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Determination of the complex refractive index of a thick slab material from its spectral reflectance and transmittance at normal incidence

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ABSTRACT

Multiple beam incoherent reflectance, transmittance and absorbance of a homogenous planar slab are derived by ray tracing and transfer matrix approaches. Two different procedures are introduced to retrieve the bulk complex refractive index analytically. The needed experimental measurements are the slab thickness, the spectral reflectance and transmittance at normal incidence. Errors of the deduced refractive indices are calculated to be of about 1×10^{-7} for imaginary and 0.013 for real refractive indices. Refractive indices of two different thicknesses and compositions glassy slabs are determined across a wide spectral range 0.22–2.2 μm.

1. Introduction

Refractive index is the fundamental optical parameter of all materials. Its real part is inversely proportional to the wave propagation velocity, while its imaginary part is related to the intensity attenuation inside the medium. Refractive indices of supporting substrates are very important for characterization of thin film materials and optoelectronic devices [1,2]. Measurements of refractive indices of bulk material are frequently needed in glass, polymer and plastic industries [3,4]. Different methods and techniques for the measurement of refractive indices of various materials have been reviewed [5]. Formulas were derived to determine the refractive index of a dielectric material from its reflectance and transmittance but numerical procedure for minimization and two samples with different thicknesses have to be used [6,7]. An iterative numerical procedure, which needs computational means and time, was adopted to retrieve the refractive indices of a slab from its spectrophotometric measurements [8]. Ray tracing approach has been used to derive expressions for the incoherent reflectance and transmittance only without an expression for absorbance [9]. Then analytical relations were derived to calculate the complex refractive index of a planer slab from its normal incidence reflectance and transmittance [9]. Unfortunately, these expressions are not widely used and experimental measurement errors were not discussed or evaluated.

In this work; two different approaches, ray tracing and transfer matrix, are used to derive the multiple beam incoherent reflectance, transmittance and absorbance of a planar thick slab. Also two different analytical procedures to retrieve the complex refractive index are introduced. Both of them use the spectral reflectance and the transmittance measurements. The errors of experimental measurements by the two procedures are discussed and evaluated. Two glassy slabs with different composition and thickness are tested experimentally across the spectral range 0.22–2.2 μm.

2. Ray tracing approach

Ray tracing or summation approach has been used to derive both the reflectance and transmittance, without absorbance, in a thick slab [9]. Multiple beam incoherent reflectance, transmittance and absorbance are derived in this work.

Consider a thick, parallel-sided, isotropic and homogeneous slab with an average thickness, t, and a complex refractive index, $\boldsymbol{n} = n - jk$, where n is the real part of the refractive index of the slab and k its imaginary part (extinction coefficient) which is related to its absorption coefficient $\alpha = 4\pi k/\lambda$. Consider a parallel beam of light, with wavelength λ, incident normally on the slab as shown schematically in Fig. 1. Since the slab is thick enough then the optical path difference between any two successive beams inside the slab is larger than the coherence length of the incident beam ($\lambda^2/(n\Delta\lambda)$). Thus there are incoherent multiple reflections inside the slab. In case of incoherent interference the beam intensities are

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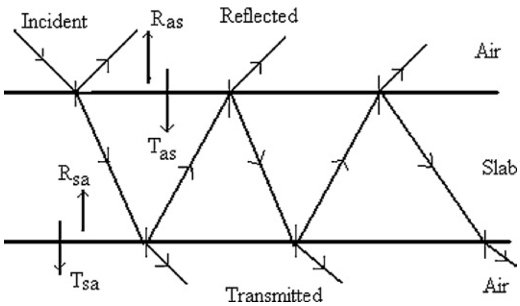

Fig. 1. Schematic diagram for ray tracing approach in a thick slab embedded in air.

