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ON THE DETERMINATION OF REFRACTIVE INDEX AND THICKNESS OF THIN DIELECTRIC FILMS FROM MEASUREMENT OF TRANSMITTANCE

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Refractive index and thickness of a transparent film (ZnS) on a transparent substrate (BK-7 glass) have been determined from measurement of normal incidence transmittance, using different methods. Some of the methods considered here are most widely used, as is apparent from the literature. The outcome of this study could help a researcher in selecting an appropriate method for such an application. The values of the refractive indices determined by different methods were found to be close to each other (within 0.5%). However, large (up to 4.4%) differences existed in the values of the thickness determined by different methods.

Keywords: Optical constants; thin films; transmittance.

PACS Number(s): Optical constants (78.20.ci), thin films (77.55.-g), transmittance (74.25.nd)

1. Introduction

There exist a number of methods[1–4] of determining optical constants (indices of refraction n and absorption k) and thickness of thin dielectric films, based on the measurement of normal incidence transmittance (T). Such a measurement can be made using a readily available commercial spectrophotometer. Most widely used methods are those of (Refs. 1 and 2), see for example (Refs. 5 and 6). In these methods, measurement of T as a function of wavelength (λ) from a dielectric film on a transparent substrate is required. However, extracting two unknown n and k from a single measurement of T cannot yield accurate values of n and k. There is no way to calculate n and k independently. On the other hand, a method[4] requiring measurement of transmittance (T_1 and T_2) from two films of a given dielectric of different thickness, yields accurate values of n and k. Therefore, the methods,[1–3] requiring measurement of T from a single dielectric film are truly applicable to a dielectric film in the spectral region in which the film is nonabsorbing (i.e. $k = 0$).

In the present work, therefore, we compare the results obtained for zinc sulfide films, in nonabsorbing spectral region, by methods of (Refs. 1 and 2) with those by the method given in (Ref. 3). On comparison, we find that the values of the refractive indices yielded by the two sets of methods are similar, however, differences in thickness up to 4.4% were observed.

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2. Experimental Details

Thin films of ZnS were deposited on polished BK-7 glass substrates (in the form of a wedge of angle 3^0) in a Leybold model L 560 box coater pumped to a base pressure of less than 10^{-6} mbar. The ZnS of 99.99% purity, supplied by Balzers, was evaporated from molybdenum boats. A quartz-crystal thickness monitor and rate controller was used to achieve a rate of evaporation of 0.7 nm/s. The source-to-substrate distance was about 40 cm. During deposition substrate was maintained at ambient temperature in the vacuum chamber.

After the films were deposited they were removed from the coating chamber and exposed to the ambient atmosphere prior to measurement of optical properties. Transmittance measurements on the films were made over the 400−850 nm wavelength range using a double beam Bausch and Lomb spectrophotometer model Spectronic 2000. The use of a wedge substrate ensured that the reflections from the back of the substrate were reflected out of the optical path of the instrument so that multiple reflections in the substrate do not affect the measurements. However, the wedge angle was sufficiently small for the transmission across the back face to be given accurately enough by the transmittance formula for normal incidence.

3. Theory

Normal incidence transmittance at a wavelength λ of a nonabsorbing film of refractive index n_1 and thickness d on a transparent substrate of refractive index n_2, is given by Heavens[7] as

$$T_f = [(n_2/n_0)(1+g_1)^2(1+g_2)^2]/[1+g_1^2g_2^2 + 2g_1g_2\cos 2\gamma], \quad (1)$$

where, $g_1 = (n_0-n_1)/(n_0+n_1), g_2 = (n_1-n_2)/(n_1+n_2), \gamma = 2\pi n_1 d/\lambda$ and $n_0 = 1$ the refractive index of air. Equation (1) gives transmittance into substrate. This equation is identical to that given in (Ref. 1) for an infinite substrate. However, in practice measurements are made for transmittance across the back face of the substrate into the air. Thus, the measured transmittance (T) is

$$T = T_f T_s, \quad (2)$$

where $T_s = 4n_0n_2/(n_0+n_2)^2$. It may be noted that multiple reflections in the substrate have been neglected for the reasons discussed earlier in Sec. 2.

