3. OPTICAL CALCULATIONS

The determination of the amplitudes and intensities of beams of light reflected or transmitted by a thin film, require to set up the Maxwell's equations and apply the appropriate boundary conditions [1]. The equations of propagation of wave entering an absorbing medium normally may be expressed in a similar form to that for transparent medium, by replacing the real refractive index (n) by complex quantity "complex refractive index" (n-ik), where n is the ratio of the velocity of the wave in vacuum to that of the wave in the medium and k represents the energy absorption in the medium.

The following discussion is limited to the calculation of the film thickness and optical constants using normal transmission data, the only experimental facility that was available to us.

3.1. MODEL FOR DETERMINATION OF THICKNESS, REFRACTIVE INDEX AND THICKNESS IRREGULARITY

Many methods have been proposed in the last decades to determine the optical parameters of thin films from transmission data [2-13], rather than using transmission and reflection data. This is due to the simplicity of calibration of the spectrophotometer, which yields accurate experimental results. One of the simplest methods was introduced by Swanepoel [2], which used the transmission envelope to solve the equation, analytically, for the thickness and refractive index. However, including the thickness variation in his formula [3] required a numerical solution for every data point. Another interesting method by Cisneros [4,5] for a uniform film includes the effect of substrate and solves an equation numerically for the optical parameters. Here we present a simple approach for determination of thickness, thickness irregularity, refractive index and extinction coefficient for semiconductor thin films.

3.1.1 THEORETICAL BACKGROUND

The expression for transmittance, including the reflection from the second interface of the substrate and the effect of a finite substrate, which is valid for transparent as well as weakly absorbing substrates [4] is

$$T = \frac{(1-\rho)T_{123}U}{1-\rho R_{321}U^2}, \tag{3.1}$$

$$R_{321} = r_{321}r_{321}^{\bullet}, \tag{3.2}$$

$$T_{123} = (n_3/n_1)t_{123}t_{123}^{\bullet}, \tag{3.3}$$

where r_{321} and t_{123} are the amplitude of the electric field of the wave reflected and transmitted in 321 and 123 directions respectively (illustrated in Fig. 3.1). These parameters are given by

$$t_{123} = \frac{t_{12}t_{23}\exp(i\psi/2)}{1+r_{12}r_{23}\exp(i\psi)}, \tag{3.4}$$

$$r_{321} = \frac{r_{32}+r_{21}\exp(i\psi)}{1+r_{32}r_{21}\exp(i\psi)}, \tag{3.5}$$

here r_{ij} and t_{ij} are the Fresnel coefficients of reflected and transmitted wave in different regions [1,4] and expressed as

$$r_{ij} = \frac{N_i - N_j}{N_i + N_j} \quad , \quad t_{ij} = \frac{2N_i}{N_i + N_j}. \tag{3.6}$$

The complex refractive index is

$N_i = n_i + ik_i$,

where n_i is the real part and k_i is the imaginary part (extinction coefficient) of the complex refractive index of air (n_1, k_1), film (n_2, k_2) and substrate (n_3, k_3). ψ is the phase difference of the wave between two interfaces,

$\psi = 4\pi N_2 d/\lambda = 4\pi n_2 d/\lambda + 4\pi k_2 di/\lambda = \phi + i\alpha d$,

where d is the film thickness, λ is the wavelength, α is the absorption coefficient and ϕ is the phase angle.

The modified Fresnel coefficient of reflected and transmitted waves at rough film surface [14], (1-2) interface, where the r.m.s. height of surface irregularity $\sigma << \lambda$, are

$$r_{12}' = r_{12}\exp[-2(2\pi\sigma/\lambda)^2 n_1^2] = \eta\, r_{12}, \qquad (3.7)$$

$$r_{21}' = r_{21}\exp[-2(2\pi\sigma/\lambda)^2 n_2^2] = \beta\, r_{21}, \qquad (3.8)$$

$$t_{12}' = t_{12}\exp[-\frac{1}{2}(2\pi\sigma/\lambda)^2 (n_1 - n_2)^2] = \gamma\, t_{12}. \qquad (3.9)$$

Substitution of equations (3.2)-(3.9) into equation (3.1) and proceeding with careful and lengthy calculation will result in an expression for transmittance in the following simplified form,

$$T = \frac{A_1\exp(\alpha d)}{B_1\exp(2\alpha d) + C_1\exp(\alpha d) + D_1} \times \frac{B_2\exp(2\alpha d) + C_2\exp(\alpha d) + D_2}{B_2\exp(2\alpha d) + C_3\exp(\alpha d) + D_3}, \qquad (3.10)$$

where,

$A_1 = \gamma^2[16n_1n_3(1-\rho)(n_2^2+k_2^2)U]$, $B_1 = st - \rho svU^2$, $B_2 = st$

$C_1 = \beta\{[2(4n_3k_2^2 - ZY)\cos\phi + 4k_2(n_3Y+Z)\sin\phi] - \rho U^2[4k_2(Z-n_3Y)\sin\phi - 2(ZY+4n_3k_2^2)\cos\phi$

$C_2 = \beta\{2(4n_3k_2^2 - ZY)\cos\phi + 4k_2(n_3Y+Z)\sin\phi\}$, $C_3 = \eta\{2(4n_3k_2^2 - ZY)\cos\phi + 4k_2(n_3Y+Z)\sin\phi\}$

$D_1 = \beta^2[uv - \rho tuU^2]$, $D_2 = \beta^2[uv]$, $D_3 = \eta^2[uv]$, $u = (n_1-n_2)^2 + k_2^2$, $v = (n_2-n_3)^2 + k_2^2$,

$s = (n_1+n_2)^2 + k_2^2$, $t = (n_2+n_3)^2 + k_2^2$, $Y = n_2^2 - n_1^2 + k_2^2$, $Z = n_2^2 - n_3^2 + k_2^2$,

$\rho = [(n_1-n_3)^2 + k_3^2]/[(n_1+n_3)^2 + k_3^2]$, $n_3 = n_1[1/T_s + (1/T_s^2 - 1)^{1/2}]$,

$U^{-1} = \frac{(1-\rho)^2}{2T_s} + [\frac{(1-\rho)^4}{4T_s^2} + \rho^2]^{1/2}$, $U = \exp(-\alpha_s d_s)$,

where T_s is the transmittance of the substrate and, for transparent substrate U=1 and k_3=0.