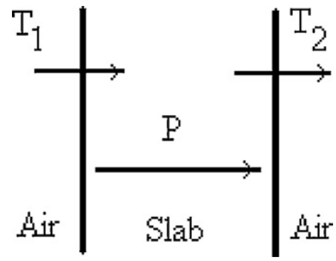

Fig. 2. Schematic diagram for transfer matrix approach in a thick slab embedded in air.

added together. The infinite summation of multiple reflected beam intensities is:

$$R = R_{as} + T_{as}R_{sa}T_{sa}\eta^2(1 + \eta^2R_{sa}^2 + \eta^4R_{sa}^4 + \cdots) \tag{1}$$

Since $\eta^2R_{sa}^2 < 1$, then:

$$R = R_{as} + T_{as}R_{sa}T_{sa}\eta^2\left(\frac{1}{1-\eta^2R_{sa}^2}\right) \tag{2}$$

The infinite summation of multiple transmitted beam intensities is:

$$T = T_{as}\eta T_{sa}(1 + \eta^2R_{sa}^2 + \eta^4R_{sa}^4 + \cdots) \tag{3}$$

The last equation can be written as:

$$T = \frac{\eta T_{as}T_{sa}}{1-\eta^2R_{sa}^2} \tag{4}$$

The infinite summation of multiple absorbed beam intensities is:

$$A = T_{as}(1-\eta)(1 + \eta R_{sa} + \eta^2R_{sa}^2 + \cdots) \tag{5}$$

The absorbance can be written as:

$$A = \frac{T_{as}(1-\eta)}{1-\eta R_{sa}} \tag{6}$$

From Eqs. (2), (4) and (6), it is obvious that the conservation of energy leads to:

$$R + T + A = 1 \tag{7}$$

In the above equations (see Fig. 1), R_{as} is the surface (interface) reflectance when the light incident from air to slab, R_{sa} is the surface reflectance from slab to air, T_{as} is the surface transmittance from air to slab, T_{sa} is the surface transmittance from slab to air and $\eta = e^{-\alpha t}$ is called the attenuation factor. It should be noted that $R_{as} = R_{sa}$, $T_{as} = T_{sa}$ and $R_{as} + T_{as} = R_{sa} + T_{sa} = 1$.

3. Transfer matrix approach

Coherent and incoherent matrices have been introduced to study multilayer structures but the coherent one is much popular with multilayer thin films [10,11]. The incoherent matrix is rarely used but it is used here since there is an incoherent interference in the thick slab. Suppose the planar slab is immersed in air and a parallel beam of light incident near normal incident from left to right as shown schematically in Fig. 2. The refraction or transmission matrix of the first slab interface is:

$$T_1 = \frac{1}{T_{as}}\begin{vmatrix} 1 & -R_{sa} \\ R_{as} & (T_{as}T_{sa} - R_{as}R_{sa}) \end{vmatrix} \tag{8}$$

The propagation matrix through the slab medium is:

$$P = \frac{1}{\eta}\begin{vmatrix} 1 & 0 \\ 0 & \eta^2 \end{vmatrix} \tag{9}$$

The refraction matrix of the second slab interface is:

$$T_2 = \frac{1}{T_{sa}}\begin{vmatrix} 1 & -R_{as} \\ R_{sa} & (T_{sa}T_{as} - R_{sa}R_{as}) \end{vmatrix} \tag{10}$$

All parameters in these matrices have the same meaning as that in the ray tracing section.

The equivalent matrix of a planar slab in air is the multiplication of the three matrices such that:

$$T_1PT_2 = \frac{1}{\eta T_{as}^2}\begin{vmatrix} (1-R_{sa}^2\eta^2) & [-R_{as} - R_{sa}\eta^2(T_{sa}T_{as} - R_{sa}R_{as})] \\ [R_{as} + R_{sa}\eta^2(T_{as}T_{sa} - R_{as}R_{sa})] & [-R_{as}^2 + \eta^2(T_{as}T_{sa} - R_{as}R_{sa})(T_{sa}T_{as} - R_{sa}R_{as})] \end{vmatrix} \tag{11}$$

Eq. (11) can be written as:

$$T_1PT_2 = \begin{vmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{vmatrix} \tag{12}$$

