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Inspection of Optical Properties of ZnO Thin Films Deposited on Different Substrates

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Abstract: *ZnO is a compound semiconductor with tetrahedral bonding configuration in a wurtzite structure. In a thin film device, it is a promising material for different optical and optoelectronic device applications. Also, among other possible applications are such as piezo-electric transducers, spin functional devices, gas sensors, transparent electronics in solar cell, UV light emitters, surface acoustic waves and smart windows etc. In this work, optical properties of ZnO Thin film deposited on three different substractes have been inspected. In order to investigate the optical properties of ZnO thin film simulation program "Matlab" was developed for its high efficiency to produce accurate graph. The optical properties of ZnO thin films were studied as a function of wavelength in the range from 300 nm to 1200 nm. The refractive index, absorption coefficient, extinction coefficient decrease with the increase in wavelength and their values are steady in the higher wavelength region. By comparing among the refractive indices of three substrates it was found that extraordinary KDP exhibits lowest refractive index. The transmittance spectra of ZnO thin films were investigated for different thicknesses (100nm, 450nm, 750nm). It was also observed that all the substrates exhibit a high transmittance of (80-95)% in the visible region. Moreover, in transmission spectra non-interference and interference effects were analyzed. No peaks in the transmission spectra reveals the evidence of non- interference effect. Interference fringes are represented by the maxima and minima in the interference term. Due to the interference effect the number of peaks increases with the increase in thickness. Thus, from the results it can be concluded that extraordinary KDP is the better substrate among other substrates for the deposition of ZnO thin film and give better causes for optoelectronic device applications.*

Keywords*: Optoelectronics, Thin Film, ZnO, Simulation, Matlab*

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I. Introduction

Zinc oxide is a II-VI compound semiconductor material with great potential for a variety of practical applications, such as piezoelectric transducers, optical waveguides, surface acoustic wave devices, varistors, phosphors, transparent conductive oxides, chemical and gas sensors, spin functional devices, and UV-light emitters.[[1]] Its wide bandgap 3.37 eV at room temperature makes ZnO a promising material for photonic applications in the UV or blue spectral range, while the high exciton-binding energy 60 meV [[2],[3],[4]] allows efficient excitonic emission even at room temperature. It also has relevantcharacteristics of a transparent conductive oxide (TCO)[[5]],which makes it very useful material for different technological applications like optical, optoelectronic devices, flat panel displays, liquid crystal displays and thin film photovoltaic devices, transparent electronics etc. [[3]-[7]]. After the improvement of nanotechnology, there is a lot of thirst to study the various important properties of this material in its nano dimensional form i.e. either in the form of nano dimensional thin film ornano structure/nano particle [[6],[7],[8],[9]]. The nano dimensional thin films attract much interest for their applications in future optical and optoelectronic applications due to their typical properties such as high optical transmittance in visible and near IR-region, high electrical conductivity and high chemical and physical stability [[8]]. Along with the experimental studies viz. synthesis and characterization of the physical and chemical properties, it is highly dispensable and important to study these properties theoretically to predict the optimized properties of the same before implementing the materials for above-mentioned applications [[9]]. Specifically, for the applications in optical and optoelectronic devices, it is extremely important to study the different optical properties like refractive index, extinction coefficient, transmittance and reflectance with varying the wavelength or energy of the incident light. For designing the modern optical and optoelectronic devices, it is also crucial to know the thickness, refractive index and extinction coefficient as a function of optical wavelength to predict the optical behavior of a device[[10],[11]].

In the present work, we start our simulation using two different model known as Sellimeier model and Cauchy's dispersion model for optical properties in the visible and near-IR region wavelength (300nm to 1200nm).Where the optical properties of ZnO thin film deposited on germania silica, extraordinary quartz and extraordinary KDP substrates for different thicknesses (100nm, 450nm, 750nm) were analyzed. The modeling is done by using Matlab code. This study is important to establish a correlation between theoretically calculated and experimentally observed properties before the implementation of this material in device fabrication.

