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Optical Properties of ZnO Thin Film: A Simulation Study for Optoelectronic Applications

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Spectroscopic ellipsometry is widely used to find the optical properties of thin film coatings with optically smooth surfaces. Theoretical modeling is developed within the Sellmeier model theory in order to analyze, understand and predict the optical behavior of a ZnO thin film. ZnO is a well-known semiconductor with possible applications in optoelectronics such as solar cells, light emitting diodes, liquid crystal displays, etc. This paper presents an analysis of the optical properties of ZnO thin films obtained by the Sellmeier method using transmission spectra. For this, the computer language MATLAB was employed to generate the transmission data, and the film was observed to exhibit 96 % transmittance in the 500-1000 nm range, superior for the solar spectrum. These transmission data were used to calculate various optical parameters such as refractive index, extinction coefficient, and optical band gap, which were calculated using different formulas with respect to wavelength in the UV-visible region. It is found that the direct band gap transition is 3.23 eV, while the refractive index and extinction coefficient show variation up to 400 nm. This sort of research work will help us find the best thin film coating technology for designing optoelectronic devices. Simulation and comparison of the optical properties help to optimize the best material/property ratio for promising devices. The present investigation can provide an environment friendly and low-cost tool for optoelectronic and solar cell devices.

Keywords: Optoelectronics, Sellmeier model, Thin film, ZnO, MATLAB simulation.

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1. INTRODUCTION

Generally, wide band gap semiconductor thin films (ZnO, TiO_2, CdO, SnO_2 etc.) are extensively studied for optical and electrical characteristics because of their excellent chemical and physical properties [1]. Among many semiconductors, ZnO is the most widely used material due to its large band gap (3.40 eV), huge exciton binding energy (60 MeV), better thermal stability, and, more importantly, its absorption edge is in the ultraviolet (UV) range [2]. In recent years, a significant number of research papers have been published on the designing optical thin films and claiming their potential applications in the field of optoelectronics [3, 5]. The structure of a thin film is manifested in the optical properties in the wavelength range from UV to infrared (IR) region [6, 7]. In this communication, ZnO based thin films are a very useful material for different technological applications such as optical, optoelectronic devices, flat panel displays, liquid crystal displays and thin film photovoltaic devices, etc. [8-11].

In this work, the optical properties of ZnO thin film deposited on glass substrates of 700 nm were investigated using the MATLAB simulation program. This study is important to establish a correlation between theoretically calculated and experimentally observed properties before the implementation of this material in device fabrication.

2. THEORETICAL MODEL

Fig. 1 shows a schematic model of ZnO thin film with thickness d deposited on a glass substrate. The thickness of the substrate is considered several orders of magnitude higher than that of the film. In the figure, the refractive index of the film is shown as n, that of the substrate is shown as s, and the refractive index of air is taken as $n_0 = 1$. The vertical arrow shows incident light, where some light is reflected from the top surface (shown by R_1) and some is reflected from the surface of the substrate (shown by R_2). The final ray (shown by T) represents the transmitted light from ZnO thin film on the transparent substrate after multiple reflections. Here, it is mentioned that the reflection is considered negligible at the interface between the substrate and air.

2.1 Sellmeier Model

An empirical model known as the Sellmeier model is used to describe the variation of the refractive index in the transparent region [12] with wavelength of incident light. In this model, the extinction coefficient k is taken to be zero, which, in turn, assumes that the subband absorption is also zero. The formula for the refractive index of a thin film n is given by:

$$n^2(\lambda) = A + \frac{B\lambda^2}{\lambda^2 - C^2} + \frac{D\lambda^2}{\lambda^2 - E^2}, \quad (1)$$

where A, B, C, D and E represent the fitting parame-

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ters, λ is the wavelength of light (nm). The Sellmeier coefficients of ZnO are given in Table 1 [13].

Table 1 – Fitting parameters of the Sellmeier relation for ZnO

A	*B*	*C* (nm)	*D*	*E* (nm)
2.0065	$1.5748 \cdot 10^6$	$1 \cdot 10^7$	1.5868	260.63

With the help of the above fitting parameters, the refractive index of ZnO was studied using simple MATLAB software.

