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IMPACT OF THICKNESS AND SUBSTRATE ON OPTICAL PROPERTIES OF ZnO THIN FILMS

S. DAS[1], S. SULTANA[2], L. AKTER[1], S. C. MAZUMDAR[1*], M. A. RAHMAN[1] AND K. KALI[1]

[1]*Department of Physics, Comilla University, Cumilla-3506, Bangladesh*

[2]*Department of Information & Communication Technology, Comilla University, Cumilla-3506, Bangladesh*

**Corresponding author e-mail: sajalf@gmail.com*

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ABSTRACT

During the last decades, ZnO has emerged as the most promising material in optoelectronic and optical applications in the visible region as well as in the infrared and UV region. It is because of the broad direct band gap of 3.37 eV at ambient temperature and high exciton binding energy of 60 meV allowing it to utilize the ultraviolet region. In this investigation, the optical characteristics of ZnO thin film of various thicknesses (300 nm, 600 nm, 900 nm) deposited on Quartz, Fused silica and Sapphire have been studied as a function of wavelength and photon energy. To obtain this, the equations for thin film have been derived, simulated and visualized by Matlab coding language. It is observed that with the increase in the photon energy, the refractive index and extinction coefficient show an increasing tendency. The results represent that among three substrates Fused silica has the lowest refractive index, reflectance and absorbance. In the visible region, the transmission spectra show that the average transmittance of all films is 85%-95%, which is superior for solar continuums. The performance of Fused silica as transparent conducting material is better than other substrates. The present investigation might provide an environment friendly and low cost material for optoelectronic and solar cell devices.

Keywords: ZnO, Thin Film, Visible Region, Matlab.

1. INTRODUCTION

Over the past few years, there has been a huge increasing interest in nanomaterials owing to their indistinguishable difference in properties from macroscopic and bulk materials. It mainly focused on the synthesis, characterizations and applications of nanometer-sized metals, semiconductors and ceramics [1]. As the properties of nanomaterials play a momentous role on the performance of devices, it is an important issue for engineering applications [2]. Due to this reason, ZnO nanostructures have been studied intensively and expansively over the last decade not only for their outstanding chemical and physical properties but also for their diverse, present and future technological applications [3]. ZnO is a non-toxic, abundant and II-VI compound semiconductor [4-6]. These put it down within the visible region having high optical transmission suitable for solar spectrum [4]. As a result, it has potential applications in transparent electrode in display, window layers in solar cells, field emitters, ultraviolet laser emission, photodetectors, piezoelectricity, bio-sensors, short wavelength light emitting diode and information technology [7-14]. Besides these, in designing modern optoelectronic devices, it is important to know the thickness, refractive index, absorption and transmission as a function of wavelength to envisage the photoelectric performance of a device. In this paper, optical properties of ZnO thin films of various thicknesses and deposited in three different substrates have been observed by using a simulation program “Matlab”.

2. METHODS

Figure 1 represents the model of thin absorbent films which is deposited on a transparent thick substrate. Here d and n denote the thickness and refractive index of the films, respectively. The refractive index of the substrate is s and thickness of the substrate has the several orders of magnitude greater than the film thickness. Moreover, n_o=1 defines the refractive index of surrounding air, R_1 is the intensity of the reflected light on the interface between air and film and R_2 is that on the interface between the film and substrate. The reflection at the air under substrate interface between the substrate and interface between the substrate is not considered here [15].

The sellmeier equation for the refractive index n of ZnO thin film as a function of wavelength is given by,

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

Fitting Parameters are A, B, C, D and E, the wavelength of light (nm) is λ. Fitting parameters (Table-1) are calculated at different powers for different thickness, as deposit varies significantly [15]. The sellmeir coefficients of ZnO is given in Table-2:

