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# ON THE ERROR OF THE ABSORPTION COEFFICIENTS OF WEAKLY ABSORBING THIN LAYERS, DETERMINED FROM TRANSMITTANCE MEASUREMENTS

By

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The absorption coefficient, k(λ), calculated from the transmittance is very sensitive to the errors in thickness and refractive index. The error in k(λ) is relatively small at the wavelengths of the extrema of transmittance but more pronounced between them, yielding a characteristic wobbling in the absorbance spectrum calculated.

The fringe pattern of the measured transmittance spectrum can be used to determine the optical constants (refractive index n(λ) and absorption coefficient k(λ)) of semiconductor or insulator layers. We earlier proposed an improved [1] method for the determination of the optical constants and thickness of weakly absorbing (n >> k) films deposited on thick transparent substrates [2, 3]. In a recent paper [4], we showed that the coefficient of absorbance, k can be determined with high accuracy in a wide range of wavelengths when the index of refraction, n = n(λ) satisfies the disper-

sion relation of the classical oscillator model [5].

In the present work, we discuss the influences of the error in measured transmittance, $n(\lambda)$ and d on the $k(\lambda)$ spectrum determined using the method outlined in [4]. Instead of making complicated and not very impressive error calculations we will call attention to the effects of the mentioned errors by presenting simple numerical results obtained by analysis of simulated trasmittance spectra.

*The method*

In the usual thin-film geometry a weakly absorbing layer ($n >> k$) deposited onto a thick transparent substrate ($d_s >> \lambda$) should be considered (Fig. 1). The transmittance of

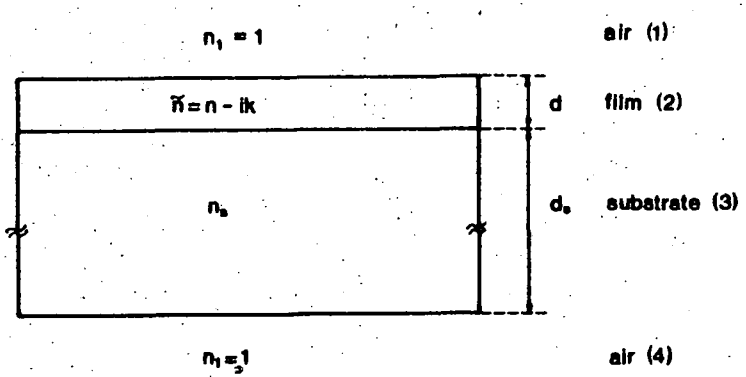


*Figure 1.:* Typical sample structure for transmittance measurement on a thin film. The refractive index is denoted by n, the absorption coefficient is k and the thickness of the film is d.

a thin, weakly absorbing film on a non-absorbing substrate is described in [6] as follows:

$$T = \frac{T_{31}T_{34}}{1-R_{31}R_{34}} , \tag{1}$$

where $T_{31}$ denotes the transmittance of the light travelling from the air through the film into the substrate, and $R_{31}$ is the reflectance of the same surface. $T_{34}$ and $R_{34}$ relate to the substrate/air interface. These quantities can be calculated as follows:

$$T_{31} = \frac{n_s\tau_{12}^2\tau_{23}^2}{\exp(\delta)+\rho_{12}^2\rho_{23}^2\exp(-\delta)-2\rho_{12}\rho_{23}\cos(\varphi_{12}+\varphi_{23}+\alpha)} \tag{2}$$

$$R_{31} = \frac{\rho_{12}^2\exp(\delta)+\rho_{23}^2\exp(-\delta)-2\rho_{12}\rho_{23}\cos(\varphi_{23}-\varphi_{12}+\alpha)}{\exp(\delta)+\rho_{12}^2\rho_{23}^2\exp(-\delta)-2\rho_{12}\rho_{23}\cos(\varphi_{12}+\varphi_{23}+\alpha)} \tag{3}$$

$$T_{34} = \frac{4n_s}{(n_s+1)^2}, \tag{4}$$

$$R_{34} = \left(\frac{n_s-1}{n_s+1}\right)^2 . \tag{5}$$

The quantities in (2) and (3) are expressed by the optical constants of the layer, n and k, and the refractive index of the substrate, $n_s$, as follows:

$$\tau_{12}^2 = \frac{4}{(n+1)^2+k^2} , \tag{6}$$

$$\tau_{23}^2 = \frac{4(n^2+k^2)}{(n_s+n)^2+k^2}, \tag{7}$$

$$\rho_{12}^2 = \frac{(n-1)^2+k^2}{(n+1)^2+k^2} \tag{8}$$

$$\rho_{23}^2 = \frac{(n_s-n)^2+k^2}{(n_s+n)^2+k^2}, \tag{9}$$

$$tg\varphi_{12} = \frac{2k}{n^2+k^2-1}, \tag{10}$$

$$tg\varphi_{23} = \frac{2kn_s}{n^2+k^2-n_s^2}, \tag{11}$$

$$\alpha = \frac{4\pi nd}{\lambda}, \tag{12}$$

$$\delta = \frac{4\pi kd}{\lambda}. \tag{13}$$

For the range of wavelengths, if the layer is weakly absorbing ($n >> k$), Eq.(1) can be simplified and the extrema of the transmittance $T(\lambda)$ can be expressed as

$$T_{extr.} = \frac{16n^2n_s\eta}{(n+1)^3(n_s^2+n)-(n-1)^3(n_s^2-n)\eta^2+(-1)^m 2(n^2-1)(n_s^2-n^2)\eta}, \tag{14}$$

where

$$\eta = \exp(-\frac{4\pi}{\lambda}kd), \tag{15}$$

and m denotes the order of interference satisfying the rela-

tion

$$\frac{4\pi}{\lambda} nd = m\pi, \tag{16}$$

or, to a good approximation

$$m = \frac{\lambda_{m+1}}{\lambda_m - \lambda_{m+1}} . \tag{17}$$

Here $\lambda_m$ and $\lambda_{m+1}$ denote the wavelengths of two neighbouring extrema.

From the measured transmittance of the system film--substrate, one can obtain the maximum and minimum values of the spectrum and the corresponding wavelengths. Using the relations (14-17) or the method presented in [2,3] at the wavelengths relating to the extrema, the optical constants and the thickness of the layer can be determined. If the refractive index of the substrate, $n_s(\lambda)$, is also unknown, it can be determined from one transmittance measurement before the deposition of the film.

If the calculated $n(\lambda_m)$ values lie on a straight line in $1/(n^2-1)$ vs $1/\lambda^2$ plot (i.e. the function $n = n(\lambda)$ behaves as predicted by the classical oscillator model [5]), then this line can be used to interpolate or extrapolate the refractive index at any wavelength. Now, Eqs (1)-(3) allow the determination of $K(\lambda) = (4\pi/\lambda)\cdot k(\lambda)$ at any wavelength, from measured $T(\lambda)$ and calculated $n(\lambda)$ and d values [4].

*Analysis of possible errors by using simulated transmittance spectra*

As the first step we constructed a transmittance spectrum (Fig. 2) from given $n(\lambda)$, $k(\lambda)$, $n_s(\lambda)$ functions and thickness d with help of Eqs (1)-(13). The $n(\lambda)$ and $n_s(\lambda)$ functions were chosen to fulfil the conditions of the clas-

