 values. Using a couple of semiconductors AC and BC, a A1-xBxC semiconductor alloy is obtained. The compound of x alloy or the lattice parameter of mole fraction of the alloy of AC is handled as aAC,, the lattice parameter of BC being aBC and the parameter of the alloy is handled as aABC(x)=xaAC+(1-x)aBC. This is called Vegard's Law [19]. The basic band gap of A is EgAC, for B it is EgBC and for the alloy, the band gap is EgABC (x)=x EgAC+(1-x) EgBC-x(1-x) Eb, here Eb is a bowing parameter and it is called bowing energy [20].

3. RESULTS AND DISCUSSION

3.1. Structural and Electronic Properties

There are eight atoms (4 pieces of Be and 4 pieces of Se) within the (F-43m) unit cell of face-centered cubic structure of BeSe compound. When we add Zn instead of Be, the simple cubic structure is (P-43m) for Be0.75Zn0.25Se ve Be0.25Zn0.75Se probable crystal structures depending on the x growth upon the Be1-xZnxSe alloy. However, there is a simple tetragonal structure for Be0.5Zn0.5Se (P-4m2). Within the Be1-xZnxSe alloy, depending on the growth of x; crystal structures and bond lengths are clearly seen in Figure 1. Bond lengths remain unmodified outside of x=0.25 for Be-Se and outside of x=0.5 for Se-Zn. As Se-Se and Zn-Be bond lengths grow in x, the (x = 0.25, 0.50 and 0.75) grows as well. All values are collected in the Table 1.

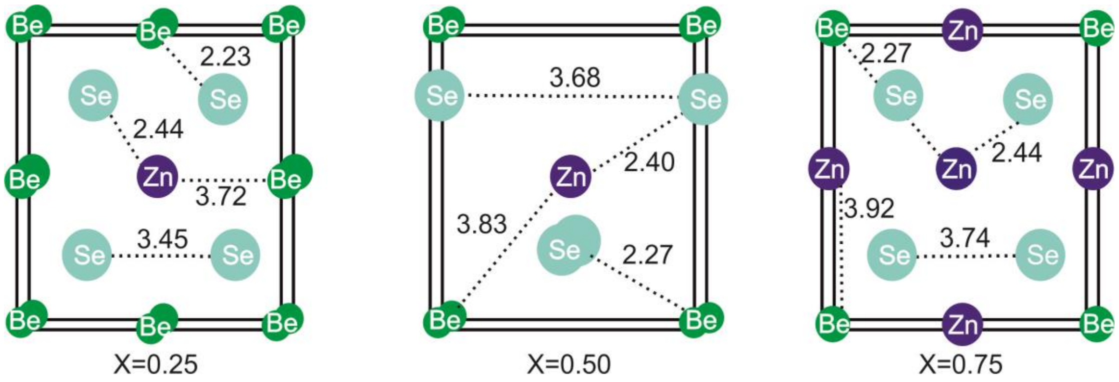

Figure 1. The Crystal structures and bond lengths (in Angstrom unit) of Be1-xZnxSe

Table 1. The crystal structures and bond lengths for Be1-xZnxSe.

Be1-xZnxSe	Space group-Structure Phase	Be-Se(Å)	Zn-Se(Å)	Se-Se(Å)	Zn-Be(Å)
Be0.75Zn0.25Se	P-43m Cubic	2.23	2.44	3.45	3.72
		2.22a	2.38a		
Be0.5Zn0.5Se	P-4m2 Tetragonal	2.27	2.40	3.68	3.83
Be0.25Zn0.25Se	P-43m Cubic	2.27	2.44	3.74	3.92
		2.25a	2.42a		

aReference [21]. Other results are DFT consequences obtained out of this study.

We initially calculated the lattice constants, cell volume and the bulk modulus by using CASTEP, for each x value of Be1-xZnxSe. Then, the same parameters for these alloys were computed semi-experimentally using the structural and elastic properties of binary components with Vegard Law. In addition, the properties of binary components can be founded in most text books. Results are shown in Table 2 in addition to the experimental and theoretical values [15,22]. For Be1-xZnxSe (x =0.25, 0.5, 0.75) alloys, lattice parameters were found as 5.26, 3.78, 3.78, 3.68 and 5.54 Å respectively [25,26]. Lattice parameters are seen to be consistent with those previously calculated. For Be1-xZnxSe, the bulk modules are 72.58 - 71.02 and 57.70GPa. The highest bulk modulus is seen for Be0.75Zn 0.25Se. Consequently, it is less compressible and its value is 0.013 1/GPa. Compressibility varies according to the increasing values of x; being Be0.75Zn0.25Se <Be0.5Zn0.5Se <Be0.25Zn 0.75Se.

Table 2. The experimental and theoretical lattice constants, bulk modulus B and cell volume for Be1-xZnxSe.