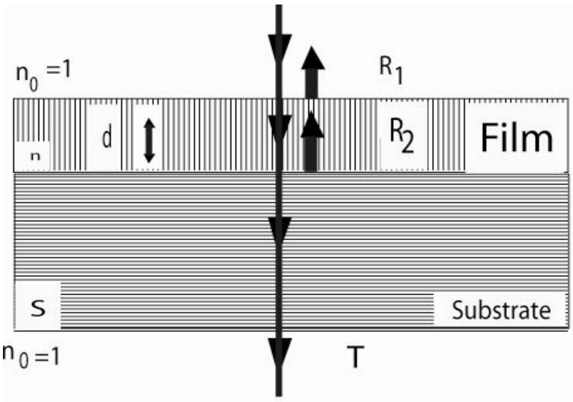


Fig. 1: Model of the thin absorbent films on a transparent thick substrate [15]

Table1: By VASE method of sellmier model fitting parameters for Zinc Oxide [15]

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

From these fitting parameters using the Matlab programme the refractive index of ZnO has been studied.

The refractive index of the substrate

$$S^2(\lambda) = 1 + \frac{A_1\lambda^2}{\lambda^2 - \lambda_1^2} + \frac{A_2\lambda^2}{\lambda^2 - \lambda_2^2} + \frac{A_3\lambda^2}{\lambda^2 - \lambda_3^2} \quad \text{.............(2)}$$

Table2: The Sellmeier Coefficients of various substrates where λ_1, λ_2, λ_3 are in nm are given below [16]

Material	A_1	A_2	A_3	λ_1 (nm)	λ_2 (nm)	λ_3 (nm)
Quartz, n_o	1.35400	0.010	0.9994	92.612	10700	9850
Fused Silica	0.696749	0.408218	0.890815	69.066	115.662	9900.559
Sapphire	1.023798	1.058264	5.280792	61.4482	110.7	17926.56

From, these coefficients with the Matlab the refractive indices of the substrates have been calculated. The extinction coefficient of ZnO is given by the following relation,

$$\mathrm{k}(\lambda) = \mathrm{F_k} e^{-G_k\left(\frac{1}{H_k}-\frac{1}{\lambda}\right)} \text{...}(3)$$

Table3: Cauchy parameters for Zinc oxide [15]

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

With the help of equation (3) and Cauchy parameters the extinction co-efficient of ZnO thin film has been determined.

After that the value of R_1 and R_2 have been calculated by the following equations

$$\mathrm{R_1} = \frac{(n-1)^2+k^2}{(n+1)^2+k^2} \text{...}(4)$$

$$\mathrm{R_2} = \frac{(s-n)^2}{(s+n)^2} \text{..}(5)$$

The absorption co-efficient of ZnO thin film is given by the following equation [2] [5]

$$\alpha = \frac{4\pi k}{\lambda} \text{...}(6)$$

The thicknesses of the films are 300 nm, 600 nm, 900 nm that are used in this research. For different thicknesses of ZnO thin films deposited on different substrates, the transmittance has been determined by Matlab programme. The expression of the transmission of ZnO thin films deposited on different substrates is given by [15],

$$\mathrm{T}(\lambda) = \mathrm{T_0}(\lambda) - 2\sqrt{R_1 R_2}\cos\left[\delta(\lambda)\right] \text{.................................}(7)$$

$$\delta(\lambda) = 2\pi \times \frac{2nd}{\lambda} + \pi \text{...}(8)$$

In equation (9), T_0 (λ) is the transmission with no interference effect.

Reflectance (R) is an elementary optical property of thin films and it means the percentage of incident light reflected from a surface. The expression of the reflectance of ZnO thin films deposited on different substrates is given by [8],

$$R+T+A=1 \text{...}(9)$$

The absorbance means the capability of light absorption of a medium passing through it. It is also known as the optical density or extinction. This is the contrary of the transmittance and is defined by [17], A= $(\log\ 1)/T$...(10)

