Determination of Optical Constants of SnO_2 Thin Film Using Matlab Curve Fitting Method

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Abstract:- ***Thin absorbing films are becoming common in optical coating applications. Such films require proper techniques to insure unique results for both thickness and optical constants. This project describes the determination of optical constant and thickness of SnO_2 thin film using MATLAB curve fitting method. Various techniques are available for determining the properties of surfaces and thin films. A versatile method for determination of the optical constants is described that can be applied to a variety of coating materials. It is based on the use of an optical thin film synthesis program to adjust the constants of dispersion equations until a good fit is obtained between measured and calculated spectral transmittance and/or reflectance curves. A method for fitting the optical transmission data using MATLAB software is presented in this paper. The sensitivity of the determination can be increased by a suitable combination of measurement quantities. Because more than the minimum amount of data can be used, sensitivity to measurement errors and the chances of obtaining multiple solutions can both be reduced. This is a multiple parameter, nonlinear-curve fitting method which is used to determine the optical constants and thickness of SnO_2 thin films. The transmission equation is customized and six constants are determined using the MATLAB curve-fitting tool box.***

Keywords: Thin Film, Spectral Transmittance or Reflectance, Optical Constants, Complex Refractive Index, Dielectric Function.

INTRODUCTION

In current years there has been an intensifying need for an accurate data of the optical constants n and k of thin absorbing films over a wavelength range. Since the optical constants of the materials have generally been completely unknown or determined only in a narrow wavelength range, proposed designs for such films have had to be tested experimentally rather than by the much more rapid method of numerical simulation. The insufficient knowledge of optical constants has thus slowed progress in its application. The refractive index of a material is the most important property of any optical system that uses refraction. It is used to calculate the focusing power of lenses, and the dispersive power of prisms. Since refractive index is a fundamental physical property of a substance, it is often used to identify a particular substance, confirm its purity, or measure its concentration. Refractive index is used to measure solids (glasses and gemstones), liquids, and gases. Most commonly it is used to measure the concentration of a solute in an aqueoussolution. A refractometer is the instrument used to measure refractive index. For a solution of sugar, the refractive index can be used to determine the sugar content. In GPS, the index of refraction is utilized in ray-tracing to account for the radio propagation delay due to the Earth's electrically neutral atmosphere. It is also used in Satellite link design for the Computation of radiowave attenuation in the atmosphere.

OPTICAL CONSTANTS AND THICKNESS OF THIN FILM USING MATLAB

The optical constants $n(\lambda)$ and $\alpha(\lambda)$ are of particular significance in knowing the optical properties of thin films. In this method measurement of the transmittance T of light through a parallel-faced dielectric film is sufficient to determine the real and imaginary parts of the complex refractive index and the thickness of thin film. Optical constants are usually determined using the envelope method where extreme values of transmission data are used. A multiparameter curve-fitting method was proposed by Xuantong (1990) for determining optical constants (refractive index n and absorption coefficient α) and the thickness‘t’ of optical films from transmission spectra. The curve-fitting method using MATLAB software is used for determining the optical constants. MATLAB provides a platform to perform parametric data fitting using toolbox- library equations or using a custom equation. Custom equation can be defined to suit the specific curve fitting requirements. The fit statistics are used to determine the goodness of fit. Analysis capabilities such as extrapolation,

differentiation and integration are other helpful features in using this toolbox. The transmission equation for uniform thickness and homogeneous film is made use of in the calculations. A non-linear least-squares-fitting has been used to fit the experimental transmittance data on the basis of dispersion models for refractive index and absorption. The goodness-of-fit results are helpful in the fitting routine to improve the accuracy of the result. Once the equation of transmission is customized, the same equation can be used for all samples by changing the boundary conditions for making the fitting procedure fast and reliable.

Curve fitting

In this homogeneous model, the transmittance T of weakly absorbing films can be expressed by the following equation

$$T = \frac{16 n_o n^2 n_s A}{C_1^2 + C_2^2 A^2 + 2C_1 C_2 A \cos(4\pi n t/\lambda)}$$

---- (1)

Where $C_1 = \frac{(n+n_o)}{(n_s+n)}$

$$C_2 = \frac{(n-n_o)}{(n_s-n)}$$

$$A = \exp(-4\pi kt/\lambda) = \exp(-\alpha t)$$

And n_s is the refractive index of substrate, no is the refractive index of ambient (air), and λ is the wavelength of the optical beam in air. The dispersion equation for n is the Cauchy's formula

$n = a + b/\lambda 2$ ---- (2)

the form chosen for α is an exponential law,

$\alpha = d\exp(-e\lambda) + f$ ---- (3)

and the thickness 't' is taken to be the fit parameter 'c'. The transmission curve of each specimen was fitted with equation 1 and the six parameters 'a to f' were determined using curve fitting toolbox. The custom equation given in the toolbox is as follows:

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fittedmodel1(x)=(24.*(a+(b./x.^2)).^2.*exp(-(d.*exp(-e.*x).*c)-(f.*c)))./((((a+(b./x.^2))+1).^2.*((a+(b./x.^2))+1.5).^2)+((((a+(b./x.^2))-1).^2.*(1.5-(a+(b./x.^2))).^2).*(exp(-(d.*exp(-e.*x).*c)-(f.*c))).^2)-(2.*((a+(b./x.^2)).^2-1).*((a+(b./x.^2)).^2-2.25).*exp(-(d.*exp(-e.*x).*c)-(f.*c)).*cos((4.*pi.*(a+(b./x.^2)).*c)./x)))
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To determine the best fit, both the graphical and numerical fit results are examined. In the graphical approach the transmission curve and the fitted curve are compared and the two should overlap each other for most of the points. The residuals are displayed graphically as a line plot and the residual from a good fit should look random with no apparent pattern. A pattern, such as a tendency for consecutive residuals to have the same sign, can be an indication that better model exists. As the graphical results cannot examine fully the goodness of a fit, the numerical fit results should be considered to evaluate the fit results. Two types of numerical fit results are displayed in the results. The first is the goodness of fit statistics which determines how well the curve fits the data. The confidence intervals on the coefficients determine their accuracy. The sum of squares due to error (SSE) and adjusted R-square statistics are useful in determining the best fit. The SSE value closer to zero indicates a better fit and the adjusted R-square value should be closer to 1 for the best fit. The parameters are determined to 95% confidence bound and the prediction bounds give the accuracy of the parameters. If there is a wider prediction bounds for the parameters then the parameters are not very accurate.

