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Optimizing ZnO Thin Films for Light Absorption Using FDTD Simulation

Mengoptimalkan Film Tipis ZnO untuk Penyerapan Cahaya Menggunakan Simulasi FDTD

Hadeel Abdalbari Hussein, hadeelabdalbari718@gmail.com, (1)

Ministry of Education General Directorate of Education in Najaf Governorate, Iraq

⁽¹⁾ Corresponding author

Abstract

General Background: The development of efficient and cost-effective photovoltaic devices relies heavily on theoptical performance of semiconductor materials. Specific Background: Zinc oxide (ZnO), a low-cost and abundant material, exhibits promising optical properties suitable for light absorption applications. Knowledge Gap: However, limited studies have simulated the impact of varying thickness and surface roughness on the optical behavior of ZnO membranes using advanced computational methods. Aims: This study aims to simulate and analyze the optical properties of three-dimensional ZnO thin films deposited on a glass substrate using the Finite Difference Time Domain (FDTD) method. Results: The simulation, conducted across wavelengths ranging from 300-800 nm, demonstrates that increasing the ZnO membrane's thickness and surface roughness enhances light absorption and reduces reflectivity. Optimal performance was observed at a membrane thickness of 5.2 µm. Novelty: This research applies FDTD-based modeling to examine both flat and rough-surfaced ZnO membranes, providing a comprehensive understanding of light interaction in nanostructured layers. Implications: The findings contribute to the design of high-performance, low-cost optical and photovoltaic devices by optimizing ZnO film characteristics for maximum efficiency.

Highlights:

B1a.ckground: ZnO films have potential in low-cost photovoltaic applications.

M2e.thod/Result: FDTD simulation shows thickness and roughness improve light absorption.

Implication: Guides efficient ZnO-based optical device design.

Keyword : Zinc Oxide (ZnO), Thin Films, FDTD Simulation, Optical Properties, Photovoltaic Devices

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Introduction

1-1 Introduction

Interest in the study of semiconductors began in the early nineteenth century, and over the subsequent years many of them were studied because of their unique shape and characteristics, as the semiconductor has conductivity affected by light, temperature, impurities of atoms and magnetic field [1]. Modern semiconductor electronic devices are a necessary aspect of normal human life activities, containing many sets such as image capture devices, LED and aviation lamps, remote sensing systems, improving the interaction of light with materials and absorbing incident light rays [2].

2-1 Thin Membranes

Thin- Membranes technology contributed significantly to the development of the study of semiconductor materials and gave a clear idea of many of their physical and chemical properties, and the term thin film describes one or several layers of atoms of matter exceeding the thickness of one micron [2,3] In 2015, thin films were made of high-temperature superconducting conductors made of unequal two-dimensional structures. Intensive research has begun to understand the behavior of the properties of electrical and optical thin films that benefit humans in their lives. [4]

3-1 Thin Membranes Preparing Methods

Technological and practical advances have helped to produce new preparation methods, which have become highly efficient and precise to suit the thickness of the thin Membranes. Diagram (1-1) shows the methods of preparing thin Membranes and each method is different from the others to obtain Membranes with suitable specifications, cheap and always available [5].



Figure 1. Thin- Membranes preparation methods

4-1 Thin Membranes Applications

The uses of thin Membranes varied in many physical fields, the most important of which are [6]:

4-1-1 Photovoltaic Applications

In the optical fields, thin Membranes have been used in the manufacture of optical fibers used in communications, solar cells, as well as in the manufacture of photoreagents and reflective coatings [7].

4-1-2 Magetic Applications

Thin Membranes were used in the manufacture of magnetic memory devices, reagents and pumps, as well as in the addition of CDs [8].

4-1-3 Thermal Applications

Thin Membranes have been used in a variety of fields, including thermal reactors and thermal fields, where they can be used using a barrier or layer that reduces heat exchange between the internal and external medium to improve the performance of reactors [9].

5-1 Thine Membranes Properties

The study of semiconductor materials has become an important part of electronics because of its unique features, for example, it is involved in the study of crystal structure and mechanical, optical and electrical properties, and these properties depend on the conditions of their manufacture and represent a challenge to other experimental methods [9,10].

