

Analysis of the Maximum and the Minimum of the Spectral Transmittance According to the Coherence Condition for Weakly Absorbing Thin Films.

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In this work the maximum T_{sam}^{max} and the minimum T_{sam}^{min} of the spectral transmittance of weakly absorbing thin films deposited on non-absorbing substrate is analyzed as a function of refractive indices of both substrate and film according to the coherence condition. Also the ratio of T_{sam} / T_w (where T_w is the transmittance of the uncoated substrate) is obtained for both homogeneous and inhomogeneous films. The results of the analysis enabled us to interpret the increment of the ratio (T_{sam} / T_w) over unity, distinguishing the inhomogeneous and homogenous films and obtaining the refractive index of the film.

Introduction

The effect of sample type on the spectrophotometric results occurs by two ways, interference within the film as well as the substrate which depends upon the coherence condition and the interaction between sample and photometer.

It is well known that the methods devoted for determining the optical constants of metal or dielectric thin films, [1], were based on analysis of the spectral scans of transmittance and reflectance. One of them based on the determination of the spectral transmittance of the coated T_{sam} relative to the uncoated substrate T_w which is defined as the observed transmittance where ($T_{obs} = T_{sam}/ T_w$) ,[2]. It was noticed experimentally that T_{obs} sometimes exceeds unity.

In this work different cases of coherency are considered. Also analysis of the spectral transmittance is driven.

Theory:

Figure (1) shows a practical situation where a parallel and monochromatic beam is incident on homogeneous, absorbing or non-absorbing, and isotropic film of thickness d_1 with a plane parallel surfaces. The substrate is being transparent with thickness d_2 .

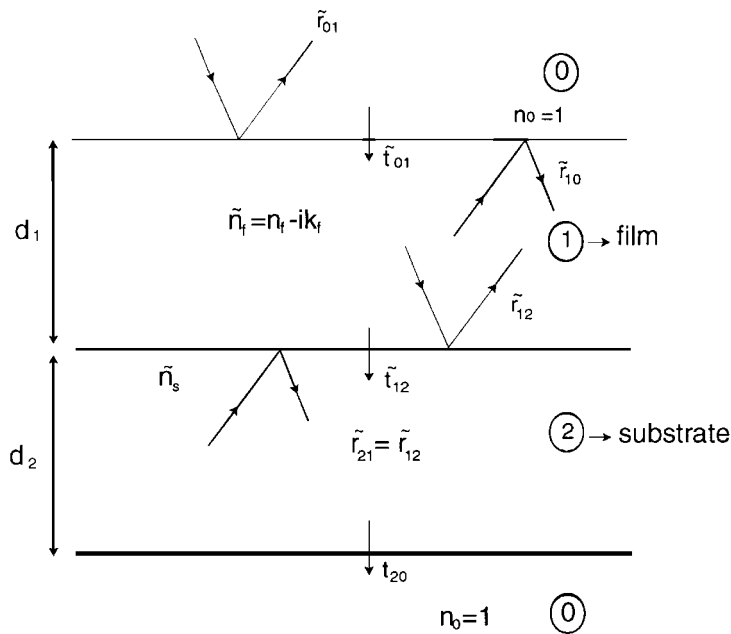


Fig. (2) The optical constants used in the calculation of transmittance

of a thin film on a nonabsorbing substrate.

Generally the transmittance T_{sam} can be expressed in terms of complex transmission (\hat{t}) as follows, [3],

$$T_{sam} = |\hat{t}_{sam}|^2 \tag{1}$$

where

$$\hat{t}_{sam} = \frac{\hat{t}_{01} \hat{t}_{12} \hat{t}_{20} e^{-i(\hat{\beta}_1 + \hat{\beta}_2)}}{(1 + \hat{r}_{01} \hat{r}_{12} e^{-2i\hat{\beta}_1}) + (\hat{r}_{12} + \hat{r}_{01} e^{-2i\hat{\beta}_1}) \hat{r}_{20} e^{-2i\hat{\beta}_2}}$$

