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OPTICAL PROPERTIES OF ZnO THIN FILM

ABSTRACT

In this work, we studied with a Matlab program, some of optical properties of zinc oxide (ZnO) deposited on glass (SiO2). The parameters studied include the refraction index, extinction coefficient, optical band gap, and complex dielectric constant versus incident photon energy, and transmittance, absorbance and reflectance spectrum of ZnO thin film deposited on glass (SiO2) for different thickness. The films were found to exhibit high transmittance (75- 95%), low absorbance and low reflectance in the visible / near infrared region up to 1000 nm. However, the absorbance of the films was found to be high in the ultra violet region with peak around 380 nm.

Keywords: ZnO, Thin film, optical properties, Sol gel deposition, Matlab.

INTRODUCTION

Zinc oxide (ZnO) is an important material in many optoelectronic devices with wide applications such as varistors, biosensors, gas sensors, transparent electrodes, etc. [1]. ZnO is a promising material due to the wide direct band gap of 3.37 eV at room temperature (RT) and high exciton binding energy of 60 mev which allow it to use in ultraviolet region with harsh condition [2]. Based on known research, various techniques are known to prepare ZnO films including the sol-gel process [3], chemical deposition [4], direct current (DC) and radio frequency (RF) sputtering [5], and pulsed laser deposition [6].

In designing modern optoelectronic and optoelectronic device, it is important to know the refractive index as a function of wavelength to predict photoelectric behavior of a device.

Therefore, an accurate knowledge of the structural and optical properties of ZnO is important for the design and analysis of various optical and optoelectronic devices.

Unfortunately, there are larger discrepancies among various studies on the optical property of the ZnO thin films. Reliable determination of the optical properties of the ZnO thin film is still an issue [7].

In this study, a simulation of Sellmeier equation was used to study the refractive index as a function of wavelength and photon energy. However, according to [8], Cauchy-like dispersion model was formulated to account for the absorption tail and exitronic structure near the direct band gap.

The optical transmission and absorption spectra for a range of samples of ZnO thin films (of different thickness) were obtained by a Matlab program.

Zinc oxide thin film was reported which has been deposited from metallic zinc target has purity (99.98 %) according to [9]. Different thin films of (nm) are deposited on glass substrates.

THE THEORY

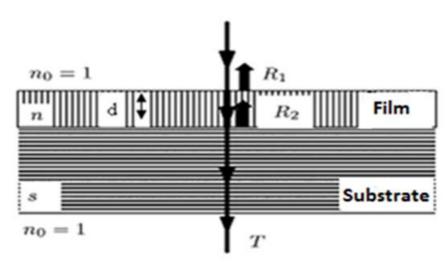


Fig. 1. Optical system consisting of a thin absorbent film on a transparent substrate thick

The brief model of thin films on a thick glass substrate is shown in figure 1, 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 expression in the transmission of all thin film / substrate is given by [9]:

$$T(\lambda) = T_0(\lambda) - 2\sqrt{R_1 R_2} \cos \left[\frac{4\pi n(\lambda)d}{\lambda} + \pi \right]$$

$$R_1 = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \quad \text{et} \qquad R_2 = \frac{(s-n)^2}{(s+n)^2}$$
(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. k is the extinction coefficient of the thin film. In equation (1), T_0 (λ) represents the term of transmission with no interference effect.

$$\mathbf{T} \square_{\mathbf{i}} \mathbf{0} (\lambda) = B/C e^{\uparrow}(-d\alpha(\lambda)))$$
 (2)

Where: $B = 16n^2s$ et $C = (1+n)^2(n+s^2)$

NUMERICAL MODEL AND RESULTS

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

$$n^{2}(\lambda) = A + \frac{B\lambda^{2}}{\lambda^{2} - C^{2}} + \frac{D\lambda^{2}}{\lambda^{2} - E^{2}}$$
(3)

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 [8]. We take in our future modeling parameters cited in reference [2].

Table 1. Fitting parameters by the method VASE of Sellmeier model for zinc oxide [2]

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

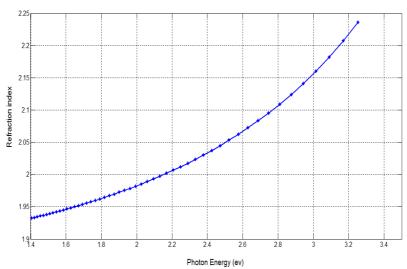


Fig. 2. Refraction index versus incident photon energy

Figure 2 shows the increasing variation in the refractive index of the ZnO thin film as a function the incident photon energy.

The extinction coefficient (also called or attenuation coefficient) of a particular substance, k, measuring the energy loss of electromagnetic radiation through that medium. It depends on the material and the wavelength. This is the imaginary part of the complex relation index. The extinction coefficient of zinc oxide is given by [10, 11, 12, 13]:

$$k(\lambda) = F_k \lambda e^{-G_k \left(\frac{1}{H_k} - \frac{1}{\lambda}\right)}$$
 (4)

Table 2. Cauchy parameters for zinc oxide [8]

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

Figure 3 shows the increasing variation of extinction coefficient of ZnO thin film with the incident photon energy. This is explained by the very little absorption of ZnO in the near ultraviolet and visible light.