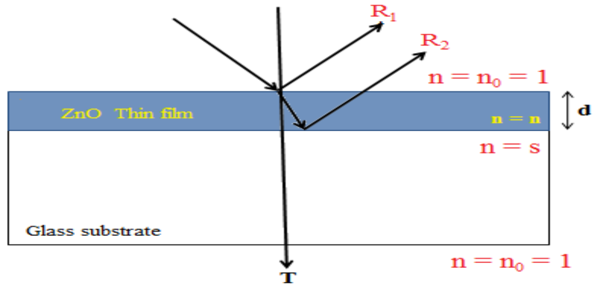

Fig. 1 – Model of a thin absorbent film on a transparent thick glass substrate

From the above model (Fig. 1), it can be seen that the ZnO film has thickness d and refractive index n, whereas the substrate has thickness several orders of magnitude greater than d and the refractive index is s. The index of surrounding air is defined as $n_0 = 1$. We consider that there is no reflection at the lower interface between the substrate and air under the substrate. Here R_1 is the intensity of the reflected light from the interface between the upper air and the film, and R_2 – from the film/substrate interface [14]. The transmission of the film/substrate can be expressed as [15]

$$T(\lambda) = T_0(\lambda) - 2\sqrt{R_1 R_2} Cos[\delta\lambda] , \quad (2)$$

where

$$\delta\lambda = \frac{2n(\lambda)d}{\lambda} \times 2\pi + \pi \quad (3)$$

(phase shift $\delta\lambda$ describes the change in the optical field as it passes through the layer),

$$R_1 = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \text{ and } R_2 = \frac{(n-s)^2}{(n+s)^2} ,$$

assuming the half wave loss in the film structure due to $n > s$ and $n < n_0$. Also, in Eq. (2), $T_0(\lambda)$ is supposed to be the term of transmission with no interference effect.

The substrate refractive index can be deduced as

$$s^2(\lambda) = 1 + \frac{B_1\lambda^2}{\lambda^2 - C_1^2} + \frac{B_2\lambda^2}{\lambda^2 - C_2^2} + \frac{B_3\lambda^2}{\lambda^2 - C_3^2} . \quad (4)$$

The transmission spectrum contains interference and non-interference terms. The interference is described in [16]:

$$T(\lambda)_i = T(\lambda) - T_0(\lambda) . \quad (5)$$

In our study, fitting is carried out in the wavelength range from 300 to 1000 nm for thin films of different thicknesses. It is worth to mention that this model is widely used in the case of UV, visible and IR regions and is mainly applicable to regions where absorption is negligible, which means that the extinction coefficient k is zero. The coefficients given in the Sellmeier relation are usually obtained by a least-squares fitting procedure, which is applied to measure refractive indices in a wide wavelength range. Therefore, it is possible to accurately determine the refractive index by using the Sellmeier equation in a wide wavelength range. These Sellmeier coefficients for many optical materials are available in databases.

$$k(\lambda) = F_k \lambda e^{-G_k\left(\frac{1}{H_k} - \frac{1}{\lambda}\right)} . \quad (6)$$

Here B_1, B_2, B_3, C_1, C_2 and C_3 are the fitting parameters, and their values taken from the literature are tabulated in the following Table 2. The Cauchy parameters for ZnO are given in Table 3 [17].

Table 2 – Constraint values of B_1, B_2, B_3, C_1, C_2 and C_3 for ZnO films

B_1	B_2	B_3
1.0396	$2.3179 \cdot 10^{-1}$	1.0104
C_1 (nm^2)	C_2 (nm^2)	C_3 (nm^2)
$6.0069 \cdot 10^3$	$2.0017 \cdot 10^4$	$1.0356 \cdot 10^8$