5-1-1 Thickness

Scientific experiments have shown that the thickness of the membrane can affect some other properties of the thin film, and there are various factors that can be developed by increasing the thickness of the membrane, and the rate of the fragmented sample is determined by the sedimentation process, as the thickness of the membrane is always preferred in electronic fields because it resists corrosion when exposed [11].

5-1-2 Surface Roughness

It consists of surfaces in the form of terrain similar to the geometric shape of the surface when building the structures of thin-film devices with a solid body and be different roughness, whether single-layer or multiple, and surface roughness is defined as a morphological characteristic of an unclear nature (random), and the composition of its surface is measured by the atomic force microscope, and the rate of surface roughness can be determined in units (RMS) [12].

6-1 Optical Properties

6-1 Reflectivity

Reflectivity (R) is defined as the ratio between the intensity of the incident radiation and the intensity of the reflected beam. Reflectivity is measured by the law of conservation of energy [13].

$$\mathscr{R} + \mathbf{A} + \mathbf{T} = 1 \quad \dots (1-1)$$

6-1-2 Permeability

Transmittance represents the ratio between the intensity of transmitting light (I_t) and incident light (I_0) and is illustrated by the following formula [14]

$$T = \frac{I_t}{I_0} \qquad \dots (2-1)$$

It can be defined as the ratio between the intensity of incident light (I_0) and absorbed light (I_A) as in the following relationship [15]

$$A = \frac{I_A}{I_0} \qquad \dots \quad (3-1)$$

7-1 Zinc oxide

It is a white inorganic compound that yellows when heated due to lattice deformations, as well as it is a non-toxic substance and it is one of the stable oxides and that the crystal structure is in it the body is centered (BCC) as shown in Figure (2-1), and it is characterized by its high absorption where its absorption coefficient is $(10^{4} \text{ [[cm]]}^{(-1)})$ at a wavelength of 500 nm, and most of the charge carriers in it are gaps [16]

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Figure 2. Zinc Oxide Crystal Structure

8-1 Research Problem

There are many difficulties that caused the research problem of thin films, including the economic cost of the materials used, methods of preparation, and the ability of the materials to reflect and absorb the incident light beam, as well as that this study takes a long time to reach a state of stability in the program used (FDTD), and when modeling complex materials, the electromagnetic constants of the material are known only over a narrow frequency range.

9-1 Importance of research

The research aims to understand the behavior of light in zinc oxide membranes and study the effect of changing surface roughness and thin film thickness on optical properties (transmittance, absorption, reflectivity) using the method of finite differences in the time domain (FDTD), and also aims to obtain a membrane with good specifications and improve its properties in a faster and cheaper way before manufacturing prototypes and taking experimental measurements and using it in the manufacture of semiconductor devices such as photovoltaic cells and photoreagents and improving them before manufacturing.

Methods

1-2 Introduction

Maxwell's equations describe the behavior and changes of electromagnetic waves and their impact on materials and their transformations from one form to another of energy, as numerical methods for searching for solutions to Maxwell's equations have become common over a huge extent, usually numerical methods of Maxwell's equations are called arithmetic electromagnetism, Computational models used in these methods provide advanced computer software used to model and simulate electromagnetic phenomena, observe their changes, and process the electromagnetic interaction between electromagnetic fields and engineering formations. The development of computational software systems is closely related to the development of the computer. The irregular (random) shape of the studied model and the unequal electric moments, as well as the boundary conditions of the material surfaces, made the solution of Maxwell's equations difficult in analytical methods, and as a result mathematical methods, approximate and other methods are used. [17]

2-2 Electromagnetic Waves

In 1820, the scientist Orested observed that if a current passes in a wire, a magnetic effect arises represented in the deviation of a magnetic needle placed next to the wire, and the discovery of Orested linked the relationship between the science of electricity and magnetism. It is named after the electromagnetic spectrum or electromagnetic radiation. Electromagnetic waves propagate in space and physical media, and the most famous types of light rays, X-rays and gamma rays are propagated. These waves consist of two electric and magnetic fields perpendicular to each other, variable, concomitant and in phase agreement [18].