3. RESULTS AND DISCUSSION

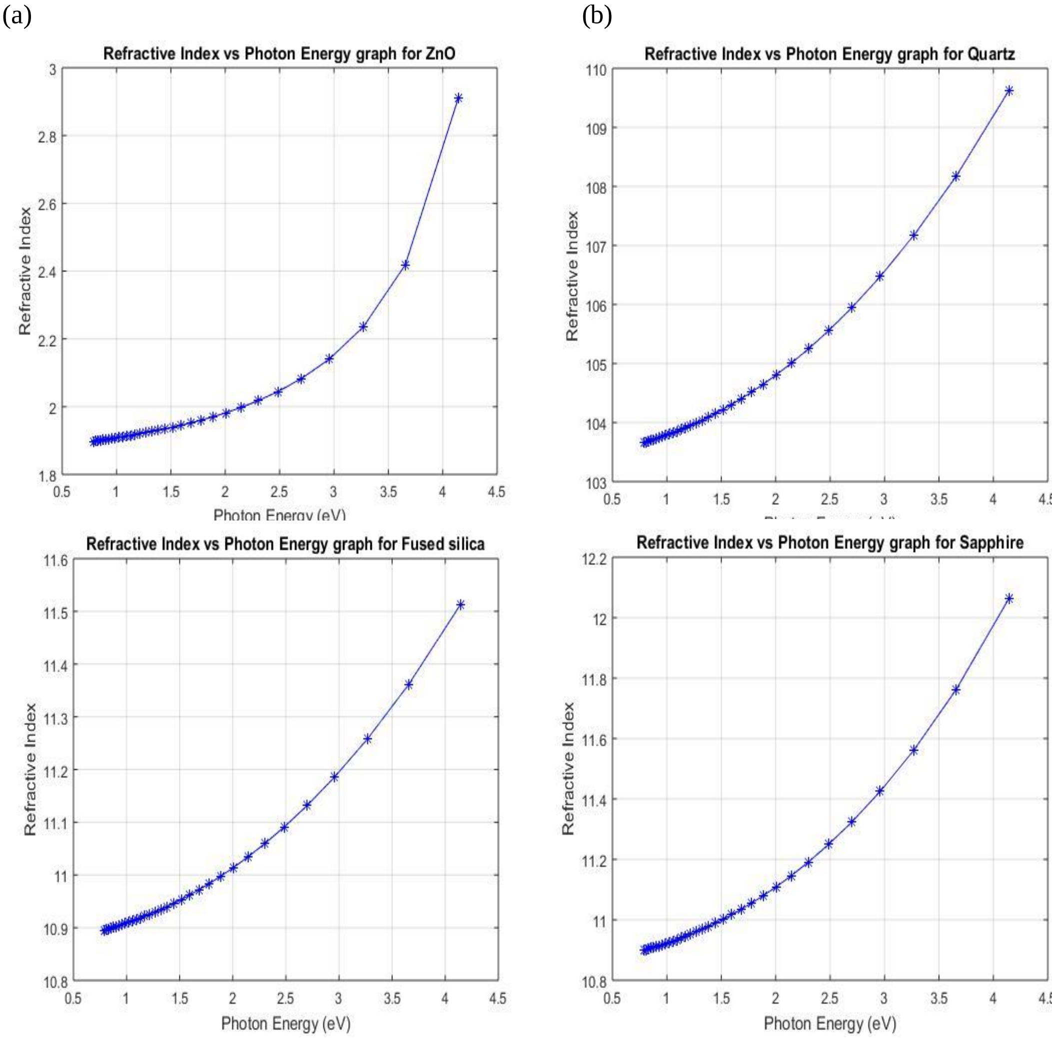


Fig. 2. Variation of refractive index as a function of photon energy for (a) ZnO (b) Quartz (c) Fused silica and (d) Sapphire.

3.1 Refractive Index Study

It is observed that the refractive indices rise gradually with the increase in photon energy in the range from 0.5 eV to 4.5 eV for all the substrates and ZnO thin film (Figure 2). It is evident from the graph that the value of refractive index goes in a single series of stages from one point to another point in the higher photon energy region. At 4.1 eV the refractive indices are 2.9, 109.63, 12.06 and 11.51

for ZnO, Quartz, Sapphire and Fused silica, respectively. By comparing the values for all substrates it is observed that Quartz exhibits highest refractive index and fused silica exhibits lowest refractive index in terms of photon energy.

3.2 Extinction Coefficient Measurements

From the Figure 3 it is clear that with the increase of photon energy the extinction coefficient increases slowly up to 1.4 eV and after that the value increases sharply to a high value. After 1.4 eV there is a sharp increase in extinction coefficient because of tremendously low absorption of light. The highest value of extinction coefficient is 82.5 above 1.6 eV.

