The Measurement of Overall Elastic Stiffness and Bulk Modulus in Solar Photovoltaic Devices

Imad Alhayek [a], Mohamed S. Gaith [b,*]

[a] *Department of Mechanical Engineering, FET, Al-Balqaa Applied University, Amman, 11134 Jordan*

[b] *Department of Applied Sciences, FET, Al-Balqaa Applied University, Amman, 11134 Jordan*

Abstract

In this study, the correlation between macroscopic and microscopic properties of the II-IV semiconductor compounds ZnX (X=S, Se, Te) manufactured in photovoltaic window layers is investigated. Based on constructing orthonormal tensor basis elements using the form-invariant expressions, the elastic stiffness for cubic system materials is decomposed into two parts; isotropic (two terms) and anisotropic parts. A scale for measuring the overall elastic stiffness of these compounds is introduced and its correlation with the calculated bulk modulus and lattice constants is analyzed. The overall elastic stiffness is calculated and found to be directly proportional to bulk modulus and inversely proportional to lattice constants. A scale quantitative comparison of the contribution of the anisotropy to the elastic stiffness and to measure the degree of anisotropy in an anisotropic material is proposed using the Norm Ratio Criteria (NRC). It is found that ZnS is the nearest to isotropy (or least anisotropic) while ZnTe is the least isotropic (or nearest to anisotropy) among these compounds. The norm and norm ratios are found to be very useful for selecting suitable materials for electro-optic devices, transducers, modulators, acousto-optic devices.

Keywords: Overall Stiffness, Bulk Modulus, Anisotropic Materials, Window Layer Compounds.

1. Introduction

Nowadays, the necessity of alternative energy use is widely accepted. In solar energy technology, thin film solar technology based on the II-IV semiconductor compounds, is very promising due to lower production costs and shorter energy pay back times [1]. For these compounds, a successful interface between absorber and buffer layers with alternative and promising non-toxic materials requires compositional and electronic material characterization as a prerequisite for understanding and intentionally generating interfaces in photovoltaic devices [1]. On the other hand, stability of ZnTe/ZnS solar cells is of concern for their application in space, where the cells have to withstand high energy particles, mainly electrons and protons that can cause severe damage in solar cells up to a complete failure. Therefore, the radiation hardness and damage mechanism of the ZnTe solar cells is associated with the overall elastic stiffness and bulk modulus [3]. Most of the elastic materials in engineering applications are, with acceptable accuracy, considered as anisotropic materials such as metal crystals (due to the symmetries of the lattice), fiber-reinforced composites, polycrystalline textured materials, biological tissues, and photovoltaic materials. The wide-gap II-VI semiconductors, well known anisotropic materials used in high technology, have received much attention in the past decades since they have important applications in short-wavelength light-emitting diodes (LEDs), laser diodes and optical detectors [3]. Moreover, semiconductor materials constitute today basic components of emitters and receivers in cellular, satellite, solar cells, and photovoltaic systems. Their electronic and structural properties of such systems are subject of considerable interest in nanotechnology as well. For the semiconductor compounds ZnS, ZnSe, and ZnTe, the zinc-blend structure (ZB) has the lowest minimum total energy. With respect to classical II- VI semiconductors, the ZnS, ZnSe, and ZnTe compounds have attracted much attention in recent years for their great potential in technological applications [3]. They have a high melting point, high thermal conductivity, and large bulk modulus. The hardness and large bulk modulus of these anisotropic materials make them ideal protective coating materials in photovoltaic applications [4]. These materials can, therefore, be used for optoelectric devices in which the availability of light sources in the mid-infrared spectral region is crucial for many applications, i. e., molecular spectroscopy and gas-sensor systems for environmental monitoring or medical diagnostics [5]. Being stable to high

temperatures and can be made of sufficiently insulating allows precise measurements of piezoelectric, elastic, and dielectric constants. For such data eventually a fully quantum-mechanical description is essential in order to serve to verify a quantative theory of piezoelectricity and elasticity in these structures.