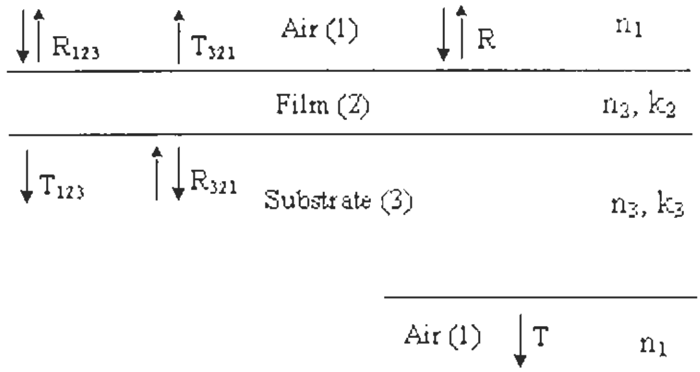

Fig. 3.1. Optical parameters and directions of the transmittance and reflectance, adopted in Eqs. 1-6.

3.1.2. SOLVING FOR d, σ, n AND α

In the transparent region of the transmission spectra maximum and minimum transmission occur at [2-6] $\phi = m\pi$, where m=1, 2, 3,.....

$$4\pi nd / \lambda_m = m\pi \, . \tag{3.11}$$

For $n_2 > n_3$, m is even at maximum transmission and odd at minima. Eq. (3.11) could be rewritten as

$$n_2(m, \lambda) = \frac{m\lambda}{4d} \, . \tag{3.12}$$

We can calculate the interference fringes order (m) by assuming that the refractive index varies slowly with the wavelength [4,5] in this region so that

$$(m-1)\lambda_{m-1} \approx m\lambda_m \approx (m+1)\lambda_{m+1} \rightarrow m \cong \frac{\lambda_{m-1}}{\lambda_{m-1} - \lambda_m} \cong \frac{\lambda_{m+1}}{\lambda_m - \lambda_{m+1}} \, . \tag{3.13}$$

Using the conditions that m is even for maxima and odd for minima makes it easy to find the value of m. In some cases, in which it is not easy to decide the value of m, for example, in thicker films, one could use a model for variation of the refractive index with the wavelength [2,3,7] as

$$n = n_0 + g/\lambda^2 , \qquad (3.14)$$

where n_0 and g are constants, and Eq.(3.12) may be written as

$$4dn_m = m\lambda_m ,\ 4dn_{m+1} = (m+1)\lambda_{m+1} ,\ 4dn_{m-1} = (m-1)\lambda_{m-1} . \qquad (3.15)$$

Substituting Eq.(3.14) in Eq.(3.15) and solving for m gives

$$m \cong \frac{\lambda_{m-1}^3\lambda_{m+1}^2 + \lambda_{m-1}^2\lambda_{m+1}^3 - \lambda_{m-1}^3\lambda_m^2 - \lambda_{m+1}^3\lambda_m^2}{(\lambda_{m+1}-\lambda_m)(\lambda_{m-1}^3\lambda_{m+1} - \lambda_{m-1}^2\lambda_{m+1}^2 + \lambda_{m-1}^3\lambda_m - \lambda_{m-1}^2\lambda_{m+1}\lambda_m - \lambda_{m-1}^2\lambda_m^2 + \lambda_{m+1}^2\lambda_m^2)} . \qquad (3.16)$$

Then m could be listed for all the spectra where the interference fringes appear. Knowing the value of m, the refractive index of the film (n_2) at the extremes in Eq.(10) is replaced with

$$n_2(m,\lambda) = \frac{m\lambda_m}{4d} . \qquad (3.17)$$

Substituting Eq.(3.17) into Eq.(3.10) and setting $k_2 = 0$ gives two equations for T_M(for m even $\rightarrow \cos(\phi)=1$) and T_m(for m odd $\rightarrow \cos(\phi)= -1$). We solved these two equations by minimizing Δ, where

$$\Delta = (T_m - T_{me})^2 + (T_M - T_{Me})^2 . \qquad (3.18)$$

T_{Me} and T_{me} are the experimental transmittance data at maxima and minima respectively. Solution of Eq. (3.18) for one consecutive maxima and minima gives the value of d and σ.Then the refractive index can be calculated from Eq. (3.17) for all maxima and minima, since this equation is valid for absorption films where the value of m could neatly be defined [4]. Fitting the values of the refractive index to some known model gives the values of the refractive index for the entire spectra.

Knowing the values of d, σ and n_2, Eq. (3.10) could be solved for k_2, by minimizing Δ_1,

$$\Delta_1 = (T(k) - T_e)^2 . \qquad (3.19)$$

Here T (k) is the transmittance formula (3.10) and T_e is the experimental transmittance value.

3.1.3 SIMULATION FOR α-Si:H

For checking the accuracy of the presented method, typical values [3,7] for n (λ), $\alpha(\lambda)$, d and σ, were used to reproduce the transmission curve using Eq. (3.10), the value were $n_2 = 2.6+3\times10^5/\lambda^2$, $Log(\alpha)=-8+1.5\times10^6/\lambda^2$, d=1000 nm, σ = 15 nm, n_3=1.53 and n_1=1. Interference fringes (m) calculated using Eq. (3.13) and listed for all extremes is shown Fig. 3.2. Solving Eq.(3.18) in the transparent region as shown in Fig. 3.3 gave d=999.63 nm and σ =15.014 nm .The value of d was used to determine the refractive index by Eq.(3.17). A plot of $n_2(\lambda)$ versus $1/\lambda^2$ is shown in Fig. 3.4. A linear fitting gives $n_2=2.60138+3.00859\times10^5/\lambda^2$.