It can be shown from Eq. (1) that maxima and minima in measured transmittance and film thickness d are given by:

$$T_{\max} = [4n_0n_2/(n_0+n_2)^2]^2 = T_s^2, \quad \text{and} \quad (3)$$

$$T_{\min} = [4n_0n_2/(n_0+n_2)^2][4n_1^2n_2/(n_1^2+n_2)^2], \quad (4)$$

$$d = \lambda_1\lambda_2/\{2[n_1(\lambda_2)\lambda_1 - n_1(\lambda_1)\lambda_2]\}, \quad (5)$$

where λ_1 and λ_2 are the wavelengths corresponding to two consecutive minima or maxima of the transmittance curve and $n_1(\lambda_2)$ and $n_1(\lambda_1)$ are the refractive indices of the film at wavelengths λ_2 and λ_1, respectively.

In the present work, the values of the refractive index (n_2) of the BK-7 glass substrate at different wavelength were calculated using the relation given below.[7]

$$n_2 = [B_1\lambda^2/(\lambda^2 - C_1) + B_2\lambda^2/(\lambda^2 - C_2) + B_3\lambda^2/(\lambda^2 - C_3) + 1]^{1/2}, \quad (6)$$

where $B_1 = 1.03961212$, $B_2 = 2.31792344 \times 10^{-1}$, $B_3 = 1.01046945$, $C_1 = 6.00069867 \times 10^{-3}$, $C_2 = 2.0\,0179144 \times 10^{-2}$ and $C_3 = 1.03560653 \times 10^2$.

4. Results and Discussion

The spectral transmittance of a ZnS film on a BK-7 glass substrate is shown in Fig. 1(a). The curve shows maxima and minima arising in the film due to multiple reflections in the film (see Eqs. (1)−(4)). The curve marked (b) in Fig. 1, represents the transmittance of

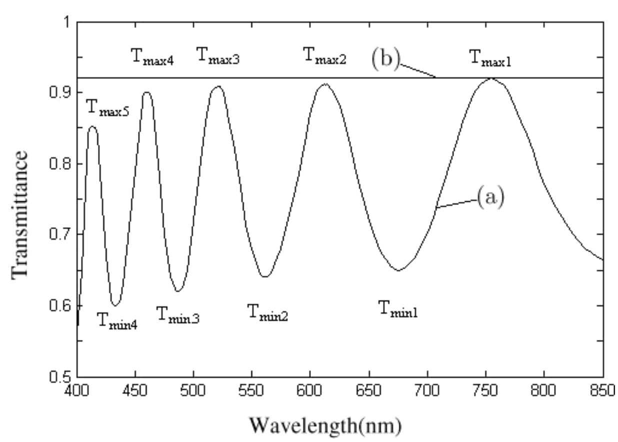

Fig. 1. Measured spectral transmittance curves: (a) for a ZnS film on a glass substrate, and (b) for an uncoated glass substrate.

an uncoated glass substrate. The transmittance of the uncoated glass substrate was calculated using $T_s^2 = [4n_0n_2/(n_0+n_2)^2]^2$ where n_2 was obtained from Eq. (6). Square of T_s is used because transmittance takes place across two faces of the substrate. A check for transparency of a film is that at maxima the curve (a) must have same value as that of an uncoated substrate (see Eq. (3)). The deviation from this condition in the lower wavelength side is not a serious problem. This deviation may be caused by some absorption in the film. However, for the thickness of the film involved in the present case absorption index was estimated to be less than 0.003. Thus, in the spectral range covered ZnS film may be taken to be transparent (see Fig. 1).

Equations (4) and (5) were used in both Refs. 1 and 2 to extract refractive index (n_1) and thickness (d) of a film, respectively. Here, we follow their method. Based on the results of Fig. 1, the magnitudes and wavelength positions of various minima in transmittance are listed in Table 1. Corresponding values of the refractive indices n_2 (obtained from Eq. (6) and n_1 (obtained from Eq. (4)) are also listed in Table 1. In order to find value of the film thickness, we may use Eq. (5) and different sets of two consecutive $T_{\min}$ or $T_{\max}$. The required refractive indices in the case of $T_{\min}$ are given in Table 1; however, in the case of $T_{\max}$ we do not have such values. This was overcome by interpolation of the data (n_1 versus λ) of Table 1, and for this purpose we need some sort of a fit to the data. We first looked for the commonly used Cauchy's relation of the type $n_1 = A + B/\lambda^2$, where A and B are constants. Satisfactory fit to the data using this relation was not obtained. However, we obtained acceptable fit to the data (see Fig. 2) using Sellmeier relation of the type

