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Determination of Optical Properties in Polycrystalline Zn O Thin Films by Theoretical Methods

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ABSTRACT

Polycrystalline ZnO thin films deposited on glass substrate, were optically characterized. The optical constants (Index of refraction n, absorption coefficient α and optical gap E_g^{opt})and the film thickness d, were determined using the transmission spectrum and Cauchy relation and sellmeier expression .the direct method and wemple-dodimenico relation are applied for calculation of the optical gap E_g^{opt} and their comparison shows that the optical band gap of Zn O thin film is direct transition.
KEYWORDS: Zno Thin Film, Optical Properties, Polycrystalline.

1. INTRODUCTION

Accurate measurements of optical constants and the thickness of semiconductor and dielectric thin films are great importance ,particularly of optical coatings and photo-optical devices .many methods for determining optical constants and the layer thickness of thin films deposited onto substrate have been published (Laaziz et al,2000,149-155;Kushev et al,1986,358-393; Vedam,1998,1-9).Minkov used the reflectance spectrum for different angles of incidence of nonpolarized or s (or p) polarized light to compute the optical constants and the thickness (Minkov,1991,306-310).Moreover optical constants and the layer thickness of a layer coated on a seminfinite transparent layer were estimated using transmission spectrum alone by Manifacier et al (so-called envelope function method of which takes into account of interference fringe pattern) (Manifacier et al, 1976,1002-1004).Swanepoel improved this method further in the case of finite substrate thickness (Swanepoel,1983,1214-1222).

In addition, the optical constants have been corresponded with the functions versus the light wavelength,such as: Cauchy relation, sellmeier expression,wimple-dodimenico function and ect. In this paper for computation of the optical constants of Zn O thin film had been used from the swanepoel, Cauchy, sellmeierand wimple-dodimenico function.

2. RESULTS AND DISCUSSION

The optical constants (the index of refraction and absorption coefficient) are usually determined by elaborated computer iteration procedures (Szezyrbowski and A.Czapla ,1977, Meredith, G.S.Buller and A.C.Walker, 1993) using both, the transmission and reflection spectra. in this work, we used the procedures by Swanepoel(Swanepoel,J.Phys.E:Sci.Instrum. 1983),Cauchy relation (poelman,P.F.Smet,J.Phys.D:Appl.Phys. 2003),sellmeier expression(P.O.Nilsson, 1968, Tatian,Ap1984) and wemple-didomenico (Didomenico,S.H.Wemple 1969, S.H.Wemple,M.Didomenico, 1971) to determine $n(\lambda)$ and $\alpha(\lambda)$ .The film thickness was determined from the interference fringes of the transmission spectrum.

3. Determination of the optical constants

This section presents results corresponding to calculation of the thickness and optical constants of the Zn O thin films by the several methods based on theory procedures.

The optical constants were obtained using the above methods and calculations based on a procedure described in details in Ref [Swanepoel,J,1983).This consist basically in the following:

a- Initially the complex index of refraction $n^* = n - ik$ are determined by simple straightforward calculations using the Swanepoel,Cauchy,sellmeier and wimple-didomenico.Fig.1. k is the extinction coefficient which can be expressed in terms of the absorption coefficient α $(k = \alpha\lambda / 4\pi)$.Fig.1.shows the Index of refraction n of Zn O film on the glass substrate obtained by Cauchy and sellmeier models. The absorption coefficient α calculated through Cauchy and sellmeier models given in the Fig.2.

