DETERMINATION OF REFRACTIVE INDICES OF THIN TRANSPARENT LAYERS FROM THE TRANSMITTANCE OR REFLECTANCE MEASURED AT THE WAVENUMBER OF AN INTERFERENCE PEAK

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1. Introduction

The thicknesses of thin transparent layers are often determined by an interference method: by varying the wavenumber or the angle of incidence of the light, the transmitted or reflected intensity varies nearly periodically because of interference and has its extreme values at the wavenumbers where the interference condition

$$4d\sqrt{n^2 - \sin^2 \vartheta} = \frac{m}{\tilde{\nu}_{ext}} \tag{1}$$

is met. (n is the refractive index of the layer, ϑ is the angle of incidence, d is the film thickness, m is the order of interference, and $\tilde{\nu}_{ext}$ is the wavenumber of an interference peak.)

In the following, a normal incidence is assumed and the transmittance or reflectance is considered as function of the wavenumber (a spectrum is recorded). Then the interference condition (1) reduces to

$$4n\,d = \frac{m}{\tilde{\nu}_{ext}} \tag{2}$$

The film thickness can be calculated from $\tilde{\nu}_{ext}$ by means of (2) if the refractive index n at $\tilde{\nu}_{ext}$ is known. It will be shown that the refractive index can be calculated relatively simply from the extreme intensities of the transmittance or reflectance spectrum in the following cases:

a) a single thin layer,
b) a thin layer on an infinitely thick substrate,
c) a thin layer on a thick substrate,
d) two thin layers of the same thickness and material on both sides of a thick substrate.

Both the thin layer and the substrate are assumed to be transparent. The term "infinitely thick substrate" means that the beam reflected from the sample contains no component from the back side of the substrate.

In the following, the expressions for transmittance or reflectance will be deduced for the four cases above, applying methods by ABELÈS and by WOLTER for stratified media [1], [2]. From the resulting formulae, expressions for extremes of intensity are determined. In cases *a)* and *b)* known formulae are arrived at. In the cases *c)* and *d)* the expressions of transmittance contain a rapidly oscillating interference term arising from the substrate. If the resolution of the spectrometer is less than the period of the dense interference fringes, the spectrometer cannot follow the rapid changes in the transmission and records an averaged spectrum. Accordingly, expressions for the average transmittance will be deduced by integrating the theoretical transmittance spectrum over one period of an interference fringe, and the extremes of this average transmittance will be determined.

Then the conditions will be discussed under which the refractive index can be determined unambiguously. Finally, the refractive indices of thermally grown silica films on silicon substrates will be calculated from the transmittance spectrum measured in the infrared region.

2. Matrix representation of a system of plan-parallel layers

Consider a plane light wave incident on the surface of a system of m layers. (See Fig. 1). A travelling wave and a reflected one appear in each medium. At normal incidence, the waves travelling into the $+z$ and $-z$ direction in the j-th medium can be represented by electric field components $E_j^+(z)$ and $E_j^-(z)$, respectively:

$$E_j^+(z) = E_j^{0+} \exp\left(-i\,\omega \frac{N_j}{c} z\right),$$

$$E_j^-(z) = E_j^{0-} \exp\left(i\,\omega \frac{N_j}{c} z\right), \tag{3}$$

where E_j^{0+} and E_j^{0-} are the complex amplitudes of the electric field intensity in the j-th layer in the waves travelling in directions $+z$ and $-z$, respectively; N_j is the complex refractive index of the j-th medium

$$N_j = n_j - ik_j \tag{3a}$$

ω is the angular frequency of the light, and c is the light velocity in vacuum.

Owing to the linearity of the Maxwell equations and of the boundary

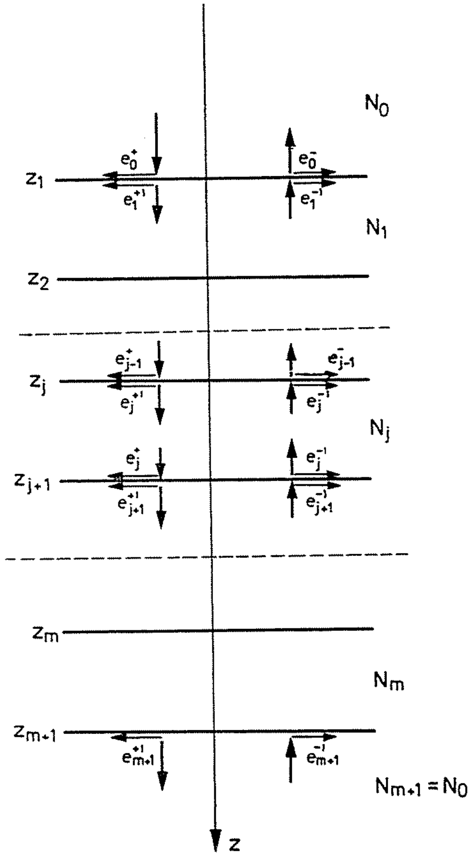

Fig. 1. Propagation of the electric field in a stratified medium

conditions, the values of the electric field components at two different points of the system are linearly related that can be expressed in matrix form.