Be1-xZnxSe	Space group-Structure Phase	Reference	a0(Å)	b0(Å)	c0(Å)	V(Å)3	B(GPa)
Be0.75Zn0.25Se	P-43m Cubic	This study	5.26	-	-	146.33	73.58
		This study(X-Ray)	5.27	-	-	147.00	68.70
		Theory	5.27b	-	-		
		Theory	5.35c	-	-		70.13c
Be0.5Zn0.5Se	P-4m2 Tetragonal	This study	3.78	3.78	5.49	78.96	71.01
		This study(X-Ray)	5.40	-	-	158.00	65.03
		Theory	5.40b	-	-		
		Theory	5.05c	-	-		65.40c
Be0.25Zn0.75Se	P-43m Cubic	This study	5.54	-	-	170.44	57.74
		This study(X-Ray)	5.54	-	-	170.44	61.71
		Theory	5.53b	-	-		
		Theory	5.63c	-	-		60.81c

bReference [22], cReference [15]

For Be1-xZnxSe alloys, by means of lattice constants calculated within ground state, electronic band structures that equal high symmetrical directions within the first Brillion region and electronic density of state structures (DOS) that equal band structures were obtained. This finding is displayed in Figure 2. Band structures and density of state were found to be computable. In this figure, it is seen that the density of (DOS) curve states compose of concise peaks upon the bands in which the energy values indicate immense stability.

The entire alloys hold a direct band transition and a semiconductor characteristic. Results counted are listed with other theoretical data in Table 3. Band profiles and band gap values are consistent with the former studies [15,22]. Band gap energies that equals to x (x=0.25, 0.5, 0.75) of Be1-xZnxSe alloy are shown in Figure 2. It is seen that the forbidden band gap tends to decrease as x increases.

Table 3. The experimental and theoretical band gaps for Be1-xZnxSe.

Be1-xZnxSe	Space group- Structure Phase	Reference	Eg(eV)
Be0.75Zn0.25Se	P-43m Cubic	This study	2.83
		Theory	3.35b
		Theory	2.75c
Be0.5Zn0.5Se	P-4m2 Tetragonal	This study	2.50
		Theory	2.54b
		Theory	2.27c
Be0.25Zn0.75Se	P-43m Cubic	This study	1.92
		Theory	1.90b
		Theory	1.64c

bReference [22], cReference [15]