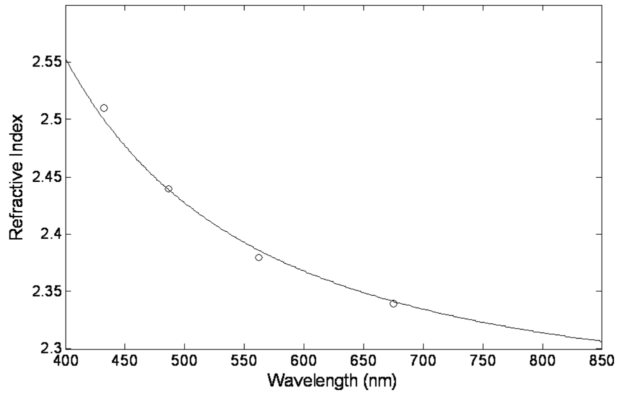

Fig. 2. Refractive index vs wavelength for the ZnS film. The dots represent the data from Table 1 and fit to the data using Sellmeier relation (details are included in the text) is presented by the continuous curve.

$$n_1^2 = 1 + a\lambda^2/(\lambda^2 - \lambda_0^2), \tag{7}$$

for the values of the constants $a = 4.07$ and $\lambda_0 = 205$ nm. Limited applicability of Cauchy's relation has been pointed out.[8] On the other hand Sellmeier relation is based on the well established idea of natural resonances.[8]

Different sets of consecutive $T_{\min}$ (or $T_{\max}$) were used to obtain the values of film thickness from Eq. (5). The values are listed together with the necessary details in Table 2. Different sets yielded different value of thickness. The average value of the thickness was 652 nm with an uncertainty of about 4.4%.

A method in which refractive index and thickness of a transparent film on a transparent substrate are determined simultaneously from measurement of transmittance was suggested earlier.[3] If T is measured

Table 1. Determination of refractive index (n_1) of ZnS film from $T_{\min}$ using the methods given in Refs. 1 and 2.

Minima as marked in Fig. 1	$T_{\min}$	Corresponding wavelength λ (nm)	Refractive index of substrate $n_2(\lambda)$*	c Refractive index of ZnS film $n_1(\lambda)$**
$T_{\min 1}$	0.650	676	1.514	2.34
$T_{\min 2}$	0.640	563	1.518	2.38
$T_{\min 3}$	0.620	488	1.522	2.44
$T_{\min 4}$	0.600	433	1.527	2.51

*Calculated from Eq. (6).
**Calculated from Eq. (4).

Table 2. Determination of film thickness from spectral positions of T_{min} and T_{max} and the corresponding refractive indices.

Minima and Maxima as marked in Fig. 1	Corresponding wavelength* λ (nm)	Corresponding refractive indices of the film $n_1(\lambda)$**	d (nm)
$T_{\min 1} = 0.650$	676	2.34	
$T_{\min 2} = 0.640$	563	2.38	653
$T_{\min 2} = 0.640$	563	2.38	
$T_{\min 3} = 0.620$	488	2.44	647
$T_{\min 3} = 0.620$	488	2.44	
$T_{\min 4} = 0.600$	433	2.51	628
$T_{\max 1} = 0.920$	755	2.32	
$T_{\max 2} = 0.912$	614	2.36	648
$T_{\max 2} = 0.912$	614	2.36	
$T_{\max 3} = 0.908$	522	2.41	648
$T_{\max 3} = 0.908$	522	2.41	
$T_{\max 4} = 0.900$	459	2.47	662
$T_{\max 4} = 0.900$	459	2.47	
$T_{\max 5} = 0.852$	414	2.53	682

*Taken from Fig. 1.
**In the case of T_{min} values of refractive indices at different wavelength were taken from Table 1. In case of T_{max} values of refractive indices at different wavelengths were obtained using Eq. (7).

as a function of λ and d and n_2 are known, then, in principle n_1 can be determined from Eq. (2). An expression giving an explicit value of n_1 cannot be obtained. However, the equation for T may be solved by a numerical method.[3] Thus, the method given in (Ref. 3) was also used in the present work. The results of the application of the above method to the data of Fig. 1(a) are shown as dots in Fig. 3. Figure 3 shows multiple solutions and proper closure of the dispersion curve.[3] A continuous curve shown in Fig. 3 represents the correct solutions while other solutions are unwanted.[3] It may be noted that the method is based on the fact that for a single uniform film with smooth surface there is only one value of the film thickness for which a continuous acceptable dispersion curve can be obtained. The film thickness used in generating results of Fig. 3 was 653 nm.