RESULT AND DISCUSSION

The fitted and transmission curve of the samples used in the present work are shown below.

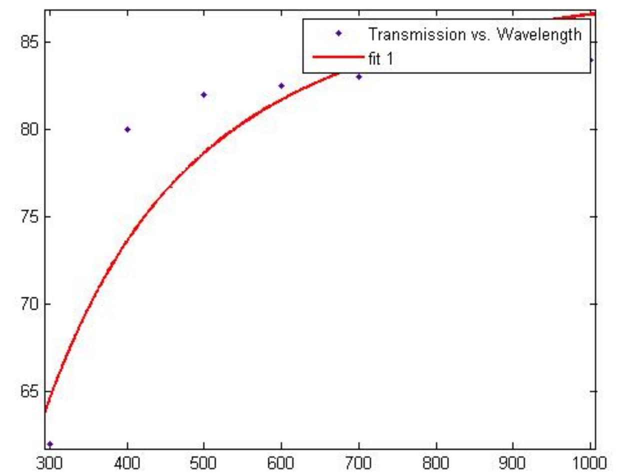

Figure1: The fitted transmission spectrum of sample SnO_2

Table1: The six parameters determined with custom equation using curve fitting toolbox

Sample	a	b (x10 $^{-14}$)	c (x10 $^{-7}$)	d (x10 ^{5})	e (x10 ^{6})	f (x10 ^{3})	R^2
SnO_2	1.518	0.330	2.52	0.039	0.5586	2.738	0.9875

The constant 'a' is the value of the refractive index in the longer wavelength region and the constant 'c' is the thickness of the sample. The sum of squares due to error (SSE) and adjusted R-square statistics are useful in determining the best fit. The SSE value closer to zero indicates a better fit and the adjusted R-square value should be closer to 1 for the best fit.

Result of absorption coefficient (α) and extinction coefficient (k) values which obtain from Beer's law

S.No.	Wavelength (nm)	Absorption coefficient(α)	Extinction coefficient(k)
1.	532	160 CM^{-1}	6.8096×10^{-4}
2.	532	155 CM^{-1}	6.5968×10^{-4}
3.	532	167 CM^{-1}	7.10752×10^{-4}

Reflectance and transmittance spectra of film using a MATLAB program

For a single thin film on a substrate we get the amplitude reflectance, r, and the amplitude transmittance, t. At normal incidence the following applies:

$$r = \frac{r_1 + r_2 e^{-2i\partial}}{1 + r_1 r_2 e^{-2i\partial}}; \qquad r_1 = \frac{N_1 - N_2}{N_1 + N_2}, \qquad r_2 = \frac{N_2 - N_3}{N_2 + N_3}$$

$$t = \frac{t_1 t_2 e^{-i\partial}}{1 + r_1 r_2 e^{-2i\partial}}; \qquad t_1 = \frac{2N_1}{N_1 + N_2}, \qquad t_2 = \frac{2N_2}{N_2 + N_3}$$

Where the phase shift, ∂, is given by

$$\partial = -\frac{2\pi}{\lambda} N_2 d \cos\varphi_2 = [\text{normal incidence}] = -\frac{2\pi N_2}{\lambda} d$$

And r_1 and t_1 are the Fresnel coefficients for the boundary between air and film and r_2 and t_2 are the corresponding coefficients for the boundary between film and substrate.

With the equations above we can calculate the intensity reflectance, R, and the intensity transmittance, T, according to

$$R = rr^* \quad \text{and} \quad T = \mathrm{Re}\left(\frac{N_3}{N_1}\right) tt^*$$

In our case, the medium through which the light is incident is air, i.e. $N_1=1$

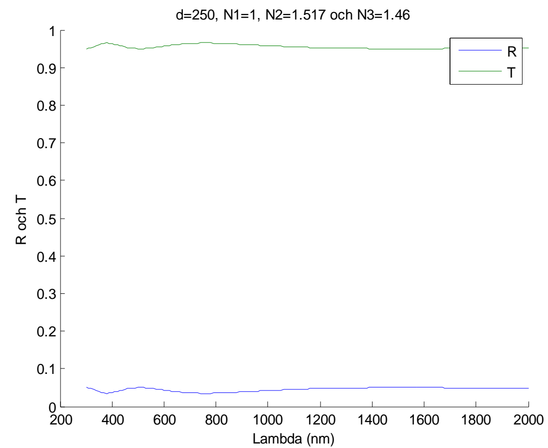

Figure2: Transmission and Reflectance spectra of SnO_2 thin film

CONCLUSION

In this project optical constant and thickness of SnO_2 thin film has been measured using MATLAB curve fitting method. It is quite simple to calculate R and T for a single film on a non-absorbing substrate using this method and to study how variations in the optical constants n and k of thin films and substrates influence R and T spectra? In order to study interference effects only, we look at dispersion free materials for which n and k are not wavelength dependent.

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