II. Materials & Methods

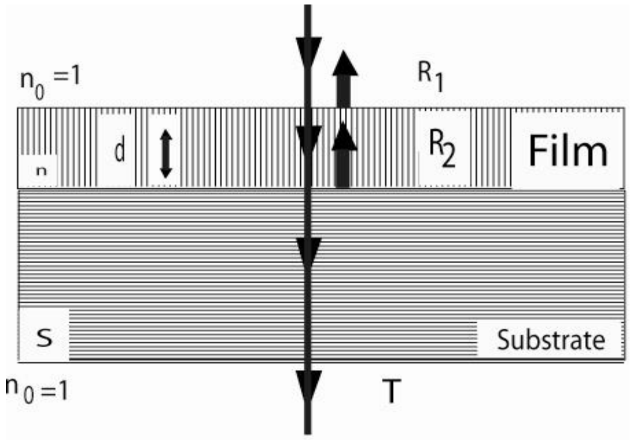

Figure 1: Model of the thin absorbant films on a transparent thick substrate.

The brief model of the thin absorbent films on a transparent thick substrate is shown in figure 4.14, where d and n is 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_o=1. R_1 is the intensity of the reflected light on the interface between air and film, and R_2 is the reflection on the interface between the film and substrate in middle. While the reflection at the interface between the substrate and air under substrate is not considered here [12] .

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

$$n^2(\lambda) = A + \frac{B\lambda^2}{\lambda^2 - C^2} + \frac{D\lambda^2}{\lambda^2 - E^2} \text{ ....(2.1)}$$

A,B,C,D and E are fitting Parameters, λ is the wavelength of light (nm). Fitting parameters are calculated for different thickness, as deposit varies significantly [13]. The sellmeir coefficients of ZnO is given in table 2.1

Table-2.1 : Fitting parameter by the method VASE of sellmeier model for Zinc Oxide [14] .

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

From this fitting parameters by the Matlab programme the refractive index of ZnO has been studied.
The refractive index of the substrate

$$S^2(\lambda) = 1 + \frac{A_1\lambda^2}{\lambda^2 - \lambda_1^2} + \frac{A_2\lambda^2}{\lambda^2 - \lambda_2^2} + \frac{A_3\lambda^2}{\lambda^2 - \lambda_3^2} \text{ .... (2.2)}$$

Table-2.2:The Sellmeier Coefficients of various substrates where $\lambda_1, \lambda_2, \lambda_3$ are in nm were given below [11]

Material	A_1	A_2	A_3	λ_1 (nm)	λ_2 (nm)	λ_3 (nm)
Germrnia Silica	0.711040	0.451885	0.704048	64.27	124.408	9425.478
Extraordinary Quartz, n_e	1.38100	0.0100	0.9992	93.505	11310	9528
Extraordinary KDP, n_e	1.13000	0.0001	0.9999	93.51	7671	12170

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

$$k(\lambda) = F_k e^{-G_k\left(\frac{1}{H_k}-\frac{1}{\lambda}\right)} \qquad \text{.............. (2.3)}$$

Table- 2.3: Cauchy parameter for Zinc oxide [13]

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

with the help of equation (2.3) and cauchy parameter the extinction co-efficient of ZnO thin film has been determined.

After that the value of R_1 and R_2 has been calculated by the following equation

$$R_1 = \frac{(n-1)^2+k^2}{(n+1)^2+k^2} \qquad \text{................................. (2.4)}$$

$$R_2 = \frac{(s-n)^2}{(s+n)^2} \qquad \text{....................................... (2.5)}$$

The absorption co-efficient of ZnO thin film is given by the following equation

$$\alpha = \frac{4\pi k}{\lambda} \qquad \text{..(2.6)}$$

The expression of the transmission of ZnO thin films deposited on different substrates is given by [12],

$$T(\lambda) = T_0(\lambda) - 2\sqrt{R_1R_2}\ \mathrm{Cos}\,[\delta(\lambda)] \qquad \text{...................(2.7)}$$

$$\delta(\lambda) = 2\pi \times \frac{2nd}{\lambda} + \pi \qquad \text{..(2.8)}$$

In equation (2.8), $T_0(\lambda)$ is considered to be the term of transmission with no interference effect.

