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Analysis of the reflection-transmission method for determining the optical constants on thin films*

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An analysis of solutions of the equation system in the reflection—transmission method for determining the optical constants of thin films is presented. The effect of errors in measured reflection, transmission and thickness of a film upon the refractive index n_1 and the coefficient of absorption k_1 is considered and a restriction on the use of the method is discussed. The analysis is illustrated by results of measurements on homogeneous film of Gd_2O_3.

The paper [1] presents two versions of an algorithm for determining the optical constants n_1 and k_1 of thin films on a transparent substrate from normal incidence reflection R and transmission T measurements. While working out the algorithm the equations in Tomlin's form [2] were used, in which the functions R and T have been replaced by their combination $\frac{1\pm R}{T}$, respectively. The refraction and absorption coefficients can be determined approximately by finding the intersection points of two curves:

$$F = f_1 - f_1'(n_1, k_1, d, \lambda, n_2, n_0) = 0, \tag{1}$$

$$\Phi = f_2 - f_2'(n_1, k_1, d, \lambda, n_2, n_0) = 0, \tag{2}$$

where:

$$f_1 = \frac{1+R}{T}, \; f_2 = \frac{1-R}{T},$$

$$f_1' = \frac{1}{4n_0 n_2 (n_1^2+k_1^2)} \Big\{(n_0^2+n_1^2+k_1^2)[(n_2^2+n_2^2+k_1^2)\times \times \cosh 2\alpha_1 + 2n_1 n_2 \sinh 2\alpha_1] + (n_0^2-n_1^2-k_1^2)\times \times [(n_1^2-n_2^2+k_1^2)\cos 2\gamma_1 - 2n_2 k_1 \sin 2\gamma_1]\Big\},$$

$$f_2' = \frac{1}{2n_2(n_1^2+k_1^2)} \Big\{n_1 [(n_1^2+n_2^2+k_1^2)\sinh 2\alpha_1 + +2n_1 n_2 \cosh 2\alpha_1 + k_1 [(n_1^2-n_2^2+k_1^2)\sin 2\gamma_1 + 2n_2 k_1 \cos 2\gamma_1]\Big\},$$

$$\gamma_1 = \frac{2\pi n_1 d}{\lambda}, \; \alpha_1 = \frac{2\pi k_1 d}{\lambda},$$

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d — thickness of the film,
n_1 — refraction coefficient of the film,
n_2 — refraction coefficient of the substrate,
n_0 — refraction coefficient of the air,
λ — wavelength,
k_1 — absorption coefficient of the film.

The first version of the computational algorithm based upon the tabulated process was applied to find the solutions of eqs. (1) and (2), respectively, within a given range of refraction coefficient n_1. This algorithm was utilized to analyse the nature of the solutions of eqs. (1) and (2), and the effects of errors in the measured quantities R, T, and d. In this paper the results for the homogeneous Gd_2O_3 films are presented.

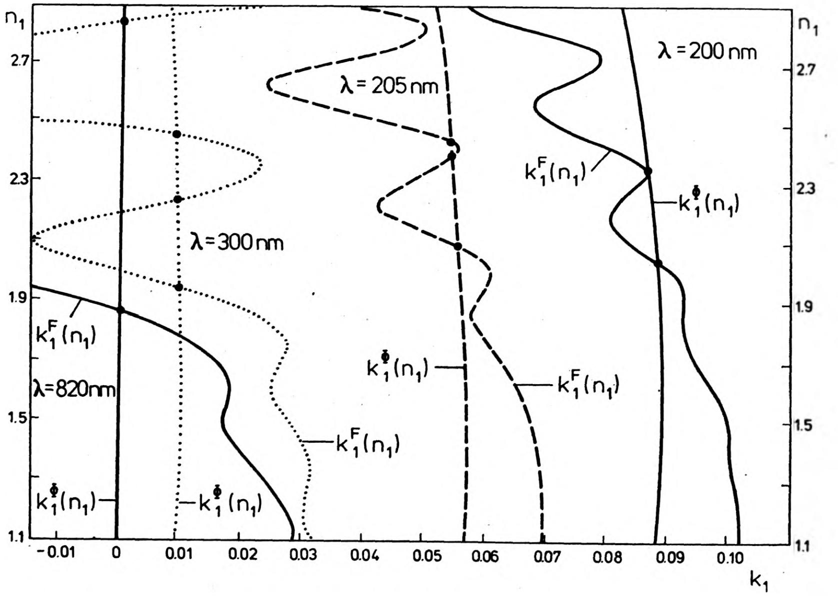

Fig. 1. A schematic diagram of the solutions of eqs. (1) and (2) for four different wavelengths, for a Gd_2O_3 film 285 nm thick on a CaF_2 substrate. Curve $k_1^F(n_1)$ — solution of the equation $F = 0$, $k_1^{\Phi}(n_1)$ — solution of the equation $\Phi = 0$