These covalent materials have been extensively studied for their intrinsic structural, optical, and elastic properties such as energy gap, charge density, lattice constants and bulk modulus [1-36]. However, bulk modulus has been found to correlate well with strength and hardness in many materials and those with largest bulk moduli are usually expected to be the hardest materials [7]. Therefore, one of the important parameters that characterize the physical property of a material system is the material stiffness and its corresponding bulk modulus which measures the degree of stiffness or the energy required to produce a given volume deformation. The bulk modulus reflects important bonding characters in the material and, for many applications, is used as an indicator for material strength and hardness. Early experimental and theoretical investigations for bulk modulus were reported in [6,8]. Cohen [6] obtained an empirical expression for the bulk modulus based on the nearest-neighbor distance. His theoretical and experimental results were in agreement. Lam et al. [8] obtained an expression for bulk modulus using the total energy method with acceptable results. The bulk modulus for the semiconductor compounds was found to be inverse proportionally correlated to the lattice constants [8,17].

Historically, the study of anisotropic elastic materials has been synonymous with study of crystals. It is, therefore, natural to seek to characterize physical properties of crystal by constants (or invariants) whose values do not depend upon the choice of the coordinate system. Using several decomposition methods, these invariants were investigated such as photo elastic coefficients [37], piezoelectric coefficient [38] and elastic stiffness coefficients [39-42]. Physical properties are intrinsic characteristics of matter that are not affected by any change of the coordinate system. Therefore, tensors are necessary to define the intrinsic properties of the medium that relate an intensive quantity (i.e. an externally applied stimulus) to an extensive thermodynamically conjugated one (i.e. the response of the medium). Such intrinsic properties are the dielectric susceptibility, piezoelectric, and the elasticity tensors. Several studies were conducted to reveal the physical properties using decomposition methods for piezoelectric and elastic tensors [37-45]. An interesting feature of the decompositions is that it simply and fully takes into account the symmetry properties when relating macroscopic effects to microscopic phenomena. One can directly show the influence of the crystal structure on physical properties, for instance, when discussing macroscopic properties in terms of the sum of the contributions from microscopic building units (chemical bond, coordination polyhedron, etc). A significant advantage of such decompositions is to give a direct display of the bearings of the crystal structure on the physical property. For the stress and strain, for instance, the decomposition allows one to separate changes in volume from changes of shape in linear isotropic elasticity; the bulk modulus relates to the hydrostatic part of stress and strain while the shear modulus relates the deviatoric part [46].

It is often useful, especially when comparing different materials or systems having different geometrical symmetries, to characterize the magnitude of a physical property. One may also have to make, in a given material, a quantitative comparison of the contribution of the anisotropy to a physical property [42-44]. The comparison of the magnitudes of the decomposed parts can give, at certain conditions, valuable information about the origin of the physical property under examination [42,44]. These problems can be dealt with by defining the norm of a tensor. The norm is invariant and not affected by any change of the coordinate system. Invariance considerations are of primary importance when studying physical properties of matter, since these properties are intrinsic characteristics which are not affected by a change of the reference frame. Tu [42] and Jerphagnon et al. [43] proposed the norm criterion to quantify and then, quantitatively to compare the effect of piezoelectricity and elasticity using irreducible tensor theory. They compared the magnitude of piezoelectricity of two materials only of the same symmetry using Cartesian and spherical framework. However, their method seemed to be valid only for elastic tensor. Gaith et al. [44] developed a decomposition procedure based on constructing orthonormal tensor basis elements using the form-invariant expressions [37-41]. They introduced a method to measure the stiffness and piezoelectricity in fiber reinforced composite and piezoelectric materials, respectively, using the norm criterion on the crystal scale. In their method, norm ratios proposed to measure the degree of anisotropy in an anisotropic material, and compare it with other materials of different symmetries. They were able to segregate the anisotropic material property into two parts: isotropic and anisotropic parts. Of the new insights provided by invariance considerations, the most important is providing a complete comparison of the magnitude of a given property in different crystals. Such a comparison could be obvious for average refractive index, even birefringence, piezoelectricity, electro-optic effects, elasticity, etc. From a device point of view, the new insights facilitate the comparison of materials; one is interested in maximizing the figure of merit by choosing the optimum configuration (crystal cut, wave propagation direction and polarization, etc); and one wants to be able to state that a particular material is better than another for making a transducer or modulator [43]. It is most suitable for a complete quantitative comparison of the strength or the magnitude of any property in different materials belonging to the same crystal class, or different phases of the same material. The norm concept is very effective for selecting suitable materials for electro-optic devices, transducers, modulators, acousto-optic devices.