From Table 3.1. which shows the calculated values of the thickness (d) and thickness irregularity (σ) for different values of the interference order (m) in transparent as well as low absorption region, one can notice that the calculated values of d are within good accuracy, better than 0.1%, whereas the accuracy of σ is better in the transparent region .

The calculated values of d, σ and n_2 are used to determine the absorption coefficient (α) from Eq. (3.19) in the transparent and in the low absorption region, whereas in the high absorption region, where the interference fringes disappear, the fitting parameters of the refractive index have been used.

Table 3.2, which gives the comparison of the calculated and exact values of the absorption coefficient for different wavelength, shows that the calculated values of α have good accuracy in high and low absorption regions, while in the highly transparent region the accuracy was less because of a small value of α ($\sim10^{-6}$-10^{-8} nm^{-1}). However, fitting the calculated values (Fig. 3.5) gave good accuracy, since the values of α in the transparent region have less weight than in the other regions.

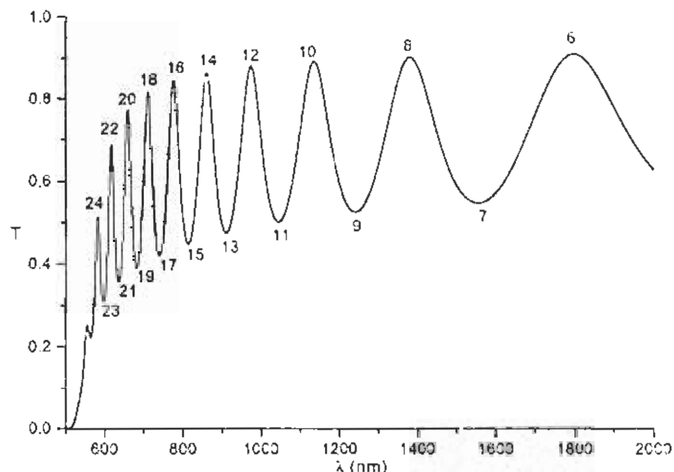

Fig. 3.2. Calculated transmittance curve of α-Si:H vs. wave-length (λ), along with interference fringes order (m).

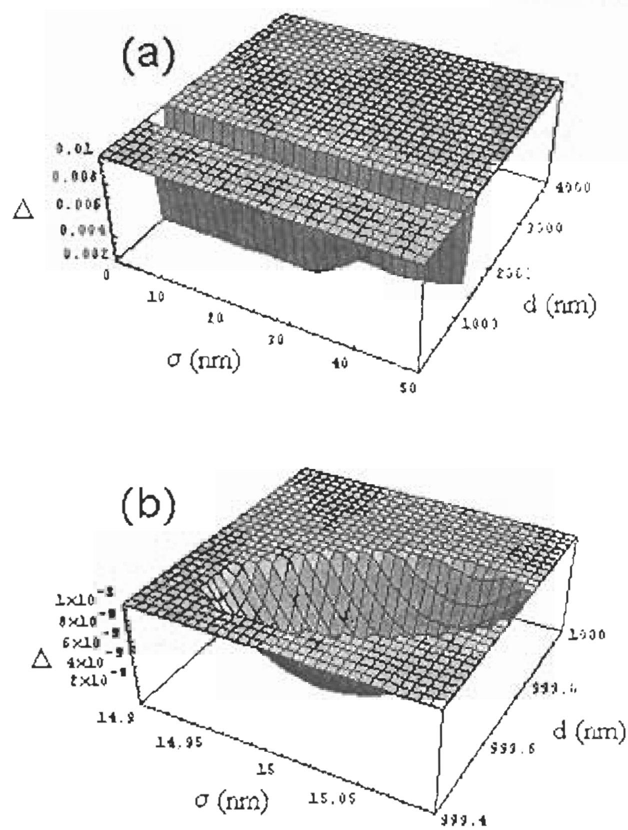

Fig. 3.3. Solution of Eq. (3.18) for σ and d large range (a) and small range (b).

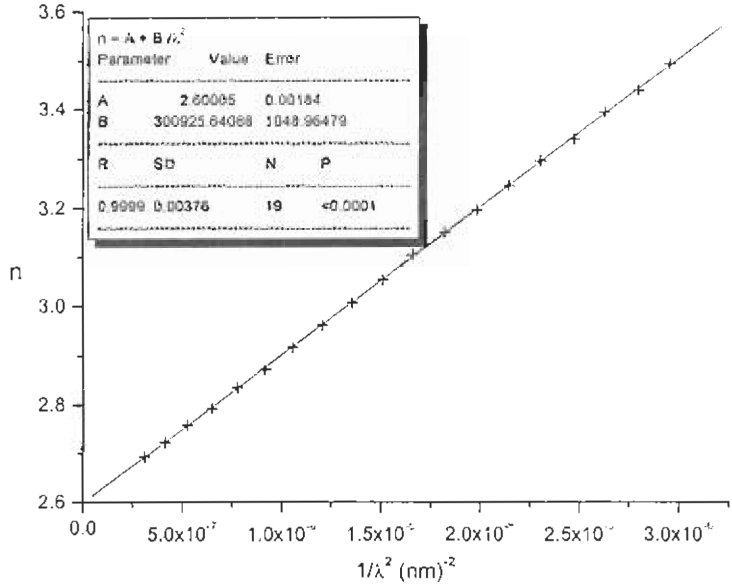

Fig. 3.4. Linear fitting of the refractive inex (n) vs. $1/\lambda^2$ for α-Si:H.

