American Journal of Optics and Photonics
2013; 1(1) : 1-5
Published online February 20, 2013 (http://www.sciencepublishinggroup.com/j/ajop)
doi: 10.11648/j.ajop.20130101.11

Simulation study of optical transmission properties of ZnO thin film deposited on different substrates

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To cite this article:
N. Bouchenak Khelladi, N. E. Chabane Sari. Simulation Study of Optical Transmission Properties of ZnO Thin Film Deposited on Different Substrates. *American Journal of Optics and Photonics.* Vol. 1, No. 1, 2013, pp. 1-5. doi: 10.11648/j.ajop.20130101.11

Abstract: ZnO is an important II-VI semiconductor material for devices with possible applications such as piezoelectric transducers, gas sensors, transparent electronic in solar cell, saw devices. Based on known research, ZnO is the most promising in optoelectronic and optical applications, especially in UV region. An understanding of the optical properties of ZnO thin film on different substrates is also needed to obtain the optimal configuration for the best performance. In this work, we start our simulation by made a Matlab code to study the Sellmeier equation. The behavior of light transmission of ZnO/BK7 glass and ZnO/Sapphire is studied. Both the variation of thickness of ZnO film and different parameters of Sellmeier model are studied. This approach helps us to determine the best configuration (thin film / substrate) to made advices for optoelectronic applications.

Keywors: ZnO, Thin film, Sellmeier equation, Matlab

1. Introduction

ZnO is a key technological material. ZnO is a wide bandgap (3.37 eV) compound semiconductor that is suitable for short wavelength optoelectronic applications. Zinc oxide (ZnO) is one of transparent conducting oxide (TCO) materials whose thin films attract much interest because of typical properties such as high chemical and mechanical stability in hydrogen plasma, high optical transparency in the visible and near-infrared region **[1-3]**. Due to these properties ZnO is a promising material for electronic or optoelectronic applications such as solar cells (anti-reflecting coating and transparent conducting materials), gas sensors, liquid crystal displays, heat mirrors, surface acoustic wave devices etc. **[4-6]**. In addition to the traditional applications ZnO thin films could also be used in integrated optics and gas sensors **[7]**.

In designing modern optoelectronic and optical devices, it is important to know the thickness, refractive index and absorption coefficient as a function of wavelength to predict the photoelectric behavior of a device. Unfortunately, there are larger discrepancies among various studies on the optical property of ZnO thin films. Reliable determination of the optical properties of ZnO thin film is still an issue **[8]**.

2. The Theory

Where d and n are the thickness and refractive index of the thin films, respectively. The substrate has a thickness of the several orders of magnitude larger than d and the refractive index is s. The index of surrounding air is defined as $n_0 = 1$. R_1 is the intensity of the reflected light on the interface air / film, and R_2 is the reflection on the interface the film / substrate. While the reflection at the interface the substrate / air under substrate is not considered here. The expression of the transmission of all thin film / substrate is given by **[9]**:

$$\mathrm{T}(\lambda) = \mathrm{T}_0(\lambda) - 2\sqrt{R_1 R_2}\,cos[\delta(\lambda)] \quad (1)$$

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

$$R_1 = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \quad et \quad R_2 = \frac{(s-n)^2}{(s+n)^2}$$

Where k is the extinction coefficient of the thin film.

In equation **(1)**, T_0 (λ) represents the term of transmission with no interference effect.

The interference term can be described as:

$$\mathrm{T}(\lambda)_\mathrm{i} = \mathrm{T}(\lambda) - \mathrm{T}_0(\lambda) \quad (3)$$

The absorption coefficient α is given by the following relations

$$\alpha = \frac{4\pi k}{\lambda} \quad (4)$$

$$\alpha(\lambda) = \frac{1}{d} ln(\frac{A}{B}\frac{1}{T_0}) \quad (5)$$

Where $A = 16n^2 s \ \ et \ \ B = (1+n)^3(n+s^2)$.

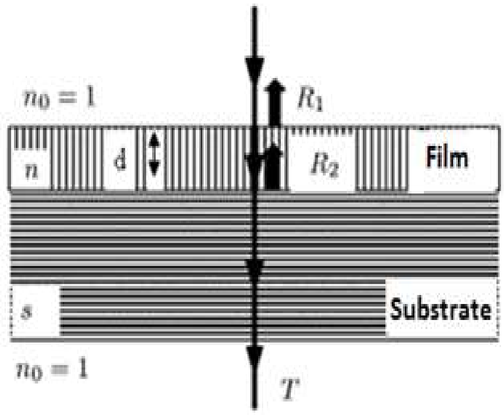

Figure 1. *Optical system consisting of a thin absorbent film on a transparent substrate thick.*

The Sellmeier equation for the refraction index, n, of ZnO thin film a function of wavelength is given by expressed:

$$n^2(\lambda) = A + \frac{B\lambda^2}{\lambda^2 - C^2} + \frac{D\lambda^2}{\lambda^2 - E^2} \quad (6)$$

A, B, C, D and E are the fitting parameters, **λ** is the wavelength of light (nm).