Where the \hat{r}_{ij} , \hat{t}_{ij} are the Fresnel coefficients for a light beam going from medium i with complex refractive index \hat{n}_i to medium j with refractive index \hat{n}_j , $\hat{\beta}_1$ and $\hat{\beta}_2$ are the complex phase factors for the two traversal media respectively.

$$\begin{aligned} \text{Also} \quad \hat{r}_{ij} &= \frac{\hat{n}_i - \hat{n}_j}{\hat{n}_i + \hat{n}_j}, & \hat{t}_{ij} &= \frac{2\hat{n}_i}{\hat{n}_i + \hat{n}_j}, \\ \hat{\beta}_1 &= \frac{2\pi}{\lambda} \hat{n}_1 d_1, & \hat{\beta}_2 &= \frac{2\pi}{\lambda} \hat{n}_2 d_2 \end{aligned} \tag{2}$$

where λ is the wavelength, For semi-finite substrate \hat{t} is given by, [4],

$$\hat{t} = \hat{t}_f \frac{t_{20} e^{-i\beta_2}}{1 - \hat{r}'_f r_{20} e^{-2i\beta_2}} = t_f t_s \tag{3}$$

where \hat{t}_f is referred to the complete transmitted amplitude of the absorbing film and \hat{t}_s is that of the substrate

$$\hat{t}_f = \hat{t}_{01} \hat{t}_{12} e^{-i\hat{\beta}_2} \times \frac{1}{1 - \hat{r}'_{10} \hat{t}_{12} e^{-2i\hat{\beta}_2}} \tag{4}$$

$$\text{and} \quad \hat{t}_s = \frac{\hat{t}_{20} e^{-i\beta_2}}{1 - \hat{r}'_f \hat{t}_{20} e^{-2i\beta_2}} \tag{5}$$

where r'_f represents the reflection amplitude of the film when the light incident from the substrate side and given by

$$\hat{r}_f = \frac{\hat{r}_{21} + \hat{r}_{10} e^{-2i\beta_1}}{1 - \hat{r}_{10} \hat{r}_{12} e^{-2i\beta_1}} \quad (6)$$

The interference occurs when the band width of the spectrophotometer $\Delta\lambda$, the thickness and optical constants of the film (or substrate) verifying the coherence condition.

$$\Delta\lambda.2\pi.n.d / \lambda^2 \ll 1 \quad (7)$$

In this case the transmittance through the film (or substrate) obtained by adding the coherent amplitudes of the multireflections in the film or substrate are denoted by $T_{f,coh}$ ($T_{s,coh}$) which can be given by equations (3,6). In the case for which the coherence condition is not valid the multiple reflections will be added incoherently and the obtained transmittance are denoted by $T_{f,incoh}$ and $T_{s,incoh}$. Then to reveal the effect of interference and inhomogeneity on the transmittance of the sample, we have to consider the cases for which $T_{f,coh}$ and $T_{s,coh}$ for homogenous and inhomogenous films. Also the influence of using $T_{s,incoh}$ is considered.

It is worth noting that all the derivations have been carried out assuming weakly absorbing film for which $K_2 \ll |n_2 - n_1|, |n_2 - n_3|$.

Case 1:

A single non-absorbing film on a non-absorbing substrate.

$T_{f,coh}$ and $T_{s,coh}$ for homogenous films.

In this case $T_{f,coh}$ can be given by equation (4) it is found that $T_{f,coh}^{max} = 4n_s/(n_s + 1)^2$. Also from equations (5) and (6) we have

$$T_{s,coh} = \frac{(1 - R_{20})}{(1 - 2|r_f'|^2 R_{20} + |r_f'|^4 R_{20})} \quad (8)$$

As the maximum value of $T_{s,coh}$ occurs at $\beta_1 = 2m\pi$ where $m = 0, 1, 2, \dots$ for which $|r_f'|^2 = R_{20}$, then $T_{s,coh}^{max}$ can be written in the following formula

$$T_{s,coh}^{max} = \frac{(1 - R_{20})}{(1 - R_{20})^2} = \frac{(n_s + 1)^2}{4n_s} \quad (9)$$