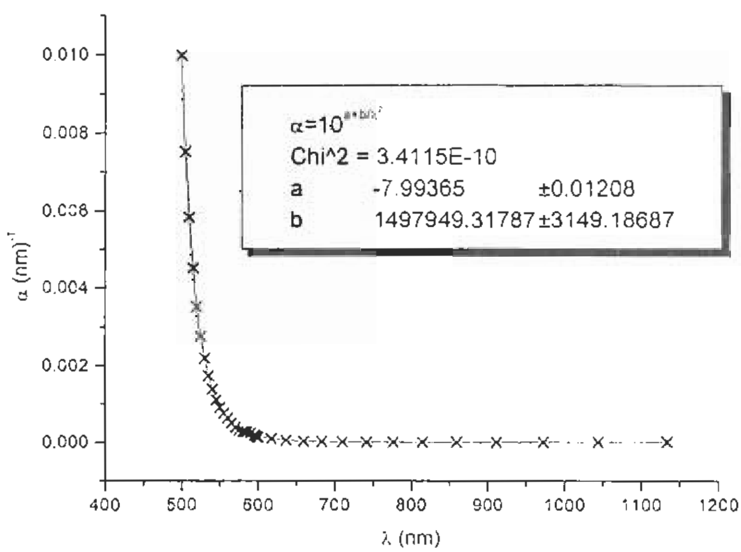

Fig. 3.5. Fitting of calculated absorption coefficient α values for α-Si:H.

Table 3.1. Calculated values of thickness (d) and thickness irregularity (σ) obtained by solving of Eq. (3.18) for different values of interference fringes orders, for α-Si:H.

Interference orders (m).	λ_M (nm)	T_M	λ_m (nm)	T_m	d (nm)	σ (nm)
6,7	1796	0.90690	1556	0.54687	999.63	15.014
8,9	1379	0.89955	1241	0.52515	999.91	15.029
10,11	1134	0.88973	1044	0.50099	999.631	15.048
12,13	973	0.87727	911	0.47532	999.764	15.098
14,15	859	0.86191	814	0.44872	999.90	15.190
16,17	775	0.84243	741	0.42120	1000.58	15.432
18,19	710	0.81564	683	0.39211	1000.60	15.996
20,21	659	0.77156	636	0.35808	1000.7	17.3682
22,23	617	0.68630	597	0.31002	1000.83	20.571

Table 3.2. Comparison between calculated and exact values of the absorption coefficient in different regions, for α-Si:H.

λ (nm)	α_{exact} (nm)$^{-1}$	$\alpha_{calculated}$ (nm)$^{-1}$	λ (nm)	α_{exact} (nm)$^{-1}$	$\alpha_{calculated}$ (nm)$^{-1}$
500	0.01000	0.00999	582	2.682E-4	2.695E-4
505	0.00762	0.00752	595	1.783E-4	1.878E-4
510	0.00585	0.00584	597	1.670E-4	1.592E-4
515	0.00452	0.00452	600	1.468E-4	1.319E-4
520	0.00353	0.00352	617	8.714E-5	8.841E-5
525	0.00277	0.00276	636	5.109E-5	5.138E-5
530	0.00219	0.00220	659	2.844E-5	2.901E-5
535	0.00174	0.00174	683	1.643E-5	1.473E-5
540	0.00139	0.00139	710	9.454E-6	9.262E-6
545	0.00112	0.00110	741	5.390E-6	3.297E-6
550	9.088E-4	8.996E-4	776	3.090E-6	2.902E-6
555	7.400E-4	7.558E-4	814	1.835E-6	1.105E-6
560	6.069E-4	6.301E-4	859	1.078E-6	9.538E-7
565	4.999E-4	5.024E-4	911	6.410E-7	2.759E-7
570	4.138E-4	3.875E-4	972	3.890E-7	3.659E-7
			1044	3.516E-6	1.878E-7
			1134	1.467E-7	9.973E-8

3.1.4. ZnTe THIN FILM

The transmission spectra of ZnTe thin film, prepared by two-sourced thermal evaporation on corning7059 glass substrate [15], recorded with a Perkin-Elmer, Lambda19, UV-VIS-NIR spectrophotometer with UV-WinLab software, for range 400-2000 nm is shown in Fig. 3.6. The interference order (m) calculated from Eq.(3.13) is also listed for all extremes in Fig. 3.6.

The solution of Eq.(3.18), gives d = 745.8 nm and σ=6.17 nm, where the refractive index of the substrate(n_3) was 1.53. The calculated refractive index of the ZnTe film, using Eq.(3.17), is shown in Fig. 3.7.

Many models [4,5,9,11,13,16-21] could be used for fitting of such film, but the single oscillator model [4,5,13,16-19] is found to have the best fitting for the refractive index values.

$$n^2 = 1 + \frac{E_m E_d}{E_m^2 - (h\nu)^2} = 1 + \frac{(n_0^2 - 1)E_m^2}{E_m^2 - (h\nu)^2}, \qquad (3.20)$$

where E_m, E_d are the oscillator and dispersive energies, h is the Planck constant, ν is the photon frequency and n_0 is the refractive index of an empty lattice at infinite wave length. The calculated values of the refractive index along with fitting to Eq. (3.20) is shown in Fig. 3.7.

The values of α, calculated by Eq. (3.19), are fitted to the Urbach relation [16,21],

$$\alpha = \alpha_0 \exp(h\nu / E_e) = \exp(a + b/\lambda), \qquad (3.21)$$

where α_0, E_e, a and b are constants related to the characteristic slope of α. It is obvious, from Fig. 3.8, that Urbach relation has good fitting for $\alpha < 0.003$ nm^{-1} (30,000 cm^{-1}).