Fig. 1 shows the graph illustrating the solutions of eqs. (1) and (2) in the plane n_1-k_1 for four fixed wavelenghts. The curve $k_1^F(n_1)$ is a solution of the equation $F = 0$, and $k_1^{\Phi}(n_1)$ is a solution of the equation $\Phi = 0$. It can be seen that the curve $k_1^{\Phi}(n_1)$ approximates a straight line in certain intervals, and in the non-absorbing spectrum range ($\lambda = 820$ nm) it covers the axis of n_1. This property of the function $k_1^{\Phi}(n_1)$ has been used while working out a more effective version of the algorithm [1]. Depending on the type of film and ratio d/λ the curve $k_1^F(n_1)$ is more or less oscillatory in the given range n_1. Coordinates of the intersection points of the curves are the desired solutions. We notice that there is a possibility of multiple solutions for one value of R and T.

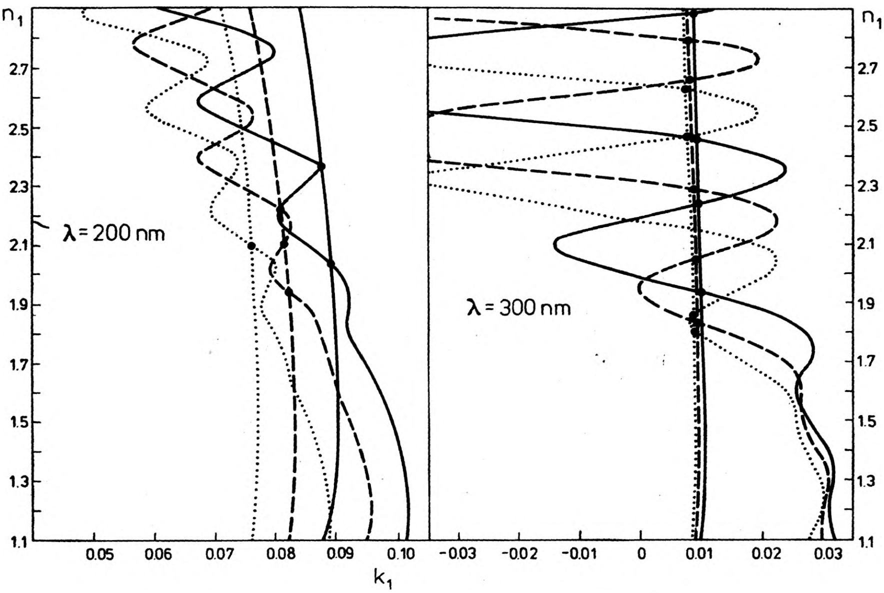

Fig. 2. The effects of errors in d on the calculated $k_1^F(n_1)$ and $k_1^\Phi(n_1)$ curves for a Gd_2O_3 film 275 nm thick on a CaF_2 substrate (—— $d = 255$ nm, – – – $d = 275$ nm, ... $d = 295$ nm)

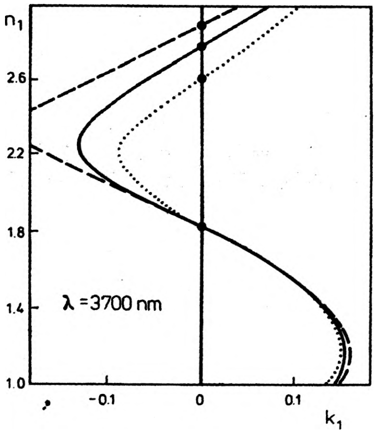

Fig. 3. The effects of errors in d on the calculated $k_1^F(n_1)$ and $k_1^\Phi(n_1)$ curves for a Gd_2O_3 film 557 nm thick on a CaF_2 substrate in the infrared region (—— $d = 557$ nm, – – – $d = 537$ nm, ... $d = 577$ nm)

Figs 2 nad 3 show how an error in the measured thickness of the film affects the solutions. Substitution of $d \pm 20$ nm changes distinctly the curves $k_1^F(n_1)$ and $k_1^\Phi(n_1)$. Consequently, the results of coordinates of the intersections as well as a number of the intersections change, too. Sometimes a slight experimental error in d causes a situation in which no solution is possible. From the analysis of the graphs of the functions $k_1^F(n_1)$ and $k_1^\Phi(n_1)$ in the plane $n_1 - k_1$, for different wavelengths and thicknesses of Gd_2O_3 films, it has been found that for a certain ration d/λ an error in d does not affect the physical solutions [3]. This situation is shown in figure 3, where the resulting solutions are illustrated for a non-absorbing Gd_2O_3 film in the infrared region. In this region the film thickness cannot be determined accurately by the adjustment of d, unless a complete dispersion curve is obtained [2].

