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MECHANICAL EVALUATION OF THE HETROJUNCTION LAYERS IN SOLAR PHOTOVOLTAIC CELLS

Mohamed S. Gaith, mgaith@coe.neu.edu Department of Mechanical Engineering, Faculty of Engineering Technology, Al Balqa Applied University, Amman, Jordan

Imad Al Hayek, imadha_99@yahooo.com Department of Applied Sciences, Faculty of Engineering Technology, Al Balqa Applied University, Amman, Jordan

ABSTRACT

Being good candidate materials for solar cell absorbers due to their high absorption and resistance to deterioration, the hetrojunction layers compounds in solar photovoltaic cells $CuInSe_2$, $CuInS_2$, $AgGaSe_2$, and $AgGaS_2$ are evaluated from the continuum mechanics point of view. Using Orthonormal Decomposition Method (ODM), namely, Orthonormal Tensor Basis Method (OTBM), the tetragonal structure is decomposed into two parts; isotropic (two terms) and anisotropic parts. The overall elastic stiffness is used for comparison among these layers compounds, and for correlation with the calculated bulk modulus and lattice constant. A scale quantitative comparison of the contribution of the anisotropy to the elastic stiffness and to quantify the degree of anisotropy in an anisotropic material is investigated using the Norm Ratio Criteria (NRC). Moreover, the norm and norm ratios are found to be very useful for selecting suitable materials for electro-optic devices, acousto-optic devices and solar photovoltaic cells.

Keywords: Solar Cells, Absorber Layer Compounds, Bulk Modulus, Overall Stiffness.

1. INTRODUCTION

The window layer compounds $CuInSe_2$, $CuInS_2$, $AgGaSe_2$, and $AgGaS_2$ have a chalcopyrite structure that is closely related those of zinc blend and wurtzite structures. These compounds are found in many applications such as fiberglass communication, thin film solar cells, and photovoltaic systems. Thin film solar cells made from ternary chalcopyrite compounds, such as the aforementioned hetrojunction layers, are characterized by low-cost and clean energy sources. Their high absorption and resistance to deterioration make them good candidate materials for solar cell absorbers. Moreover, due to their flexible optical properties and good stabilities, they are promising compounds for fabricating polycrystalline thin film hetrojunction solar cells [1-3]. Yet, the significant discrepancy in the efficiency of solar cells between the laboratory scale, over 19% [3], and the commercial one, around 13 %, is due to the lack of fundamental understanding of interface and junction properties in the film.

Various attempts have been made to correlate the bulk modulus of compound semiconductors and chalcopyrite compounds with many other physical parameters [4-18]. Nevertheless, it is found that bulk modulus interconnected well with strength and hardness in many materials [5]. Therefore, the material stiffness and its corresponding bulk modulus is one of the important factors that characterize the physical property of a material system which quantifies the degree of stiffness or the energy required to produce a given volume deformation. With a good agreement result, an empirical expression for the bulk modulus was obtained by Cohen [4] based on the nearest-neighbor distance. Using the total energy method Lam et al. [6] obtained an expression for bulk modulus with acceptable results. The bulk modulus for the semiconductor compounds was found to be inverse proportionally correlated to the lattice constants [14, 15]. Gaith et al [16-18] have studied the correlation between the bulk modulus and the over all stiffness and lattice constants for CdX and ZnX (X=S, Se, and Te) using orthonormal decomposition method (ODM) [16] from continuum mechanics point of view.

The goal of this study is to understand how qualitative ground state concepts of the hetrojunction layer compounds, $CuInSe_2$, $CuInS_2$, $AgGaSe_2$, and $AgGaS_2$, such as overall elastic stiffness, can be related to bulk modulus and lattice constants. Therefore, using the elastic coefficients for anisotropic material, an elastic stiffness scale for such anisotropic material, and a scale to quantify the isotropic elasticity within the material will be discussed.

2. THEORY

In comparison of different materials or different geometrical symmetries, or even in a quantitative comparison, for a given material, of the contribution of the anisotropy to a physical property [19-21], the magnitudes of the decomposed parts can give, at certain conditions, valuable information about the origin of the physical property under examination [19, 21]. These problems can be approached by define the norm of a tensor. The norm is invariant and not affected by any transform of the coordinate system. From a device point of view, the new insights facilitate the comparison of materials; one wants to be able to state that a particular material is better than another for making solar cells [20]. The norm concept is very effective for selecting suitable materials for electro-optic devices, transducers, modulators, acousto-optic devices. Based on building up an orthonormal tensor basis elements using the form-invariant expressions [22-26], Gaith et al. [21] developed a decomposition procedure to explore the physical understanding of materials. Hence, following the same procedure, the tetragonal symmetry tensor is decomposed into several independent orthonormal parts.