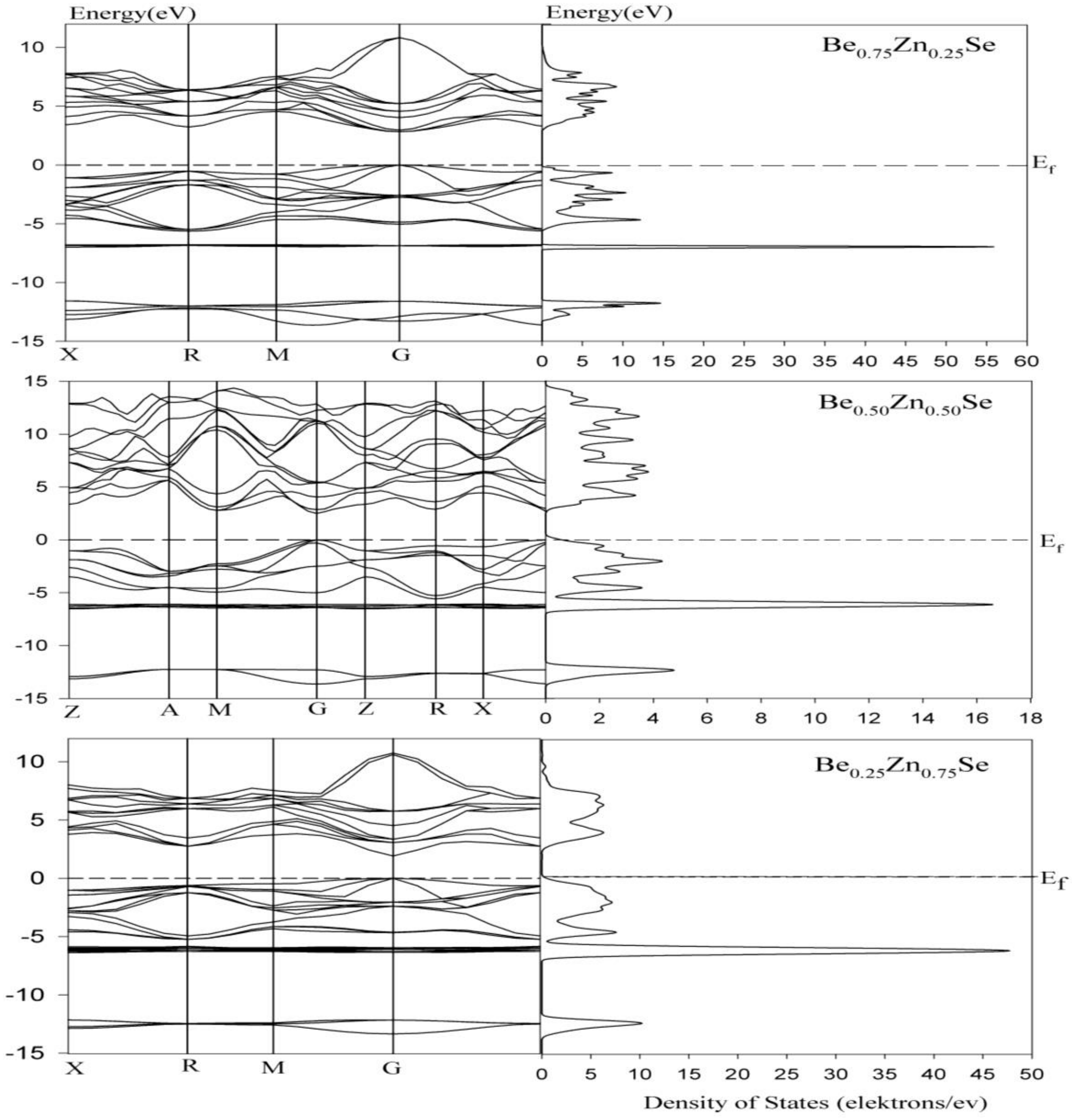

Figure 2. DOS (electronic density of state) and the band structure of Fermi level for Be1-xZnxSe.

Bulk modulus for Be1-xZnxSe through X-Ray values was calculated to be 68.70-65.03-61.71GPa. (68.70 GPa), the highest bulk modulus is found for Be0.75Zn0.25Se. It is less compressible and its value is 0.014 1/GPa. Compressibility varies as Be0.75Zn0.25Se <Be0.5Zn0.5Se <Be0.25Zn0.75Se, according to the increasing value of x.

3.2. ELASTIC PROPERTIES

The elastic constants of solids establish a connection between the mechanical and dynamic properties of crystals and give crucial information about the nature of forces in solids; hardness and stability in particular. Ab-initio calculation calls upon a precise method. Since forces and elastic constants are the first, the second orders the derivative of the potentials; they provide another control for the confirmation of solids' forces. Quadratic elastic constants are calculated through the (Cij) 'Volume -conserving' technique [23,24]. For a stable tetragonal structure, six liberal elastic constants Cij (C11, C12, C13, C33, C44 and C66) are required; for stability, it needs to maintain Born-Huang criteria [25]. C11>0, C33>0, C44>0, C66>0, (C11− C12) >0, (C11+ C33− 2C13) >0, [2(C11+ C12) + C33+ 4C13] >0, For stable cubic crystals, three liberal elastic constants Cij(C11, C12 and C44) are required and for stability[26], it is called upon to maintain (C11− C12) >0, C11>0, C44>0 and 2(C11+ C12)>0 Born-Huang criteria. For Be1-xZnxSe alloys, the elastic constants through CASTEP and X-Ray values were calculated as semi-experimental. For Be0.5Zn0.5Se2, when we calculated via CASTEP; we obtained six elastic constants for Primitive Tetragonal (P-4m2) structures. We obtained three elastic constants in that we calculated through X-Ray values as Primitive cubic (P-43m). The whole elastic constants provide all the stability conditions and were indicated in Tables 4 and 5. It is seen that the results we obtained through both methods are consistent. Through elastic constants, we calculated Bulk modulus, Shear modulus (G) [27], compressibility, B/G and Poisson ratio (ν) rate. The results calculated are listed in Tables 6 and 7.

Table 4. The elastic constants were calculated from CASTEP for Be1-xZnxSe alloys.

Be1-xZnxSe	Space group -Structure	C11	C12	C13	C33	C44	C66
Be0.75Zn0.25Se	P-43m Primitive cubic	118.51	49.62	-	-	61.07	-
Be0.5Zn0.5Se	P-4m2 Primitive Tetragonal	145.70	12.17	51.99	116.72	64.98	25.09
Be0.25Zn0.75Se	P-43m Primitive cubic	82.12	45.55	-	-	49.38	-

Table 5. The elastic constants were calculated from X-Ray values for Be1-xZnxSe alloys.