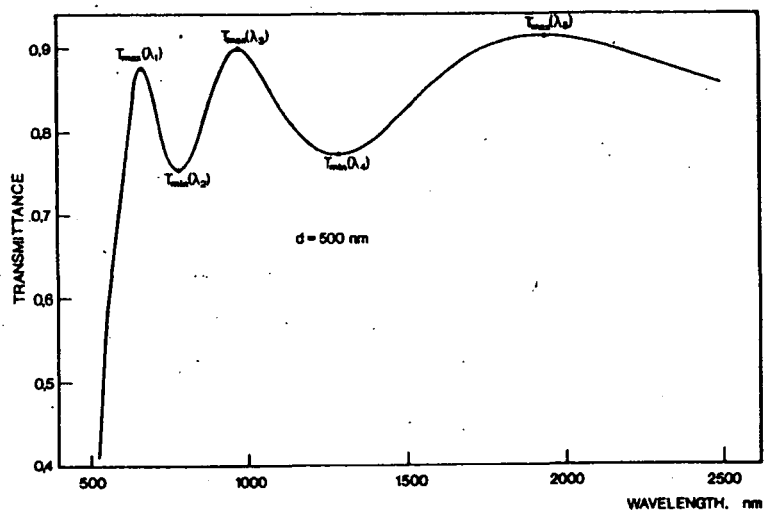


*Figure 2.:* Simulated transmittance spectrum with fringe pattern

sical oscillator model (Figs 3 and 4). The absorption coefficient is given as

$$k(\lambda) = a \cdot \exp(-b \cdot \lambda) + c$$

(where $a = 1.55 \cdot 10^6$; $b = 3.26 \cdot 10^{-2}$; $c = 4.5 \cdot 10^{-3}$). This original $k(\lambda)$ function appears as the full curve in Figs 5-7. The thickness was chosen as 500 nm. From the $T(\lambda)$ spectrum constructed in this way, the n, k and d values were determined at the wavelengths $\lambda_1$, $\lambda_2$, ... via the fringe pattern method described in [1,3]. The obtained n and k values are

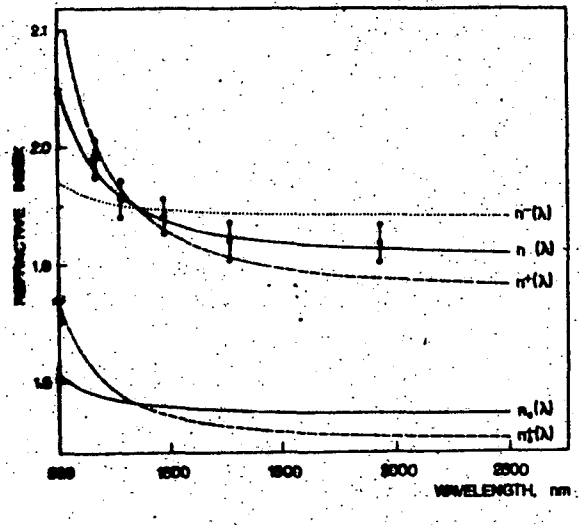


*Figure 3.:* Wavelength-dependence of the refractive indices n and $n_s$, constructed by means of the classical oscillator model.

shown as full circles in Figs 3-7. For comparison we calculated then, k and d values at the same wavelengths from the transmittance spectra

$$T^+(\lambda) = T(\lambda) + 0.003$$

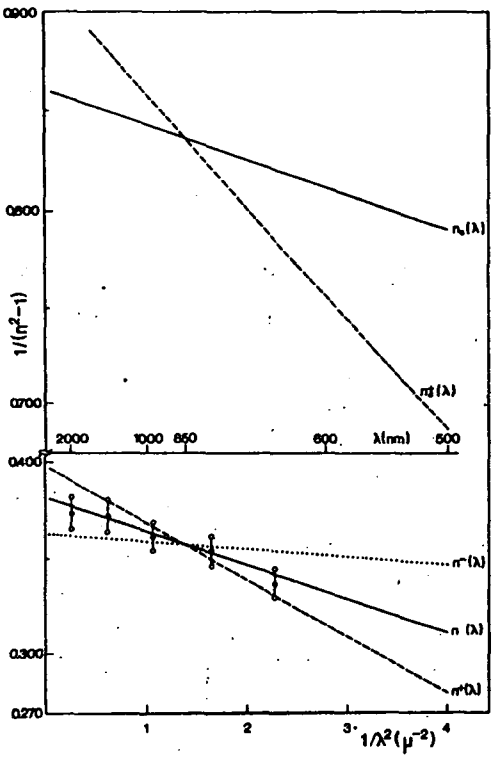


*Figure 4.:* The refractive indices n and $n_s$ of Fig. 3, replotted as $1/(n^2-1)$ vs. $1/\lambda^2$.

and

$$T^{-}(\lambda) = T(\lambda) - 0.003$$

too. The obtained values are given as empty circles in

Figs 3-7. The original and the calculated values of the optical constants and thicknesses are listed in Table I. When the data given in this Table are compared, it can be concluded that the error in the procedure is less than that caused by the uncertainty in the measurement.