The number of elements of the decomposed stiffness tensor should be equal to the number of non-vanishing distinct stiffness coefficients, i.e., six constants for tetragonal materials, that can completely describe the elastic stiffness in that medium. Thus, using Orthonormal Decomposition Method (ODM), namely, Orthonormal Tensor Basis Method (OTBM) [16, 21], the matrix representation for the elastic stiffness with tetragonal symmetry system is decomposed into a contracted form as shown in Eq. (1):

$$C_{ij}=\begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix} = A_1\begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}+$$
$$A_2\begin{bmatrix} 4 & -2 & -2 & 0 & 0 & 0 \\ -2 & 4 & -2 & 0 & 0 & 0 \\ -2 & -2 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 \end{bmatrix}+A_3\begin{bmatrix} -3 & -1 & -1 & 0 & 0 & 0 \\ -1 & -3 & -1 & 0 & 0 & 0 \\ -1 & -1 & 12 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}+$$
$$A_4\begin{bmatrix} -3 & -5 & 4 & 0 & 0 & 0 \\ -5 & -3 & 4 & 0 & 0 & 0 \\ 4 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}+A_5\begin{bmatrix} -1 & 1 & 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}+$$
$$A_6\begin{bmatrix} -1 & 1 & 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{1}$$

where

$$\begin{aligned} A_1 &= \frac{1}{90}(2C_{11}+2C_{12}+C_{33}+4C_{13}) \\ A_2 &= \frac{1}{45}(2C_{11}-C_{12}+6C_{44}+3C_{66}+C_{33}-2C_{13}) \\ A_3 &= \frac{1}{90}(-3C_{11}-C_{12}-4C_{44}-2C_{66}+6C_{33}-2C_{13}) \\ A_4 &= \frac{1}{144}(-6C_{11}-10C_{12}+8C_{44}+4C_{66}+16C_{13}) \\ A_5 &= \frac{1}{16}(-2C_{11}+2C_{12}+8C_{44}-4C_{66}) \\ A_6 &= \frac{1}{8}(-2C_{11}+2C_{12}+4C_{66}) \end{aligned} \tag{2}$$

Where A_1 to A_6 are constants in terms of elastic stiffness coefficients expressed as in Eq. (2). It can be observed clearly that the first two terms on the right hand side are identical to the corresponding well known two terms namely bulk and shear [21] which are identical to those found in literature [27] for the isotropic system [28]. Here, A_1 and A_2 defined in Eq. (2), are the Voigt average polycrystalline bulk ***B*** and shear modulus ***G***, respectively. Hence, it can be stated that the tetragonal system is discriminated into the sum of two parts: isotropic part (first two terms), and anisotropic part (other four terms). The latter part resembles the contribution of the anisotropy on elastic stiffness in the tetragonal system.

Due to the fact that the norm is invariant for the material, it was 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 [16, 19-21]. 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 [21]:

$$N = \|C\| = \left\{C_{ij} \cdot C_{ij}\right\}^{1/2} \tag{3}$$

3. RESULTS AND DISCUSSION

In solar energy technology, thin film solar technology based on the hetrojunction layer compounds $CuInSe_2$, $CuInS_2$, $AgGaSe_2$, and $AgGaS_2$, is very promising due to lower production costs and shorter energy pay back times [29]. For these compounds, the successful interface between absorber and buffer layers with alternative materials requires structural and optical material characterization as a prerequisite for understanding interfaces in photovoltaic devices [29]. On the other hand, stability of these compounds in solar cells is of concern due to 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 hetrojunction layer compounds solar cells is associated with the overall elastic stiffness and bulk modulus [30]. The materials elastic stiffness coefficients and lattice constants for $CuInSe_2$, $CuInS_2$, $AgGaSe_2$, and $AgGaS_2$ are presented in Table 1. The correlation trend between overall elastic stiffness ***N*** and bulk modulus ***B*** for each group, i.e. ($CuInS_2$, $CuInSe_2$) and ($AgGaS_2$, $AgGaSe_2$) is clearly shown in Figure 1; the overall elastic stiffness increases as the calculated bulk modulus ***B*** increases. Besides, the calculated bulk moduli are in good agreement with those found by theory of anisotropy [28] and experimental values [13]. Also, the bulk modulus for each group is inversely proportional to lattice constants ***a***, as shown in Figure 2, which was confirmed in several studies [14-15, 31-32]. Consequently, the overall elastic stiffness ***N*** is inversely proportional to lattice constants ***a***, as shown in figure 3. $CuInS_2$ and $AgGaS_2$ have larger elastic stiffness, largest bulk modulus, and lower lattice constant than those for $CuInSe_2$ and $AgGaSe_2$, respectively. 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 [33], and thereafter the overall elastic stiffness can be cited as well [16].