Be1-xZnxSe	Space group - Structure	C11	C12	C13	C33	C44	C66
Be0.75Zn0.25Se	P-43m Primitive cubic	114.78	45.67	-	-	65.34	-
Be0.5Zn0.5Se	P-4m2 Primitive cubic	103.90	45.60	-	-	57.10	-
Be0.25Zn0.75Se	P-43m Primitive cubic	93.350	45.90	-	-	49.15	-

Bulk modulus, Shear (slip) modulus (G), compressibility, B/G and poisson ratio (ν) are important qualities for the hardness and durability of the material [28]. If B/G is >1.75 the alloy is ductile; if B/G <1.75 then the alloy is brittle [29]. The alloy, the Bulk modulus (B) of which is bigger, is less compressible (if the alloy has bigger bulk modulus (B) it is less compressible, vice versa). If Poisson ratio is (ν) ≤0.1, the alloy is covalent; if Poisson ratio is (ν) ≥ 0.25, then the alloy displays ionic characteristics [30]. Poisson ratio (ν)= 0.25 and (ν) = 0.5 values are lower and upper the limit of force in the center of solids [31]. Kleinman parameter ξ defined as internal strain is an important parameter. This parameter couldn't be compared for x= 0.5 as the parameter can be calculated for cubic structures, although it could not be done for tetragonal structures. Reference [32] is related to maximum strains. If it is ξ=0, the atom remains in the centre on distorted four-faced. If ξ =1, a bond twist appears [33]. Kleinman parameters could not compared for x = 0.5 because this parameter can be calculated for cubic structures but it cannot be done tetragonal structures. Ref. [32], is related to maximum stresses.

Table 6. The Bulk modulus, Shear modulus (G), Compressibility, B/G and Poisson ratio (ν) results were calculated from the CASTEP for Be1-xZnxSe alloys.

Be1-xZnxSe	Poisson ratio (ν)	Shear modulus (G)	B/G	Compressibility (1/GPa)	Kleinman parameter (ξ)
Be0.75Zn0.25Se	0.29	48.53	1.43	0.013	0.554
Be0.50Zn0.50Se	0.32	46.35	1.53	0.014	-
Be0.25Zn0.75Se	0.35	33.16	1.56	0.017	0.670

Table 7. The Bulk modulus, Shear modulus (G), Compressibility, B/G and Poisson ratio (ν) results were calculated from X-Ray values for Be1-xZnxSe alloys.

Be1-xZnxSe	Poisson ratio (ν)	Shear modulus (G)	B/G	Compressibility (1/GPa)	Kleinman parameter (ξ)
Be0.75Zn0.25Se	0.28	50.59	1.29	0.014	0.53
Be0.5Zn0.5Se	0.31	43.59	1.41	0.015	0.57
Be0.25Zn0.75Se	0.33	36.69	1.58	0.016	0.62

3.3. Optical properties

When electromagnetic radiation is dispatched upon the material; optical phenomenons arise as a result of the interaction of photons with the electrons of atoms. If the energy of the photons dispatched equals the forbidden energy gap (Eg), the electron of the material is stimulated to a higher energy level. If it is smaller than the energy gap, then photons are replaced by absorption and the material is called transparent [33]. From a quantum mechanics perspective, the stimulation of electrons as a result of the interaction of a photon with an electron should be defined to be dependent upon time. The absorption and emission of photons causes transitions between the two of the filled and unfilled phenomenons. In this study, in order to analyse the optical behaviour of Be1-xZnxSe we need to define the way the dielectric function reacts in a linear sense to the electromagnetic radiation related to the interaction of ε(ω) with photons and electrons. Matrix components of momentum may be calculated through the selection rule of ε2(ω) for filled and unfilled wave functions which is known to be the imaginary part of the dielectric function. The real part of the dielectric function ε1(ω) is associated with Kramers-Kronig relations. Other optical properties were derived from the complex part of the dielectric function. The definitions for dielectric functions, refraction index n(ω), extinction coefficient , absorption coefficient energy loss function L(ω) is shown below: [34,35]

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

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

stands for the incident photon energy, p stands for momentum operator, stands for the energy eigen value together with the wave function, along with and standing for Fermi distribution function.

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

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

$$L(\omega) = \mathrm{Im}\left[\frac{-1}{\varepsilon(\omega)}\right] = \varepsilon_2(\omega)/\left[\varepsilon_1^2(\omega)+\varepsilon_2^2(\omega)\right] \tag{5}$$

$$\alpha(\omega) = \sqrt{2\omega}\left[\sqrt{\varepsilon_1^2(\omega)+\varepsilon_2^2(\omega)}-\varepsilon_1(\omega)\right]^{1/2} \tag{6}$$

Relations used here, the definitions for dielectric functions ε1(ω), ε2(ω), refraction index n(ω), extinction coefficient, absorption coefficient and energy loss function were calculated. Results were shown in Figures 2, 3, 4 and 5. The refraction subscript and dielectric constants are important in determining the optical and electrical features of crystal. A few experiments interrelate between the band gap and refraction subscripts of semiconductors. This experimental relation is given by Herve and Vandamme [36,37].

$$n = \sqrt{1+(\frac{\mathrm{A}}{\mathrm{E}_g+\mathrm{B}})^2} \tag{7}$$

This equation is known as the Herve equation, where A=13.6 eV and B=3.4 eV.