So it is easy to show that the maximum value of the sample transmittance T_{sam}^{max} in this case is equal to unity. On the other hand, the maximum value of $T_{w,coh}$ for the uncoated substrate is equal to unity and the minimum value is given by,[6],

$$T_{w,coh}^{min} = \frac{4n_w^2}{(n_w^2 + 1)^2} \tag{10}$$

The minimum value of the transmittance can be obtained using $T_{f,coh}^{min}$ from equation (4) and $T_{s,coh}^{min}$ using equation (5). Then T_{sam}^{min} can be written as

$$T_{sam}^{min} = \frac{4n_1^2}{(n_1^2 + 1)^2} \tag{11}$$

Then using equation (10) we have.

$$T_{obs}^{min} = \frac{n_1^2(n_w^2 + 1)^2}{n_w^2(n_1^2 + 1)^2} \tag{12}$$

It is clear that T_{obs}^{max} is equal to unity in this case , therefore $T_{obs}^{max} > 1$ is not probable in such a case. From equation (11) it is clear that T_{sam}^{min} independent on n_s and the variations of T_{sam}^{min} , T_{obs}^{min} and the quantity $(T_{obs}^{max} - T_{obs}^{min})$ with n_f are considerable and illustrated in table (1) .

Case 2 :

Inhomogeneous film, $T_{f,coh}$ and $T_{s,incoh}$.

In case of inhomogeneous film on a transparent substrate. According to, [8] ,it is assumed that the refractive index of a film at the film/air interface n_f and at the film/substrate interface n_b are different, then T_f can be determined for such case.

$$T_f = \frac{16n_f n_b n_s A}{C_1^2 + C_2^2 A^2 + 2C_1 C_2 A \cos(4\pi n_m d/\lambda)} \tag{13}$$

Where $C_1 = (n_f + n_o) (n_1 + n_b)$, $C_2 = (n_f - n_o) (n_1 - n_b)$, $A = \exp(-\alpha d_1)$ α denotes the absorption coefficient of the film and n_m is the mean refractive index of the film having thickness d_1 .

Putting $A=1$ in the case of weakly absorbing films, then from equation (4), we can write

$$T_{f,coh}^{max} = \frac{4n_f n_b n_s}{(n_s n_f + n_b)^2} \quad (14)$$

From equation (14), it is clear that $T_{f,coh}^{max}$ is dependent on $\Delta n = (n_f - n_b)$. Also according to equation (5) a formula for $T_{s,incoh}^{max}$ in this case is given by

$$T_{s,incoh}^{max} = \frac{(n_s n_f + n_b)^2}{(n_s^2 n_f n_b + n_s^2 n_f^2 + n_b^2 + n_f n_b)} \quad (15)$$

Then

$$T_{sam}^{max} = \frac{4n_f n_b n_s}{(n_s^2 n_f n_b + n_s^2 n_f^2 + n_b^2 + n_f n_b)} \quad (16)$$

Since $T_{s,incoh}$ in this case then we have $T_{w,incoh}$ which determined by,[9],

$$T_{w,incoh}^{max} = \frac{2n_w^2}{n_w^2 + 1} \quad (17)$$

$$T_{obs}^{max} = \frac{2n_f n_b (n_s^2 + 1)}{(n_f n_b n_s^2 + n_s^2 n_f^2 + n_b^2 + n_f n_b)} \quad (18)$$

To obtain T_{sam}^{min} we must have $T_{f,coh}^{min}$, $T_{s,incoh}^{min}$. So from equation (4) we have

$$T_{f,coh}^{min} = \frac{4n_f n_b n_s}{(n_f^2 n_b^2 + 2n_f n_b n_s + n_s^2 n_0^2)} \quad (19)$$

Then from equations (5) and (6) we have

$$T_{s,incoh}^{min} = \frac{(n_f n_b + n_s)^2}{(n_f n_b + n_s^2)(n_f n_b + 1)} \quad (20)$$

$$T_{sam}^{min} = \frac{4n_f n_b n_s}{(n_f^2 n_b^2 + n_f n_b n_s^2 + n_f n_b + n_s^2)} \quad (21)$$