The effect of errors in reflection and transmission for two Gd_2O_3 films of different thicknesses is illustrated in figs. 4 and 5. From fig. 4 it may be concluded that an alternation of the experimental values of R and T by ±0.01 only slightly influences the solutions. However, this effect increases visibly near the maxima or minima of the $R=f(\lambda)$ and $T=f(\lambda)$ curves. In this region even the replacing of the alternation

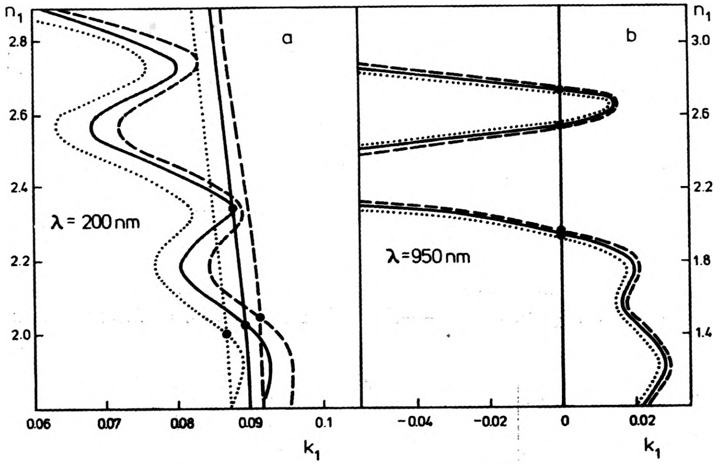

Fig. 4. Effect of ±0.01 reflection and transmission errors on the solution branches for Gd_2O_3 film on a CaF_2 substrate: (a) $d = 285$ nm, $R = 0.11$, $T = 0.22$, (b) $d = 570$ nm, $R = 0.105$, $T = 0.895$ (––– $R+0.01$, $T-0.01$; ... $R-0.01$, $T+0.01$)

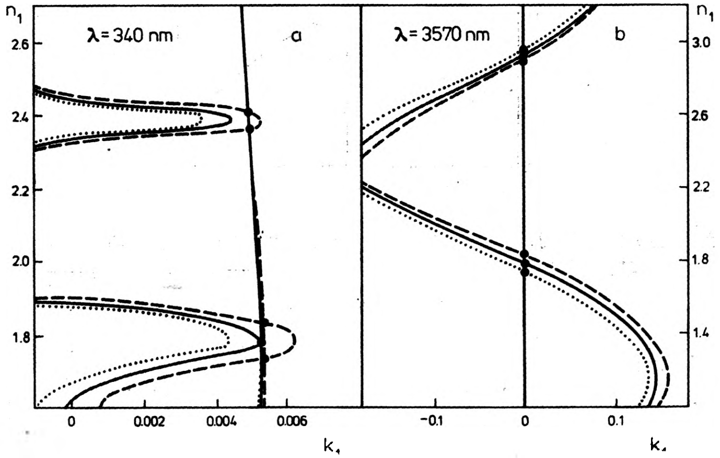

Fig. 5. Effect of errors in R and T on the solution branches for the same films as shown in fig. 4, for the wavelength range, where the curves $R=f(\lambda)$ and $T=f(\lambda)$ have extremes: (a) $R = 0.035$, $T = 0.91$, (b) $R = 0.15$, $T = 0.85$ a. (—— $R+0.005$, $T-0.005$; ... $R-0.005$, $T+0.005$); b. (–––$R+0.01$, $T-0.01$, ... $R-0.01$, $T+0.01$)

of the respective values of R and T by ± 0.005 changes drastically the solution branches, which can be observed in fig. 5a. Much less effect of R and T errors is visible in fig. 5b. Errors equal to ± 0.01 change the physical value of n_1 from 1.74 to 1.84, but do not change the number of roots.