The goal of this study is to understand how qualitative ground state concepts, such as overall elastic stiffness, can be related to bulk modulus and lattice constants, An important observation for studying the respective semiconductors is the clear difference in the bulk modulus and lattice constants going from the group-IV to III-V and II-VI semiconductors. The relationship of the macroscopic characteristics of a covalent crystal (dielectric and elastic constants) and the microscopic ones (band gap, covalent,

atomic charge densities and lattice constants) is of interest. Therefore, using the elastic constant for anisotropic material, an elastic stiffness scale for such anisotropic material, and a scale to measure the isotropic elasticity within the material will be discussed. Besides, the microscopic origin of the overall elastic stiffness and bulk modulus calculation will be correlated with the structural properties parameter, i.e. lattice constant a, which represents some fundamental length scale for the chemical bond of the unit cell.

2. Decomposition and Norm concept

The Orthonormal Decomposition Method (ODM) [44] is established through constructing an orthonormal tensor basis using the form-invariant expressions [37-39]. The basis is generated for the corresponding symmetry medium of the tensor, and the number of basis elements should be equal to the number of non-vanishing distinct stiffness coefficients that can completely describe the elastic stiffness in that medium. Accordingly, based on the Orthonormal Decomposition Method, the basis elements for isotropic material is obtained and consisted of two terms; shear and bulk moduli [44] and they are identical to those found in literature [46]. The elastic stiffness matrix representation for the isotropic system can be decomposed in a contracted form as:

$$
C_{ij} = \begin{bmatrix} 2C_{44}+C_{12} & C_{12} & C_{12} & 0 & 0 & \\ C_{12} & 2C_{44}+C_{12} & C_{12} & 0 & 0 & \\ C_{12} & C_{12} & 2C_{44}+C_{12} & 0 & 0 & \\ 0 & 0 & 0 & C_{44} & 0 & \\ 0 & 0 & 0 & 0 & 0 & C_{44} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}
$$

$$
= A_1 \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} + A_2 \begin{bmatrix} 4 & -2 & -2 & 0 & 0 & 0 \\ -2 & 4 & -2 & 0 & 0 & 0 \\ -2 & -2 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 \end{bmatrix} \quad (1)
$$

where

$$
A_1 = \frac{1}{3}(C_{11} + 2C_{12}), \quad C_{11} \quad 2C_{44} \quad C_{12} = \quad +
$$
$$
A_2 = \frac{1}{15}(C_{11} - C_{12} \quad 3C_{44}) \qquad + \quad (2)
$$

where A_1 and A_2 are the Voigt average polycrystalline bulk B and shear G modulus, respectively. The decomposed parts of Eq. (1) designated as bulk and shear modulus are identical to those found in literature [46-48].

For cubic crystals such as the II-VI semiconductor compounds, there are only three independent elastic stiffness coefficients C_{11}, C_{12} and C_{44} that can describe the mechanical elastic stiffness for these materials. The elastic coefficient C_{11} is the measure of resistance to deformation by a stress applied on the (100) plane, while C_{44} represents the measure of resistance to deformation with respect to a shearing stress applied across the (100) plane. These elastic coefficients are function of elastic material parameters, namely, Young's modulus, shear modulus, and Poisson's ratio. Thus, using the orthonormal decomposition procedure [44], the elastic stiffness matrix

representation for cubic system can be decomposed in a contracted form as:

