Study the Effect of Thickness on the Optical Properties of Copper Oxide Thin Films by FDTD Method

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Abstract: In this work, we present the optical modeling results of film thickness effect on the optical properties of CuO thin film based devices. The finite-difference time-domain (FDTD) method were used to predict the optical properties of CuO thin films on glass substrate with deferent thicknesses (100 nm- 3 µm). The absorption, transmittance, and reflectance are detected over a wavelength range of 300–800 nm. FDTD simulation results indicated that the optical absorption increased with increasing CuO film's thickness. In addition, a numerical simulation predicted that the CuO active layer with thickness 1.5 µm has a higher absorption spectrum. On the other hand, the further increase of CuO thickness (2, 2.5, and 3 µm) showed no more effect on the absorptance, where their absorption spectra behave similarly to each other. This study can be useful to develop highly efficient and low cost thin film based optoelectronic devices.

Keywords: FDTD Simulation, Copper Oxide (CuO), Thin Films, Thickness, Optical Properties.

1. Introduction

Thin film semiconductors are getting an intensive interest in a very wide range application in various fields such as solar cells, sensors, transistors, thermoelectric devices, medical equipment, and so on. Besides, Thin films are utilized in many and environmental applications, tools coating, self-cleaning and antireflective layer on lenses, optical devices, photovoltaic [1, 2]. This is due to the useful physical and chemical properties of the semiconducting thin films since they can respond to energy conversion, sensing and mechanical effects in addition to their unique behaviors in the optical coatings [1, 3]. Thin film based device efficiency is strongly dependent on the films morphology, thickness, and stability, which are directly related to the synthesis conditions and materials nature [3, 4]. The effect of film thickness on the surface morphology and optical properties has been widely studied by many researchers in the last decades. Studies showed that the probability of light absorption in the thin film optoelectronic devices can increase by increasing the active layer thickness [5]. Accordingly, thin film device weight and cost will increase too, where thin film thickness ranges from several nanometers to few micrometers. Therefore, numerical study are commonly used to improve the optical devices design processes by testing and optimizing device components dimensions and their structures before fabrication. Moreover, applying simulations before fabrication process can help to avoid a significant amount of production costs as well as to save effort and time [6]. Finally, understanding light-matter interaction behavior can help to increase light absorption by controlling device geometric parameters.

Several simulation approaches have been utilized for simulating thin film optical based devices to achieve better light absorption efficiency [7]. For example, finite-difference time-domain (FDTD) method has been used widely as a numerical simulation technique to investigate light propagation within materials that used in optoelectronic structures. I t can be performed with 2D and 3D designs, simulate a wide range of wavelengths at one time and fast efficiency. Therefore, studies showed that the FDTD approach has become the most popular and efficient numerical simulations method that offers accurate results of the optoelectronics field [7-9].

Cupric oxide (CuO) thin film has recently received a considerable interest due to its remarkable optical, electrical and mechanical properties. There are several applications used in CuO semiconductor, such as catalysis, solar cells, sensors, and optoelectronic devices [1].

In this work, the influence of the thicknesses variation on the optical properties of the CuO film layer was investigated by using FDTD simulation method in order to achieve an optimized design for CuO based photonic devices. Research has performed to understand the physics behind light absorption and reflection in the CuO thin film structure with deferent thicknesses.

2. Finite difference Method and Structure Under Investigation

The commercially available software FDTD Solutions by Lumerical Inc. (http://www.Lumerical.com) has been used in this study. We focused on the light propagation inside the various CuO film thickness on glass substrates. The finite difference method (FDTD) solves Maxwell's equations in the time domain, therefore this method can describe electromagnetic phenomena in any structure where Maxwell's equations explain the necessary physics.

There is a wide range of applications for this method including: LEDs, solar cells, biomedical device, optical switches, semiconductor-based photonic devices, sensors, meta-materials, and so on [10, 11]. FDTD simulation has been successfully used to find out the performance of the optical devices with more than two-component and multi layers [12]. CuO thin film structures on glass substrates were modeled by using a three-dimensional (3D) FDTD simulations. Figure 1 shows (a) perspective view of the simulation setup and (b) 3D simulation region, light source, monitors and CuO/glass structures without the top metal contact layer. The thin film layers have thicknesses in the range of 100 nm to 2.5 μm and the structures were excited by a broadband (300 nm- 800 nm) polarized plane. The plane wave light source placed normally to the samples along the z-axis. In addition, the perfectly matched layer (PML) boundary condition in the Z-direction was employed with periodic boundary conditions in the x and y directions. The size of the simulation region was set to 5 × 5 × length from 0.3 to 7 μm^3.