The thickness of the films were 100nm, 450nm, 750nm which are used in this project. For different thickness of ZnO thin films deposited on different substrates,the transmittance have been determined by Matlab programme.

On the other hand,the transmission spectrum can be divided into two terms.They are (1) non-interference term (2) interference effect term.

The transmission of all ZnO thin film deposited on different substrates have been determined from the following formula [14],

$$\alpha(\lambda) = \frac{1}{d}\ln\left(\frac{A}{B}\frac{1}{T_0}\right) \qquad \text{..................................... (2.9)}$$

Where, $A = 16n^2s$

$B = (1+n)^3 (n+s^2)$

From the equation (2.9),transmittance(without interference effect), T_0 for all ZnO thin films have been determined by Matlab programme for different thickness(100nm, 450nm, 750nm) of the film.

The transmittance(with interference effect) can be expressed as [12],

$$T(\lambda)_i = T(\lambda) - T_0(\lambda) \qquad \text{...(2.10)}$$

From the equation (2.10), transmittance (with interference effect), $T(\lambda)_i$ for all ZnO thin films have been determined by Matlab programme for different thickness(100nm, 450nm, 750nm) of the film.

III. Results and Discussion

The optical properties of ZnO thin films were investigated as a function of wavelength in the region of 330-1200nm.

3.1. Refractive index

The variation of refractive indices with wavelength for ZnO and different substrates were shown in Fig 2(a) to 2(d) shows a decreasing tendency of refractive index with the increasing wavelength ranged from 300 nm to 1200 nm.All the curves are plotted using sellmeier equation.At 300 nm ZnO and all substrates indicates the highest refractive index which is 2.92 for ZnO,1.5165 for Ge-Si,1.5902 for extraordinary Quartz and for extraordinary KDP it is 1.5003.By comparing all substrates it was observed that extraordinary Quartz exhibits highest refractive index while extraordinary KDP exhibits lowest refractive index.