With this method, the dielectric constant and refraction subscript, which were obtained by CASTEP for this compound, were compared in Table 8. It was observed that the results for every two methods were in good harmony. Zn with the 3d10s2 valence electrons shows the sd hybridization. Due to the increase in the number of free electrons, the metallic bonds are occurred easily and ionic properties increases and then the forbidden band gap is reduced as shown in last column of Table 8.

Table 8. Refractive index n and the real part of dielectric function for Be1-xZnxTe.

Be1-xZnxSe	Reference	n(0)	$\varepsilon(0)$	Eg(eV)
Be0.75Zn0.25Se	In this study(Herve equality)	2.41	5. 81	2.83
	(CASTEP)	2.48	6.15	2.83
Be0.5Zn0.5Se	In this study (Herve equality)	2.48	6.31	2.50
	In this study(CASTEP)	2.66	6.90	2.50
Be0.25Zn0.75Se	In this study (Herve equality)	2.74	7.72	1.92
	(CASTEP)	2.59	6.78	1.92

The key peaks of the real part of dielectric function is obtained as 4.89-3.54-5.15 eV respectively for x=0.25-0.50-0.75 doping values from Figure 3. For ε1(ω)= 0 frequency value, 6.24-6.96 -6.78 eV gives the static dielectric constant respectively for x=0.25-0.50-0.75 from this figure. The imaginary part of the dielectric constant, according to the doping values, starts to absorb around 2.71-2.47-1.9 eV; an approximate value for the band gap energy. This represents the optical transition between the conductance band and the valence band. The alloy acts to be a transparent substance up until the dispersion value begins to rise and it is in the region where dispersion is poor. The maximum values of the imaginary part of the dielectric constant is 6.0-5.6-5.4 eV respectively for x=0.25-0.50-0.75 doping values. These values correspond to inter band transitions [38, 39].

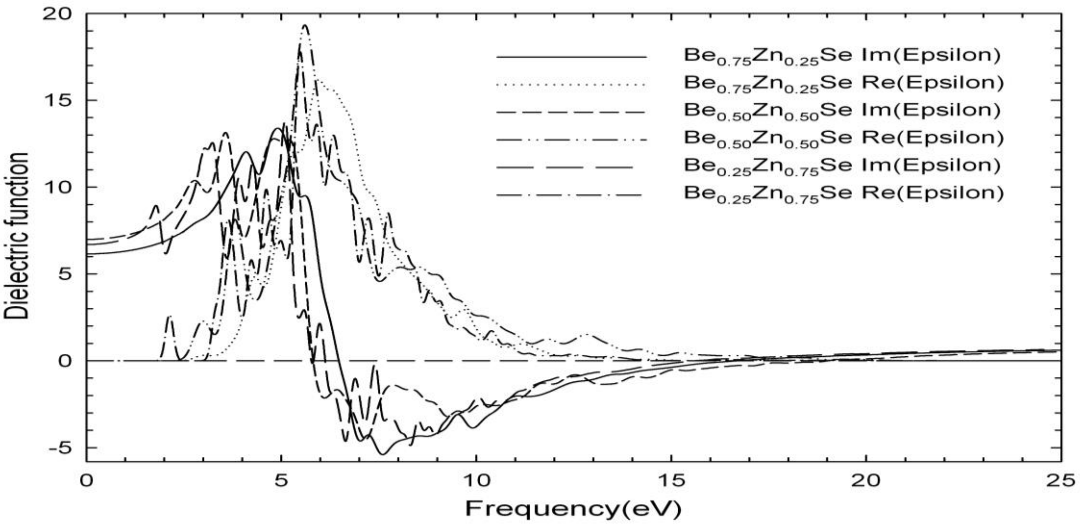

Figure 3. The real and imaginary parts of the Dielectric Constant for Be1-xZnxSe alloys.

Considering Be1-xZnxSe, the dispersion curve of the refraction index, for each x compound, the refraction indexes in n(0) were found to be 2.48-2.66-2.59 and displayed in Figure 4. As the Zn value grows, the refraction index varies. For Be1-xZnxSe, according to the x doping values, extinction coefficient values were calculated to be 2.8-2.5-1.9, respectively. The real part of the dielectric function and the refraction coefficient is seen to be consistent with the imaginary part of the dielectric function and the extinction coefficient

