Correction of optic spectra on a absorption substrate

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Abstract. Analysis of possibility of determination optical constants of films by numerical and analytical methods is done. It’s shown, that universal method of minimization quality function does not get a unique solution. Methods of consistent approximation is proposed to use for determining optical constants. These methods are: correction spectra for absorption in the substrate; correction spectra of films for its absorption; using additional numerical and analytical methods. Method of correction substrate’s absorption for determining spectra of films on substrate without absorption is proposed.

Spectra of films are show important information about optic constants of film’s material: refraction coefficient $n(\lambda)$ and extinction coefficient $k(\lambda)$ (or absorption coefficient $\alpha(\lambda)$). Spectrophotometric methods are widely used. This methods based on calculation optic constants of films from refraction and transmission spectra. Numerical [1] and analytical[2] methods for calculation optic constants on substrate without absorption are known.

The first group involves finding convenient analytical expressions for the direct calculation of optical constants in various particular cases. Examples of this approach are works [3-5]. In these works, values of optical constants are found at the points, which coincide to extremes of transmission and reflection of absorption films.

Let’s analyze reflection spectra of films on the substrate without absorption. In this case, reflection coefficient of film is

$$R_{1,3} = \frac{r_{1,2}^2 + r_{2,3}^2 + 2r_{1,2}r_{2,3} \cos (-\Delta_{1,2} + \Delta_{2,3} - 4\pi n_2 h_2/\lambda)}{1 + r_{1,2}^2 r_{2,3}^2 + 2r_{1,2}r_{2,3} \cos (\Delta_{1,2} - \Delta_{2,3} + 4\pi n_2 h_2/\lambda)}$$

(1)

$$\Delta_m$$ – phase shift of reflection on the border $lm$. $r$ – Frenel’s amplitude coefficients of reflection on the borders film (2) – air (1) and film (2) – substrate (3)

$$r_{1,2} = (n_1 - n_2)/(n_1 + n_2) = (1 - n_2)/(1 + n_2)$$

(2)

$$r_{2,3} = (n_2 - n_3)/(n_2 + n_3)$$

(3)

Reflection of film $R_0$, transmission $T_0$, at absence of absorption $R_0 + T_0 = 1$. 


Let’s analyze possibility of finding solution of equation (1) concerning $n_2$. Let’s use calculated spectra of films for analysis. Transmission spectra of films with different refraction coefficients ($n_2=1.30-1.50$) and the same geometric thickness on the ZnSe substrate $n_3\approx2.42$ are shown on the figure 1.

As shown at the figure, big amount of solutions coincide for the same wavelength at the one geometric thickness. We showed graphic with rarefied $n$ spectra. But series of ranges have several solutions. For example, value of refraction coefficient coincides for 3 lines better 0.003 at the wavelength $6.67$ μm. It’s showed impossibility finding the unique solution of equation (1) concerning refraction coefficient $n_2$. From this analysis clear, the unique solution is could be not found.

![Figure 1](image)

**Figure 1.** The dependence of the transmittance spectra on the wavelength and refraction coefficient. Solid lines on the 3d graphic are lines of the equal transmittance.

The second group is based on different numerical methods. In the work[6] method of determining optical constants is proposed. This method based on solution system of nonlinear equations for energetic coefficients of reflection and transmittance of the system air-substrate at the wavelength $\lambda$ by minimization of quality function. Quality function $F$ is could be specified for $T$ as:

$$
F_T (n_2, h_2, k_2, \lambda_i) = \frac{1}{L} \sum_{i=1}^{L} \left| T(\lambda_i) - T_0(n_2, h_2, k_2, \lambda_i) \right|^2
$$