$$
C_{ij} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix} = A_1 \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}
$$
$$
+ A_2 \begin{bmatrix} 4 & -2 & -2 & 0 & 0 & 0 \\ -2 & 4 & -2 & 0 & 0 & 0 \\ -2 & -2 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 \end{bmatrix} + A_3 \begin{bmatrix} -4 & 2 & 2 & 0 & 0 & 0 \\ 2 & 4 & -2 & 0 & 0 & 0 \\ 2 & 2 & -4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix} \quad (3)
$$

where

$$
A_1 = \frac{1}{3}(C_{11} + 2C_{12})
$$
$$
A_2 = \frac{1}{15}(C_{11} - C_{12} \quad 3C_{44}) \qquad + \quad (4)
$$
$$
A_3 = \frac{1}{10}(C_{12} - C_{11} \quad 2C_{44}) \qquad +
$$

It can be shown that the sum of the three orthonormal parts on the right hand side of Eq. (3) is apparently the main matrix of cubic system [47]. Also, the first two terms on the right hand side are identical to the corresponding two terms obtained in Eq. (1) for the isotropic system [47]. Hence, it can be stated that the cubic system is discriminated into the sum of two parts: isotropic part (first two terms), and anisotropic part (third term). The latter term resembles the contribution of the anisotropy on elastic stiffness in the cubic system. On the other hand, the first term on the right hand side of Eqs (1) and (3), designated as the bulk modulus, is identical to Voigt bulk modulus [47].

Since the norm is invariant for the material, it can be used for a Cartesian tensor as a parameter representing and comparing the overall stiffness of anisotropic materials of the same or different symmetry or the same material with different phases [42-44]. The larger the norm value is, the more the elastic stiffness of the material is. The concept of the modulus of a vector, norm of a Cartesian tensor is defined as [44]:

$$
N = \|C\| = \quad C_{ij} \square C_{ij} \quad {}^{1\!/_2} \quad (5)
$$

3. Results and Discussion

Table 1 presents the materials elastic stiffness coefficients, calculated bulk B and overall elastic stiffness N moduli for the II-VI semiconductor ZnX (X=S, Se, and Te) compounds. Figure 1 shows clearly the correlation between overall elastic stiffness N and bulk modulus B. Quantitatively, the overall elastic stiffness increases as the calculated bulk modulus B increases. Besides, the calculated bulk moduli are identical to those found by theory of anisotropy [47], and are in agreement with experimental values [6] with maximum error of 8.5 % for ZnTe. The calculated bulk moduli obey the cubic stability

conditions, meaning that $C_{12} \leq B \leq C_{11}$. Figure 2 shows that the bulk modulus is inversely proportional to lattice constants a which was confirmed in several studies [8,14,17,21]. Consequently, from Figure 3 the overall elastic stiffness N is inversely proportional to lattice constants a, as well. Figures 1-3 indicate that among the three compounds under examination, ZnS has the largest elastic stiffness, largest bulk modulus (lowest compressibility), and lowest lattice constant, while ZnTe, in contrary, has the smallest elastic stiffness, smallest bulk modulus, and largest lattice constant. Therefore, the overall elastic stiffness and bulk modulus, the only elastic moduli possessed by all states of matter, reveal much about interatomic bonding strength. The bulk modulus also is the most often cited elastic constant to compare interatomic bonding strength among various materials [48], and thereafter the overall elastic stiffness can be cited as well.

For the isotropic symmetry material, the elastic stiffness tensor is decomposed into two parts as shown in Eq. (1), meanwhile, the decomposition of the cubic symmetry material, from Eq. (3), is consisted of the same two isotropic decomposed parts and a third part. It can be verified the validity of this trend for higher anisotropy, i.e., any anisotropic

Table 1 Elastic coefficients *(GPa)*[4], overall stiffness N *(GPa),* bulk modulus B *(GPa)*, and lattice constants a *(nm)*.