For the isotropic symmetry material, the elastic stiffness tensor is decomposed into two parts [12, 26-28]; meanwhile, the decomposition of the tetragonal symmetry material, from Eq. (1), is consisted of the same two isotropic decomposed parts and other four terms. The Norm Ratio Criteria (NRC) used in this paper is similar to that proposed in [16, 21]. For isotropic materials, the elastic stiffness tensor has two parts, so the norm of the elastic stiffness tensor for isotropic materials is equal to the norm of these two parts, Eq. (3), i.e., $N = N_{iso}$. Hence, the ratio $\frac{N_{iso}}{N}$ is equal to one for isotropic materials.

For tetragonal symmetry materials, the elastic stiffness tensor has the same two parts that consisting the isotropic symmetry materials and the other four terms, will be designated as the other than isotropic or the anisotropic part. Hence, two ratios are defined as: $\frac{N_{iso}}{N}$ for the isotropic parts and $\frac{N_{aniso}}{N}$ for the anisotropic parts. The norm ratios can also be used to assess the degree of anisotropy of a material property as a whole. The following criteria are implemented [16]: when N_{iso} is dominating among norms of the decomposed parts, the closer the norm ratio $\frac{N_{iso}}{N}$ is to one, the more isotropic the material is. When N_{iso} is not dominating, norm ratio of the other parts, $\frac{N_{aniso}}{N}$, can be used as a criterion. But in this case the situation is reversed; the closer the norm ratio $\frac{N_{aniso}}{N}$ is to one, the more anisotropic the material is.

The norms and norm ratios for the hetrojunction layer compounds $CuInSe_2$, $CuInS_2$, $AgGaSe_2$, and $AgGaS_2$ are calculated and shown in Figures 4 and 5; as the isotropic ratio $\frac{N_{iso}}{N}$ increases, the anisotropic ratio $\frac{N_{aniso}}{N}$ decreases and this confirms the definitions of these two ratios, and the bulk modulus increases at the same time.

Therefore, $CuInS_2$ is a closer material to isotropy (or less anisotropy), with $\frac{N_{iso}}{N}$ = 0.9859, and larger bulk modulus $\boldsymbol{B}$ = 64.43 *GPa* than those for $CuInSe_2$. Similarly, $AgGaS_2$ possesses a closer material structure to isotropy and larger bulk modulus $\boldsymbol{B}$ than those for $AgGaSe_2$.

Table 1 Elastic coefficients *(GPa)* and lattice constants ***a*** (*nm*) for the hetrojunction layers compounds

	C_{11}	C_{12}	C_{44}	C_{13}	C_{33}	C_{66}	***a***
CuInS$_2$[34]	83.7	54.4	34.5	54.8	84.5	33.9	0.5532[37]
CuInSe$_2$[34]	71.0	45.3	45.5	45.3	63.3	47.4	0.5782[38]
AgGaS$_2$[35]	87.9	58.4	24.1	59.2	84.5	30.8	0.5759[39]
AgGaSe$_2$[36]	89.8	65.7	21.7	45.1	63.3	13.3	0.5993[39]