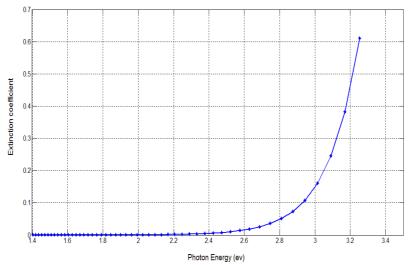


Fig. 3. Extinction coefficient versus incident photon energy

The absorption coefficient α and the extinction coefficient k are related by the formula [11]

$$\alpha = \frac{4\pi k}{\lambda} \tag{5}$$

The optical energy gap Eg and absorption coefficient α are related by the equation

$$\alpha h v = K (h v - E_g)^{\frac{1}{2}} \tag{6}$$

Where K is constant, h is Planck's constant, hv is the incident photon energy.

The optical band gap is determined by extrapolating the straight line portion of the spectrum to $(\alpha h v)^2 = 0$ [10], Eg = 3.11 ev. (Figure 4).

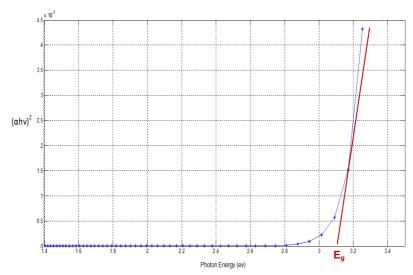


Fig. 4. Optical band gap of the ZnO thin films determined from $(\alpha hv)^2$ versus incident photon energy

The real and imaginary parts of the dielectric constant were determined using the relation [15].

$$\boldsymbol{\varepsilon}_c = \boldsymbol{\varepsilon}_r + \boldsymbol{\varepsilon}_i = (n + tk)^2 \tag{7}$$

Where \mathcal{E}_r is the real part and is the normal dielectric constant, \mathcal{E}_i is the imaginary part and represents the absorption associated of radiation by free carrier.

Figures 5 and 6 shows the variations in the real and imaginary parts of the dielectric constant with the incident photon energy.

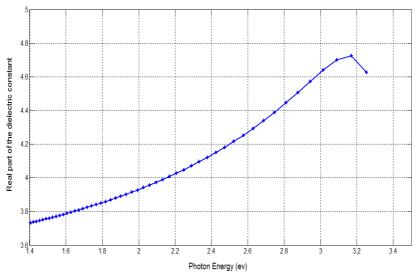


Fig. 5. Real part of the dielectric constant versus incident photon energy

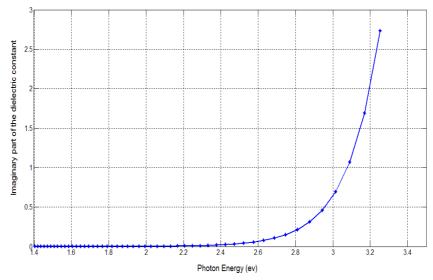


Fig. 6. Imaginary part of the dielectric constant versus incident photon energy

The refractive index of the substrate (glass SiO₂) is given by the Sellmeier equation

$$S^{2}(\lambda) = 1 + \frac{B_{1}\lambda^{2}}{\lambda^{2} - C_{1}} + \frac{B_{2}\lambda^{2}}{\lambda^{2} - C_{2}} + \frac{B_{3}\lambda^{2}}{\lambda^{2} - C_{3}}$$
(8)

Table 3. Sellmeier coefficients for SiO2 glass [16]

| Glass | B_1 | B_2 | B_3 | $C_1(nm^2)$ | $C_2(nm^2)$ | $C_3(nm^2)$ |
|------------------|------------------------|-------------------------|------------------------|----------------------|----------------------|------------------------|
| SiO ₂ | 6.694×10 ⁻¹ | 4.3458×10 ⁻¹ | 8.716×10 ⁻¹ | 4.4801×10^3 | 1.3284×10^4 | 9.5341×10^{7} |

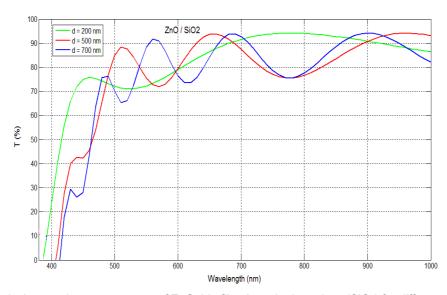


Fig. 7. Optical transmittance spectrum of ZnO thin film deposited on glass (SiO₂) for different thickness.

The figure 7 shown the transmittance optical interference effect of various thicknesses of ZnO thin films (≥ 200 nm) deposited on glass (SiO₂). We see interference fringes with minima and maxima. These interference fringes due to multiple reflections of light occurring between the lower surface in contact with the substrate and the free surface of the layer.