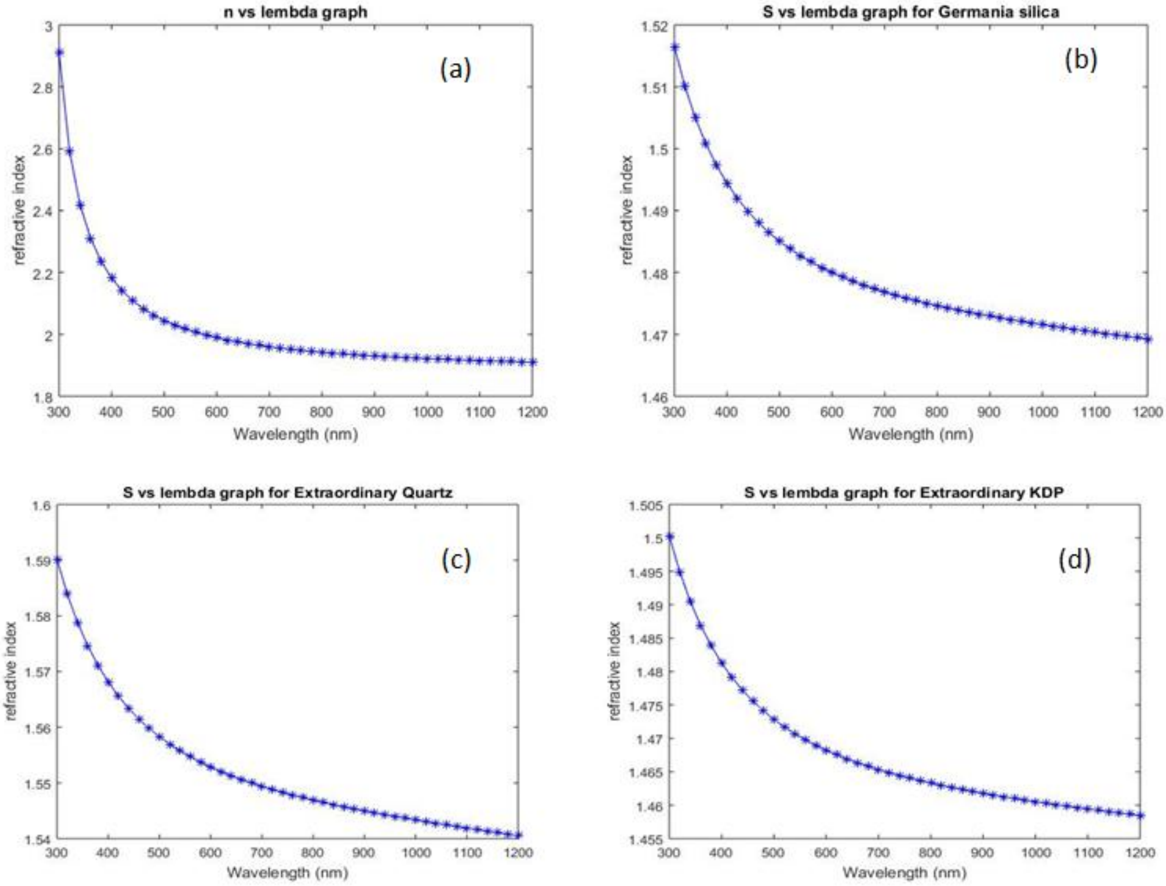

Figure2: Variation of refractive index as a function of wavelength for (a)ZnO, (b)Ge-Si, (c)Extraordinary Quartz, (d)Extraordinary KDP.

3.2. Absorption coefficient and Extinction Coefficient

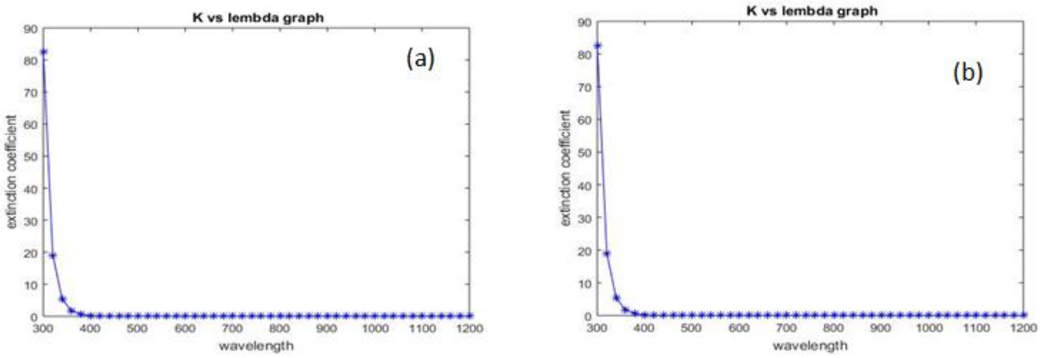

Figure 3: Variation of (a) coefficient co-efficient and (b) extinction coefficient as a function of wavelength for ZnO thin film.

Fig 3(a) and 3(b) represent the variation of absorption coefficient and extinction coefficient with the wavelength for ZnO thin film.The curve of Fig 3(a) shows that the absorption coefficient decreases sharply with the increase in wavelength which indicates that the ZnO film is the most absorbent in the UV region but low absorbant towards the visible region.The value of absorption coefficient is found to be almost zero for visible range while can be understand as the high transmittance value of the films for visible region.

From Fig 3(b), it can be clearly observed that ZnO thin film shows the highest absorbance for lower value of wavelengths.It can be seen from the curve that at around 370 nm,the value of extinction coefficient tends to zero which occurs due to small absorption by ZnO in the near ultra-violet and visible region.