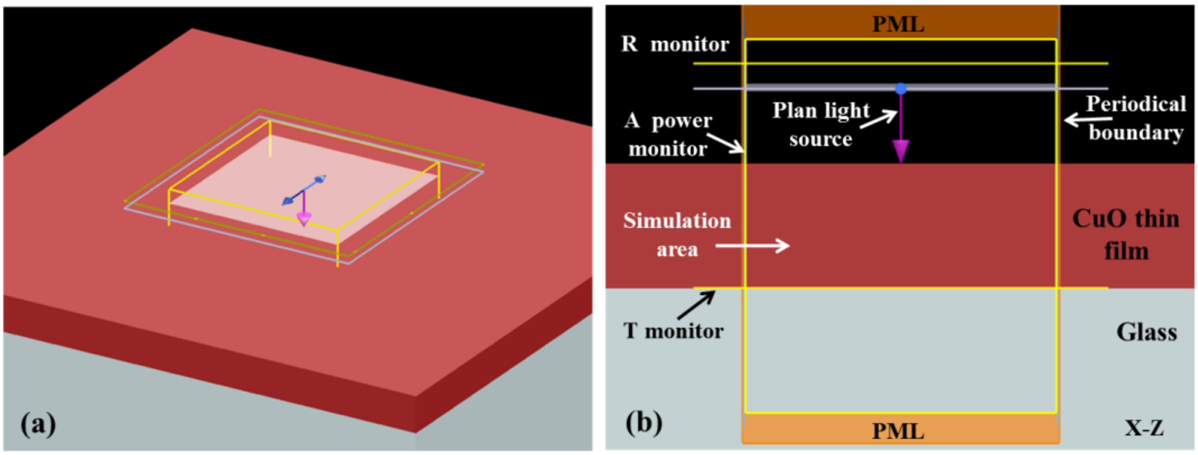

Figure 1. The setup of FDTD simulations, (a) perspective view (b) 3D simulation region, light source, monitors and CuO thin film on glass structure.

A field monitor and a power monitor were set as shown in figure 1(b) to collect the propagated light rays. The low frequency domain field monitors was used to calculate transmission (T) and reflectance (R) at different locations of the simulated structure. Where the absorption (A) can determined from the T and R calculated values (A+T+R=1) [13].

The refractive index (N) may be defined to be complex and can express as:

$$N = n - ik \tag{1}$$

The real part (n) relates to the velocity of light in the medium at the given frequency. It can determine from the reflectance (R) using the relation [7]:

$$n = \frac{1+R+\sqrt{R}}{1-R} \tag{2}$$

While the imaginary part (k) or an extinction coefficient is related to the attenuation of the wave amplitude due to absorption, therefore k can be calculated using the following equation [14]:

$$k = \frac{\alpha\,\lambda}{4\,\pi} \tag{3}$$

Where, λ is the wavelength, (α) is the absorption coefficient and can be found by using the equation [7]:

$$\alpha = \frac{2.303\,A}{t} \tag{4}$$

where (A) is the light absorptance and (t) is the sample thickness.

In this work, The optical constants (n and k) of CuO were calculated based on the experimental R and T measurements that extracted from [15].

The power absorptance per unit volume (Pabs) can be calculated by using the equation [7]:

$$Pabs = -0.5\,\omega\,|E^2|\,imag\,(\varepsilon) \tag{5}$$

Where $\omega = 2\pi f$, f is the frequency, $|E|$ is the absolute magnitude of the total electric field, and ε is the imaginary part of the permittivity.

3. Results and Discussion

Different thickness (0.1, 0.5, 1.0, 1.5, 2.0, 2.5, and 3.0 µm) of the planar copper oxide films model are simulated to calculate reflectance, transmission and absorption. The results of the simulated absorptance, transmittance, and reflectance as a function of CuO film thickness are shown in figures 2, 3, and 4. Figure 2 shows the variation of absorptance that the calculated through the relation A = 1-T-R over a wavelength spectrum of λ= 300 nm - 800 nm at various film thicknesses. It can see that as the film thickness increased from 0.1 to 1.0 µm, there is a remarked increase in light absorptance in both of UV and visible range of CuO thin films spectrum. Whereas, at thickness above 1.0 µm, the absorptance spectrum increased slightly till the thickness of CuO layer reaches to 2.0 µm and then the absorptance remain constant as shown in figure 2. The increasing light absorptance with a thin film thickness increasing can be attributed to an increase of the effective optical path length with increasing film thickness [16, 17]. This is as expected because the film packing density increase with increasing film thickness [18, 19]. This study revealed that the optimal thickness of CuO film for high absorption was 1.5 µm, which help to produce economical light harvesting devices with low- cost semiconductor materials and high efficiency.