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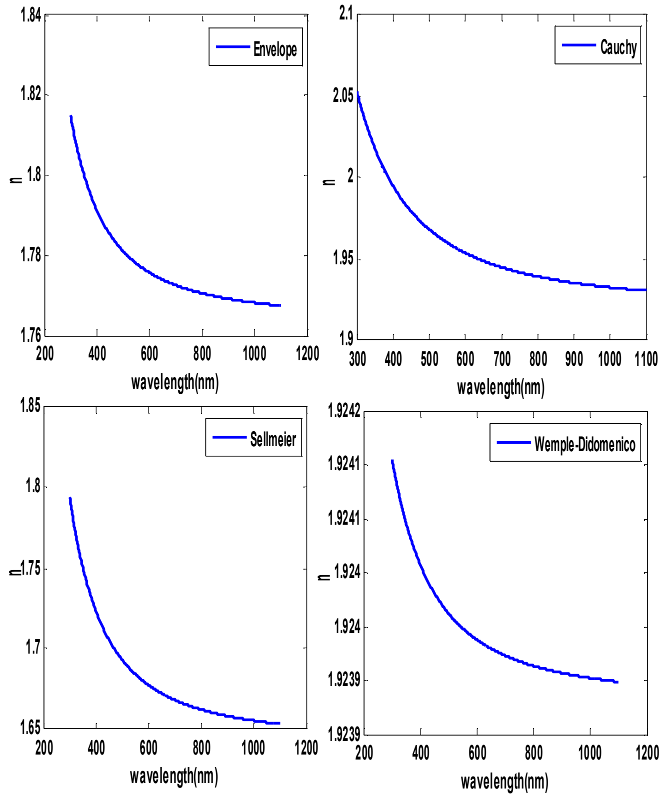

Fig.1. Dispersion curve of refractive index (n) for ZnO film calculated by Envelope, Cauchy, Sellmeier and Wimple-Dodimenico model.

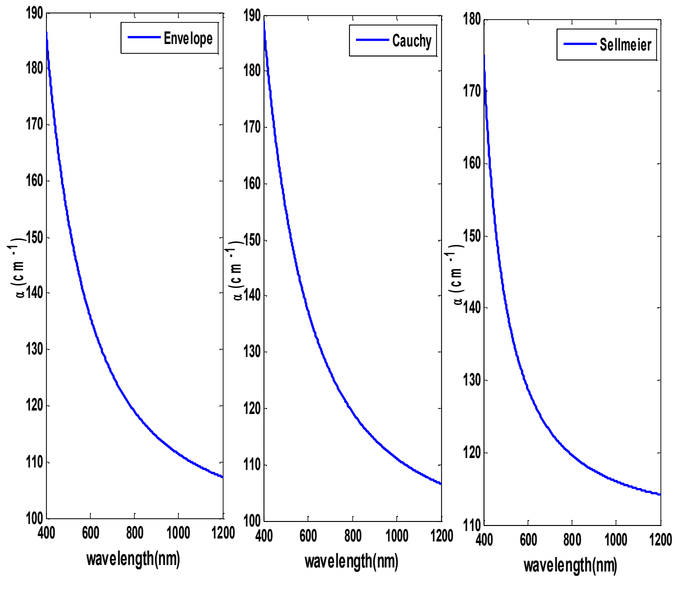

Fig.2. Dispersion curve of absorption coefficient for ZnO film calculated by Envelope, Cauchy and Sellmeier.

b- Subsequently, the optical gap E_g^{opt} is determined through the relation: $(\alpha h\upsilon) = A(h\upsilon - E_g^{opt})^m$, where A is the a constant and m determines the type of transition. The parameter m has the value ½ for the direct allowed transition, has the value 1 for the direct forbid transition, has the value $3/2$ for the indirect forbid transition and has the value 2 for the indirect allowed transition. E_g^{opt} determined by extrapolating the straight line portion of the spectrum to $\alpha h\upsilon = 0$. from this drawing ,the optical energy gap $E_g^{opt} = 3.29$ eV is deduced for the Zn O thin film.Fig.3 shows that the type of transition is direct allowed. This value of energy

gap is very good agreement to exact value for Zn O thin film at temperature 400^{c}.the value energy gap calculated by one method in the next section that it is near to the value calculated with above method.
to obtain the thickness and the values n and α from transmission spectra(swanepoel),it is necessary to analyze them as follow:

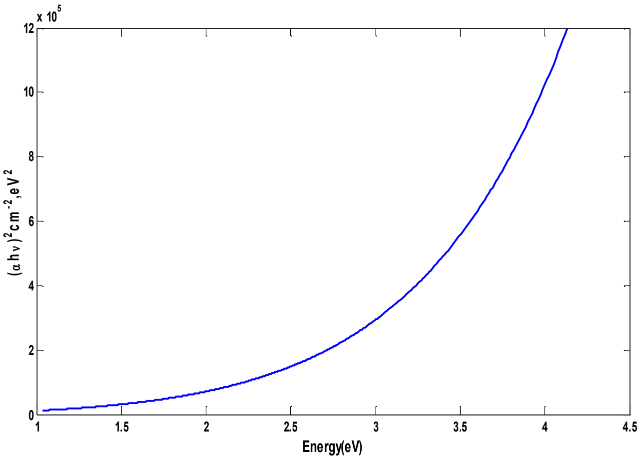

Fig 3.Dependence of $(\alpha h\upsilon)^{2}$ on the photon energy for ZnO thin film (thickness 500nm)

4. Interference Zone

Assuming that the interference are fully coherent, the location of the interference maxima and minima are related to the real part of the index of refraction n, through the expression:

$$2nd = m\lambda \qquad (1)$$

Where the interference order m is an integer for maxima and half integer for minima. There is no way of obtaining information on either n or d separately using Eq.(1); however, these parameters can be determined as follows:

In the transparent region (far below the band gap energy) where $\alpha = 0$, the n value at a minimum is given by the following relation (Swanepoel, J.Phys.E:Sci.Instrum, 1983):

$$n = [M + (M^{2} - s^{2})^{1/2}]^{1/2}$$

$$M = (s^{2} + 1)/2 + 2s(T_{\max} - T_{\min})/T_{\max}T_{\min} \qquad (2)$$

Where s is the index of refraction of substrate (glass) which is a function as wavelength λ:

$$s = [1 + 1/(0.7568 - 7930/\lambda^{2})]^{1/2}$$

T_{max} and T_{min} are maxima and minima transmittance at the same wavelength in the fitted envelope curves on the transmittance spectrum. Therefore the index of refraction can obtained solving Eq. (2).The index of refraction of Zn O film(thickness 500) given in the Fig.1.

Finally, the absorption coefficient of Zn O thin film in the low absorption region of the interference zone can be calculated using the following relation (Swanepoel, J.Phys.E:Sci.Instrum, 1983), Fig.2.

$$\alpha = -\{\ln[E_{M} - [E^{2}{}_{M} - (n^{2} - 1)^{3}(n^{2} - s^{4})]^{1/2}]\};$$

$$E_{M} = 8n^{2}s/T_{M} + (n^{2} -)(n^{2} - s^{2}\ ) \qquad (3)$$

The absorption coefficient can be obtained from Manifacier model by following relation:

$$\alpha = -\frac{1}{d}\ln(n-1)(n-s)[(\frac{T_M}{T_m})^{1/2}+1]/(n+1)(n+s)[(\frac{T_M}{T_m})^{1/2}-1] \qquad (4)$$

The thickness d of the thin film was calculated using the following relation:

$$d = \lambda_1\lambda_2 / 2[n(\lambda_1)\lambda_2 - n(\lambda_2)\lambda_1] \qquad (5)$$

where $n(\lambda_1)$ and $n(\lambda_2)$ are the index of refractions at the two adjacent maxima (or minima) at λ_1 and λ_2.The Zn O thin film thickness was found to be 500nm.

5. Interference Zone

In this region, the index of refraction is determine by extrapolating the curve of n vs λ obtained previously at λ values within the interference zone. for that ,the n versus λ curve is fitted to a polynomial equation of the following forms (Cauchy equation and sellmeier relation respectively):

$$n = A + B/\lambda^2 \qquad (6)$$

$$n = [1 + 1/(A + B/\lambda^2)]^{1/2} \qquad (7)$$

Where A and B are constant parameters.