The absorbance measures the ability of a medium to absorb light passing through it. It is also called optical density or extinction. This is the inverse of the transmittance, is defined by:

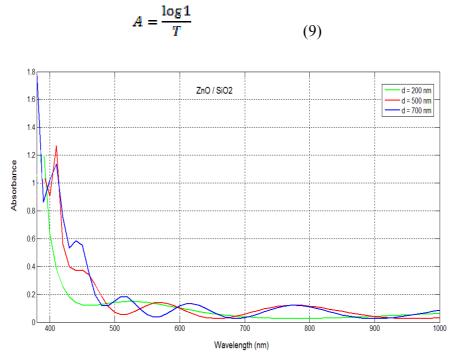


Fig. 8. Absorbance spectrum of ZnO thin film deposited on glass (SiO₂) different thickness.

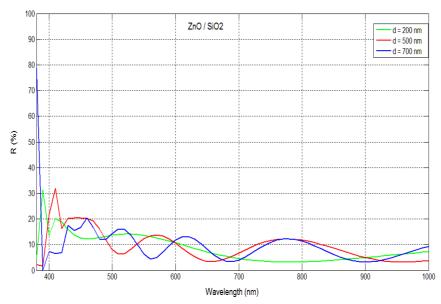


Fig. 9. Optical reflectance spectrum of ZnO thin film deposited on glass (SiO₂) for different thickness

The absorbance spectrum of the thin films of ZnO, having different thickness, is shown in figure 8. These spectrums reveal, have low absorbance in the visible and near infrared regions. However, absorbance in the ultraviolet region is high.

$$R + T + A = 1 \tag{10}$$

The optical reflectance spectrums R for ZnO present in Figure 9 confirm the low optical reflection of thin films. We observe that reflectivity is of 10% in the visible range. It decreases with increasing wavelength in the range 500 to 1000 nm. The reflectance has been found by using the relation (10).

CONCLUSION

The film properties investigated include the refraction index, extinction coefficient, optical band gap, complex dielectric constant, and transmittance, absorbance and reflectance spectrum of ZnO thin film deposited on glass (SiO₂) for different thickness. The films were found to exhibit high transmittance (75- 95%) in the visible range. This result is very important for transparent thin films that are used for applications in optoelectronic devices, low absorbance and low reflectance in the visible / near infrared region up to 1000 nm. However, the absorbance of the films was found to be high in the ultra violet region with peak around 380 nm.

REFERENCES

- 1. M. Willander, et al., Nanotechnology, 20 332001 (2009).
- 2. X. Sun and H. Kwork, J. of Appl. Phys, 86 408 (1999).
- 3. Hsin-Chiang You and Yu-Hsien Lin, Int. J. Electrochem. Sci., 7 9085 9094 (2012).
- 4. Feng Shi and Chengshan Xue, Cryst. Eng. Comm, 14, 4173-4175 (2012).
- 5. Li Shao-Juan, He Xin, Han De-Dong, Sun Lei, Wang Yi, Han Ru-Qi, Chan Man-Sun and Zhang Sheng-Dong, CHIN. PHYS. LETT., Vol. 29, No. 1 018501 (2012).
- 6. Lorenz M., Hochmuth H., Grüner C., Hilmer H., Lajn A., Spemann D., Brandt M., Zippel J., Schmidt-Grund R., Wenckstern H. and Grundmann M., Laser Chemistry, Hindawi Publishing Corporation, 1-27 (2011).
- 7. Hu W.S et al J.Phy.Chem.Solids 58853 (2003).
- 8. Ahmad A., Alsaad A., Eur. Phys. J. B 52, p 41–46 (2006).
- 9. Wang Ming- Dong et al. Chin. Phys. Lett, Vol. 25, No. 2, p 743-746 (2008).
- 10. Holden T., Ram P., Pollak H., Freeouf J., Yang B., Tamargo M., Phys.Rev. B56, 4037 (1997).
- 11. Yoshikawa H., Adachi S. Jpn Appl. Phys. I 36, 6237 (1997).
- 12. Teng C., Muth J., Ozgur U., Bergmann M., Everitt H., Sharama A., Jin C., Narayan J., Appl. Phys. Lett. 76, 979 (2000).

- 13. Bai L., Xu Ch., Schunemann P., Nagashio N., Feigelson R., Giles N., J. Phys. Condens. Matter. 17, 549 (2005).
- 14. Zebbar N., Aida M.S., Hafdallah A., Daranfad W., Lekiket H., and Kechouane M., Materials Science Forum, 609, 133-137 (2009).
- 15. Chopra K.L., Thin Film Phenomena, McGraw Hill Book Company, USA, p.729 (1969).
- 16. Rosete-Aguilar M., et al. Investigacion, Rev. Mex. Fis, 54 (2), 141-148 (2008).