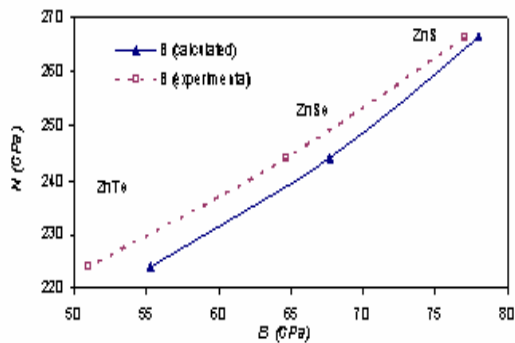|	C_{11}	C_{12}	C_{44}	N	B	B_{exp}[6]	a[13]
ZnS	104	65	46.2	266.5	78	77	0.54
ZnSe	95.9	53.6	48.9	244.0	67.7	64.7	0.57
ZnTe	82	42	55	224.0	55.3	51	0.61

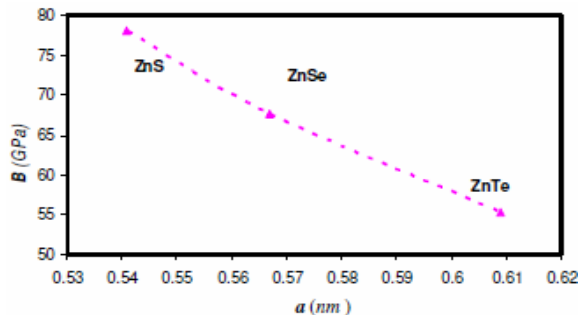Figure 1 The overall elastic stiffness N versus bulk modulus B for ZnX (X=S, Se, Te).

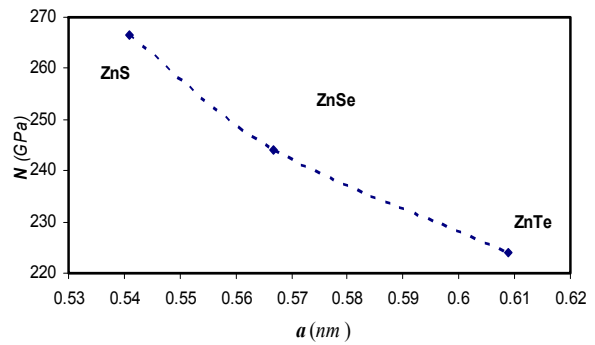Figure 2 The bulk modulus B versus the lattice constants a for ZnX (X=S, Se, Te).

Figure 3 The overall stiffness N versus the lattice constants a for ZnX (X=S, Se, Te).

elastic stiffness will consist of the two isotropic parts and anisotropic parts. Their total parts number should be equal to the number of the non-vanishing distinct elastic coefficients for the corresponding anisotropic material. Anisotropic materials with orthotropic symmetry, for example, like fiber reinforced composites should have two isotropic parts and seven independent parts. Consequently, The Norm Ratio Criteria (NRC) used in this paper is similar to that proposed in [44]. For isotropic materials, the elastic stiffness tensor has two parts, Eq.(1), so the norm of the elastic stiffness tensor for isotropic materials is equal to the norm of these two parts, Eq.(5),

i.e., $N = N_{iso}$. Hence, the ratio $\dfrac{N_{iso}}{N}$ is equal to one for isotropic materials. For cubic symmetry materials, the elastic stiffness tensor has the same two parts that consisting the isotropic symmetry materials and a third, will be designated as the other than isotropic or the anisotropic part. Hence, two ratios are defined as: $\dfrac{N_{iso}}{N}$

for the isotropic parts and $\dfrac{N_{aniso}}{N}$ for the anisotropic part(s). For more anisotropic materials (like orthotropic composites), the elastic stiffness tensor additionally contains more anisotropic parts, and then $\dfrac{N_{aniso}}{N}$ is

defined for all the anisotropic parts. The norm ratios can also be used to assess the degree of anisotropy of a material property as a whole. In this paper the following criteria are proposed: when N_{iso} is dominating among norms of the decomposed parts, the closer the norm ratio $\dfrac{N_{iso}}{N}$ is to one, the more isotropic the material is. When N_{iso} is not dominating, norm ratio of the other parts,

