Method of correction optical spectra for absorption

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Abstract. A new method for determining optical constants of films is proposed. The method is based on correction optical spectra for absorption. Free from absorption bands spectra can be used for determining optical constants by the known methods. The new method is illustrated by an example of barium fluoride spectrum at the range 1.5–12 μm.

There are a number of spectrophotometric methods for determining optical constants of films that are based on the measurement of reflectance and transmittance spectra [1–3]. These methods are applicable for unabsorbing films, when there exist analytical solutions for optical constants at the transmittance extremum points [3]. However, application of these analytical methods is impossible in the presence of absorption bands. In this case, different numerical-analytical methods are used. These methods are based on using the minimization quality function. Note that this problem is an inverse one and, as a rule, it has several solutions.

A method of correction of the optical spectra of films is proposed. It allows one to exclude absorption from the spectra. The method is based on additivity of the law of energy conservation absorbed in the film and the possibility to separate it into the energy in transmittance and the energy in reflectance. After this correction we obtain transmittance and reflectance spectra without absorption, which allows us to use the known methods for determining optical constants of unabsorbing films.

Let us consider the correction method for absorption $A$ of the optical spectra of reflectance $R$ and transmittance $T$. The value of the film’s absorption $A$ can be calculated (if we know the thickness $h$ and the refraction coefficient $n$) through the extinction coefficient $k$ (or absorption coefficient $\alpha$). All these variables depend on a wavelength. $R$, $T$ and $A$ spectra are related by the law of energy conservation. Absorption $A$ introduces some distortions into the reflectance and transmittance spectra. Since $A$ is an additivity variable, we can present absorption $A$ as the sum of its contributions in the reflectance $A_R$ and in the transmittance $A_T$:

$$ A = A_R + A_T, $$

Here $A_T$ and $A_R$ are defined as:

$$ A_T = T_0 - T; \quad T_0 = T + A_T; $$

$$ A_R = R_0 - R; \quad R_0 = R + A_R, $$

where $R_0$, $T_0$ are the reflectance and transmittance coefficients of the unabsorbing film that has the same values of the refraction coefficient as the absorbing film. If we know $A_R$ and $A_T$, we can correct the spectra for absorption by adding these variables to the reflectance and transmittance coefficients for each wavelength.
To calculate \( A_R(\lambda) \) and \( A_T(\lambda) \) we use the correction functions \( f_R \) and \( f_T \) that determine the contribution of the total absorption \( A \) to \( A_R(\lambda) \) and \( A_T(\lambda) \). Let us introduce these correction functions \( f_R \) and \( f_T \):

\[
f_R = \frac{R_0 - R}{A}, \quad f_T = \frac{T_0 - T}{A}.
\]

We can separate the absorption \( A \) into two parts \((A_R \text{ and } A_T)\). The correction functions show the contribution of the distortions introduced by the absorption \( A \) into the reflectance and transmittance spectra. Therefore the sum \( A_R + A_T = 1 \).

The corrected reflectance and transmittance spectra are calculated by the equations:

\[
R_{\text{cor}} = R + f_R A, \quad T_{\text{cor}} = T + f_T A.
\]

It follows from (5) that in order to find \( f_R \) and \( f_T \) we have to know \( R_0 \) and \( T_0 \), i.e. the spectra free of absorption. Actually, it is our aim to determine these spectra. To find analytical equation for the optical constants of the spectra free of absorption is not possible because there are several solutions. To produce a model of the absorption spectrum corresponding to the real one seems to be impossible because it is an inverse problem with the same difficulties as the one of determining optical constants.

The following method is proposed to calculate the correction functions. We introduce the model of an absorbing film, with its spectra approximately corresponding to the spectra of the film considered. Then the spectra \( R, T \) and \( A \) of this model are calculated. In addition, the reflectance and transmittance spectra of the film’s model without absorption, but with the same refraction coefficients as the absorbing film are also calculated and then their spectra \( R_0 \) and \( T_0 \) are calculated as well. After calculating \( R_0, T_0, R, T \) and \( A \) the correction functions \( f_R \) and \( f_T \) are to be calculated using (5) for different film models. The correction functions \( f_R \) and \( f_T \) are to be used to correct the experimental spectra of the films. The calculation of \( R_0, T_0, R, T, A, f_R \) and \( f_T \) spectra has been performed by the program FilmMgr [4], which provides the possibility to introduce both the dispersion of the refraction coefficients and the absorption of the films.

The calculated correction functions \( f_R \) and \( f_T \) depend on the film’s parameters and the form of its absorption spectrum. The impact of an amplitude and an absorption spectra form on the correction function has been analyzed. Absorption spectra with different amplitudes and widths have been considered.

The correction functions for film’s models with the refraction coefficient 1.35, the thickness 3.14 \( \mu m \) on ZnSe substrate at the range 2–4 \( \mu m \) are shown in figure 1. Graphs 1 correspond to the absorption amplitude 8 %, graphs 2 – 16 %, graphs 3 – 30 %.

![Graphs 1](image1.png)

**Figure 1.** The correction functions \( f_R (a) \) and \( f_T (b) \) for different models of films.

Figure 1 shows that the main character of the correction functions is connected with the extrema of the film’s transmittance. Note that the thickness of this film should be found with the minimal error. It follows from the figures 1(a), (b) that the errors of the spectra correction do not exceed 0.2 % when using the correction functions for 30 % absorption. This error corresponds to the accuracy of the
spectra amplitude measurements. In other words, the accuracy of the spectra resulting from the correction corresponds to the accuracy of the spectra measurements regardless of the absorption spectrum form.

As an unabsorbing substrate we have used ZnSe plates of CVD make, on which the films of barium fluoride with the thickness 3.14 µm have been applied by the resistive coating method. The spectra of the films have been measured by spectrophotometer FSM-1201 with the accuracy of 0.2 %.

Figure 2 shows the reflectance (1), transmittance (2) and absorption (3) spectra of the barium fluoride on the ZnSe substrate. The corrected spectra of reflectance (4) and transmittance (5) are shown in the same figure.

The refraction and absorption coefficients are found from the corrected spectra by the method described in [4]. The results of the refraction coefficient calculations are shown in figure 3.

The reflectance and transmittance spectra of the film with absorption have been calculated by the already determined data of the refraction and absorption coefficients. They are shown in figure 2 and coincide with the corrected spectra (graphs 1 and 2) with ±0.3 % accuracy.

![Figure 2](image1.png)  ![Figure 3](image2.png)

**Figure 2.** The spectra of reflectance (1), transmittance (2) and absorption (3). The corrected reflectance (4) and transmittance (5) spectra.

**Figure 3.** The dependence of the refraction coefficient of BaF₂ on a wavelength.

The proposed method of spectra correction allows one to recalculate the reflectance and transmittance spectra so as to exclude the effect of absorption from the optical spectra. This correction technique allows one to apply the methods developed for determining optical constants of unabsorbing films for the absorbing ones.

**References**

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