3.3 .Transmittance Analysis

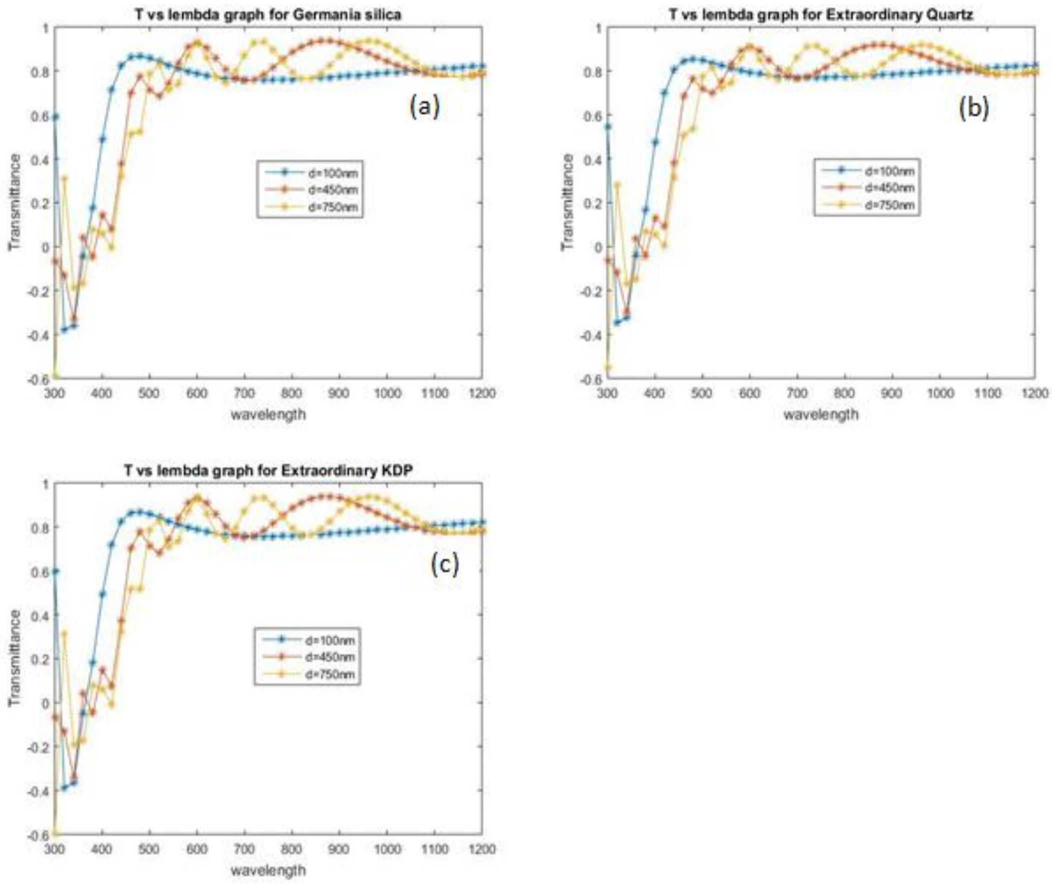

Figure 4: Transmission spectrum of ZnO thin film for different thicknesses deposited on (a) Germania Silica,(b) extraordinary quartz, and (c)extraordinary KDP.

Figure 4(a) to 4(c) show the optical transmittance spectra of thin film substrates Germania Silica, extraordinary quartz and extraordinary KDP for different thickness (100nm, 450nm and 750nm). It is clearly seen that all the substrates exhibit about a high transmittance of 80-90% in the visible region with a sharp absorption edge near ~380 nm. For all the substrates maximum peak is found in for the thickness of 750nm. It is observed from Fig 4(a)to 4(c) that the highest transparent region lies within the range from 420nm to 1200nm. On the other hand, the strong absorption region lies between 300-380nm which is in the UV region. In the UV region transmittance is low because of high photon energy. At the wavelength 700nm, Germania Silica showed transmittance about 87.17%, extraordinary quartz about 86.38% and extraordinary KDP showed about 87.28%. By comparing the transmittance among all substrates it can be concluded that extraordinary KDP is the best substrate for the deposition of ZnO thin film. Moreover, transmission spectra were analyzed for non-interference and interference effect.

