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Effect of Experimental Errors on the Determination of Optical Constants of Thin Films

By

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Introduction The determination of the optical constants (i.e. refractive index n and absorption coefficient α) and of the thickness d of a thin film deposited on a thick non-absorbing substrate is a topic of fundamental importance. Such a determination by a photometric method requires the measurement of the transmission T and of the reflections R and R' from the air–film and from the air–substrate interfaces, respectively [1]. The optical constants and the thickness are then obtained from the data by an inversion of the nonlinear equations for T, R, and R' [1 to 6]. For a given wavelength λ, this procedure yields multiple solutions. From a theoretical point of view the physical solution may be easily found since the dispersion curve of the refractive index is continuous [7, 8]. However, there is any continuous solution for actual cases because of experimental errors. The effect of experimental errors is studied with a theoretical model and a procedure is suggested which allows the best estimation of the optical constants.

Effect of experimental errors on the solutions of a theoretical model The transmission t and reflections r and r' corresponding to a thin film deposited on a non-absorbing substrate of infinite thickness may be easily obtained from T, R, and R' [1 to 3] and they will be considered in the following.

We consider a non-absorbing film of thickness $d = 1000$ nm and of refractive index $n_0 = 2.5$ deposited on a substrate of refractive index $n_s = 1.5$. The considered wavelengths are between 1150 and 1550 nm. As recently pointed out [1], the ratio $(r + r')/2t$ is very sensitive to the refractive index and will be used in the following. For a non-absorbing film, $r = r'$ and $t = 1 - r$ and we consider r/t whose computed values are taken as the experimental data. The inversion of the nonlinear equation yields the solutions plotted in Fig. 1. Besides the physical branch there are two other branches which are degenerated with the former at λ_1 and λ_2 where r/t is minimum and close to a maximum, respectively. In Fig. 2a and b we have plotted the solutions corresponding to an experimental error ε on r of $+0.02$ and -0.02, respectively. The degeneracy of the branches has been lifted and there is any continuous solution. The physical branch is now hybridized with the nonphysical ones. It is worthwhile to note that an error in the thickness of the film has a similar effect.

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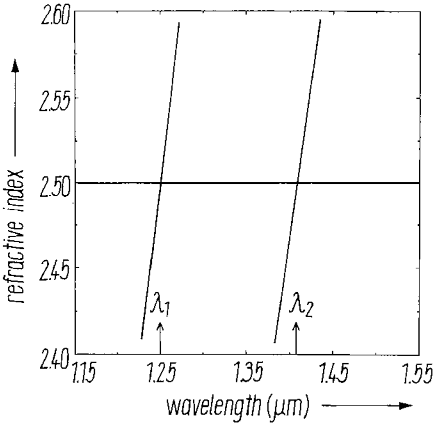

Fig. 1. Solutions of the nonlinear equation close to the physical one $n_0 = 2.5$. The arrows correspond to the wavelengths λ_1 and λ_2 where the solutions are degenerated

Discussion of the results The previous results may be easily explained by writing the nonlinear equation (see [1]) as

$$\cos(2\varphi) = f(n) + \mu g(n), \tag{1}$$

where the phase factor is

$$\varphi = 2\pi n \frac{d}{\lambda} \tag{1a}$$

and where g is a negative function while μ is approximately $\varepsilon/(rt)$. Looking for solutions close to the physical one, we expand (1) near n_0 up to second order in $(n - n_0)$. We then obtain

$$n - n_0 = \frac{-B \pm \sqrt{B^2 - 2Ag(n_0)\,\mu}}{A}, \tag{2}$$

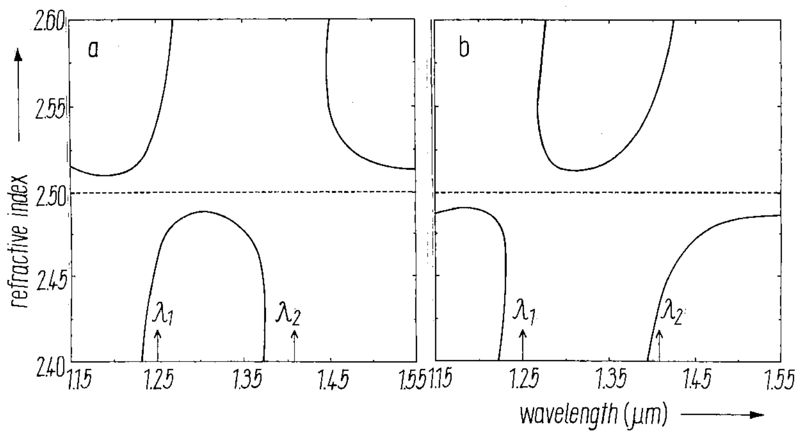

Fig. 2. Solutions of the nonlinear equation close to the physical one $n_0 = 2.5$ which is indicated by the horizontal dashed lines. The errors of measurement are a) $+0.02$ and b) -0.02. The arrows correspond to the wavelengths λ_1 and λ_2 where the solutions are degenerated in the absence of experimental errors

where

$$A = \frac{d^2f}{dn_0^2} + \left(\frac{4\pi d}{\lambda}\right)^2 \cos(2\varphi_0) \tag{2a}$$

and

$$B = \frac{df}{dn_0} + \frac{4\pi d}{\lambda} \sin(2\varphi_0)\,. \tag{2b}$$

Terms in $\mu(n - n_0)$ and $\mu(n - n_0)^2$ have been neglected.

Let us first consider the case $\mu = 0$. There are two solutions, the physical one

$$n = n_0$$

and

$$n = n_0 - \frac{2B}{A}\,. \tag{3}$$

The second solution becomes degenerated with the physical one at each wavelength where B vanishes. The sign of B/A may be found by the examination of Fig. 1 and the sign of A changes between λ_1 and λ_2.

We now consider the effect of the experimental error. Far away from λ_1 and λ_2 one has approximately

$$n - n_0 = -\mu \frac{g(n_0)}{B} \tag{4a}$$

and

$$n - n_0 = -\frac{2B}{A} + \mu \frac{g(n_0)}{B}\,. \tag{4b}$$

The solution (4a) is the shift of the physical solution, while (4b) corresponds to the nonphysical branch. The sign of the solution (4a) depends on the sign of μ and for a given μ changes at λ_1 and λ_2 in agreement with Fig. 2a and b.

At wavelengths λ_1 and λ_2 (2) reads

$$n - n_0 = \pm \frac{\sqrt{-2Ag(n_0)\,\mu}}{A}\,. \tag{5}$$

If $Ag(n_0)\,\mu$ is positive, there is no solution close to the physical one. This occurs at λ_2 for $\mu > 0$ and at λ_1 for $\mu < 0$ since the sign of A changes between λ_1 and λ_2 while g is always negative.

Conclusion We have shown that the nonlinear equations for the transmission and for the reflection have discontinuous solutions owing to experimental errors. The discontinuity arises from the degeneracy of the physical branch with nonphysical ones at wavelengths corresponding to or being close to the extrema of the reflection or of the transmission. The error in the refraction index of the film is rather small far away from the extrema, the relative error is about ten times smaller than the relative error in the reflection for the example we have considered. From a practical point of view we suggest to consider those wavelengths where the reflection or the transmission is far away from their extrema. The solutions of the nonlinear equations are computed for these wavelengths, and the physical branch is close to the curve resulting from the interpolation between the computed values of n that show the smoother variation for small changes of the wavelength. We have considered a non-absorbing film, but our conclusions still hold for weakly absorbing films at least, since the ratio $(r + r')/2t$ does not depend on the absorption coefficient α up to terms of second order in α [1].

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