Then using equation (12) considering $n_s = n_w$, then we have;

$$T_{obs}^{min} = \frac{2n_f n_b (n_s^2 + 1)}{(n_f^2 n_b^2 + n_f n_b (n_s^2 + 1) + n_s^2)} \quad (22)$$

The calculations of T_{obs}^{max} and T_{obs}^{min} versus Δn for different values of n_m show that T_{obs}^{max} is dependent on Δn and n_m only. The results of calculations is illustrated in Fig. (2). Also it has been found that the quantity ($T_{obs}^{max} - T_{obs}^{min}$) markedly varies with n_m and slightly with Δn as illustrated in Tables (2).

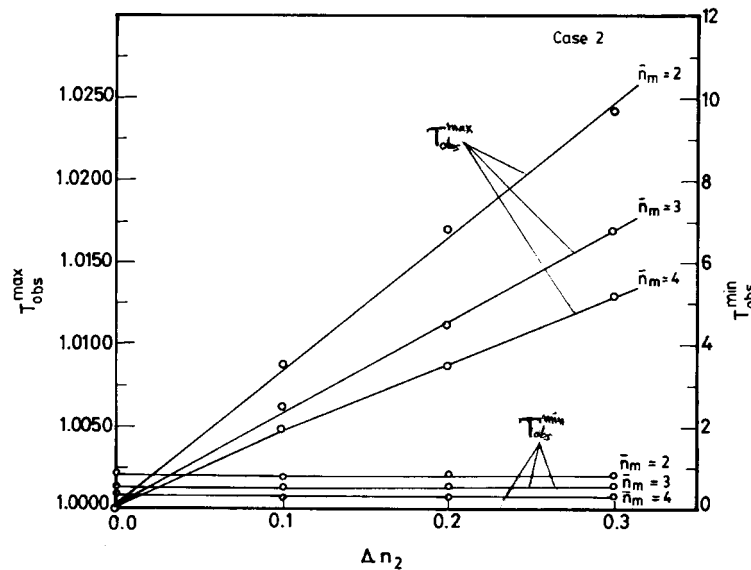


Fig. (2) Shows the effect of inhomogeneity of the film on the value of T_{obs}^{max} , T_{obs}^{min} in case 2.

Case 3:

$T_{f,coh}$ and $T_{s,coh}$ for inhomogenous films :

In this case $T_{f,coh}^{max}$, $T_{f,coh}^{min}$ as in the previous case. But to obtain $T_{s,coh}^{max}$ we must obtain $r_f' l^2$ as a function of n_f and n_b . So considering $\beta_1 = 2m\pi$ where $m = 0, 1, 2, 3, \dots$, then by substituting in equation (6) by n_f and n_b instead of n_2 we have

$$|r_f'|^2 = \frac{(n_1 n_f - n_b)^2}{(n_1 n_f + n_b)^2}$$

Then from equation (5) we have

$$T_{s,coh}^{max} = \frac{(n_1 n_f + n_b)^2}{n_1 (n_f + n_b)^2} \quad (23)$$

Accordingly

$$T_{sam}^{max} = \frac{4n_f n_b}{(n_f + n_b)^2} \quad (24)$$

$$T_{obs}^{max} = \frac{4n_f n_b}{(n_f + n_b)^2} \quad (25)$$

Also to obtain the minimum transmittance in this case we have to obtain $|r_f'|^2$ corresponding to $\beta_2 = (2m + 1)\pi$. So by replacing n_f, n_b instead of n_2 in equation (6) we have

$$|r_f'|^2 = \frac{(n_b n_f - n_s)^2}{(n_b n_f + n_s)^2}$$

Then from equation (5) we have

$$T_{s,coh}^{min} = \frac{(n_f n_b + n_s)^2}{n_1 (n_f n_b + 1)^2} \quad (26)$$

Hence we can obtain T_{sam}^{min} by using equation (19) and (26) as follows

$$T_{sam}^{min} = T_{f,coh}^{min} \cdot T_{s,coh}^{min} = \frac{4n_f n_b}{(n_f n_b - 1)^2} \quad (27)$$