Table 3 – Cauchy constraints for ZnO films

F_k (nm^{-1})	G_k (nm)	H_k (nm)
0.0178		

3. RESULTS AND DISCUSSION

3.1 Optical Properties

Optical characteristics of the material play a significant role in the fabrication of modern optoelectronic devices. The current study expresses the systematic calculation of optical parameters such as band gap, refractive index, extinction coefficient, linear and nonlinear susceptibilities with the help of standard relations. The absorbance spectra of ZnO thin film were derived from the transmission data as a logarithmic function of T (%): $A = \log_{10}(1/T)$. It is also called optical density. Fig. 2 shows the combined transmittance and absorbance spectra of ZnO thin film of a thickness of 700 nm deposited on a glass substrate. It is seen from the spectra that the film has a transmittance of 96 % in the 500-1000 nm range which means high transparency of the film in the visible region and low in the UV region. Absorbance and transmittance intersect each other in the band gap regime. Absorbance shows that the ZnO film on the glass substrate is most absorbing at lower wavelength values, while absorbance decreases with increasing wavelength towards the visible region. Here, 0 % absorbance and 96 % transmittance of materials towards higher wavelengths (> 430 nm) are expected to aid in the design and selection of a suitable substrate for ZnO thin film for potential applications in optoelectronic devices.

From the absorption edge, we can calculate the band of the material using the well-known Einstein photon energy relation [18]:

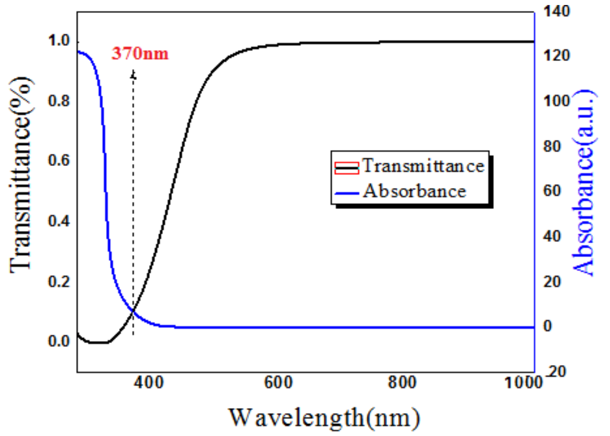

Fig. 2 – Transmittance and absorbance spectra versus wavelength of ZnO thin film

$$E_g = \frac{hc}{\lambda s}, \quad (7)$$

$$E_g = \frac{1240}{\lambda_s} eV, \quad (8)$$

where h is the Planck constant, c is the velocity of light, and λ_s (393 nm) is the excitonic absorption edge. The calculated energy band gap is ~ 3.35 eV. This value is suitable for optoelectronics devices such as LEDs, solar cells, sensors, etc.

Further, to identify whether the optical transition is direct or indirect, allowed or forbidden, the optical absorption data were analyzed, and for this, the famous Tauc relation is usually employed [19]:

$$\alpha h\nu = B(h\nu - E_g)^n, \quad (9)$$

where B is a constant, $h\nu$ is the photon energy, E_g is the energy band gap, n is a constant that depends on the optical transition and is equal to 0.5 and 2 for the allowed direct and indirect transitions, respectively. The optical band gap values are obtained by extrapolating the photon energy ($h\nu$) along the x-axis versus the linear region of the graph $(\alpha h\nu)^2$ along the y-axis for ZnO film. The band gap turns out to be 3.35 eV, this value is in good agreement with that obtained from the relation [18] and is shown in Fig. 3.

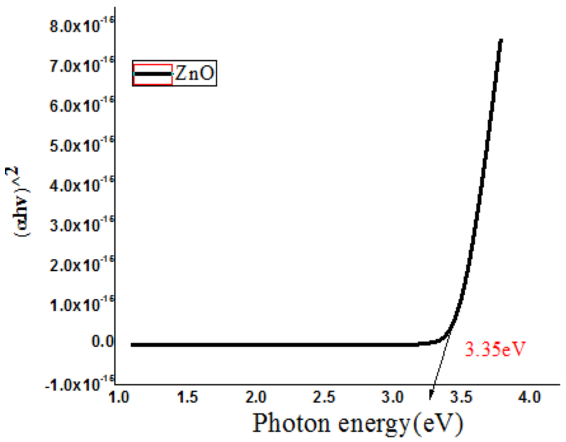

Fig. 3 – Tauc plot for the optical band gap

3.2 Refractive Index and Extension Coefficient

It is important to pay more attention to the refractive index (n) and extinction coefficient (k). These parameters mainly provide information about the suitability of the material for the fabrication of various optoelectronic devices and were obtained from reflectance data (not shown here). The refractive index (n) and extinction coefficient (k) were calculated using the relations below [20, 21]:

$$n = \left(\frac{1+R}{1-R}\right) + \sqrt{\frac{4R}{(1-R)^2} - K^2}, \quad (10)$$

$$\kappa = \frac{\alpha\lambda}{4\pi}, \quad (11)$$

where λ is the wavelength of the incident photon, α is the absorption coefficient, and R is the reflectance.