$\dfrac{N_{aniso}}{N}$, can be used as a criterion. But in this case the situation is reversed; the closer the norm ratio $\dfrac{N_{aniso}}{N}$ is

to one, the more anisotropic the material is.
The norms and norm ratios for ZnS, ZnSe, and ZnTe are calculated and presented in Table 2. From the table, interesting phenomena are observed; as the isotropic ratio

$\frac{N_{iso}}{N}$ increases, the anisotropic ratio $\frac{N_{aniso}}{N}$ decreases, which confirms the definitions of these two ratios, and the bulk modulus increases at the same time. Therefore, the nearest material to isotropy (or least anisotropy) is ZnS, with $\frac{N_{iso}}{N}$ = 0.9830, in which corresponds to the largest bulk modulus B = 78 GPa. The least isotropic (or nearest to anisotropy) is ZnTe, with $\frac{N_{iso}}{N}$ = 0.9581, in which corresponds to the smallest bulk modulus B = 55.3 GPa. Since the cubic system is the nearest to isotropy among the anisotropic systems, the calculated values of isotropic norm ratio, $\frac{N_{iso}}{N}$, in Table 2 are very close to one (i.e., 0.9581 - 0.9830). Hence, it can be concluded that the closer the material is to isotropy, the larger the bulk modulus for the material is. A reverse trend correlating the norm ratios and lattice constants can be seen from the table; the closer the material is to isotropy, the smaller the lattice constant for the material is.

Table 2 The overall elastic stiffness N (*GPa*) and norm ratios for the II-IV semiconductor compounds ZnS, ZnSe, and ZnTe

	N_{iso}	N_{aniso}	N	$\frac{N_{iso}}{N}$	$\frac{N_{aniso}}{N}$	B	a
ZnS	262	49	266.5	0.9830	0.1836	78	0.54
ZnSe	238.7	50.9	244.0	0.9780	0.2084	67.7	0.57
ZnTe	214.6	64.2	224.0	0.9581	0.2865	55.3	0.61

4. Conclusions

An interesting feature of the decompositions is that it simply and fully takes into account the symmetry properties when relating macroscopic effects to microscopic phenomena. Therefore, the decomposition of elastic stiffness for cubic system materials into two parts; isotropic (two terms) and anisotropic parts is presented. A scale for measuring overall elastic stiffness is introduced and correlated with lattice constants and calculated bulk modulus. The overall elastic stiffness of II-IV semiconductor compounds ZnS, ZnSe, and ZnTe is calculated and found to be directly proportional to bulk modulus and inversely proportional to lattice constants. Among these compounds, ZnS has the largest overall elastic stiffness and bulk modulus and the smallest lattice constant. Meanwhile, ZnTe has the smallest overall elastic stiffness and bulk modulus and the largest lattice constant. The Norm Ratio Criteria (NRC) is introduced to scale and measure the isotropy in the cubic system material among the semiconductor compounds ZnS, ZnSe, and ZnTe. Hence, a scale quantitative comparison of the contribution of the anisotropy to the elastic stiffness and to measure the degree of anisotropy in an anisotropic material is proposed. ZnS is the nearest to isotropy (or least anisotropic) while ZnTe is the least isotropic (or nearest to anisotropic) among these compounds. These conclusions will be investigated on the II-IV semiconductor compounds CdX (X=S, Se, Te) in the next paper.

References

[1] C.H. Fischer, M. Batzer, T. Glatzel, I. Lauermann, M.C. Lux-Steiner, "Interface engineering in chalcopyrite thin film solar devices", Solar Energy Materials and Solar Cells Vol. 90, 2006, 1471-1585.

[2] D.L. Bätzner, A. Romeo, M. Terheggen, M. Döbeli, H. Zogg, A.N. Tiwari, "Stability aspects in CdTe/CdS solar cells", Thin Solid Films, Vol. 451, 2004, 536-543.