10	10 ¹³	10*	10*	10.3	10°	103	10° λ (n
Gar	mma rays	X-rays	Infra	red Micro	wave	Radio	
1024	10 ²¹	10"*	lo ¹⁰	10 ¹²	10° Ir	10° hcreasing Fre	10 ¹ v (H quency (v)
100	200	300	400	500	600	700	
•—	- Ultraviolet	spectrum —			spectrum		

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Figure 3. Electromagnetic waves and the relationship between frequency and their wavelengths [18]

3-2 Visual Design

It is one of the most important modern programs at the present time and plays a good role in improving designs, and this helps in programs in the engineering and scientific fields and works by giving the correct information intended by the designer. Design programs work to give effort, sufficient time and the percentage of loss it contains. The efficient functioning of the optical apparatus improves the physical properties, the most important of which are the type of material, structures, many layers, coatings, distortion and geometric shape of the surface [19].

4-2 Limited time domain differences method

The method of finite differences in the time domain (FDTD) is one of the applications (FDM) and it is frequently used in solving Maxwell's equations and works to find the components of the electric and magnetic fields through time, and it is also considered one of the best and most used methods to form values for the interactions that occur between light and materials used in optical devices, especially after the advent of the computer, due to its distinct physical properties such as flexibility and accuracy during work, This method is a powerful tool for the formation of optical devices and materials of complex composition and have two or three-dimensional shapes and Maxwell's equations are written in the following mathematical form [20]:

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Figure 4.

The physical meaning of equation (2-2a) means the spacing of an electric field equal to the density of the electric charge, the equation (2b-2) means the divergence of a magnetic field equal to zero, equation 2c-2)) means the change of magnetic field density with respect to time gives us an electric field in a closed circuit, and the equation ((2d-2) means the flow of current in the case of alternating current generates a magnetic field in a closed circuit.

5-2 Previous studies

1-In 2009, Liu, G. et al. [21] conducted a theoretical study to develop a finite time-domain differences algorithm to simulate the propagation of light on a rough surface and calculate its spectral properties. 2. In 20110, Lacombe, J [22] and others modeled light propagation in solar cells of thin silicon films to study the effect of surrounding, light retention and absorption in three-dimensional semiconductor layers and modeling light propagation using the finite difference method in the time domain. The expected results of the optical generation rate of charge carriers from amorphous silicon membranes and rough interlayers were compared with the experimental results. 3- In 2014, Fairus Atida and his team [23] used the finite difference method FDTD to study the metal films used in three-dimensional biological sensors of different thicknesses, and the results showed that the silver membrane with a thickness of 100 nm shows the highest reflectivity at the wavelength of 644 nm, while in the thin zinc and aluminum membranes it shows less reflectivity. 4. In 2016, Jia-Sheng [24] used an optical simulation method to study the effect of surface roughness on the optical performance of LEDs and ...

3- Practical Aspect

1-3 Introduction

This chapter deals with the design of zinc oxide membrane structures in three dimensions ((X, Y, Z)) using the finite differences in time domain (FDTD) method, and through the use of the FDTD method, zinc oxide (ZnO) membranes of different thickness were simulated on the glass base, as well as changing the surface roughness of the thin film to study the effect of thickness and surface roughness on the optical properties of zinc oxide thin films. [26]

2-3 Optical modeling of thin-film structures using FDTD simulation

The optical simulation steps by the FDTD method begin by determining the values of the real part (n) and the imaginary part (k) of the complex refractive index (N) as a function of the wavelength, the values of n and k are determined depending on the practical values of the pre-measured transmittance and reflectivity of the zinc oxide membrane that is of different thickness, the complex refractive index is used to describe the reflection of light from the surface separating two mediums with different refractive indexes[27].