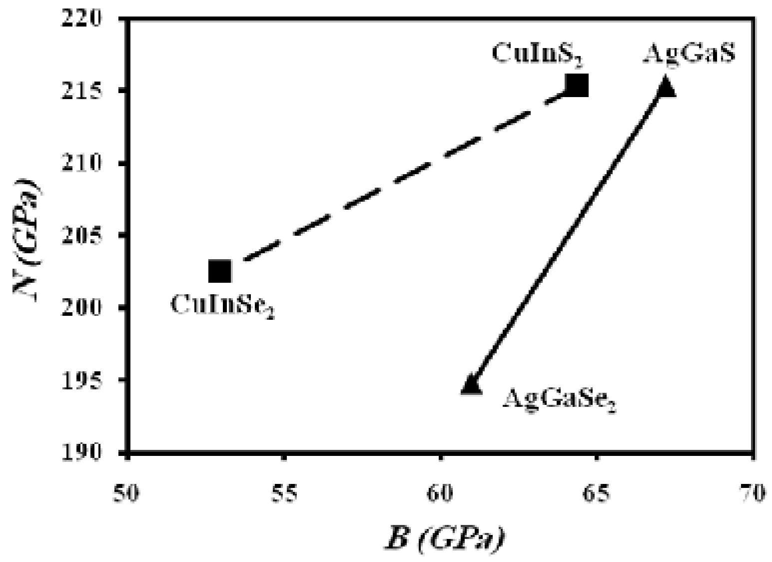

Figure 1 The relation between the overall elastic constant ***N*** and bulk modulus ***B*** for the hetrujction layer compounds.

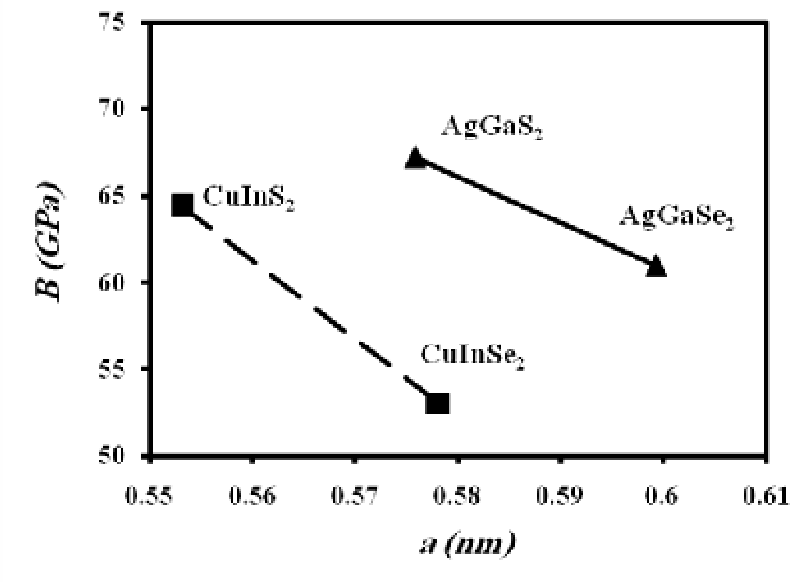

Figure 2 The relation between the bulk modulus ***B*** and lattice constant ***a*** for the hetrujction layer compounds.

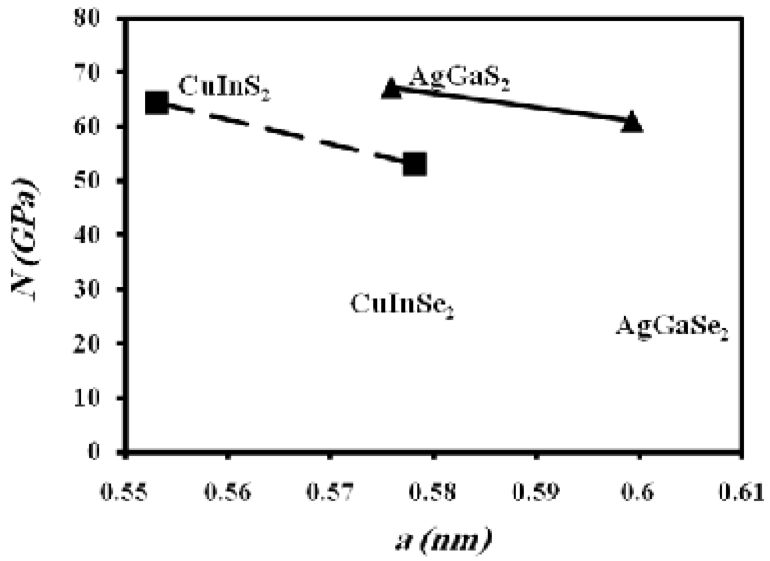

Figure 3 The relation between the overall elastic constant ***N*** and lattice constant ***a*** for the hetrujction layer compounds.