Near the absorption edge the optical energy gap (E_g) for allowed direct transition could be calculated, using the well-known dependence [22] $\alpha^2 \sim (h\nu - E_g)$. The energy gap is obtained by means of extrapolating the square of the absorption coefficient (α^2) versus incident photon energy ($h\nu$). Fig. 3.9 shows the energy gap using the values of α

calculated by Eq. (3.19), E_g =2.47 eV, and α is calculated using the following approximation [23-25] near the absorption edge.

$$T \sim \exp(-\alpha d)\,. \qquad (3.22)$$

E_g obtained was 2.234 eV. Fig. 3.10 shows the transmittance curve reproduced by Eq. (3.10) using calculated values of d and σ and the fitting parameters of n_2 and α, in the Urbach region, along with experimental transmission data, which have a good matching.

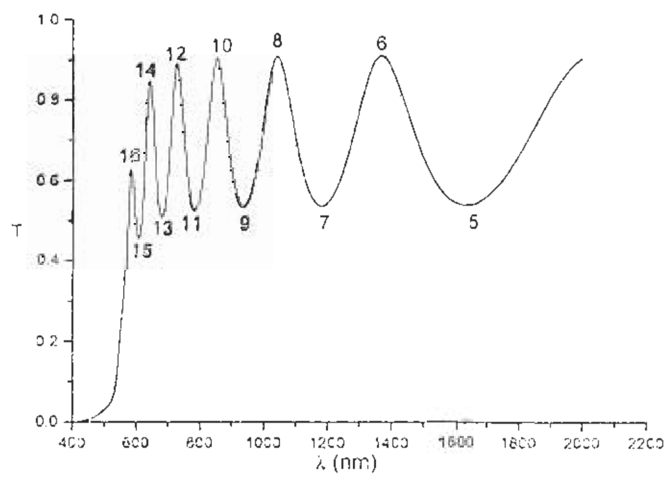

Fig. 3.6. Experimantal transmission spectra of ZnTe film with interference fringes order (m).

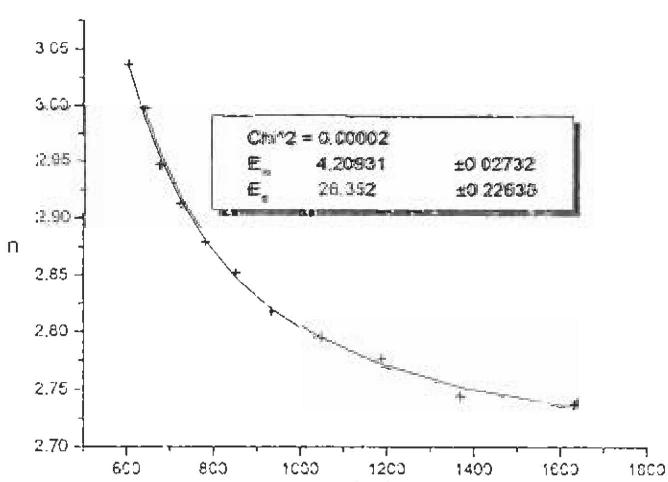

Fig. 3.7. Calculated values of the refractive index of ZnTe film, with fitting to Eq. (20).

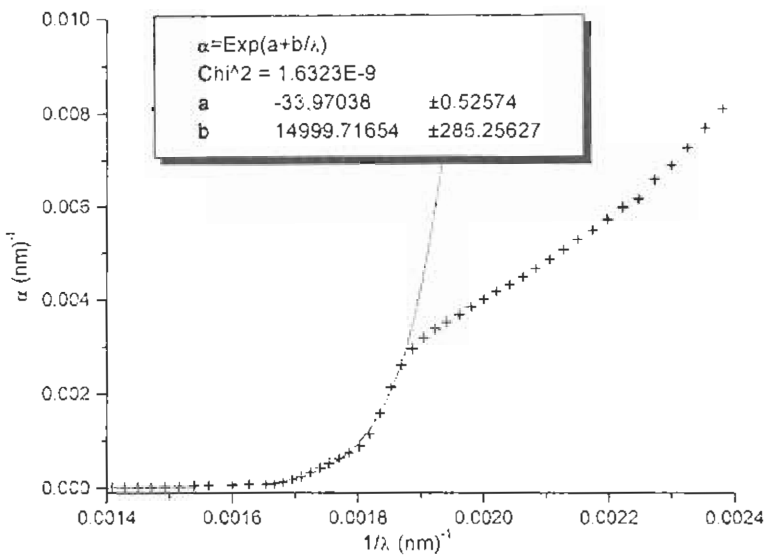

Fig. 3.8. Calculated values of the absorption coefficient, with fitting to Urbach relation.

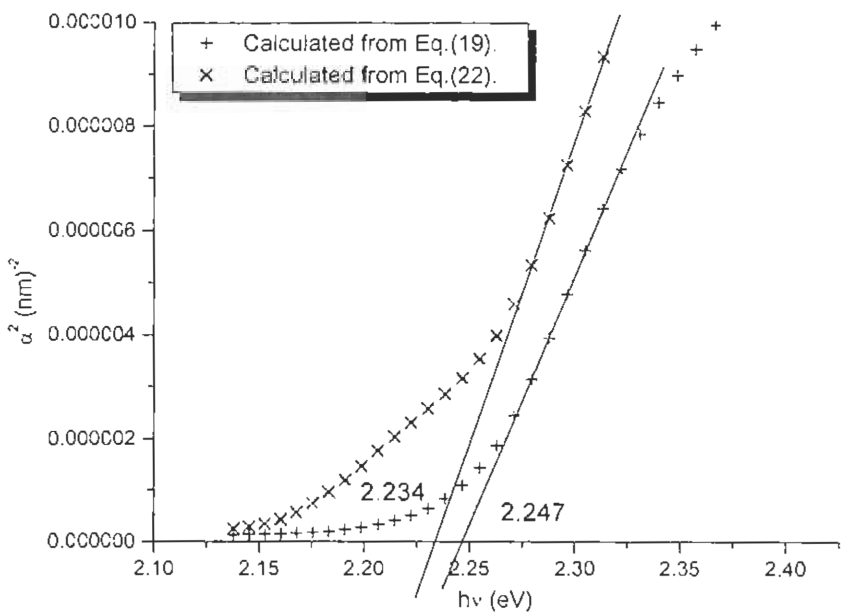

Fig. 3.9. Plot of α^2 vs. photon energy ($h\nu$) for ZnTe film.