For the same frequency region, where T is very small ($T \sim 1\%$) eqs. (1) and (2) have no solutions. An example of this kind of situation is shown in fig. 6. To improve the situation we were trying to enlarge the error interval by factor of 2 (to be sure that also the uncontrolled effects are included) hoping to find solution for these broadening intervals of permissible measuremental value. Unfortunately, no intersection of $k_1^F(n_1)$ and $k_1^\Phi(n_1)$ curves was observed.

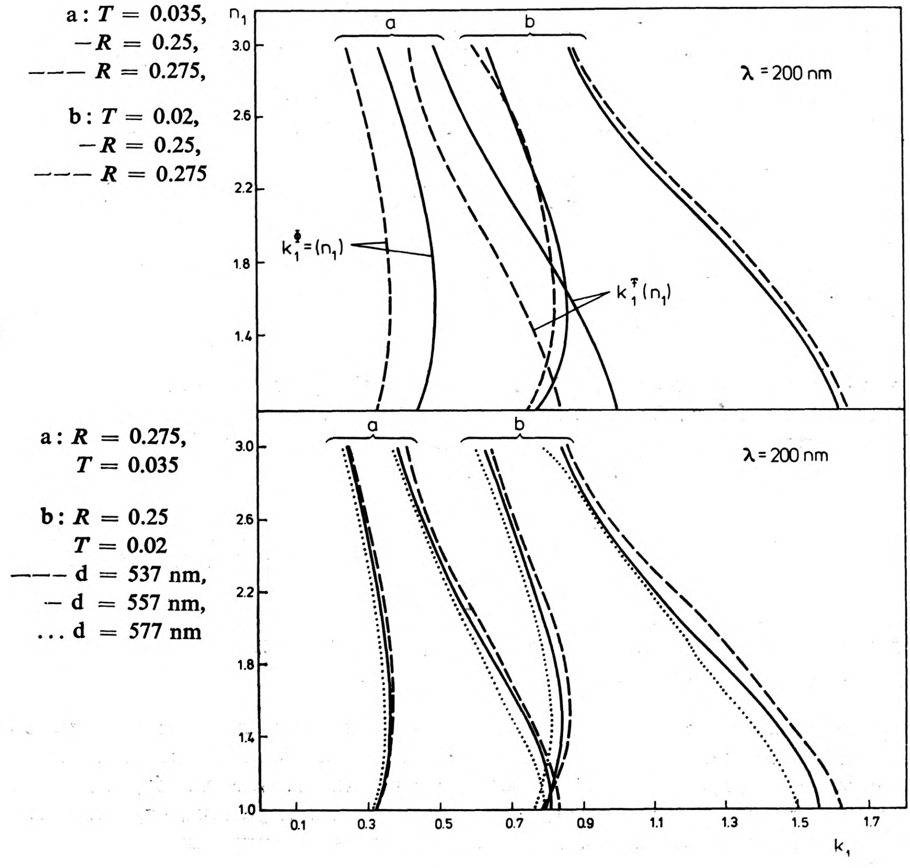

Fig. 6. Calculated $k_1^F(n_1)$ and $k_1^\Phi(n_1)$ curves for a 557 nm thick film of Gd_2O_3 on a CaF_2 substrate in the spectral region, where transmission is very small ($T \sim 0.01$)

The analysis of the graph of the solutions in the $n_1 - k_1$ plane was also performed for other homogeneous films (Sb_2O_3, ThF_4, LaF_3). The results were similar to those shown above.

Conclusions

The conclusions resulting from the carried out analysis are summarized below:

1. The value of the thickness used in the calculation of the optical constants (especially n_1) is extremely important.

2. There is a spectral region where the physically relevant values of n_1 and k_1 are insensitive to errors in the film thickness.

3. The errors in R and T strongly influences the solutions near the extremities of the plots $R = f(\lambda)$, $T = f(\lambda)$. Therefore, in this wavelength region, the reflected and transmitted intensities must be measured very carefully.

4. In some regions, especially where T is small, the iterative R-T method for determining the optical constants of thin films does not converge and another method should be used, for example Kramers-Kronig analysis of the transmission data [4].

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Анализ определения оптических постоянных тонких слоёв по отражению и пропусканию

Представлен анализ решений системы уравнений в методе определения оптических постоянных тонких слоёв по отражению и пропусканию. Обсуждено влияние погрешностей измерения отражения, пропускной способности, а также толщины слоя на коэффициент преломления n_1 и коэффициент абсорбции k_1. Обсуждены также условия, ограничивающие применяемость этого метода. Анализ проиллюстрирован результатами для однородных слоёв Gd_2O_3.