2-3-1 Thin Membranes Structures

To build a simulation model of thin films with a flat surface in three dimensions, cuboids of geometric shapes with different thicknesses of 0.1, 0.3, 0.5, 0.7, 1, 1.5, 2, 2.5, 3 μ m and dimensions of (10 μ m ×10 μ m) were placed on a glass substrate, and to create a coarse thin film surface of zinc oxide, we used the rough surface unit of geometric shapes in the program with a thickness of 500 nanometers (nm) as shown in Figure (1-3).

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Figure 5. Structure of the zinc oxide thin film model for the rough surface

2-3-2 Electromagnetic radiation sources

In this study, photosimulation of zinc oxide (ZnO) membranes was performed using a wide range of wavelengths ranging between (300 nm-800 nm) by the polarized planar wave source along the z-axis, and planar sources are used to obtain uniform electromagnetic waves, the simulation area is surrounded along the x, y axis under boundary conditions, where the state of the limits of the completely symmetrical absorption layer (PML)) of the simulation area was used to prevent any reflections issued to an acceptable level. [28] Figure (2-3) shows the numbers on which the simulation process was based.



Figure 6. Simulation process settings

The effective layer (light absorption layer) is illuminated from above by the light incident on the source perpendicular to the length of the Z plane, transmittance (T) and reflectance (R) are calculated by tow frequency domain field and power monitors, which are 2D virtual detectors. Absorptance (A) is calculated using relation (1-3) [29].

Results and Discussion

Chapter IV discusses and presents the results obtained using the theoretical study of the optical properties of zinc oxide (ZnO) membranes prepared by the method of finite differences in the time domain (FDTD), and this part contains measurements of optical properties, including absorbency reflectivity and permeability of a number of roughness and various thickness of the zinc oxide membrane (ZnO).

1-4 Effect of Thickness Change on Optical Properties Of Zinc oxide

We used a simulation of a variety of thickness (3, 2.5, 2.0, 5, 1.0, 0.5, 0.3 and 0.1) micrometers for a sample of zinc oxide membranes and figure ((1-4) shows the results to simulate absorption as a function of the thickness of the zinc oxide membrane (ZnO), and Figure (1-4) shows that the absorption values that were calculated from the previous mathematical relationship (1-3) with a wavelength extending from 800) - (300 nm), their value rises with increasing the thickness of the thin film in order to increase the number of atoms in the membrane and this leads to the formation of the opportunity to absorb a lot of fast photons. [30] The results show that the absorbance gradually increases with the thickness of the zinc oxide (ZnO) layers from 0.1 µm to 1.0 µm in the regions of the light range and ultraviolet radiation from electromagnetic radiation. [31]



Figure 7. *FDTD results of absorbency (A) in zinc oxide (ZnO) thin film structures on glass substrate in a wavelength range of (800-300) nm.*

Figure (4-2) shows the permeability (T) with the difference in wavelength with a range of (800-300) nm for various thickness numbers of the zinc oxide membrane ZnO 3), 2.5, 2.0, 1.5, 1.0, 0.5, 0.3 and 0.1) micrometers In general, it has been shown that the decrease is clearly in all permeability values with high membrane thickness, and the transmittance spectrum is characterized by its behavior being different from the absorption spectrum[32].



Figure 8. FDTD results of T-permeability in zinc oxide (ZnO) thin film structures on glass substrate in wavelength range (800-300) nm.

Figure (3-4) shows the change of reflectivity (R) as a function of the wavelength of zinc oxide membranes (ZnO) with different thickness and wavelength range (800-300) nm, we note that the difference in thickness led to a decrease in the reflectivity values of the values $(1.0, 0.5, 0.3 \text{ and } 0.1) \mu m$.

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Figure 9. FDTD results of reflectivity (R) in zinc oxide (ZnO) thin film structures on glass substrate in the wavelength range nm (800-300) nm.