The reflectance is deduced from the last equation as:

$$R = \frac{M_{21}}{M_{11}} = R_{as} + T_{as}R_{sa}T_{sa}\eta^2\left(\frac{1}{1-\eta^2R_{as}^2}\right) \tag{13}$$

The transmittance is:

$$T = \frac{1}{M_{11}} = \frac{\eta T_{as}T_{sa}}{1-\eta^2R_{sa}^2} \tag{14}$$

The absorbance is:

$$A = \frac{M_{11} - M_{21} - 1}{M_{11}} = \frac{T_{as}(1-\eta)}{1-\eta R_{sa}} \tag{15}$$

Since $R_{as} = R_{sa}$ and $T_{as} = T_{sa}$, the equations for multiple beam incoherent reflectance, transmittance and absorbance are;

$$R = R_{as}\left(1 + \frac{\eta^2T_{as}^2}{1-\eta^2R_{as}^2}\right) \tag{16}$$

$$T = \frac{\eta T_{as}^2}{1-\eta^2R_{as}^2} \tag{17}$$

$$A = \frac{(1-\eta)T_{as}}{1-\eta R_{as}} \tag{18}$$

4. First procedure for analytical formulas for refractive indices

Analytical formulas for the slab refractive indices can be derived from the spectral reflectance and transmittance as follows. Using Eqs. (16) and (17) we get:

$$\eta = \frac{R - R_{as}}{TR_{as}} \tag{19}$$

Substituting by $T_{as} = 1 - R_{as}$ and η in Eq. (17), a second-degree algebraic equation is obtained and its acceptable solution is:

$$R_{as} = \frac{[2+T^2-(1-R)^2] - \left\{[2+T^2-(1-R)^2]^2 - 4(2-R)R\right\}^{1/2}}{2(2-R)} \tag{20}$$

The imaginary part of the refractive index is deduced from Eq. (19) as:

$$k = \frac{\lambda}{4\pi t}\ln\left[\frac{T\{[2+T^2-(1-R)^2] - \{[2+T^2-(1-R)^2]^2 - 4(2-R)R\}^{1/2}\}}{[2(2-R)R + \{[2+T^2-(1-R)^2]^2 - 4(2-R)R\}^{1/2} - (2+T^2) + (1-R)^2\}}\right] \tag{21}$$

The surface (interface) reflectance between air and slab material, in case of normal incidence, is:

$$R_{as} = \frac{(1-n)^2 + k^2}{(1+n)^2 + k^2} \tag{22}$$

From the last equation, real part of the refractive index is:

$$n = \frac{(1+R_{as})}{(1-R_{as})} + \left[\frac{4R_{as}}{(1-R_{as})^2} - k^2\right]^{1/2} \tag{23}$$

The first step is to measure the slab thickness, t, its spectral reflectance, R, and spectral transmittance, T, with a spectrophotometer. Secondly; R and T are substituted in Eq. (20) to get R_{as}. Thirdly, t, T, R, R_{as} and λ are introduced in Eq. (21) to find k. Finally, n is calculated from Eq. (23) using R_{as} and k. It should be noted that this procedure has been suggested [9] and was not widely used.

5. Second procedure for analytical formulas for refractive indices

Analytical formulas for the slab refractive indices can be derived from the spectral reflectance and transmittance as follows. Using Eqs. (16) and (17) we get:

$$R = R_{as}(1 + \eta T) \tag{24}$$

Substituting by: $T_{as} = 1 - R_{as}$, $R_{as} = R/(1+\eta T)$ and $A = 1 - R - T$ in Eq. (18), a second-degree algebraic equation is obtained for the attenuation factor and its acceptable solution is:

$$\eta = \frac{[T^2 - [(1-R)^2] + \{[T^2-(1-R)^2]^2 + 4T^2\}^{1/2}}{2T} \tag{25}$$

The absorption coefficient can be written as:

$$\alpha = -\frac{1}{t}\ln\left\{\frac{[T^2 - [(1-R)^2] + \{[T^2-(1-R)^2]^2 + 4T^2\}^{1/2}}{2T}\right\} \tag{26}$$