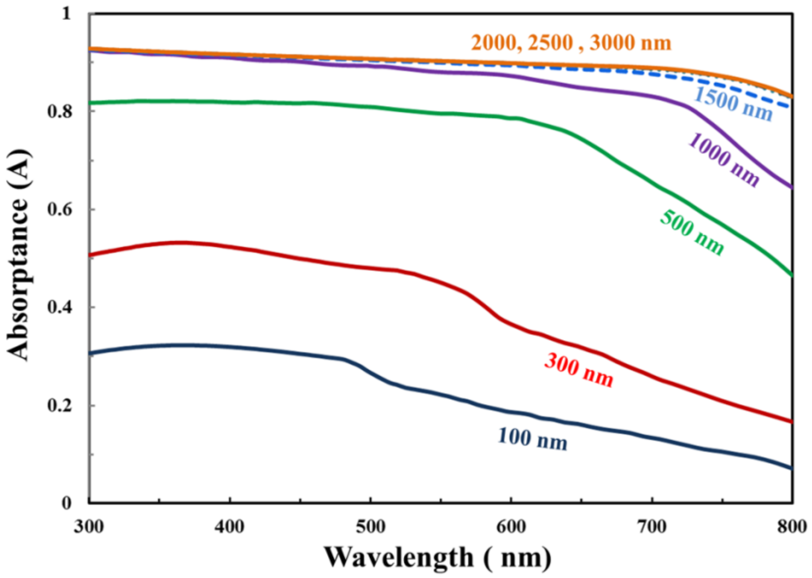

Figure 2. Absorptance (A) FDTD simulation results of CuO thin film structures on glass substrate. The measurements have been taken in the wavelength range 300-800 nm

Figures 3 presents the variation of transmission as a function of wavelength at various CuO film thicknesses. It was observed that the transmittance values in the visible light region decrease rapidly as the film thickness increases. This behaviors can be linked to increasing absorptance values and thickness affect. According to Beer−Lambert Law, the relationship between transmittance (T) and sample thickness (t) can be expressed as $(T = \exp(-t\alpha))$ [18-21]. From this equation, the transmittance decreases exponentially with light propagation through the material and the absorption coefficient α. However, the low absorption coefficient means that the light is poorly absorbed, and the material will appear transparent to that wavelength when its thickness is thin enough [22, 23]. Figure 3 also demonstrates that the predicted transmittance spectra showed almost no dependence on film thickness at 2, 2.5, and 3 µm, they have relatively similar behavior. In addition, CuO film with 1 µm thickness showed relatively lower transmittance at (300-600) nm spectral regions. These results could possibly be because of CuO films texture change with increasing thickness.

Figure 4 illustrates that the reflectance spectra for film thicknesses range between 100 nm- 1 µm decrease with increasing CuO film thickness. While films with thicknesses more than 2 µm exhibit a different behavior as reflectance results increase with increasing CuO layer thickness. This behavior can be attributed to the to an increase in CuO layer packing density and increasing absorption with increasing thickness [18, 24]. The optical results indicate that CuO films with a certain range of thickness have favorable performance as an optical active layer.