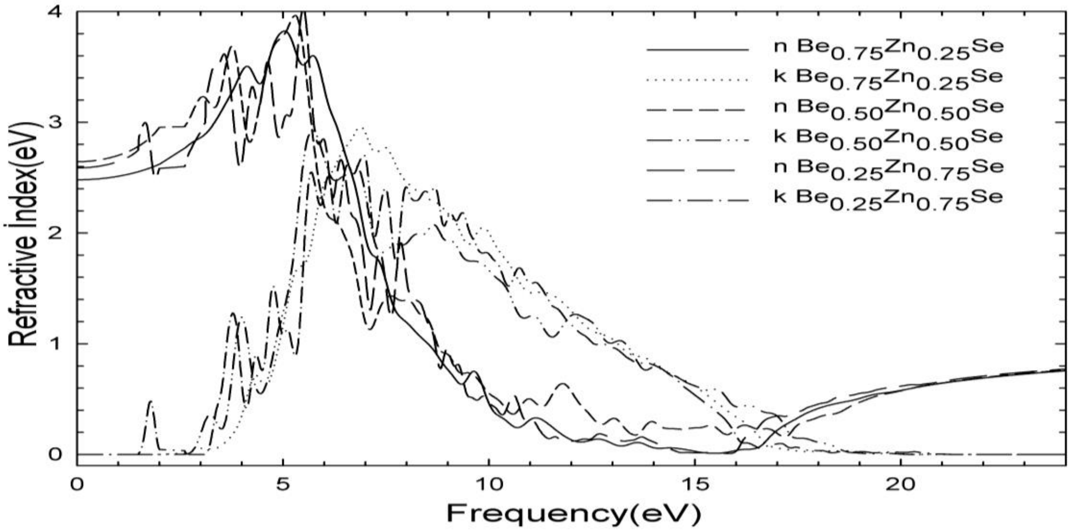

Figure 4. Refraction (n) and Extinction Constants (k) for Be1-xZnxSe alloys.

For Be1-xZnxSe, according to the x doping values, absorption coefficient values were calculated to be 2.8-2.5-1.9 eV from Figure 5, respectively. It is seen that the point where the absorption coefficient began to rise is equivalent to the imaginary part value of the dielectric function and the extinction coefficient began to rise.

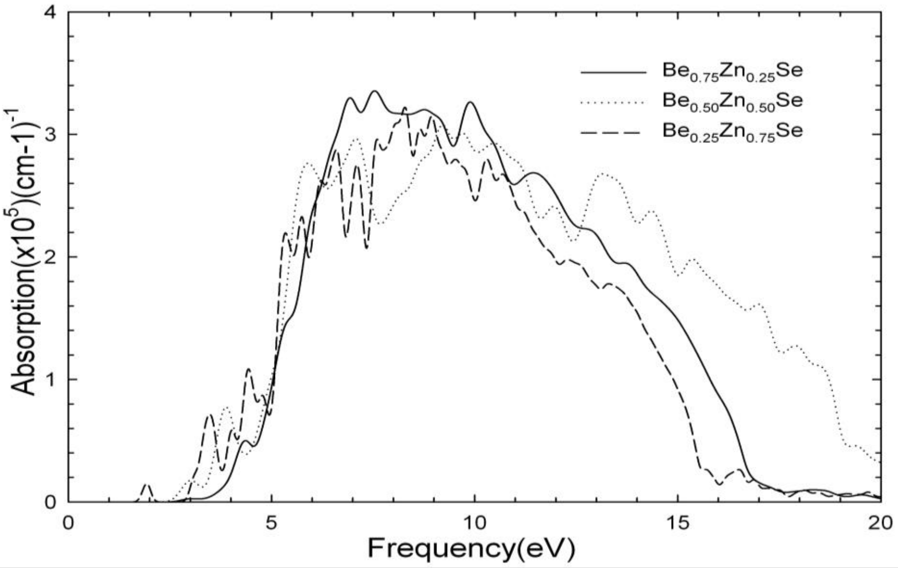

Figure 5. Absorption Coefficients for Be1-xZnxSe alloys.

To conclude; out of the real and imaginary part of the dielectric function, the loss function of electron was obtained and Figure 6 indicates the results. The loss function in range of 15-20 eV owns various peaks. The basic peak of loss function is called Plasmon frequency. Upon the value that the peak is at its maximum, the imaginary part of the dielectric constant is at its minimum. Based on X (x=0.25-0.5-0.75), Plasmon frequency holds the values of 16.68-19.01-15.52eV. While the alloy value of which is major than the peak, acts as insulators, for minor values it acts as a metal. When we look at the figure, it is seen that absorption range does not exist due to the imaginary part of the dielectric constant absorbing within this frequency range [40,41]