3.4. Transmittance without Interference Effect

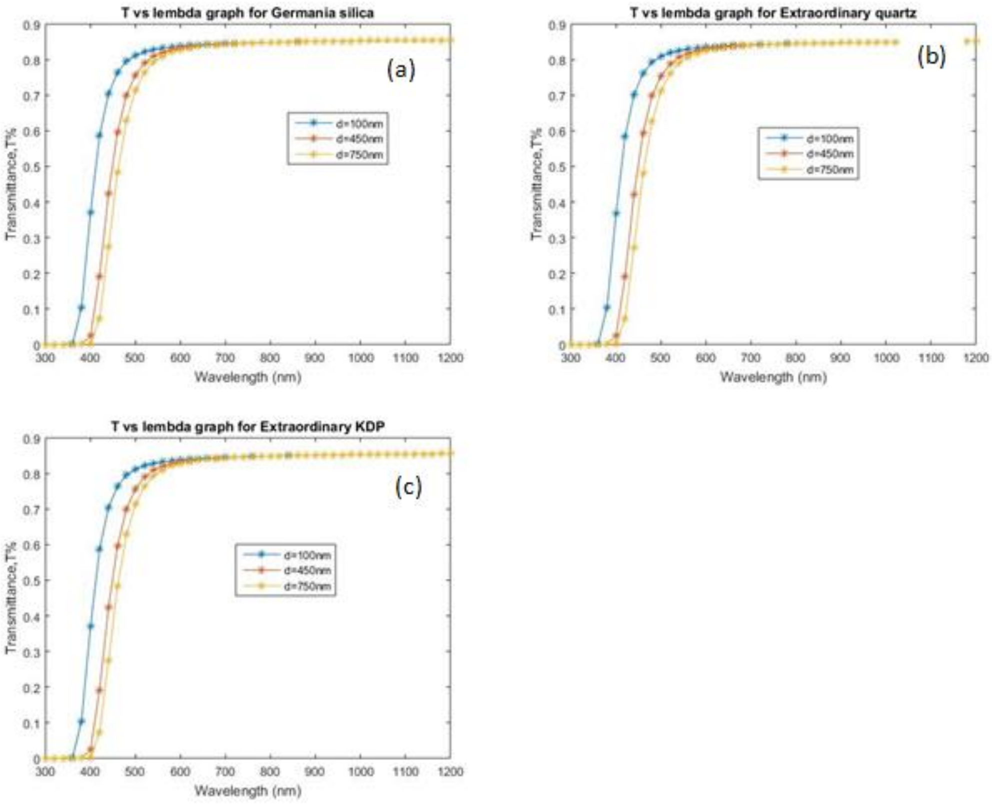

Figure 5: Transmission spectrum without interference effect of ZnO thin film for different thicknesses deposited on (a) Germania Silica,(b) extraordinary quartz, and (c)extraordinary KDP.

The graphs shown in figure 5(a) to 5(c) are the transmittance spectra for substrate of Germania Silica, extraordinary quartz and extraordinary KDP at different thicknesses at room temperature. In the graphs, the transmittance of the specimens varies in the same manner that it increases with wavelength. For all cases, the transmittance in the UV region (lower wavelength or high photon energy region) remains negligible and then starts to increase near the visible region. After the wavelength 500nm, all the spectra of different thickness remains stable upto 1200nm. At wavelength greater than 500nm, the transmittance is about 82.18% for Germania Silica, 81.92% for extraordinary quartz and 82.20% for extraordinary KDP in this region. Comparing among various substrates it can be concluded that extraordinary KDP exhibited highest transmittance and extraordinary quartz exhibited lowest transmittance in the visible region. After this, it shows no maxima and minima which is the evidence of non-interference effect. A consistent increase in transmittance is observed throughout the wavelength range for all films.