Fitting parameters calculated at different powers for different thicknesses of deposit varies very significantly [10]. We take in our future modeling parameters cited in reference [11].

Table 1. *Fitting parameters by the method VASE of Sellmeier model for zinc oxide [11].*

A	B	C (nm)	D	E (nm)
2.0065	1.5748×10^6	1×10^7	1.5868	260.63

The extinction coefficient of zinc oxide is given by the following relation:

$$k(\lambda) = F_k \lambda e^{-G_k(\frac{1}{H_k} - \frac{1}{\lambda})} \quad (7)$$

Table 2. Cauchy parameters for zinc oxide [10].

F_k (nm^{-1})	G_k (nm)	H_k (nm)
0.0178	7327.1	337.87

The refraction index of the substrates

$$\boldsymbol{s^2(\lambda) = 1 + \frac{B_1\lambda^2}{\lambda^2 - C_1} + \frac{B_2\lambda^2}{\lambda^2 - C_2} + \frac{B_3\lambda^2}{\lambda^2 - C_3}} \quad (8)$$

Table 3. *Sellmeier coefficients for BK7 glass [12].*

Glass	B_1	B_2	B_3	C_1 (nm^2)	C_2 (nm^2)	C_3 (nm^2)
BK7	1.0396	2.3179×10^{-1}	1.0104	6.0069×10^3	2.0017×10^4	1.0356×10^8

Table 4. *Sellmeier coefficients for Sapphire [13]*

Material	A_1	A_2	A_3	λ_1 (nm)	λ_2 (nm)	λ_3 (nm)
Sapphire	1.0237	1.0582	5.2807	6.1448×10^1	1.107×10^2	17.9265

$$\boldsymbol{s^2(\lambda) = 1 + \frac{A_1\lambda^2}{\lambda^2 - \lambda_1^2} + \frac{A_2\lambda^2}{\lambda^2 - \lambda_2^2} + \frac{A_3\lambda^2}{\lambda^2 - \lambda_3^2}} \quad (9)$$

3. Results and Discussion

Figure 2 shows the decreasing variation of the refractive index (n) of the ZnO thin film as a function of the wavelength in the range [380-1000] nm. After 1000 nm, the evolution of the refractive index has à linear behavior.

According to Figure 3 which describes the variation of the extinction coefficient (k) ZnO thin film as a function of the wavelength. It is observed that from 450 nm k tends to zero; this is explained by the very small absorption of ZnO in the near ultraviolet and visible light.

Figures: 4, 5 shown the optical transmission (with interference effect) of different thicknesses of ZnO thin films (200 nm or more) deposited on glass (BK7), and sapphire. We observe interference fringes with minima and maxima. These are interference fringes due to multiple reflections of light taking place between the lower surface in contact with the substrate and the free surface of the film.

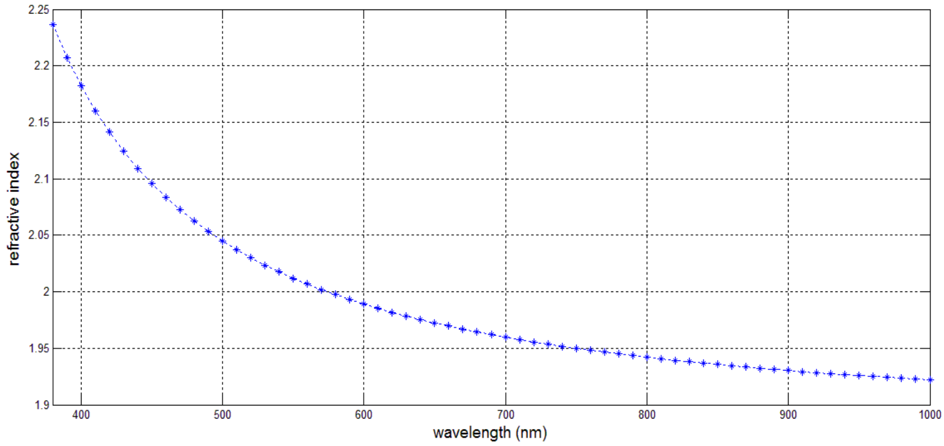

Figure 2. *Variation of the refractive index of ZnO thin film a function of the wavelength.*