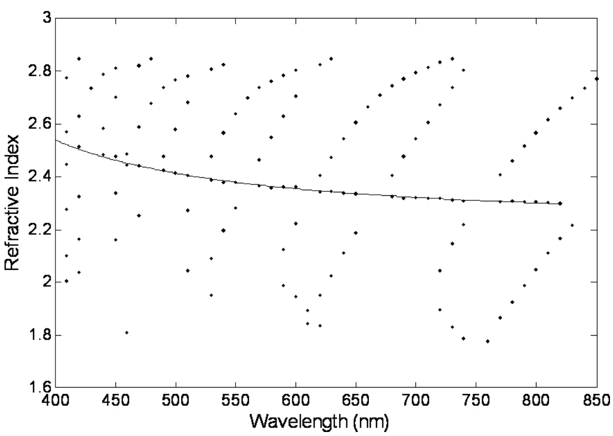

Fig. 3. The dispersion curve for the ZnS film, derived from the data of Fig. 1 using the method of Ref. 3. The continuous curve shown here represents the correct solutions while other solutions are unwanted.[3]

The dispersion curves obtained by two different methods Figs. 2 and 3 are compared in Fig. 4 by overlaying the two. The spectral region that covered the two curves show similar behavior. Moreover, the difference between the values of the refractive indices given by the two curves at any wavelength is less than 0.5%.

Another convenient way to determine the refractive index (n_1) of a transparent film on a transparent substrate (n_2) is by using tabulated values of n_1 as a function of T_{min}. This can be achieved by assuming a constant value of n_2 (independent of wavelength) and then calculating n_1 as a function of T_{min} using Eq. (4). It may be noted that the values of n_2 (obtained from Eq. (6)) at extreme values of the spectral region

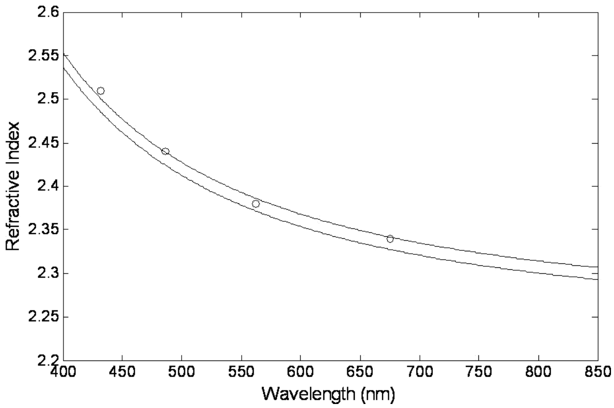

Fig. 4. Comparison of dispersion curves (of Figs. 2 and 3) obtained by two different methods.

Table 3. n_1 as a function of $T_{\min}$ calculated using Eq. (4) for n_2.

$T_{\min}$	n_1	$T_{\min}$	n_1	$T_{\min}$	n_1
0.555	2.67	0.605	2.49	0.655	2.33
0.560	2.65	0.610	2.48	0.660	2.31
0.565	2.63	0.615	2.46	0.665	2.30
0.570	2.61	0.620	2.44	0.670	2.28
0.575	2.60	0.625	2.43	0.675	2.27
0.580	2.58	0.630	2.41	0.680	2.25
0.585	2.56	0.635	2.39	0.685	2.24
0.590	2.54	0.640	2.38	0.690	2.22
0.595	2.53	0.645	2.36	0.695	2.20
0.600	2.51	0.650	2.34	0.700	2.19

covered were 1.53 at $\lambda = 400\,\text{nm}$ and 1.51 at $\lambda = 850\,\text{nm}$. In the present work a constant value of $n_2 = 1.52$ was assumed for the calculation of the data n_1 versus $T_{\min}$, given in Table 3. The values of n_1 thus obtained from Table 3 for the corresponding values of the magnitude of $T_{\min}$ from Table 1, were found to exactly match the values of n_1 that are given in Table 1.

5. Conclusion

The refractive index and thickness of a transparent film on a transparent substrate have been determined by two different methods. The values of the refractive indices determined by different methods were found to be close to each other (within 0.5%). As far as the refractive index is concerned, it will not make any difference if any of the above method is used. However, large (up to 4.4%) differences may exist in the values of the thickness. When an accurate value of the thickness of a film is desired, then in this case the method of (Ref. 3) may be used. This method yields a single accurate value of the thickness.

Acknowledgments

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