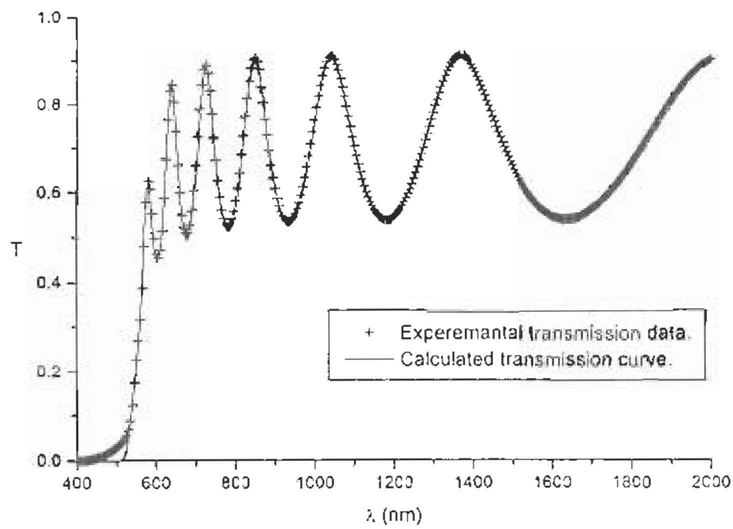

Fig. 10 . Calculated transmittance curve, with experimental transmission data, versus wavelength for ZnTe film.

3.1.5 DISCUSSION AND COMMENTS

1. The formulas include most of the film and substrate parameters, which affect the transmission spectra, are given in a simplified form.

2. The values of the interference fringes order (m), for films of thickness below ~2000 nm, could simply be determined using relation (3.13) by approximating the resulting value to the closest even integer for maxima and odd integer for minima. For thicker films where the interference fringes are so close, relation (3.16) could be used.

3. The thickness, thickness irregularity, and the refractive index of the film (with good accuracy) can be calculated by simple solution of one numerical equation.

4. Calculated values of the absorption coefficient or the extinction coefficient of the film, in the absorption region, where the interference fringes no longer exist, depend on the selection of model for the refractive index. While in the transparent region it is calculated by using the values of the refractive index calculated in this region.

5. Simulation of a tested theoretical model proved that there is no significant error due to approximation used, consider k=0 in transparent region and m is exactly integer, even at wavelength below 1000 nm (but not at lower wave-length where the absorption is too high).

3.2 APPROXIMATION APPROACH

In Eq (3.10) the transmittance formula included most of the parameters which could effect the transmission of light from thin film on partially transparent substrate (i.e. absorption of the light by the film and the substrate, irregularity of the film surface, reflection from the back side of the substrate, etc.). In case of smooth surface film (the thickness irregularity ignorable, i.e. $\sigma \sim 0$) Eq. (3.10) become,

$$T = \frac{A\ \exp(\alpha d)}{B\ \exp(2\alpha d) + C\ \exp(\alpha d) + D}, \qquad (3.23)$$

where,

$A = 16 n_1 n_3 (1-\rho)(n_2^2 + k_2^2)U$, $B = st - \rho s v U^2$

$C = [2(4n_3k_2^2 - ZY)\cos\phi + 4k_2(n_3Y + Z)\sin\phi] - \rho U^2[4k_2(Z - n_3Y)\sin\phi - 2(ZY + 4n_3k_2^2)\cos\phi]$

$D = uv - \rho t u U^2$, $u = (n_1 - n_2)^2 + k_2^2$, $v = (n_2 - n_3)^2 + k_2^2$,

$s = (n_1 + n_2)^2 + k_2^2$, $t = (n_2 + n_3)^2 + k_2^2$, $Y = n_2^2 - n_1^2 + k_2^2$, $Z = n_2^2 - n_3^2 + k_2^2$,

$\rho = [(n_1 - n_3)^2 + k_3^2]/[(n_1 + n_3)^2 + k_3^2]$, $n_3 = n_1[1/T_s + (1/T_s^2 - 1)^{1/2}]$,

$$U^{-1} = \frac{(1-\rho)^2}{2T_s} + [\frac{(1-\rho)^4}{4T_s^2} + \rho^2]^{1/2}, U = \exp(-\alpha_s d_s).$$

The above equation was derived by Cisneros [4] and used in his method to find numerical solution for the optical constants. In case of the transparent substrate (i.e. $k_2 = 0$, $U = 1$) Eq. (3.23) could be written (after rearranging the terms) as

$$T = \frac{A' x}{B' - C' x + D' x^2}, \qquad (3.24)$$

where,

$A' = 16s(n^2 + k^2)$, $B' = [(n+1)^2 + k^2][(n+1)(n+s^2) + k]$,

$C' = [(n^2 - 1 + k^2)(n^2 - s^2 + k^2) - 2k^2(s^2+1)]2\cos\varphi - k[2(n^2 - s^2 + k^2) + (s^2+1)(n^2 - 1 + k^2)]2\sin$

$D' = [(n-1)^2 + k^2][(n-1)(n - s^2) + k^2]$,

$\varphi = 4\pi n d/\lambda$, $x = \exp(-\alpha d)$, $\alpha = 4\pi k/\lambda$.