[3] H. Okuyama, T. Miyajima, Y. Moringa, F. Hiei, M. Ozawa, K. Akimot, "ZnSe/ZnMgSSe blue diode", Electronics Letters, Vol. 28, 1992, 1798-1799.

[4] S. Reich, A.C. Ferrari, R. Arenal, A. Loiseau, I. Bellom, J. Robertson, "Resonant raman scattering in cubic and hexagonal boron nitride", Physical Review B, Vol. 71, 2005, 205201-205212.

[5] R.L. Leitsmann, L.E. Ramos, F. Bechstedt, "Structural properties of PbTe/CdTe interfaces from first principles", Physical Review B, Vol. 74, 2006, 085309-085316.

[6] M.L. Cohen, "Calculation of bulk moduli of diamond and zinc-blende solids", Physical Review B, Vol. 32, 1985, 7988-7991.

[7] E. Kim, C. Chen, "Calculation of bulk modulus for highly anisotropic materials", Physics Letters A, Vol. 326, 2004, 442-448.

[8] P.K. Lam, M.L. Cohen, G. Martinez, "Analytic relation between bulk moduli" and lattice constants, Physical Review B, Vol. 35, 1987, 9190-9194.

[9] D. Berlincourt, H. Jaffe, L.R. Shiozawa, "Electroelastic properties of the sulfides, selenides, and tellurides of zinc and cadmium", Physical Review, Vol. 129, 1963, 1009-1017.

[10] Phillips, J.C. Bonds and bands in semiconductors. SD: Academic Press; 1973.

[11] P.K. Pandey, "Study of temperature dependence of interatomic separation and bulk modulus for ionic solids", Journal of Physics and Chemistry of Solids, Vol. 59, 1998, 1157-1160.

[12] S.B. Zhang, M.L. Cohen, "High-pressure phases of iii-v zinc-blende semiconductors", Physical Review B, Vol. 35, 1987, 7604-7610.

[13] J.R. Chelikowsky, "High-pressure phase transitions in diamond and zinc-blende semiconductors", Physical Review B, Vol. 35, 1987, 1174-1180.

[14] N.E. Christensen, O.B. Christensen, "Electronic structure of ZnTe and CdTe under pressure", Physical Review B, Vol. 33, 1986, 4739-4746.

[15] N.E. Zein, V.P. Antropov, "Self-consistent green function approach for calculation of electronic structure in transition metals", Physical Review Letters, Vol. 89, 2002, 126402-126405.

[16] S.R. Krishnakumar, R.N. Shanthi, D.D. Sarma, "Electronic structure of millerite Nis", Physical Review B, Vol. 66, 2002, 115105-11510.

[17] Y. Al-Douri, H. Abid, H. Aourag, " Empirical formula relating the bulk modulus to the lattice constant in tetrahedral semiconductors", Materials Chemistry and Physics, Vol. 87, 2004, 14-17.

[18] R. Dornhaus, G. Nimtz, W.Richter. Solid State Physics. Berlin: Springer; 1976.

[19] Harison, W.A. Electronic structure and the properties of solids. Toronto: General Publishing Company; 1989.

[20] T. Kobayasi, H. Nara. Bull. Coll. Sci., Tohuku University 2; 1993.

[21] H. Ledbetter, "Relationship between bulk-modulus temperature dependence and thermal expansivity", Physica Status Solidi B, Vol. 181, 1994, 81-85.

[22] Y. Al-Douri, H. Abid, H. Aourag, "Correlation between the bulk modulus and the charge density in semiconductors", Physica B, Vol. 305, 2001, 186-190.

[23] M. Ferhat, A. Zaoui, B. Khelifa, H. Aourag, "Band structure calculations of gexsi1−x", Solid State Communications, Vol. 91, 1994, 407-411.

[24] M. Kumar, "Temperature dependence of interatomic separation and bulk modulus for ionic solids", Physica B, Vol. 205, 1995, 175-179.

[25] A.M. Sherry, M. Kumar, "Analysis of thermal expansion for alkali halide crystals using the isobaric equation of state", Journal of Physics and Chemistry of Solids, Vol. 52, 1991, 1145-1148.