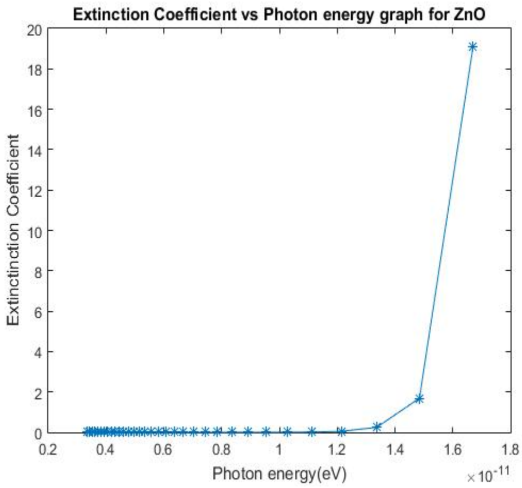
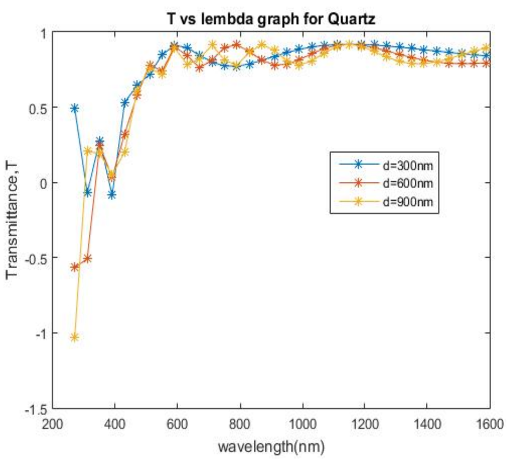


Fig. 3. Variation of extinction coefficient as a function of photon energy for ZnO thin film.

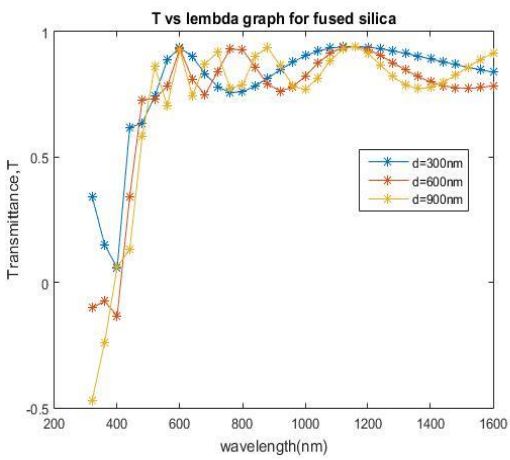
3.3 Transmittance Analysis

Figure 4 reveals that the transmittance rate is high that is about 80% -95% above the 580 nm of wavelength and it can be said that 580-1600 nm is a transparent region. On the other hand, below 300 nm of wavelength the transmittance rate is 0 and somewhere it is about -0.5 to -1 which is due to the influence of higher absorption. So, the region below 300 nm is strong absorption region. The rise and fall of peaks exhibit interference fringes which are produced because of multiple reflection of light between the top surface and bottom surface of the film. At the wavelength 1150 nm, Quartz shows transmittance of about 92%, Sapphire about 86% and Fused silica about 94%. By comparing the transmittance of these substrates it is found that fused silica exhibits highest transmittance whereas sapphire exhibits lowest transmittance.

(a)



(b)



(c)

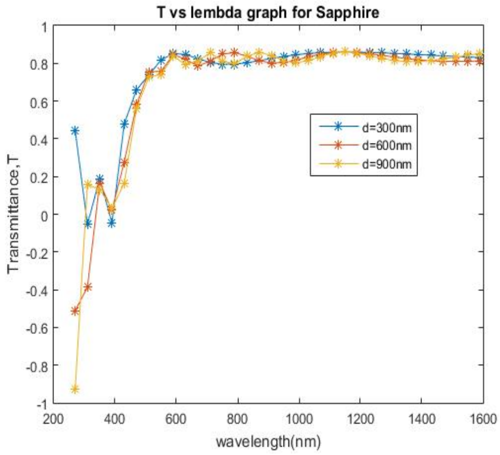


Fig. 4. Transmission spectra of ZnO thin film for different thicknesses deposited on (a) Quartz (b) Fused silica and (c) Sapphire substrates.