Here n, d, k are the thickness, refractive index and the extinction coefficient of the film, and s is the refractive index of the substrate. For $k^2 << n^2$, which is the case of the semiconductor films under investigation (see sec.3), Eq. (3.24) becomes,

$$T = \frac{A^{''}x}{B^{''} - C^{''}x + D^{''}x^2}, \tag{3.25}$$

where,

$A^{''} = 16n^2 s$, $B^{''} = (n+1)^3(n+s^2)$, $C^{''} = 2(n^2-1)(n^2-s^2)\cos\varphi$,

$D^{''} = (n-1)^3(n-s^2)$, $\varphi = 4\pi nd/\lambda$, $x = \exp(-\alpha d)$, $\alpha = 4\pi k/\lambda$.

The above equation was used by Swanepoel [3] for calculating the thickness variation of the film surface (Δd) by integrating Eq.(3.25) in the transparent region (i.e. $\alpha \approx 0$):

$$T_{\Delta d} = \frac{1}{\varphi_1 - \varphi_2}\int_{\varphi_1}^{\varphi_2} \frac{A^{''}}{B^{''} - C^{''} + D^{''}} d\varphi, \tag{3.26}$$

where

$\varphi_1 = 4\pi n(\bar{d} - \Delta d)$ and $\varphi_2 = 4\pi n(\bar{d} + \Delta d)$,

By performing the above integration Swanepoel found two equation for T_M (Maximum Transmittance) and T_m (minimum transmittance) as:

$$T_M = \frac{\lambda}{2\pi\Delta d}\frac{a}{(1-b^2)^{1/2}}\tan^{-1}\left[\frac{1+b}{(1-b^2)^{1/2}}\tan\left(\frac{2\pi n\Delta d}{\lambda}\right)\right], \tag{3.27a}$$

$$T_m = \frac{\lambda}{2\pi\Delta d}\frac{a}{(1-b^2)^{1/2}}\tan^{-1}\left[\frac{1-b}{(1-b^2)^{1/2}}\tan\left(\frac{2\pi n\Delta d}{\lambda}\right)\right], \tag{3.27b}$$

where,

$$a = \frac{A^{''}}{B^{''} + D^{''}}, \quad \text{and} \quad b = \frac{C^{''}}{B^{''} + D^{''}},$$

Using the method of transmission envelope [4] we can have two values for the transmittance, from the transmission spectra, at every wavelength value. However, this required numerical solution of Eq. (3.27) at every data point (n is function of wavelength). On the other hand using the phase angle and calculating the interference order (as done in sec. 3.1) n could be replaced by d in Eq. (3.27). In this case (since d is constant) we can solve for d and Δd by simply using consecutive maxima and minima without need to make transmission envelope around the transmission spectra. Knowing the values of d and m (as done in sec. 3.1) the value of n could be calculated for the entire spectra. But in this case the solution of the transmittance equation is limited to the transparent region. In order to calculate α in high absorption region (which is required for band gap determination) we have to consider the loss of light intensity (in this region) due to scattering from the film surface negligible as compared with the loss of light intensity due to absorption by the film. In this case the values of α could be calculated from Eq. (3.25).

Using the above procedure and solving for the optical constant of the same ZnTe film used in the previous section (using model for refractive index as Eq. (3.20), the results are:

d=744 nm, Δd = 14 nm, E_m=4.204 eV, E_d=26.32 eV, n_0=2.70, E_g=2.246 eV,

It is clear that this approach provides good result for transparent film with low thickness variation. However it is to be noted that the value of Δd calculated here is almost double than σ calculated in the previous section and this could be due to the definition of these parameters in the two equations.

3.3 NONLINEAR CURVE FITTING

For easy and fast fitting of the transmittance spectra, the transmittance equation should contain as minimum parameters as possible, with condition of good accuracy of the fitting.

3.3.1 FITTING PROCEDURES

Starting from Eq. (3.25) and assuming that the refractive index varies slowly with the wavelength within two consecutive maxima ($\cos\varphi = 1$) and minima ($\cos\varphi = -1$) and solving T_M (maximum transmission) and T_m(minimum transmission) for n gives:

$$n = \frac{[N + (N^2 - 4s^2)^{\frac{1}{2}}]}{2} , \qquad (3.28)$$

$$N = 1 + s^2 + 4s(\frac{T_M - T_m}{T_M T_m}) ,$$

$$d = \frac{\lambda_M \lambda_m}{4n(\lambda_M - \lambda_m)} . \qquad (3.29)$$

The values of n and d, calculated from equations (2.28) and (2.29), are used as initial least square fitting parameters for equation (2.25). For good fitting appropriate model for n and α should be used (see next section). For calculation of α in the high absorption region, (which needed for the determination of the band gap) the values of n and d from fitted curve are used. The exact solution of equation (3.23) for x is,

$$x = \frac{(C^{''} + A^{'}/T) - [(C^{'} + A^{''}/T)^2 - 4B^{''}D^{'}]^{1/2}}{2D^{''}} , \qquad (3.30)$$

where all the constants have been defined already.

3.3.2 MODELS USED FOR n AND α

Single oscillator model or W-D model is found to be good model for the refractive index of ZnTe (sec 3.1) and other materials [18]

$$n^2 = 1 + \frac{E_m E_d}{E_m^2 - (h\nu)^2} = 1 + \frac{(n_0^2 - 1)E_m^2}{E_m^2 - (h\nu)^2} , \qquad (3.20)$$

and could be re-written as :

$$n^2 = 1 + \frac{(n_0^2 - 1)\lambda^2}{\lambda^2 - \lambda_0^2} , \qquad (3.31)$$

where $\lambda_0 = \frac{hc}{E_m}$, $n_0 = \left(1 + \frac{E_d}{E_m}\right)^{1/2}$.