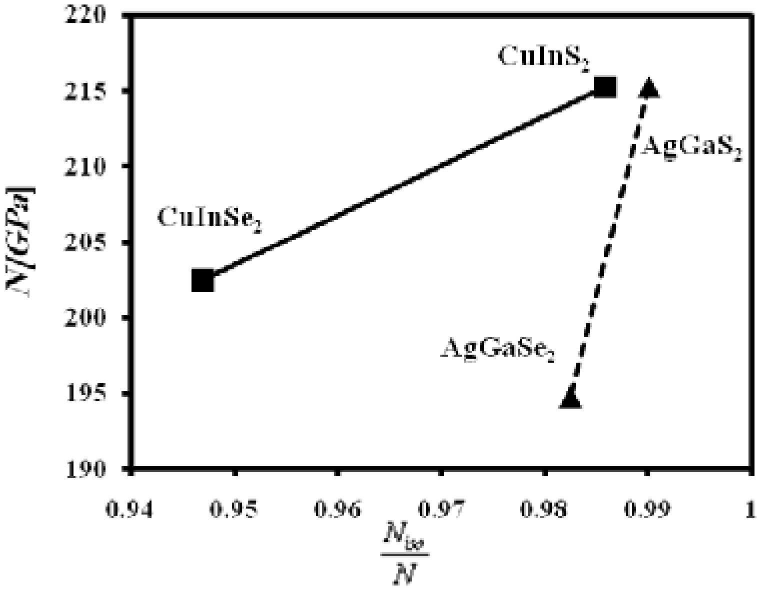

Figure 4 The relation between the overall elastic constant ***N*** and isotropy ratio $\frac{N_{iso}}{N}$ for the hetrujction layer compounds.

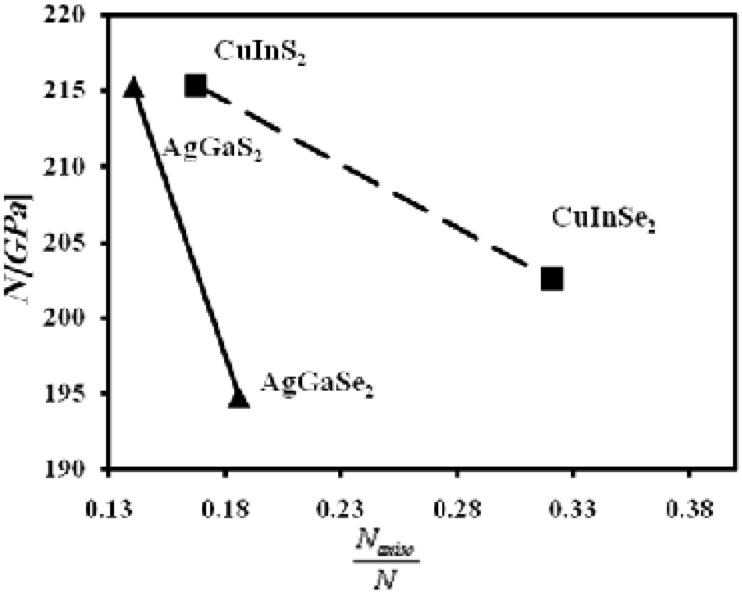

Figure 5 The relation between the overall elastic constant ***N*** and anisotropy ratio $\frac{N_{aniso}}{N}$ for the hetrujction layer compounds.

4. CONCLUSIONS

A significant contribution of this decomposition method is the direct correlation between the macroscopic and microscopic features of a material by means of symmetry properties. Based on the Orthonormal Tensor Basis Method (OTBM), the elastic stiffness for tetragonal system materials into two parts; isotropic (two terms) and anisotropic (four parts) is presented. The overall elastic stiffness is calculated and correlated with lattice constants and calculated bulk modulus for the hetrojunction layer compounds $CuInSe_2$, $CuInS_2$, $AgGaSe_2$, and $AgGaS_2$. The overall elastic stiffness is quantified and correlated to bulk modulus and inversely proportional to lattice constants. $CuInS_2$ and $AgGaS_2$ have larger overall elastic stiffness and bulk modulus and the smaller lattice constant than $CuInSe_2$ and $AgGaSe_2$, respectively. Based on the Norm Ratio Criteria (NRC), the hetrojunction layer compounds $CuInS_2$ and $AgGaS_2$ are closer to isotropy (or less anisotropic) than $CuInSe_2$ and $AgGaSe_2$.

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