We shall examine now the change in the $k(\lambda)$ spectrum calculated from $T(\lambda)$ when the values of $n(\lambda)$, $n_s(\lambda)$ and d differ from the originals. The deviations in $n(\lambda)$ and $n_s(\lambda)$

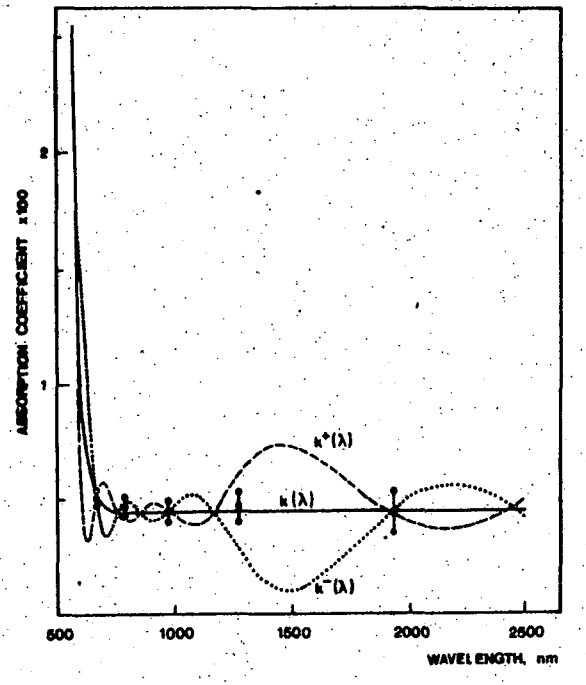


*Figure 5.:* Absorption spectra. Full line: original curve, constructed with the expression $a \cdot \exp(-b \cdot \lambda) + c$; dotted and dashed lines: calculated from the transmittance, using $n^+(\lambda)$ and $n^-(\lambda)$.

where chosen according to the following conditions: the difference between the original and new values is 2 per cent at $\lambda$ = 600 nm and zero at $\lambda$ = 850 nm; and the dispersion relation also holds for the new set of data. The new functions are denoted by $n^+$, $n^-$ and $n_s$ in Figs 3 and 4. The new thicknesses are 490 and 510 nm, corresponding to a 2 per cent change.

The $k(n, n_s, d, T)$ values were calculated by using the new set of data. The $k^+(\lambda)$ and $k^-(\lambda)$ curves (Fig. 5) were obtained by using the new $n^+(\lambda)$ and $n^-(\lambda)$ values, while the data in Figs 6 and 7 were calculated with new d values and

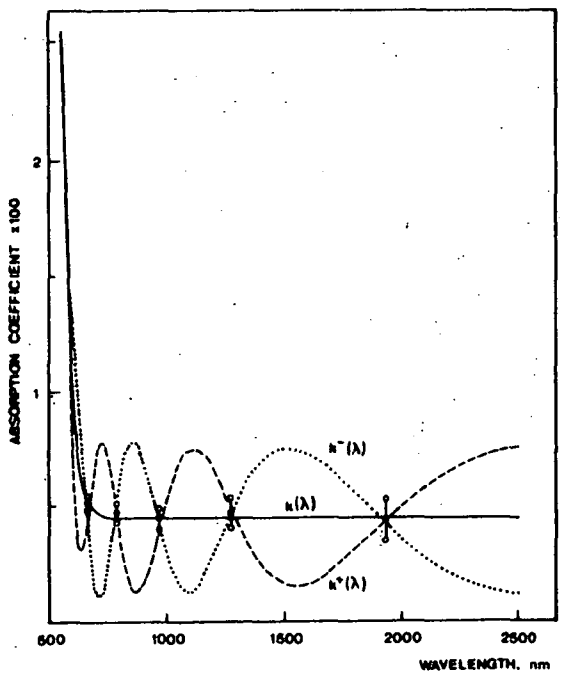


*Figure 6.:* Adsorption spectra. Full line: original; dotted and dashed lines: calculated, using $d^+$ and $d^-$.