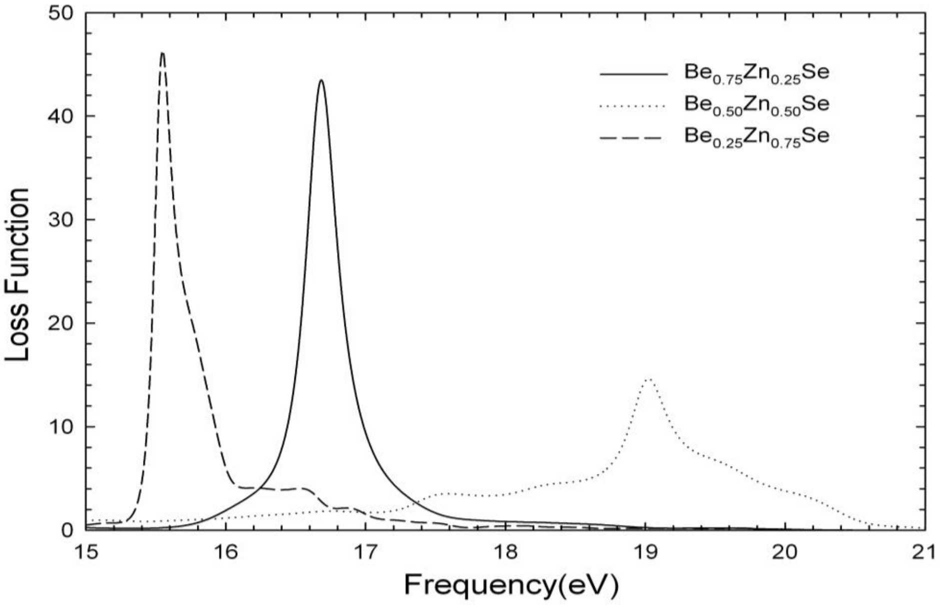

Figure 6. Loss functions for $Be_{1-x}Zn_xSe$ alloys.

4. CONCLUSIONS

In this study, Be1-xZnxSe structural, electronic, optical properties and elastic constants were analysed using the CASTEP program based on DFT. GGA was also used [38]. Through CASTEP and X-Ray values for zero pressure elastic constants, depending on elastic constants; Bulk modulus, Shear modulus (G), Compressibility, B/G and Poisson ratio (v) were calculated. Conclusions obtained through both of these methods for alloys are as follows:

a) For all alloys, B/G rate of 1.75 is small. Therefore it is brittle.

b) The Poisson ratio (v) values are greater than 0.25. Therefore they have ionic structures.

c) Poisson ratio (v) size is between the range of 0.25 and 0.5 therefore interatomic forces are predominantly the central forces.

d) For Be1-xZnxSe, the maximum bulk modulus measured through CASTEP is for (72.58 GPa) Be0.75Zn0.25Se and is the least compressible one. Its value is 0.013 1/Gpa. The maximum bulk modulus measured via X-Ray is for (68.70 GPa) Be0.75Zn0.25Se and is the least compressible. Its value is 0.014 1/GPa. In both methods, compressibility varies according to the increasing value of x. Be0.75Zn0.25Se< Be0.5Zn0.5Se < Be0.25Zn0.75Se.

e) All alloys possess a direct band transmission and display the characteristics of a semiconductor. It is seen that the values of the absorption coefficient, the imaginary part of the dielectric function and the extinction coefficient that began to increase are indistinguishable and they are fairly close to the forbidden band gap. The refractive index and real part of the dielectric constant is seen to display similar features.

f) The basic peak of loss function has received the value of x= 0.5 de 19.01 eV to the maximum energy value of Plasmon peak frequency.

g) For alloys, the Kleinman parameter ξ was calculated and the twist between bindings of atoms was observed. Finally, the results obtained with CASTEP and X-Ray, are in good harmony.

Information

This work was supported by the Ministry of Development of TR under Project No: 2011K120290 and BSTB under Project No: 0586.STZ.2013-2.

CONFLICT OF INTEREST

No conflict of interest was declared by the authors.

REFERENCES

[1] R. Gunshor, A.Nurmikko, Mater. Res. Bull., 15, (1995).

[2] C. Verie, J. Cryst. Growth 184-185, 1061, (1998).

[3] K. Maruyama, K. Suto, and J.-I. Nishizawa, J. Cryst. Growth, 214/215, 104, (2000).

[4] I.L. Kuskovsky, Y. Gu, M. van der Voort, C. Tian, B. Kim, I.P. Herman, G.F. Neumark, S.P. Guo, O. Maksimov, and M.C. Tamargo, Phys. Stat. Sol. (b), 2291, 239–243, (2002).

[5] A. Waag, Th. Litz, F. Fischer, H.-J. Lugauer, T. Baron, K. Schüll, U. Zehnder, T. Gerhard, U. Lunz, M. Keim, G. Reuscher, G. Landwehr, Journal of Crystal Growth, 184-185, l-10, (1998).

[6] Y. Baş , P. Demirel , N. Akın , C. Başköse , Y. Özen , B. Kınacı , M. K. Öztürk , S. Özçelik& E.

Özbay,Journal of Materials Science: Materials in Electronics,25, 9, 3924-3932, (2014).

[7] S. Çörekçi, K Kızılkaya, T. Asar, M. K Öztürk, M. Çakmak, S. Özçelik, ActaPhysicaPolonica A, 121,1, 247-248, (2012).

[8] M. K. Öztürk, S. Çörekçi, M. Tamer, S. S Çetin, S. Özçelik, E. Özbay, Applied Physics A-Materials Science & Processing,114, 4, 1215-1221, (2014).

[9] S.P Guo, Y Luo, W Lin, O Maksimov, M.C Tamargo, I Kuskovsky, C Tian, G.F Neumark, Journal of Crystal Growth, 208, 205-210, (2000).