3.5. Transmittance with Interference Effect

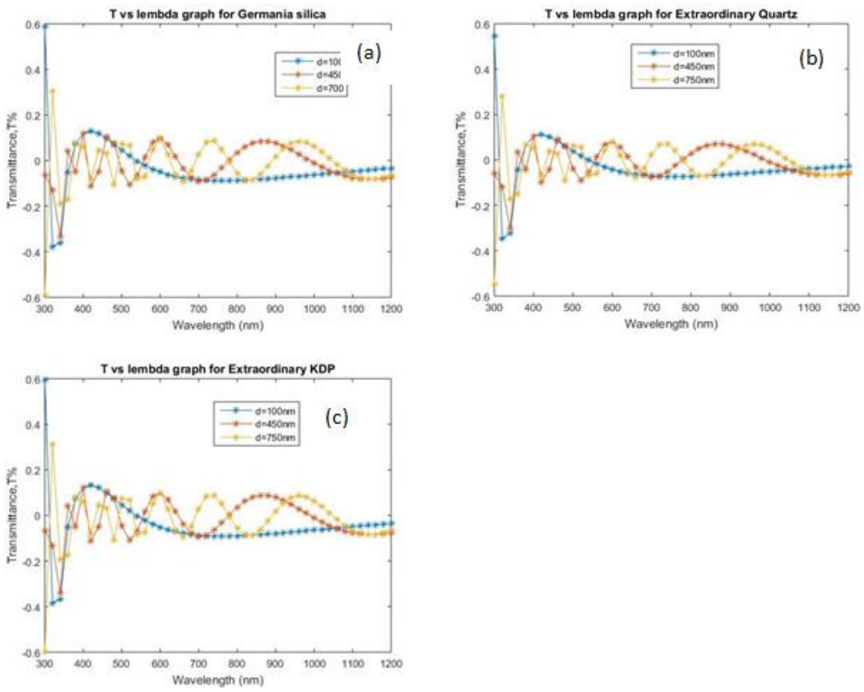

Figure 6 : Transmission spectrum(with interference effect) of ZnO thin film for different thicknesses deposited on (a) Germania Silica,(b) extraordinary quartz, and (c)extraordinary KDP.

The graphs shown in figure 6(a) to 6(c) are the transmittance spectra for substrate of Germania Silica, extraordinary quartz and extraordinary KDP at different thicknesses at room temperature.. In the graphs, the transmittance of the specimens varies in the same manner that it increases with wavelength. At 340nm it remains almost negligible for all films, and then first increase is noted at around 365nm. For all cases, there are interference fringes with maxima and minima. This is the evidence of the smoothness and highly reflectance of the film surface. These fringes occur due to the multiple reflection of light happening between the top surface of the film which is in contact with air and the bottom surface that is in contact with the substrate.

IV. Conclusions

ZnO thin films have been used for several years in making electronic devices, optical coatings, instrument hard coatings, and decorative parts. In this study, the optical properties of the ZnO thin films have been investigated as well as the refractive indices, absorption coefficient, extinction coefficient and transmission spectra of ZnO thin film for different thicknesses (100nm, 450nm, 750nm) deposited on three different substrates. The refractive indices, extinction coefficient and absorption coefficient decrease with the increase in wavelength and are almost consistent in the higher wavelength region. By comparing among three substrates it is observed that at 300nm extraordinary quartz exhibits highest refractive index of 1.5902 and extraordinary KDP exhibits lowest refractive index of 1.5003. This indicates that light travels faster through extraordinary KDP than other substrates. All the substrates exhibit high transmittance (80-90)% in the visible region with a sharp absorption edge near 380nm. Moreover, the non-interference and interference effect were observed in transmission spectra. After 520nm of wavelength there are no peaks in the transmission spectra because here the effect of reflectance and interference is totally neglected. In the interference effect term there exist maxima and minima which are the evidence of interference effect. This interference is due to the multiple reflections at the interface of films/substrate and at the interfaces of film/air. Moreover, the number of peaks increases with the increase of thickness. These also happens due to interference effect. Finally, it can be concluded that extraordinary KDP is the best substrates for the deposition of ZnO thin film in respect of highest transmittance and low refractive indices. High transmittance and low absorbance of these substrates ensures its usability in a variety of optoelectronic devices.Thus, these studies would be very helpful for selecting and designing proper substrate of ZnO thin film and for the potential application of optoelectronic devices.

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