Then using equation (10) we have

$$T_{obs}^{min} = \frac{n_f n_b (n_w^2 + 1)^2}{(n_f n_b + 1)^2 n_w^2} \quad (28)$$

The calculations of T_{obs}^{max} with Δn for different values of n_m show that T_{obs}^{max} varies slightly with Δn . The result of calculations of $T_{obs}^{max}, T_{obs}^{min}$ against

Δn for different values of n_m is illustrated in tables (3a,3b ,3a',3b'). Also the variation of the quantity ($T_{obs}^{max} - T_{obs}^{min}$) versus n_m is illustrated table (3c).

Conclusions

- 1- The condition $T_{obs}^{max} > 1$ i.e T_{max} higher than $T_w = 0.923$ for $n_2 = 1.5$ can be used to distinguish the homogeneous and inhomogeneous films. Also the data illustrated in Figure (2) can be used to determined the degree of inhomogeneity Δn .
- 2- The increase of the quantity ($T_{obs}^{max} - T_{obs}^{min}$) for weakly absorbing films is more pronounced in the case 1 and case 3, this can be explained by the occurrence of interference in the substrate {see Tables (1)& (3)}.
- 3- The data illustrated in Figure (2) can be used to determine n_m for inhomogeneous films.

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Table (1). Variation of T_{\min} & T_{obs}^{\min} and the quantity $(T_{\text{obs}}^{\max} - T_{\text{obs}}^{\min})$ versus n_2 in case 1.

n_2	4	3.4	2	1.6
T_{\min}	0.221	0.293	0.640	0.808
T_{obs}^{\min}	0.260	0.344	0.751	0.948
$(T_{\text{obs}}^{\max} - T_{\text{obs}}^{\min})$	0.740	0.656	0.249	0.051

Table (2a). Variation of the quantity $(T_{\text{obs}}^{\max} - T_{\text{obs}}^{\min})$ versus n_m for $\Delta n = 0.3$ in case 2.

n_m	4	3.4	2	1.6
$(T_{\text{obs}}^{\max} - T_{\text{obs}}^{\min})$	0.680	0.581	0.190	0.054

Table (2b). Variation of the quantity $(T_{\text{obs}}^{\max} - T_{\text{obs}}^{\min})$ versus Δn for $n_m = 2$ in case 2.

Δn	0.3	0.2	0.1	0.0
$(T_{\text{obs}}^{\max} - T_{\text{obs}}^{\min})$	0.190	0.184	0.176	0.168

Table (3a). Variation of T_{\min} and T_{obs}^{\min} versus Δn as $n_m=2$ in case 3.

Δn	n_m	T_{\min}	T_{obs}^{\min}
0.3	2	0.644	0.754
0.2	2	0.643	0.753
0.1	2	0.642	0.752
0.0	2	0.640	0.751

Table (3b). Variation of T_{\max} and T_{obs}^{\max} versus Δn as $n_m=3.4$ in case 3.

Δn	n_m	T_{\max}	T_{obs}^{\max}
0.3	3.4	0.9979	0.9979
0.2	3.4	0.9991	0.9991
0.1	3.4	0.9998	0.9998
0.0	3.4	1	1

Table (3b'). Variation of T_{\min} and T_{obs}^{\min} versus Δn as $n_m=3.4$ in case 3

Δn	n_m	T_{\min}	T_{obs}^{\min}
0.3	3.4	0.294	0.345
0.2	3.4	0.293	0.344
0.1	3.4	0.292	0.343
0.0	3.4	0.291	0.34

Table (3c'). Variation of the quantity $(T_{\text{obs}}^{\max} - T_{\text{obs}}^{\min})$ versus n_m for $\Delta n = 0.3$ in case 3.

n_m	4	3.4	2	1.6
$(T_{\text{obs}}^{\max} - T_{\text{obs}}^{\min})$	0.738	0.653	0.240	0.039