where $T(\lambda_i)$ – experimental value of transmittance coefficient, $T_0(n_2, h_2, k_2, \lambda_i)$ – calculated value of transmittance coefficient with absorption, $L$ – amount points of spectrum. This method is universal, but, as rule, finding optical constants has big difficults by reason of absence of the unique solution, because equation (1) is transcendental and has a lot of solutions for the same values reflection and transmittance coefficients.
Third group of methods [7-8] based on correction spectra of films for absorption, which allows to ignore absorption in films. This simplifies determining optical constants. Idea of method is calculating reflection and transmittance spectra for ignoring effect absorption in film. So, obtained spectra depends on only one variable and this simplifies calculating. Besides, in work [2] is proposed to determine thickness of film in range without absorption. Method of determining \( k \) is described in works [1]. However, in this case, the unique solution does not exist, as shown at the figure 1. Therefore, we have to do some additional steps. For example, we can set dispersion dependence refraction coefficient on the wavelength. The other method is determining refraction coefficient at ranges without absorption. Determined value of \( n \) is used as initial approximation at neighboring ranges of spectrum.

Absorption in the substrate complicates determining optical constants, so method of determining spectra of films on absorption substrate with correction this is proposed. In the beginning, measurement of reflection, transmittance and absorption spectra of the substrate is made. Absorption coefficient \( \alpha \) and refraction coefficient \( n_2 \) [3] may be determine from these spectra. This correction allows to calculate spectra of films (reflection \( R_0 \) and transmittance \( T_0 \)) on the substrate without absorption. Let’s consider this method in detail.

Recurrent method was used for calculating refraction and transmission spectra on absorption substrate. Refraction \( R \) and transmission \( T \) are calculated by:

\[
R = R_0 + \frac{T_0^2 \rho_0 e^{-2\alpha d}}{1 - \rho_0 R_0 e^{-2\alpha d}}, \quad T = \frac{T_0 \tau_0 e^{-\alpha d}}{1 - \rho_0 R_0 e^{-2\alpha d}}
\]

(5)

\( \rho_0 \) – refraction, \( \tau_0 \) – transmission on border film-substrate. \( R_0 \) – refraction, \( T_0 \) – transmission of film on substrate without absorption, \( \alpha \) – absorption coefficient.

Decision of system (1) for \( R_0 \) and \( T_0 \) is:

\[
R_0 = \frac{-B \pm \sqrt{B^2 - 4AC}}{2A}, \quad C = R - \left( \frac{T}{\tau_0} \right)^2 \rho_0, \quad B = 1 - R \rho_0 e^{-2\alpha d} + 2 \left( \frac{T}{\tau_0} \right)^2 \rho_0^2 e^{-2\alpha d}, \quad A = \rho_0 e^{-2\alpha d} - 2 \left( \frac{T}{\tau_0} \right)^2 \rho_0^2 e^{-4\alpha d}.
\]

(6)

\[
T_0 = \frac{T}{\tau_0} e^{\alpha d} - \frac{T}{\tau_0} R_0 \rho_0 e^{-\alpha d}
\]

(7)

Obtained equations allow calculate spectra \( T_0 \) of films on the substrate, which does not have absorption.

Analysis of possibility using proposed method was done by using model, which includes film on the absorption substrate. As model, approximated values of real silicon plate were used. The following spectra are showed on the figure 2: transmittance spectra on substrate without absorption (line 1); absorption spectra on substrate with absorption (line 2); transmission of substrate (line 3); absorption of substrate (line 4).
Figure 2. Transmittance and absorption spectra of model

Transmittance spectrum of film, which corrected by equations (6,7) is shown at the same figure (line 5). This spectrum coincides with spectra on substrate without absorption up to 0.001. This demonstrates possibility of correction spectra of films for absorption by this method.

In the future, line 5 is could be used for determining optical constants by one of the described method: analytical or numerical.

Conclusions
Analysis of possibility of determination optical constants of films by numerical and analytical methods is done. It’s shown, that universal method of minimization quality function does not get a unique solution. Methods of consistent approximation is proposed to use for determining optical constants. These methods are: correction spectra for absorption in the substrate; correction spectra of films for its absorption; using additional numerical and analytical methods.

For applying this group of methods, reflection and transmittance spectra on the absorption substrate are recalculated for obtaining spectra of films on the substrate without absorption.[1]

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