4-2 Effect of Surface Roughness Difference on Optical Properties of Zinc Oxide Membranes

To study the difference in absorbance value with surface roughness (RMS) of zinc oxide (ZnO) membranes, samples

of zinc oxide with a thickness of $0.5 \,\mu\text{m}$ and RMS values equal to (50, 10,30, 90 and 70) nm were measured by lightpolarizing linear waves perpendicular to a range of wavelengths ranging from (300-800) nm. Figure (4-4) shows that the absorption gradually changes with the roughness of the surface of the zinc oxide (ZnO) membranes, so the absorption increases with increasing RMS rates for wavelengths of 400 nm, 600 nm and 800 nm and that these results are identical to the results of the researchers. [33]



Figure 10. Change in absorbance of films with different surface roughness of zinc oxide (ZnO) for wavelengths (600, 400, and 800) nm.

Figure (a,b (5-4) shows the results of the transmittance and reflectivity of zinc oxide membranes on a glass substrate with different roughness values (0.9., 0.7, 0.5, 0.3 and 0.1) μ m. The coarse zinc oxide (ZnO) structures strengthen the light scattering, which leads to an increase in the length of the optical path, improving its transmission and absorption, thus reducing light reflection and transmittance [34].



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Figure 11. *Results of simulation of finite differences of zinc oxide (ZnO) membrane on glass substrate for different surface roughness values (a) permeability, (b) reflectivity.*

Table 4-(1) shows the different proportions of reflectivity, transmittance and optical absorption. The results explained that the best value for the thickness of the high absorbent ZnO membrane is 5 2. and 3 μ m, and that both ratios favoring permeability and absorption are lower than other membranes and it was found that the membrane with a thickness of 1.0 μ m takes the smallest percentage of reflectivity.

3	2.5	2.0	1.5	1.0	0.5	0.3	0.1	سمك الغشاء
								μm
89.5	89.5	89.4	89.0	88.8	78.5	45.5	26.3	الامتصاصية %
4.1	4.1	4.4	4.6	7.0	16.5	46.6	64.1	النفاذية %
6.4	6.4	6.2	6.4	4.2	5.0	7.9	9.6	النفاذية %

Table 1. Ratios of Absorbency (A), Permeability (T) and Reflectivity (R) of Zinc Oxide Films

Table (4-2) shows a comparison between the values of absorbance, permeability and reflectivity of ZnO membranes with roughness values of (90, 50 and 10) nm and different angles of incidence (60° , 40° , 20° and $\theta = 0^\circ$).

Table (4-2) Values of absorbency, permeability and reflectivity of membranes with roughness values ZnO (90, 50 and (10 nm and different angle of incidence (60 \circ , 40 \circ and 20 \circ and $\theta = 0 \circ$).

						-			_			
10 nm		10 nm			10 nm			10 nm			RMS	
0	-60	•	6 = 40°			0 = 20°			Θ = σ=			زاوية السقوط
R	т	A	R	т		R	т	^	R	т	•	تخاصية البصرية
28	9	63	15	10	75	9	12	79	6	13	81	تسبة تمزية %
50 nm			50 nm		50 nm		50 nm			RMS		
R	Ŧ		R	т		R	т	•	R	т	•	الغاصية البصرية
26	7	67	13	9	78	9	10	81	5	13	82	تسبة المزية %
90 nm		90 nm			90 nm			90 nm			RMS	
R	т	A	R	т		R	т	^	R	т	•	تغامية اليصرية
15	7	78	9	10	81	6	11	83	4	12	84	تسبة تموية 50

Figure 12.

The table above shows that the membrane with a thickness of 0.5 μ m and a surface roughness of 90 nm showed the largest percentage of reflectivity and the smallest percentage of absorbance when the light incident is at an angle to its direction parallel to the column based on the surface ($\theta = 0$ °). When θ rates increase to 20° and 40°, the absorbance values decrease and the reflectivity values of all roughness rates (90, 50 and 10) nm increase.

Conclusion

1- The finite difference method in the time domain can be used to study the optical properties of various photovoltaic devices based on semiconductor membranes.

2- The increase in thickness and roughness of the surfaces of the ZnO membrane leads to an improvement in the absorption of light incident in the membrane layer and a decrease in the reflectivity of light inside the surface.

3- The fall of the polarized light beam at a large angle decreases the absorption rate and increases the reflectivity.

4- Helps to produce and configure electrical and optical devices with low-cost semiconductor materials economically and highly efficient.

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