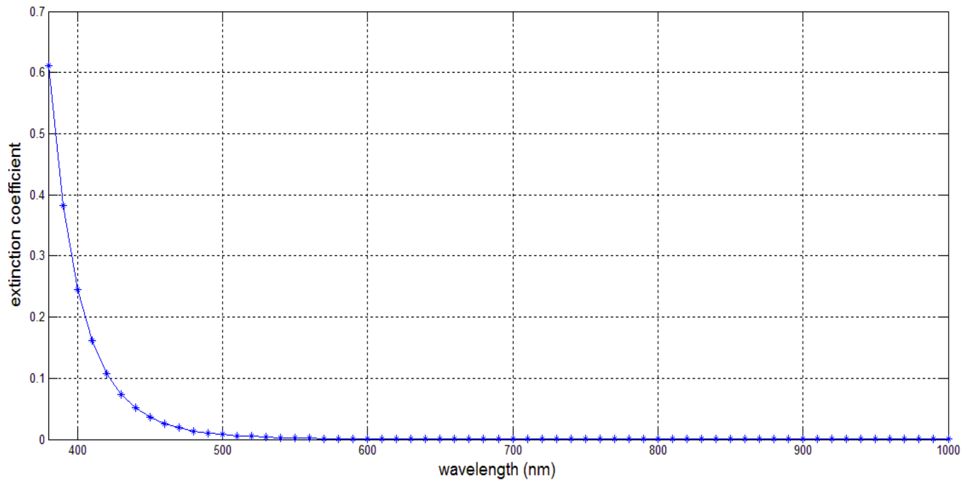

Figure 3. *Variation of the extinction coefficient of ZnO thin film a function of the wavelength.*

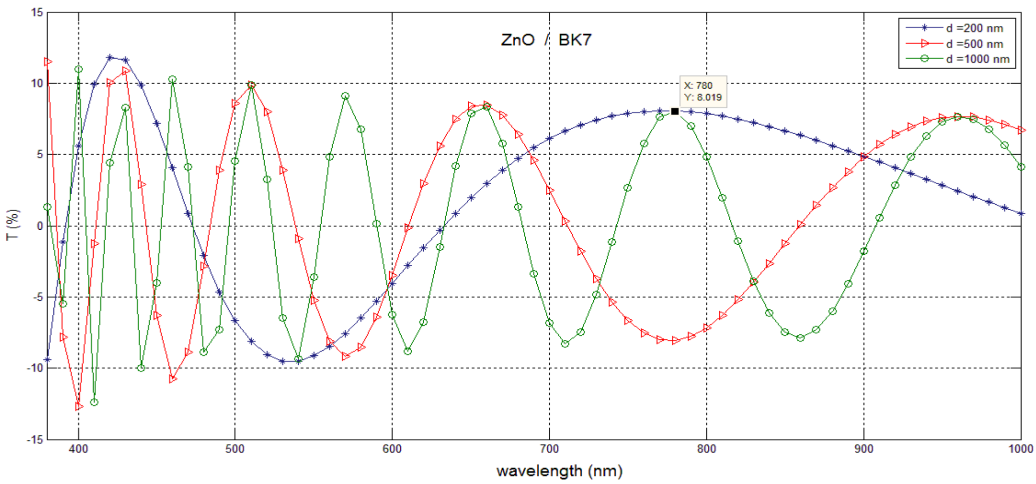

Figure 4. *Optical transmission spectrum (interference effect) of the ZnO thin films of different thickness deposited on glass (BK7).*

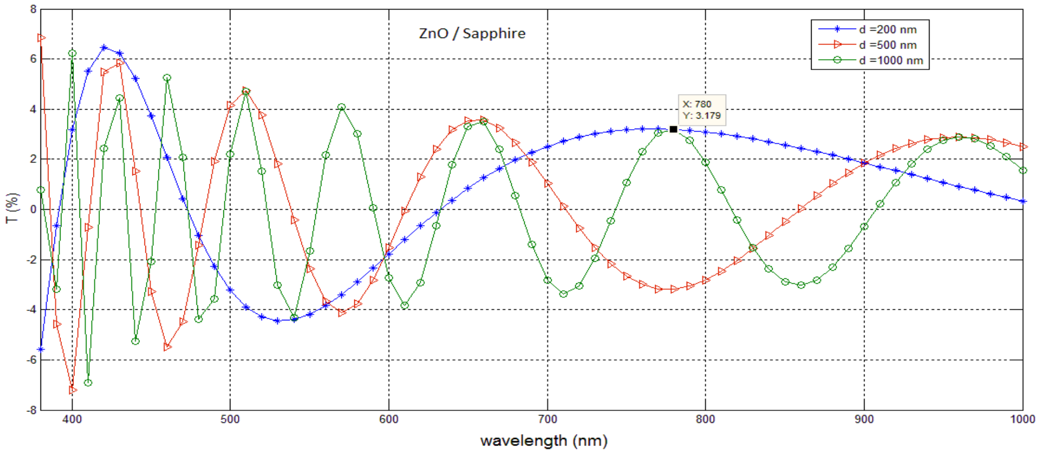

Figure 5. *Optical transmission spectrum (interference effect) of ZnO thin films of different thicknesses deposited on the sapphire.*

Figures 6 and 7 shows the optical transmission spectrum of ZnO thin film deposited on different types of substrate by varying the thickness of the layer.