The imaginary part of the refractive index is deduced from the absorption coefficient as:

$$k = \frac{-\lambda}{4\pi t}\ln\{\frac{[T^2-(1-R)^2] + \{[T^2-(1-R)^2]^2 + 4T^2\}^{1/2}}{2T}\} \tag{27}$$

The surface (interface) reflectance between air and slab material, in case of normal incidence, is:

$$R_{as} = \frac{R}{1 + [[T^2-(1-R)^2] + \{[T^2-(1-R)^2]^2 + 4T^2\}^{1/2}]/2} \tag{28}$$

The real part of the refractive index is:

$$n = \frac{(1+R_{as})}{(1-R_{as})} + \left[\frac{4R_{as}}{(1-R_{as})^2} - k^2\right]^{1/2} \tag{29}$$

The first step is to measure the slab thickness, t, its spectral reflectance, R, and transmittance, T, with a spectrophotometer. Secondly; R and T are substituted in Eq. (25) to get η. Thirdly: η and t are introduced in Eq. (26) to find α. Then k is deduced from Eq. (27). Finally, n is calculated from Eq. (29) using R_{as} and k. This procedure is suggested and used here for the first time to our knowledge.

6. Errors of measurements and surface roughness correction

An estimation of the errors of the slab material refractive indices for first procedure can be written as:

$$\Delta R_{as} = \sqrt{\left(\frac{\partial R_{as}}{\partial R}\Delta R\right)^2 + \left(\frac{\partial R_{as}}{\partial T}\Delta T\right)^2} \tag{30}$$

$$\Delta k = \sqrt{\left(\frac{\partial k}{\partial \lambda}\Delta\lambda\right)^2 + \left(\frac{\partial k}{\partial t}\Delta t\right)^2 + \left(\frac{\partial k}{\partial T}\Delta T\right)^2 + \left(\frac{\partial k}{\partial R_{as}}\Delta R_{as}\right)^2} \tag{31}$$

$$\Delta n = \sqrt{\left(\frac{\partial n}{\partial R_{as}}\Delta R_{as}\right)^2 + \left(\frac{\partial n}{\partial k}\Delta k\right)^2 + 2\frac{\partial n}{\partial R_{as}}\frac{\partial n}{\partial k}\Delta R_{as}\Delta k} \tag{32}$$

An estimation of the errors of the slab material refractive indices for the second procedure can be written as:

$$\Delta\eta = \sqrt{\left(\frac{\partial \eta}{\partial R}\Delta R\right)^2 + \left(\frac{\partial \eta}{\partial T}\Delta T\right)^2} \tag{33}$$

$$\Delta R_{as} = \sqrt{\left(\frac{\partial R_{as}}{\partial R}\Delta R\right)^2 + \left(\frac{\partial R_{as}}{\partial T}\Delta T\right)^2} \tag{34}$$

$$\Delta k = \sqrt{\left(\frac{\partial k}{\partial \lambda}\Delta\lambda\right)^2 + \left(\frac{\partial k}{\partial t}\Delta t\right)^2 + \left(\frac{\partial k}{\partial R}\Delta R\right)^2 + \left(\frac{\partial k}{\partial T}\Delta T\right)^2} \tag{35}$$

$$\Delta n = \sqrt{\left(\frac{\partial n}{\partial R_{as}}\Delta R_{as}\right)^2 + \left(\frac{\partial n}{\partial k}\Delta k\right)^2 + 2\frac{\partial n}{\partial R_{as}}\frac{\partial n}{\partial k}\Delta R_{as}\Delta k} \tag{36}$$

A computer program (Mathcad PLUS 6.0) has been used to evaluate symbolically these differentiations (Eqs. (30) and (31) and (33)–(36)). Also it is used for substituting by the values: $\Delta R = 0.003$, $R = 0.093$, $\Delta T = 0.003$, $T = 0.734$, $\Delta t = 0.001$ mm, $t = 5.190$ mm, $\Delta\lambda = 0.1$ nm and $\lambda = 1200$ nm in the resulting equations. The errors for the two procedure are $\Delta k = 1 \times 10^{-7}$ and $\Delta n = 0.013$.