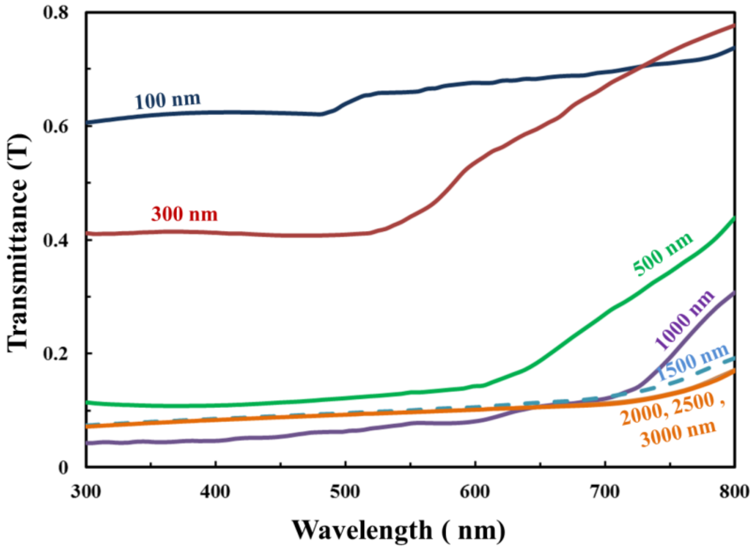

Figure 3. Transmittance (T) FDTD simulation spectra of the CuO/ glass structures

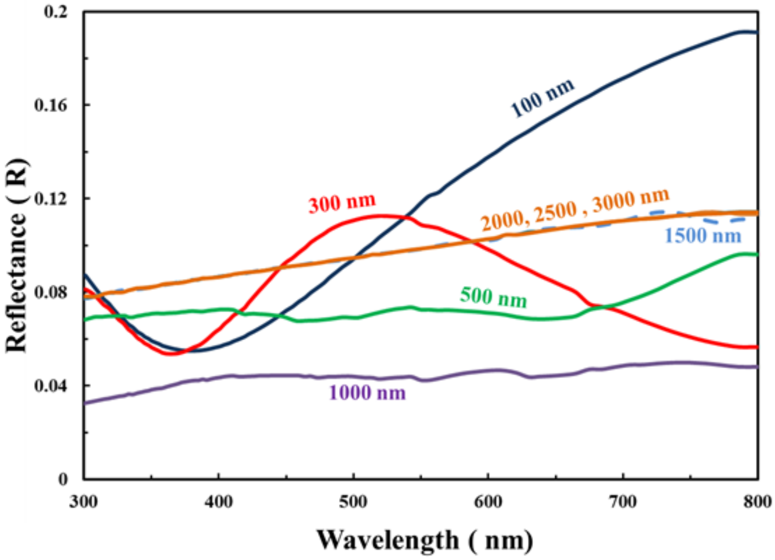

Figure 4. Reflectance (R) FDTD simulation results of CuO thin film structure on glass substrate

The calculated optical power absorption per unit volume (Pabs) profiles using the 3D FDTD method for all mimicked CuO samples illustrate in Figure 5 (a). The predicted absorption-per-unit-volume within the simulated CuO film layers was performed for wavelengths with range (300–800 nm). According to the equation (5), the absorbed power is directly proportional to the electric field intensity and the imaginary part of the permittivity. Thus, the FDTD absorbed-power distribution is necessary to obtain the better information of the light absorption mechanism within the optical device components to enhance its performance in the visible spectrum. The FDTD simulation results in figure 5 along XZ plane illustrated that the light absorption increased rapidly with increasing CuO film thickness, and the most absorption occurs at the top of the CuO film structure especially in thicker one. It is evident from the light intensity distribution images (300-800) in figure 6 that the more than 500 nm exhibit broad band absorption. Also, in CuO thin film, the shorter wavelengths such as λ = 300 nm almost absorb at the ~90 nm region, while most of light with wavelengths λ = 500 and 800 nm can be absorbed in ~120 and ~1300 nm, respectively regions. Therefore, thin film longer than 1.5 µm value might not be needed which help to estimate the optimal active layer thickness before real light harvesting device producing. Increased absorption of the CuO thin films with increasing film thickness can be attributed to the electric field confinement within the copper oxide structure [7, 25].