This spectrum can be divided into four regions:

The transparent region (450 - 1000 nm): the absorption coefficient is zero; the transmission is determined by both n and s through multiple reflections.

The region of weak absorption (430-450 nm): α is small but begins to reduce transmission.

The region of medium absorption (380-430 nm): the decrease of the transmission is mainly due to the effect of absorption.

The region of strong absorption (below 380 nm): drastic decrease of the transmission is caused by the film absorption due to the transition between the valence band and conduction band.

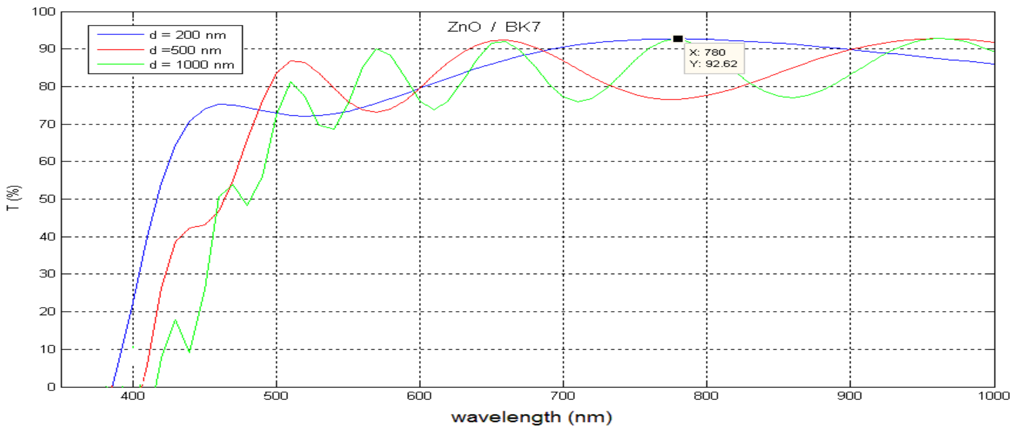

Figure 6*. optical transmission spectrum of ZnO thin film deposited on glass (BK7) for different thickness.*

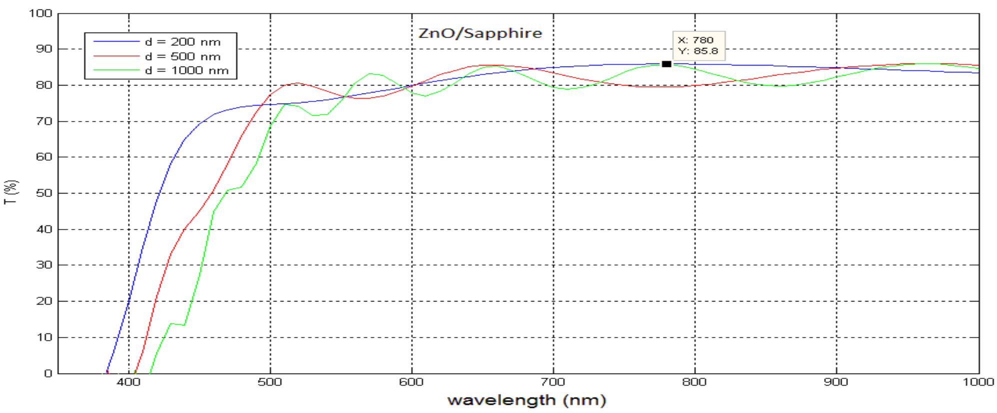

Figure 7. *optical transmission spectrum of ZnO thin film deposited on Sapphire for different thickness.*

4.Conclusion

In this work, the simulation of the Sellmeier equation to study the behavior of light transmission of ZnO on BK7 glass and Sapphire substrates shows that the optical transmission (with interference effect) of different thicknesses of ZnO thin films (200 nm or more) have interference fringes with minima and maxima. It's due to multiple reflections of light taking place between the lower surface in contact with the substrate and the free surface of the film. By varying the thickness's ZnO layer, the numerical approach shows that the optical transmission spectrum can be divided into four different regions. In each of these, we show the relation and behavior of absorption coefficient and transmission effect. Finally, this study gives us lot of important information about some important optical parameters of different configurations (thin film/ substrate). For our future works, all the results of our simulation will be used to choose the optimal structure to study and simulate different nanostructure optoelectronic devices.

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