The slab sample has to be optically flat plane parallel plate at the point of measuring the reflectance and the transmittance with

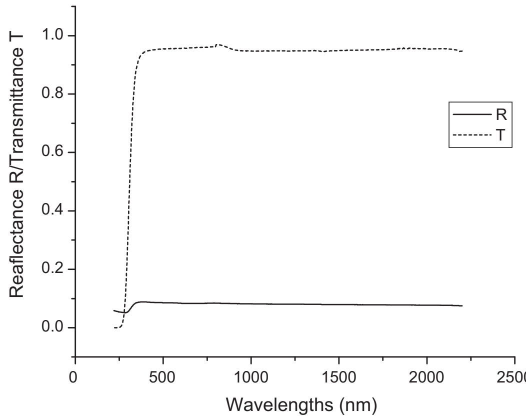

Fig. 3. Reflectance and transmittance of Corning glass sample.

a spectrophotometer. If the slab surface is rough with root mean square roughness, σ, then the measured reflectance, R_m, and transmittance, T_m, have to be corrected using the next two equations [12]:

$$R = R_m \exp\left\{-\frac{16\pi^2\sigma^2}{\lambda^2}\right\} \quad (37)$$

$$T = T_m \exp\left\{-\frac{16\pi^2\sigma^2}{\lambda^2}\right\} \quad (38)$$

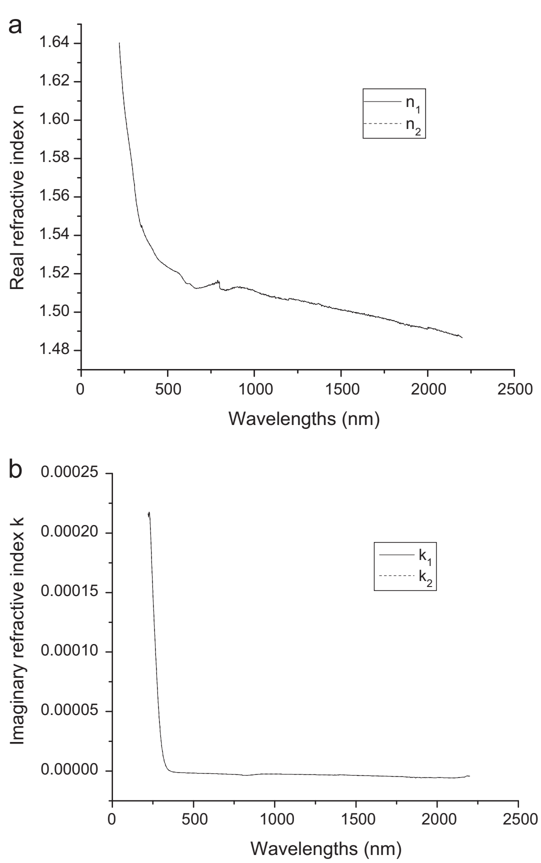

Fig. 4. (a) Real refractive indices of Corning glass sample. (b) Imaginary refractive indices of Corning glass sample.

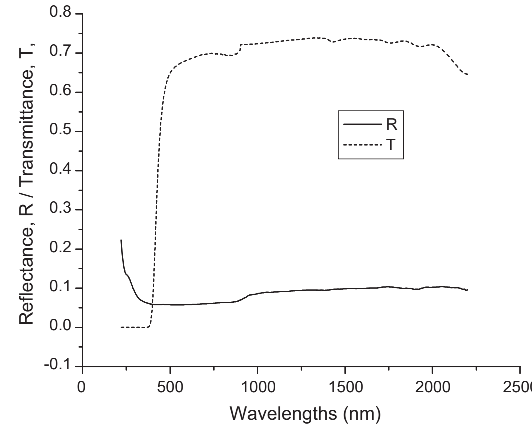

Fig. 5. Reflectance and transmittance of the Borate glass sample.