*Table I*

| $\lambda_m$ (nm) | ORIGINAL | | | CALCULATED from T | | | CALCULATED using T $\pm$ $\Delta$T | | |
|---|---|---|---|---|---|---|---|---|---|
| | n | $k \cdot 10^3$ | d | n | $k \cdot 10^3$ | d | n | $k \cdot 10^3$ | d (nm) |
| 663 | 1.981 | 5.2 | 500 nm | 1.991 | 5.1 | 499 | 1.974-2.006 | 4.0-5.4 | 504-496 |
| 780 | 1.958 | 4.5 | | 1.956 | 4.9 | 498 | 1.940-1.972 | 4.7-5.5 | 503-494 |
| 970 | 1.938 | 4.5 | | 1.941 | 4.5 | 500 | 1.926-1.956 | 4.0-4.9 | 504-496 |
| 1270 | 1.924 | 4.5 | | 1.920 | 4.8 | 496 | 1.903-1.935 | 4.4-5.6 | 501-492 |
| 1935 | 1.913 | 4.5 | | 1.918 | 4.5 | 504 | 1.902-1.933 | 3.5-5.3 | 509-501 |

$n_s(\lambda)$ function, respectively. All the other parameters were kept unaltered.

Comparison of $k(\lambda)$ with $k^+(\lambda)$ and $k^-(\lambda)$ (Figs 5-7) reveals that in the range of weak absorption there is a considerable and characteristic deviation. From Figs 5-7, it is apparent that relatively small deviations from the original $n(\lambda)$ and $d$ values result in dramatic changes in the $k(\lambda)$ spectra, while the uncertainty in $n_s(\lambda)$ causes only minor

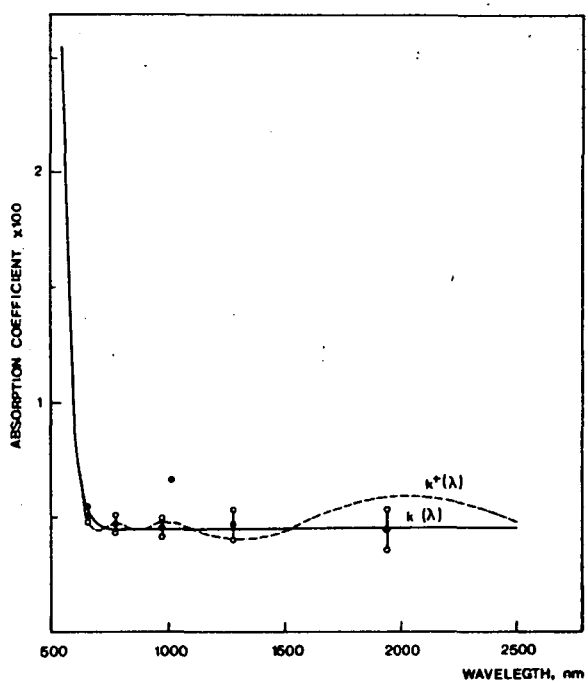


*Figure 7.:* Absorption spectra. Full line: original; dashed line: calculated using $n_s$.

differences. This effect is less pronounced in the range of strong absorption. The characteristic periodicity in the $k^+(\lambda)$ and $k^-(\lambda)$ spectra is due to the fact that, the insertion of inappropriate $n(\lambda)$ and d values into the interference term of Eqs (2) and (3) results in large deviations in arc.

The results of the above model calculations confirm that the method described in [1] in well suitable for the determination of $k(\lambda)$, if the d and $n(\lambda)$ data used are correct enough. Any fluctuation calls for a revision of the precision of the n and d values used. On the other hand, the difference between two adjacent minima and maxima of $k(\lambda)$ can be regarded as the error of the absorption constant determined.

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# О НЕТОЧНОСТИ КОЭФФИЦИЕНТА ПОГЛОЩЕНИЯ СЛАБО ПОГЛОЩАЮЩИХ ТОНКИХ ПЛЕНОК, ОПРЕДЕЛЕНОГО ПО ИЗМЕРЕНИИ СПЕКТРА ПРОПУСКАНИЯ

Л. Михайлович, М. И. Терек и И. Хевеши

Коэффициенты поглощения $\kappa(\lambda)$ рассчитанные по пропусканию очень чувствительны к неточностям определения толщины слоя и показателя преломления.

Ошибка в $\kappa(\lambda)$ относительно мала при экстремальных значениях пропускания и более значительна между ними которое приводит к характерным неровностям в рассчитанном спектре.