[10] S.H. Park, J.H. Chang, M.N. Jung, Y.K. Park, K. Goto, T. Yao, J. Cryst. Growth 278,1-4, 311-315,(2005).

[11] I. Kuskovsky, C.Tian, C.Sudbrack, G. F. Neumark, S.P.Guo, and M. C. Tamargo, J. Cryst. Growth, 214,335, (2000).

[12] M. R. Buchley, F. C. Peiris, O. Maksimov, M. Muňoz, and M. C. Tamargo, Appl. Phys. Lett. 81, 5156, (2002).

[13] J. P. Faurie, V. Bousquet, P. Brunet, and E. Tournie, J. Cryst. Growth, 184, 11, (1998).

[14] A. Gültekin, M. K. Öztürk, M. Tamer, and T. Baş, Materials Science in Semiconductor Processing 39, 629 (2015).

[15] H. Baaziz, Z. Charifi, F. El Haj Hassan, S. J. Hashemifar, and H. Akbarzadeh Phys. Stat. Sol. (b), 243, 6, 1296–1305, (2006).

[16] M. D. Segall, P. J. D. Lindan, M. J. Probert, C. J. Pickard, P. J. Hasnip, S. J. Clark and M. C. Payne, J. Phys.:Condens. Matter,14,2717, (2002).

[17] T. H. Fischer and J. Almlof, J. Phys. Chem.,96,9768, (1992).

[18] N. Troullier and J. L. Martins, Phys. Rev.B, 43,3, 1993-2006, (1991).

[19] M. Androulidaki, N. T. Pelekanos, K. Tsagaraki, E. Dimakis, E. Iliopoulos, A. Adikimenakis, E. Bellet-Amalric, D. Jalabert and A. Georgakilas, Phys. Stat. Sol. (c),3, 6, 1866–1869, (2006).

[20] 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).

[21] A.V. Postnikov, O. Pages, T. Tite, M. Ajjoun and J. Hugel, Materials Science, 78, (1-3), 219-228, (2005).

[22] S. Kumar, Tarun K. Mauryaand S. Auluck, J. Phys.: Condens. Matter, 20,075205, (2008).

[23] N. W. Ashcroft and N. D. Mermin, Solid StatePhysics, Philadelphia, PA: Saunders College, (1976).

[24] J. F. Nye, Physical Properties of Crystals, Oxford: Clarendon, (1957).

[25] M. Born and K. Huang, Dynamical Theory of Crystal Lattices, Oxford: Clarendon (1956).

[26] Z. J. Wu, E.J. Zhao, H. P. Xiang, X. F. Hao, X. J. Liu, and J. Meng, Phys. Rev.B, 76,054115, (2007).

[27] H. Zhai, X. Li, J. Du, Materials Transactions, 53, 7, 1247-1251, (2012).

[28] 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).

[29] D. Errandonea, Ch. Ferrer-Roca, D. Martínez-Garcia, A. Segura, O. Gomis, A. Muñoz, P. Rodríguez-Hernández, J. López-Solano, S. Alconchel, and F. Sapiña, Phys. Rev. B, 82, 174105, (2010).

[30] H. Fu, D. Li, F. Peng, T. Gao and X. Cheng, Comput. Mater. Sci., 44,774, (2008).

[31] Y. Shena and Z. Zhou, J. Appl. Phys.,103,074113, (2008).

[32] L. Bing, L. Rong-Feng, Y. Yong and Y. Xiang-Dong, Chin. Phys. B, 19(7), 076201, (2010)

[33] Y. Mogulkoc, Y. O. Ciftci, M. Kabak, K. Colakoglu, Cumhuriyet University Faculty of Science Journal (CSJ), 34(3), (2013)

[34] Mark Fox, Optical Properties of Solids, Oxford Master Series in Condensed Matter Physics, Oxford University Press, (2001).

[35] M. Dadsetani and A. Pourghazi, Phys. Rev.B, 73,195102, (2006).

[36] J. P. L. Herve and L. K. J. Vandamme, Infrared Phys. Technol., 35, 609 (1994)

[37] S. M. Hosseini, Physica B, 403, (10-11),1907–1915, (2008).

[38] F. Wooten, Optical Properties of Solids, New York: Academic, (1972).

[39] R. Khenata, A. Bouhemadou, M. Sahnoun and A. H. Reshak, H. Baltache, M. Rabah, Comput., Mater. Sci. 38, 29-38, (2006).

[40] Z. Hongsheng, Y. Tao, W Deqi, Journal of Ningxia University,(Natural Science' Edition), 33, 1, (2012).

[41] G. Surucu, K. Colakoglu, E. Deligoz, N.Korozlu, "The electronic and optical properties of Zn1-xCaxSe mixed alloys", Solid State Communications, 150: 1413-1418 (2010)