Power series expansion of Eq. (3.20) gives:

$$n = n_0 + \frac{E_d}{2n_0 E_m^3}(h\nu)^2 + n_0\left(\frac{E_d}{2n_0^2 E_m^5} - \frac{E_d^2}{8n_0^2 E_m^6}\right)(h\nu)^4 + \cdots\cdots\cdots$$

Using the values of ZnTe film calculated in section 3.1 gives:

$$n = 2.695 + \frac{1.008\times10^5}{\lambda^2} + \frac{6.866\times10^9}{\lambda^4} + \frac{5.027\times10^{14}}{\lambda^6} + \frac{3.836\times10^{19}}{\lambda^8} + \cdots\cdots \quad (\lambda \text{ in nm}).$$

It is obvious that the terms above the 2nd term is comparatively very small (λ range 500-2000 nm), using approximation up to 2nd terms gives:

$$n = n_0 + \frac{b}{\lambda^2} \ . \qquad (3.32)$$

Which is the model used by Swanepoel [2,3] for his calculation.

The absorption in the transparent region in the film could be due to Urbach tail, defect absorption, multi-phonon absorption and light scattering etc. As a matter of fact, the wavelength dependence of the absorption process is complicated and could not be written in a simplified formula. However, as was seen in section 3.1 the exponential dependence (Urbach relation) is good and can give good fitting for transparent film as:

$$\alpha = \alpha_0 \exp(h\nu / E_e) = \exp(c + f/\lambda), \qquad (3.33)$$

where α_0, E_e, c and f are constants related to the characteristic slope of α, or other similar model [2,3],

$$\alpha = 10^{c + \frac{f}{\lambda^2}} \ , \qquad (3.34)$$

where c and f are constants .

In case of doped films a term representing the absorption due to impurity could be added to Eq. (3.33) or Eq.(3.34) as:

$$\alpha = g + \exp(a + b/\lambda), \qquad (3.35)$$

and

$$\alpha = g + 10^{c+\frac{f}{\lambda^2}} \quad . \qquad (3.36)$$

In Eq.(3.36) the constants g and c could be correlated in one constant. It is clear that at $\lambda \to \infty$, $\alpha \to 0$ so Eq. (3.36) could be written as:

$$\alpha = \alpha_0 (10^{\frac{f}{\lambda^2}} - 1)$$

In general if total absorption coefficient is small (low and medium absorption region). α may be developed in Taylor series around photon energy far from any absorption line. If only terms up to second degree are included (α varies slowly with λ), then the relation for α could be written as:

$$\alpha = c + \frac{f}{\lambda} + \frac{g}{\lambda^2}, \qquad (3.37)$$

where c, f and g are constants.

3.3.3 COMPARISON BETWEEN DIFFERENT MODELS

i. FITTING OF DIFFERENT TRANSMITTANCE FORMULAS

In this case the model used for refractive index is Eq.(3.31) and for α is Eq. (3.33), Table (3.3) summaries the results.

Table (3.3) Fitting results of different transmittance formulas.

Transmittance equation.	d (nm)	σ (nm)	n_0	$(\lambda_0)^2$ $(nm)^2$	c $(nm)^{-1}$	f $(nm)^{-2}$
3.10	745.8	2.6	2.703	8.699E4	-31.18	1.348E4
3.24	742.9	-	2.705	8.699E4	-30.94	1.335E4
3.25	743.3	-	2.706	8.660E4	-31.07	1.342E4

Table 3.3 shows that the optical constants obtained from fitting the different formulas are quite close. This indicates that for such type of films, on transparent substrate, the approximation used (i.e ignoring the thickness irregularity of the film surface, assuming $k \ll n^2$, and the substrate absorption) does not effect the determined values of the

optical constants and thickness. Substituting the values of the refractive index and thickness determined by fitting Eq. (3.25) and calculating the values of α in the high absorption region was used to determine the band gap (see section 3.1). The value of E_g was found to be 2.249 eV, i.e. the difference is only 0.002 eV (using sec 3.1). It is to be noted here that the value of σ determined by fitting Eq. (3.10) is not accurate, due to fitting the entire spectrum. It is difficult to distinguish between the intrinsic absorption of the film and loss of the light intensity due to the light scattered from rough surface.

ii. COMPARISON OF MODELS FOR REFRACTIVE INDEX

Here the transmittance equation used is Eq.(3.25) and the model for σ is Eq.(3.33). the results are given in Table (3.4).

Table (3.4) Fitting results of different models for n.

Eq. used for n	d (nm)	n_0	$(\lambda_0)^2$ $(nm)^2$	B $(nm)^2$	n at λ=2000 nm	n at λ=1000 nm	n at λ=700 nm	n at λ=530 nm
3.31	743.3	2.706	8.660E4	----------	2.732	2.815	2.946	2.184
3.32	744.1	2.692	---------	1.247E5	2.737	2.831	2.96	2.150

The results show that the difference between the calculated values of the refractive index using the approximated model (Eq. 3.32), in the wavelength region used for calculation the optical constants and the band gap, is less than 1%. The value of the energy gap detected from α plot, was the same for both models.

ii. COMPARISON OF MODELS FOR α:

Here Eq. (3.25) was used as transmittance formula for fitting of the transmission spectra, and Eq. (3.31) was used as a model for the refractive index. Fitting results for different α models are given in Table (3.5).

Table (3.5) Fitting results of different models for α .

Eq. Used as Model for α	d (nm)	n_0	$(\lambda_0)^2$ $(nm)^2$
3.33	743.3	2.706	8.660E4
3.34	742.6	2.697	8.709E4
3.37	744.6	2.700	8.654E4

It could be seen that all the three models work good for fitting , and the resulting values of d and n are quite similar. The resulting value of thickness using relation 3.37 is closer to that calculated in section 3.1. It could be due to the fact that the polynomial approximation work for loss of transmitted light intensity due to absorption as well as the light scattered from the film surface.

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