[26] J.L. Tallon, "The thermodynamics of elastic deformation—I: equation of state for solids", Journal of Physics and Chemistry of Solids, Vol. 41, 1980, 837-850.

[27] M. Kumar, S.P. Upadhyaya, "Analysis of the thermal expansion coefficient and its temperature dependence for alkali halides", Physica Status Solidi B, Vol. 181, 1994, 55-61.

[28] Q. He, Z. Yan, "Study of temperature dependence of bulk modulus and interatomic separation for ionic solids", Physica Status Solidi B, Vol. 223, 2001, 767-771.

[29] H. Ledbetter, "Sound velocities, elastic constants: temperature dependence", Materials Science and Engineering A, Vol. 442, 2006, 31-34.

[30] J.C. Collins, G.K. White, J.A. Birch, T.F. Smith, "Thermal expansion of ZnTe and HgTe and heat capacity of HgTe at low temperatures", Journal of Physics C, Vol. 13, 1980, 1649-1656.

[31] J.C. Jamieson, H.H. Demarest, "A note on the compression of cubic ZnS", Journal of Physics and Chemistry of Solids, Vol. 41, 1980, 963-964.

[32] S.H. Wei, A. Zunger, "Role of metal d states in II-VI semiconductors", Physical Review B, Vol. 37, 1980, 8958 - 8981.

[33] G.E. Engel, R.J. Needs, "Calculations of the structural properties of cubic zinc sulfide", Physical Review B, Vol. 41, 1990, 7876-7878.

[34] M.P. Tosi' Solid State Physics. Vol. 16, 1964, 1

[35] R. Khenata, A. Bouhemadou, M. Sahnoun, A. Reshak, H. Baltache, M. Rabah, "Elastic, electric and optical properties of ZnS, ZnSe, and ZnTe under pressure", Computational Materials Sciences, Vol. 38, 2006, 29-38.

[36] Landolt-Bornstein. Numerical data and functional relationships in science and technology—crystal and solid state physics. Vol. 22. Berlin: Springer-Verlag; 1987.

[37] T.P. Srinivasan, S.D. Nigam, "Invariant forms", J.ournal of Mathematical and Physical Sciences, Vol. 2, 1968, 311-320.

[38] T.P. Srinivasan, "Invariant piezoelectric coefficients for crystals", Physica Status Solidi B, Vol. 41, 1970, 615-620.

[39] T.P. Srinivasan, "Invariant elastic constants for crystals", Journal of Mathmatics and Mechanics, Vol. 19, 1969, 411-420.

[40] T.P. Srinivasan, "Invariant acoustic gyrotropic coefficients", Journal of Physics C, Vol. 18, 1985, 3263-3271.

[41] Spencer, A.T.M. Continuum mechanics. London: Longmans; 1983.

[42] Y.O. Tu, "The decomposition of anisotropic elastic tensor", Acta Crystallographica A, Vol. 24, 1968, 273-282.

[43] J. Jerphagnon, D.S. Chemla, R. Bonnevile, "The decomposition of condensed matter using irreducible tensors", Advances in Physics, Vol. 27, 1978, 609-650.

[44] M. Gaith,, C.Y. Akgoz, "A new representation for the properties of anisotropic elastic fiber reinforced composite materials", Review of Advance Material Sciences, Vol. 10, 2005, 138-142.

[45] S. Sutcliffe, "Spectral decomposition of the elasticity tensor", Journal of Applied Mechanics, ASME Vol. 59, 1992, 762-773.

[46] W. Voigt, "The relation between the two elastic moduli of isotropic materials", Annals of Physics, (Leipzig) Vol. 33, 1889, 573.

[47] Hearmon, R.F.S. An introduction to applied anisotropic elasticity. Oxford: University Press; 1961.

[48] C. Pantea, I. Mihut, H. Ledbetter, H.,J.B.Betts, Y.Zhao, L.L. Daemen, H. Cynn, A. Miglori, "Bulk modulus of osmium", Acta Materialia Vol. 57, 2009, 544-548.