The absorption coefficient in the high absorption region of the interference free zone is calculated using the following Eq:

$$\alpha = -1/d\ln(T)$$

Where T is the normalized transmittance.

6.Dispersion energy parameters of ZnO thin film

Wimple and Didomenico (M.Didomenico,S.H.Wemple,1969, S.H.Wemple,M.Didomenico, 1971) use a single oscillator description of the frequency dependent optical constants to define a 'dispersion energy' parameters E_d and E_0. The index of refraction of the Zn O thin film studied can be fitted by the Wemple and Didomenico. The dispersion plays an important role in the research for optical materials, because it is a significant factor in optical communication and in designing devices for spectral dispersion. The relation between the index of refraction n, and the single oscillator strength below the band gap is given by the expression (M.Didomenico,S.H.Wemple,1969, S.H.Wemple,M.Didomenico, 1971):

$$n = 1 + E_0E_d/(E_o^2 - (h\upsilon)^2) \qquad (8)$$

Where E_0 and E_d are single oscillator constants, E_0 is the energy of the effective dispersion oscillator, E_d the so-called dispersion energy, which measures the average strength of inter band optical transitions. The oscillator energy E_0 is an average of the optical band gap, E_{opt}, can be obtained from the Wemple-didomenico model.

Experimental verification of Eq.(3) can be obtained by plotting $(n^2-1)^{-1}$ versus ($(h\upsilon)^2$ as illustrated in Fig.4. for Zn O thin film, which yields a straight line for normal behaviour having the slope $(E_0E_d)^{-1}$ and the intercept with the vertical axis equal to E_0/E_d.But the obtained curves in Fig.4. ,show positive deviation from linearity. A positive curvature deviation [] from linearity at longer wavelength is usually observed due to the negative contribution of lattice vibrations on the index of refraction. The values of the parameters E_0 and E_d can be estimated from Fig.4.

The optical band gap values E_g^{opt}, were also calculated from Wemple-didomenico dispersion parameter, E_0, using $E_{opt}^{WD} \approx E_0 / 2$ relation [13,14]. The E_{opt}^{WD} values obtained from Wemple- Didomenico model agree with that determined by the Fig.3.

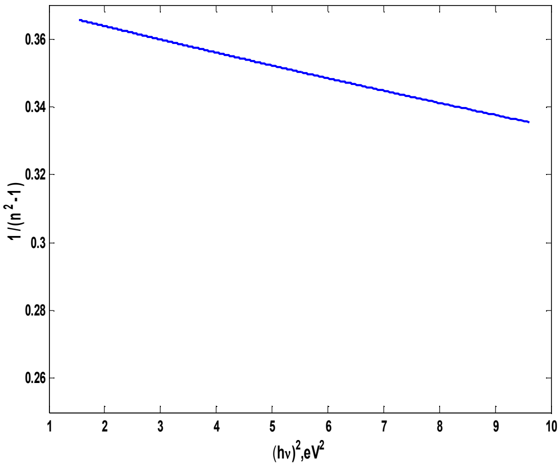

Fig 3. Plot of $1/(n^2 - 1)$ against $(h\upsilon)^2$ for Zn O thin film (thickness 500nm).)

7. Conclusions

The film thickness d, index of refraction n, and absorption coefficient $\alpha(h\upsilon)$ for the energies higher than the optical can be determined by using the optical transmission $T(\lambda)$ spectra with a method proposed by Swanepoel. On the basis of the optical investigations of the thin film, the following results were obtained. In terms of Tauc method and Wemple Didomenico model agree with that determined by the Fig.3.

Didomenico model the optical band gap was calculated. The E_g^{WD} value obtained from the Wemple-Didomenico model is in agreement with those determined from the Tauc model. The type of optical transition responsible for optical absorption was direct transitions.

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