3.4 Reflectance Analysis

Figure 5 shows the reflectance spectra of ZnO thin films of different thicknesses (300 nm, 600 nm and 900 nm) deposited on Quartz, Fused silica and Sapphire substrates. It is found that the films exhibit highest reflectance at the UV region. At the wavelength 270 nm, Quartz showed reflectance of about 205%, Sapphire about 189% and Fused silica about 211%. At 300 nm the reflectance decreases suddenly below the zero level and after that it increases slowly at about 20% and remains consistent from 420 nm to 1600 nm for all the substrates. At 1150 nm the reflectance for Sapphire, Quartz and Fused silica substrates are 7.44%, 4.33% and 3.21%, respectively. Comparison reveals that the ZnO thin film deposited on Fused silica exhibits lowest reflectance.

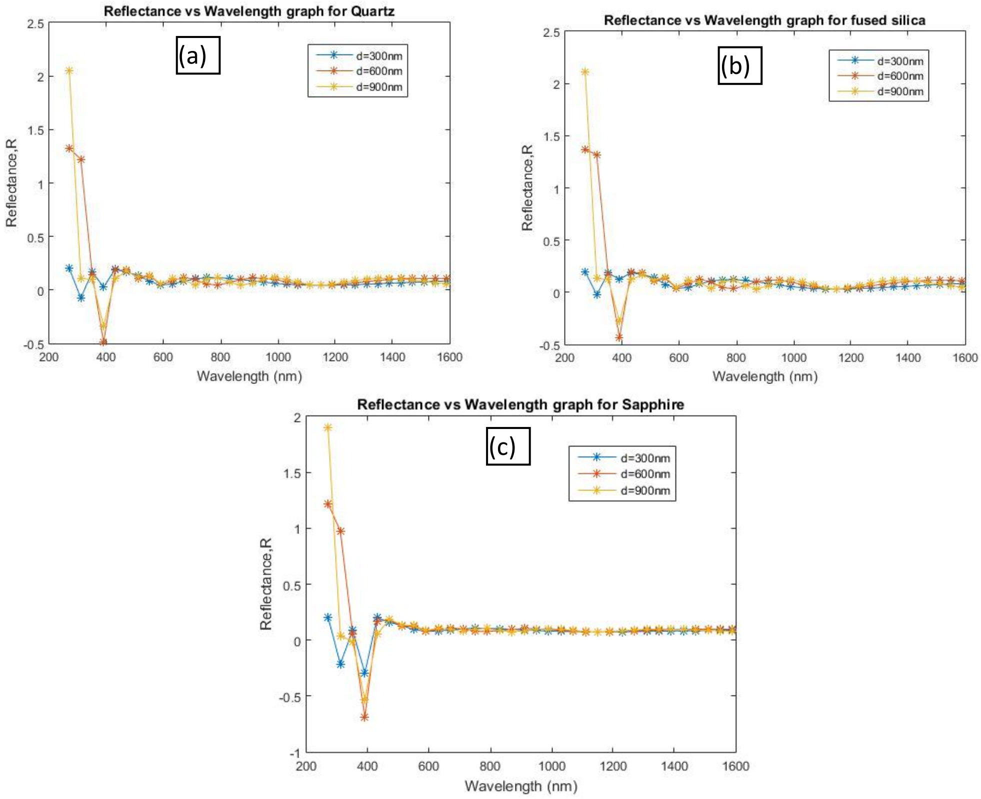


Fig. 5. Reflectance spectrum of ZnO thin film for different thicknesses deposited on (a) Quartz (b) Fused silica and (c) Sapphire substrate.

