1. Introduction

The properties and efficiency of a semiconductor thin film depend on the state of stress and defects in the film structure. When the film is growing layer by layer, the elastic energy due to deformation stress between the substrate and the film is released partly due to the formation of dislocations in the critical thickness deformation. In this paper, we present a finite element analysis of the stress state in a thin film of Cu$_3$BiS$_3$ as a function of thickness and elastic energy release by nucleation of dislocations. Initially, we analyze the stress contours associated with the epitaxial growth and dislocation nucleation and then combine these two in order to study the effective potential energy state of the system. Finally, the tool wxAMPS is today an important application for simulation of solar cells with high reliability and an improved design over its analysis of microelectronic and photonic structures predecessor, incorporating physical principles concerning photovoltaic phenomena and uses a new method for solving algorithms, combining Newton and Gummel approaches, which provides greater stability and speed of computation.

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2. Dislocation energy

Elastically stored energy in a coherent isotropic film parallel to crystallographic plane (0 0 1), (1 1 1) or (0 1 1) is given by

$$E_h = 2Gf_m^2h \left( \frac{1 + v}{1 - v} \right),$$  \hspace{1cm} (1)

where $f_m$ is the strain rate of the lattice, $h$ is the film thickness, $G$ and $v$ correspond to the shear modulus and Poisson’s ratio, respectively, of thin film material, $E_h$ is the strain energy per unit area of the sample. Edge dislocation decreases the maximum strain rate, which is proportional to the Burgers vector $b$, while a pure helical dislocation does not contribute to this reduction. The energy per unit length of an edge dislocation, such as that obtained from the theory of elasticity, using a Volterra cut is given by [6]:

$$E_{dl} = \frac{Gb^2}{4\pi(1 - v)} \left[ 2 + \ln \left( \frac{70b}{b} \right) \right],$$  \hspace{1cm} (2)

where $70b$ represents the size of the control volume and is taken such as $70b$ approximate and $E_{dl}$ is the energy per unit length of the dislocation line. The total energy in the thin film in presence of dislocations is

$$E_{total} = E_h + E_{dl}.$$  \hspace{1cm} (3)

It is noted that $E_h$ has units of energy per unit area and $E_{dl}$ is expressed in units of energy per unit length, this implies that $E_{dl}$ should be normalized with a length and may make corresponding operation with $E_h$.

Carrying out a division by using this length and $70b = h$ can be successfully established $E_{total}$ that is a function of the thickness of the thin film. This is emphasized that this length has been chosen by some authors as the Burgers vector [7]. Since the core radius is often greater than this length, it would be more appropriate to consider a distance from the power supply which dislocation formation, this length is taken such as $3b$ [4]. This value is approximately equal to the lateral expansion of the area under tension [8].

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3. Finite element analysis

3.1. Coherent of thin film growth

It is expected that the linear relationship of $E_h$ with $h$ is true for any thin film (Eq. (1)) [9]. As the growth proceeds, the upper layers will be of more relaxed energy than the layers closest to the substrate [10], although there is no evidence geometric relaxation. Consequently, the energy per unit area of the sample should increase with the thickness, but presents a significant decrease [11].

3.2. Simulation of the nucleation of a strain dislocation

To carry out the simulation, we propose a rectangular domain of 200 Å × 150 Å, discretized with a mesh of $50 \times 50$ quadrangular finite elements of standard type [12]. Figure 1 shows the location of the dislocations, where are presented with two states at different times for a configuration of sources 30 and 900 planes, showing the displacement and annihilation of dislocations and the deformation of the mesh.

Fig. 1. Location of dislocations in step (a) 1000 and (b) 5000. The deformation of the mesh with 30 planes and 900 strains is displayed.

4. Results and discussion

4.1. Critical thickness

The equilibrium theory of Frank and Van der Merve [3] takes into consideration only the energy in the sample. Using this magnitude in the finite element simulation [13], it is possible to determine the critical thickness of the thin film proposed for analysis. To accomplish this purpose it is convenient to effect a diagram that represents the energy per unit area at the interface both before and after introduction of a dislocation in the system [14].

By reference to the graph shown in Fig. 2, at distances of $b/2$ and $5b/2$ energy per unit area is between about 0.56 and 0.02 J/m², respectively. The thickness, in that the stored energy in the film tensioned by unit area of the interface, exceeds the threshold limits corresponding to two critical values that can be termed as peaks and correspond to the critical thickness [15]. For the case of a thin film of Cu₃BiS₃ through the finite element method is a 6b critical thickness. Additionally, it is expected that the level of metastability of the film depends on the configuration of the same, either metallic or semiconductor, which at the same time determines the extent of dislocation nucleation and density dislocations existing.

4.2. Current-voltage characteristic

This feature could play a significant part in the semiconductor solar cells [16], due to the low toxicity of bismuth compared with of CuInGaSe₂ (CIGS), the ternary Cu₃BiS₃ constitutes a favorable option for the development of new materials applied photovoltaic devices. Finally, the tool wxAMPS is today an important application for simulating solar cells with high reliability and improved design over its analysis of microelectronic and photonic structures (AMPS) predecessor [17], which incorporates physical principles concerning photovoltaic phenomena and uses a new method algorithms for solving combining Newton and Gummel approaches, which provides greater stability and computing speed.

However, in this work we used a computer PowerEdge T320 with Intel @ Xeon @ processor, 8 GB RDIMM, 500 GB 7.2 k RPM HD, OS Red Hat Enterprise Linux (RHEL 6.0), the Linux version of the wxAMPS free software distributed from the University of Illinois and the Linux version of the SCAPS software. On the other hand, the numerical simulation was attended with known photovoltaic parameters in order to estimate unknown quantities and associated diagrams.

Fig. 2. Variation of energy per unit area (film-substrate interface).

Fig. 3. Bands diagram (a) and I-V characteristic (b) of solar cells based on the Cu₃BiS₃ compound.

Figure 3 shows the diagrams obtained with wxAMPS and SCAPS for the Cu₃BiS₃ absorber layer of solar cell. In Fig. 3a it can be seen the energy band diagram showing a bias voltage of 0.845 V under illumination, while the diagram of Fig. 3b shows the current-voltage curves in conditions dark/light.
In wxAMP's initial conditions predicted for solar cell of Cu$_3$BiS$_3$ compound that was used such as an absorbent layer, obtained a $V_{oc} = 0.712$ V, $J_{sc} = 36.25$ mA/cm$^2$, $FF = 79.54\%$, and an efficiency of 19.86%, which allows us to infer Cu$_3$BiS$_3$ that constitutes an outstanding alternative to the design of photovoltaic devices.

5. Conclusions
We used the finite element method to simulate the nucleation of dislocations of Cu$_3$BiS$_3$ thin film. Based on a previously defined model, simulated a helical dislocation and through the analysis of energy conditions there was obtained critical thickness value for the sample semiconductor $6b$. Moreover, it is noted that large photovoltaic conversion efficiencies can occur, with a new material with properties similar to CIGS.

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