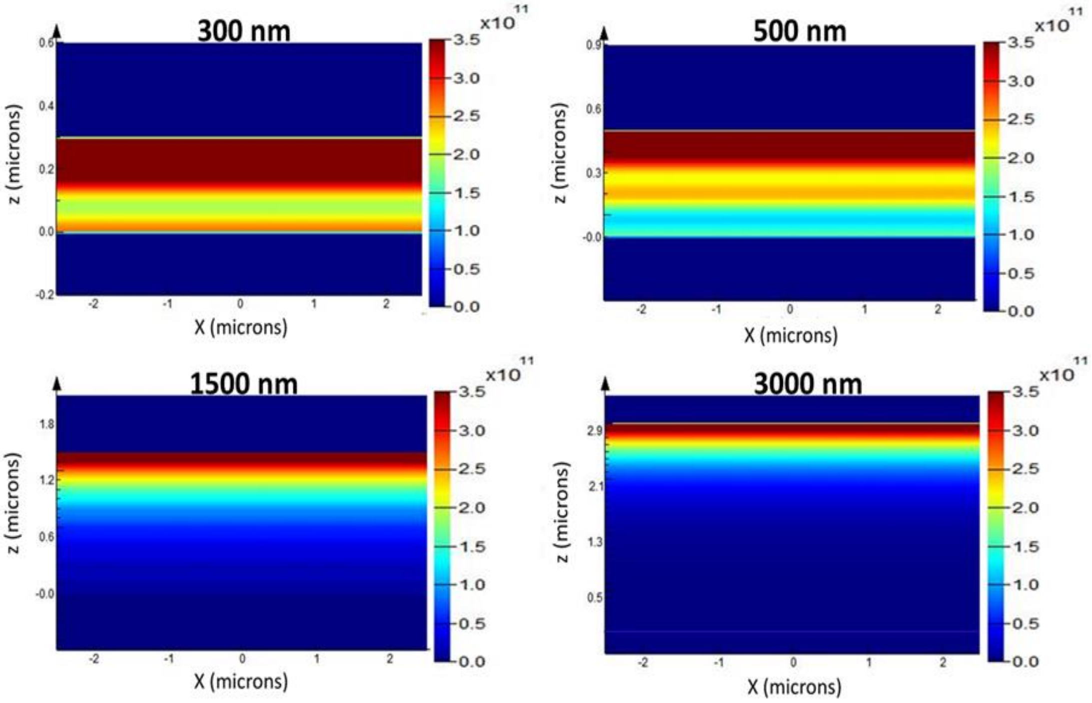

Figure 5. FDTD simulation of the optical power absorption per unit volume of CuO with 0.3, 0.5, 1.5, and 3 µm thickness over the wavelength range of 300 to 800 nm.

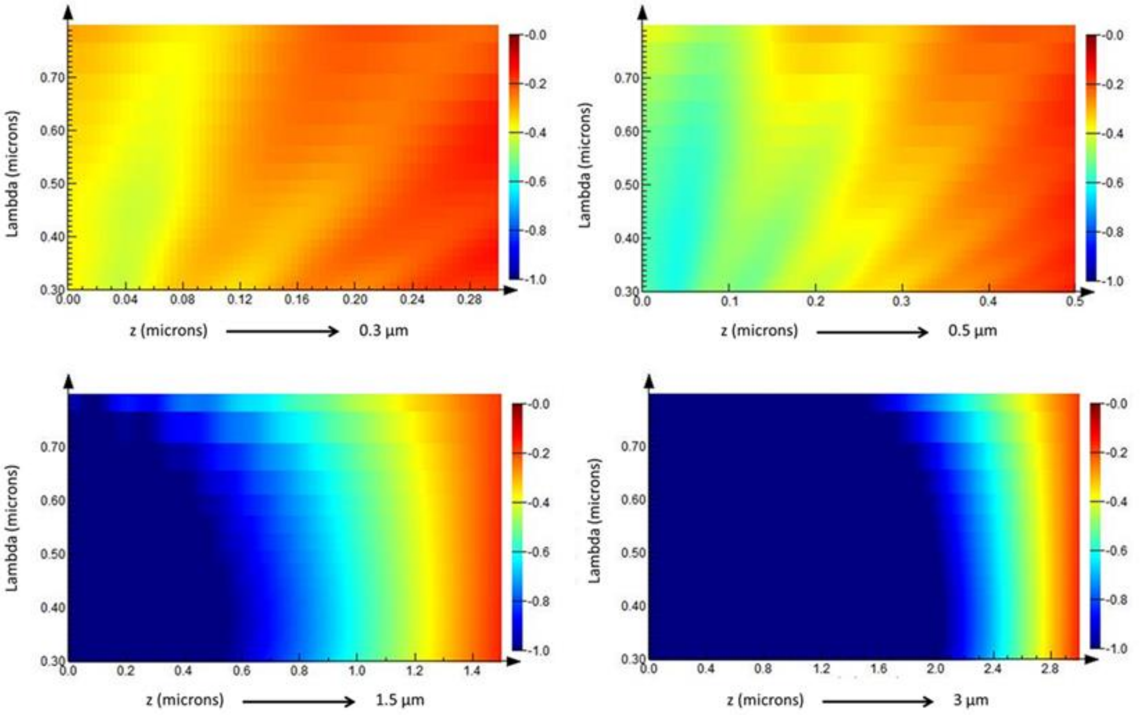

Figure 6. light-spectrum absorption distributions for CuO on glass samples

4. Conclusions

In summary, the FDTD mathematical modeling method was used to perform an optimization study for planar array to achieve better optical properties inside the copper oxide thin film based devices. FDTD simulation was successfully employed to investigate the effect of thickness on the absorptance, transmittance, and reflectance for CuO film with thickness range from 0.3 to 3µm. The predicted results indicated that the CuO film of 1.5 µm thickness exhibits the optimum optical absorption. However, device with 1.5 µm CuO layer showed a broad band absorption rate in the visible spectrum and uniform distribution of light intensity within the active layer. This study can help to optimize the optical parameters before device fabrication to enhance device performance.

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