3.5 Absorption analysis

Figure 6 illustrates the absorbance spectra of ZnO thin films of different thicknesses (300 nm, 600 nm and 900 nm) deposited on various substrates. It has been observed from Figure 6 that the films exhibit highest absorbance between UV and visible region. At the wavelength 390 nm, Quartz shows absorbance about 146%, Sapphire about 167% and Fused silica about 139%. After 400 nm it declines sharply because of lowest photon energy. At the wavelength of 1100 nm the absorbance moves nearly towards zero and all the substrates show lowest absorbance. Comparison among these substrates shows that the Fused silica exhibits lowest absorbance

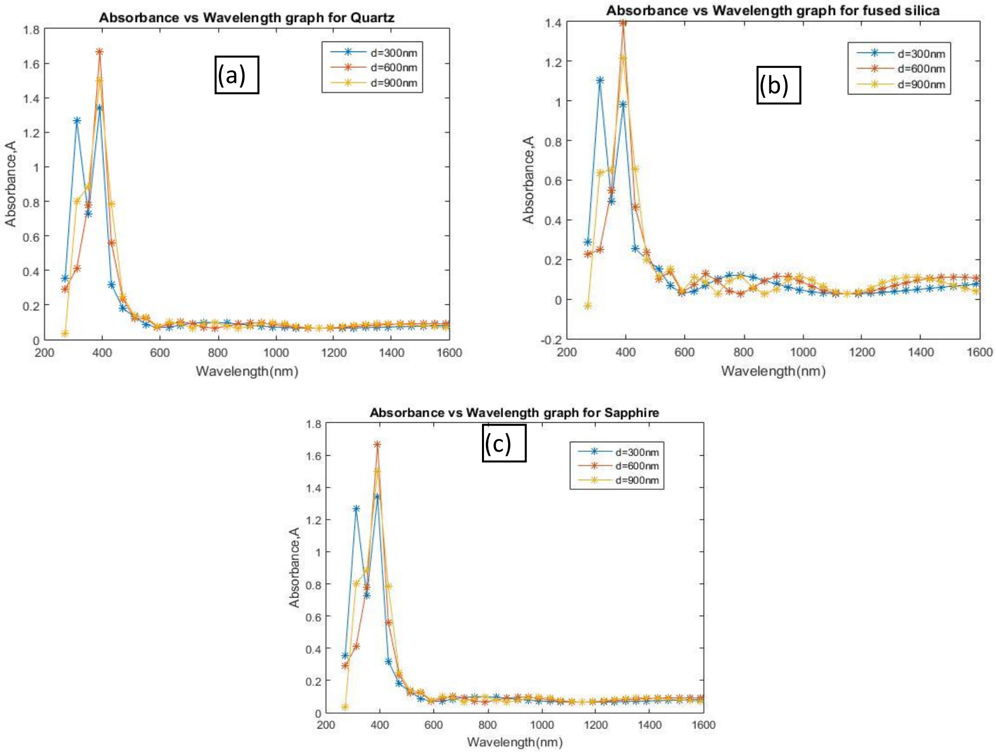


Fig. 6. Absorbance spectra of ZnO thin film for different thicknesses deposited on (a) Quartz (b) Fused Silica and (c) Sapphire substrates.

4. CONCLUSIONS

In this research, the optical properties of the ZnO thin films have been investigated for different thicknesses (300 nm, 600 nm and 900 nm) deposited on Quartz, Fused silica and Sapphire substrates by the simulation program "Matlab''. These properties are investigated as a function of photon energy and wavelength. For the calculation of refractive index of ZnO and for all substrates sellmeiers dispersion formula is used. The refractive index and extinction coefficient increase with the increase in photon energy. Comparison among the substrates reveals that Fused silica exhibits lowest refractive index which indicates that light travels faster through fused silica than other substrates. The films are found to possess highest transmittance of 85%-95% in the visible and near infrared region (IR). Among these substrates Fused silica is highly transparent. Most of the applications of fused silica exploit its wide transparency range, which extends from the UV to the near IR. All the substrates represent highest reflectance and absorbance in the UV region and consistent in the visible and IR. Moreover, in reflectance and absorbance spectra, fused silica has been found to show lowest reflectance and absorbance than the other two substrates. This substrate is highly desirable because of its small effects of absorption. From the above circumstances, it can be concluded that Fused silica is better than others for the deposition of ZnO thin film in terms of highest transmittance, lowest reflectance, refractive index and absorbance. These studies are very much expected to aid in the design, deposition and selection of proper substrate of ZnO thin film for the potential optoelectronic device applications.

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