7. Experimental

Two glassy slab samples are tested experimentally. The first sample is a Corning glass of thickness 0.920 mm and the other is a Borate glass with thickness 5.190 mm. A computer controlled two-beam spectrophotometer (JASCO Corp., Japan) is used to record the spectral reflectance R, and the spectral transmittance T, data of the slab plane parallel samples. The accuracy of measuring photometric reflectance and transmittance is ± 0.003 with an incidence angle of $5.0 \pm 0.1^\circ$ to the normal to external slab faces. The propagation angle inside the slab samples is reduced below 5° due to refraction. The measurements are carried out at room temperature for the entire spectral range 2200–220 nm. The base line reflectance and

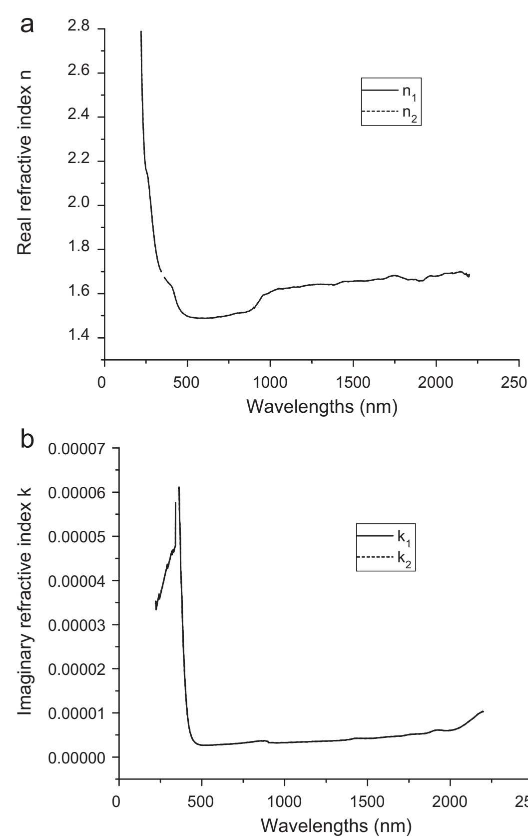

Fig. 6. (a) Real refractive indices of the Borate glass sample. (b) Imaginary refractive indices of the Borate glass sample.

transmittance of the spectrophotometer are recorded and used for normalization of the samples measurements.

8. Results

Figs. 3 and 5 show the measured reflectance and transmittance of the Corning and Borate glass samples respectively. It is clear that, the transmittance exhibits a steep depression at extreme ultraviolet end of spectrum indicating the existence of strong absorption band. The cutoff wavelength of the absorption band for the Corning sample exists at 220 nm while for the Borate sample at 358 nm. Also the two samples show high transmittance and low reflectance across the measured spectral range. Figs. 4(a and b) and 6(a and b) show the deduced real (n_1 and n_2) and imaginary (k_1 and k_2) refractive indices of the two glass samples across the measured spectral range. The first procedure gives n_1 and k_1 while the second one gives n_2 and k_2. The two procedures retrieve exactly the refractive indices for the two glass samples. It is clear that, the measured refractive indices exhibit normal dispersion away from the absorption band. The extracted refractive indices data are in a good agreement with published ones for Corning [8] and Borate [13] glasses.

9. Conclusion

Spectrophotometers (UV–VIS-IR) with high accuracy for measuring spectra across a wide range of wavelengths are available in different labs. Optical spectrophotometers work in different modes to measure optical density, absorbance, transmittance or reflectance [14]. Spectral reflectance, transmittance of a thick planar slab can be easily measured at normal incidence. Analytical expressions for slab refractive indices in terms of reflectance, R, and transmittance, T, at normal incidence have been deduced by two procedures. The two procedures can be used for transparent and semitransparent materials but not for nontransparent ones. These two procedures are applicable for thick slabs which give no interference fringes. Other researchers are encouraged to use the proposed procedures for the refractive indices determination with spectrophotometric measurements.

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