Fig. 4 shows the variation of the refractive index and extension coefficient versus the wavelength of ZnO film. As seen, the refractive index increases, whereas the extension coefficient decreases with wavelength up to 400 nm and then remains constant. The refractive index is 1.2 and the extension coefficient is $4.1 \cdot 10^{-8}$. Hence, this type of variation in n and k in the UV-visible region makes them proficient in designing optoelectronic devices [22].

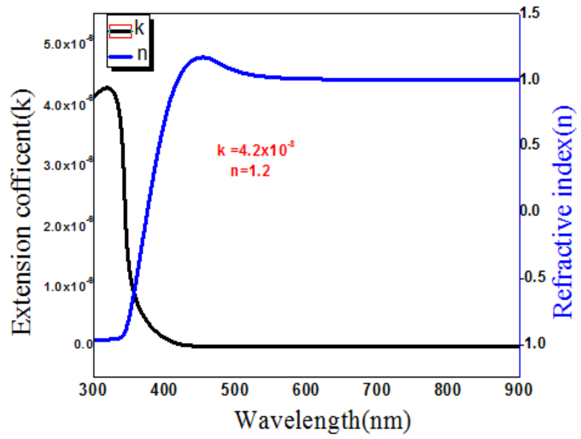

Fig. 4 – Variation of refractive index and extension coefficient versus wavelength

4. CONCLUSIONS

In this work, the optical properties of ZnO thin film, including refractive index, extinction coefficient, and band gap, have been investigated using the Sellmeier empirical dispersion formula by MATLAB coding. ZnO thin films have been deposited on glass substrates with a thickness of 700 nm theoretically. The band gap energies calculated from the Tauc plot are found in the 3.39 eV range, which agrees with the experimental results. The refractive index and extinction coefficient changed with optical conductivity up to 400 nm wavelength. So, the study shows that the Sellmeier formula is not only appropriate for investigating the optical properties of ZnO thin film, like a wide band gap material, but also more efficient for the window material of solar cells and gives better spectral fitting.

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Оптичні властивості тонкої плівки ZnO: імітаційне дослідження для оптоелектронних застосувань

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Спектроскопічна еліпсометрія широко використовується для дослідження оптичних властивостей тонкоплівкових покриттів з оптично гладкими поверхнями. Теоретичне моделювання розроблено в рамках теорії моделі Селмейера з метою аналізу, розуміння та прогнозування оптичної поведінки тонкої плівки ZnO. ZnO є добре відомим напівпровідником з можливістю застосування в оптоелектроніці, наприклад, в сонячних елементах, світловипромінюючих діодах, рідкокристалічних дисплеях тощо. У роботі представлений аналіз оптичних властивостей тонких плівок ZnO, отриманих методом Селмейера за допомогою спектрів пропускання. Для цього був використаний пакет MATLAB для генерування даних стосовно пропускання, і було помічено, що плівка демонструє 96 % пропускання в діапазоні 500-1000 нм, що є найкращим показником для сонячного спектру. Ці дані стосовно пропускання були використані для розрахунку різних оптичних параметрів, таких як показник заломлення, коефіцієнт екстинкції та оптична ширина забороненої зони, які були отримані за різними формулами в залежності від довжини хвилі в УФ і видимій областях. Встановлено, що прямий перехід забороненої зони становить 3,23 еВ, а показник заломлення та коефіцієнт екстинкції змінюються до 400 нм. Така дослідницька робота допоможе нам знайти найкращу технологію тонкоплівкового покриття для розробки оптоелектронних пристроїв. Моделювання та порівняння оптичних властивостей допомагає оптимізувати найкраще співвідношення матеріал/властивості для перспективних пристроїв. Дане дослідження може забезпечити екологічно чистий і недорогий інструмент для оптоелектронних пристроїв і пристроїв на сонячних елементах.

Ключові слова: Оптоелектроніка, Модель Селмейера, Тонка плівка, ZnO, Моделювання MATLAB.