Let us denote the values of electric field components on the boundaries of the j-th medium by $e_j^{+\prime}$, $e_j^{-\prime}$, e_j^+, e_j^-,

$$e_j^{+\prime} \equiv E_j^+(z_j) \qquad e_j^+ \equiv E_j^+(z_{j+1})$$
$$e_j^{-\prime} \equiv E_j^-(z_j) \qquad e_j^- \equiv E_j^-(z_{j+1}) \tag{4}$$

where z_j is the co-ordinate z of the boundary between the $j-1$-th and j-th media.

The relationship between the electric field components at the two sides of the j-th boundary can be expressed in the following form

$$\begin{bmatrix} e_{j-1}^+ \\ e_{j-1}^- \end{bmatrix} = \frac{1}{t_{j-1,j}} \begin{bmatrix} 1 & r_{j-1,j} \\ r_{j-1,j} & 1 \end{bmatrix} \begin{bmatrix} e_j^{+\prime} \\ e_j^{-\prime} \end{bmatrix} \equiv A_{j-1,j} \begin{bmatrix} e_j^{+\prime} \\ e_j^{-\prime} \end{bmatrix} \tag{5}$$

where $t_{j-1,j}$ and $r_{j-1,j}$ are defined as the transmission and reflection coefficients (or Fresnel coefficients) of the j-th boundary with respect to the $+z$ direction. By normal incidence, they are

$$t_{j-1,j} = \frac{2\,N_{j-1}}{N_{j-1}+N_j}; \qquad r_{j-1,j} = \frac{N_{j-1}-N_j}{N_{j-1}+N_j} \tag{6}$$

Between the electric field components at the first and second boundary of the j-th medium, the following relations exist:

$$\begin{bmatrix} e_j^{+\prime} \\ e_j^{-\prime} \end{bmatrix} = \begin{bmatrix} e^{i\delta j} & 0 \\ 0 & e^{-i\delta j} \end{bmatrix} \begin{bmatrix} e_j^{+} \\ e_j^{-} \end{bmatrix} \equiv \mathbf{B}_j \begin{bmatrix} e_j^{+} \\ e_j^{-} \end{bmatrix} \tag{7}$$

where

$$\delta_j = 2\pi\tilde{\nu}\; N_j\, d_j \tag{8}$$

and d_j is the thickness of the j-th layer.

The matrix representing the system of m layers will be the product of the respective matrices A and B.

$$\begin{bmatrix} e_0^{+} \\ e_0^{-} \end{bmatrix} = \mathbf{C} \begin{bmatrix} e_{m+1}^{+\prime} \\ e_{m+1}^{-\prime} \end{bmatrix}; \qquad \mathbf{C} \equiv \left(\prod_{j-1}^{m} \mathbf{A}_{j-1}\, \mathbf{B}_j \right) \mathbf{A}_{m,\, m+1} \tag{9}$$

The elements of matrix $\mathbf{C}$ are related to the transmission and reflection coefficients of the whole system:

When the light enters the system from direction $-z$, there is no reflected beam in the $m+1$-th medium. The reflection and transmission coefficients of the whole system referring to the direction $+z$, can be defined as

$$t^{+} \equiv \left. \frac{e_0^{+\prime}}{e_0^{+}} \right|_{e_{m+1}^{-\prime} = 0}; \qquad r^{+} \equiv \left. \frac{e_0^{-}}{e_0^{+}} \right|_{e_{m+1}^{-\prime} = 0} \tag{10a}$$

When the light enters from the direction $+z$ there will be no reflected beam in the 0-th medium, and the transmission and reflection coefficients with respect to the $-z$ direction are

$$t^{-} \equiv \left. \frac{e_0^{-}}{e_{m+1}^{-\prime}} \right|_{e_0^{+} = 0}; \qquad r^{-} = \left. \frac{e_{m+1}^{+\prime}}{e_{m+1}^{-\prime}} \right|_{e_0^{+} = 0} \tag{10b}$$

From (10a) and (10b) and by definition of the matrix $\mathbf{C}$, the elements of $\mathbf{C}$

can be expressed by the transmission and reflection coefficients of the whole system:

$$c_{11} = \frac{1}{t^{+}} \qquad c_{21} = \frac{r^{+}}{t^{+}}$$

$$c_{1} = \frac{r^{-}}{t^{+}} \qquad c_{22} = \frac{t^{-}t^{+} + r^{-}r^{+}}{t^{+}} \tag{11}$$

Since intensity can be measured, expressions for the light intensity are needed. The expressions for the intensity of the incident, reflected and transmitted light beams are [with notations in (4)]:

$$I_0 = \frac{1}{2c\,\mu_0} n_0 \,|\, e_0^{+} \,|^2$$

$$I_t = \frac{1}{2c\,\mu_{m+1}} n_{m+1} \,|\, e_{m+1}^{+\prime} \,|^2$$

$$I_r = \frac{1}{2c\,\mu_0} n_0 \,|\, e_0^{-} \,|^2 \tag{12}$$

The transmittance of the system is defined as the ratio of transmitted to incident light intensity and equals:

$$T \equiv \frac{I_t}{I_0} = \frac{|\, e_{m+1}^{+1} \,|^2}{|\, e_0^{+} \,|^2} = |\, t^{+} \,|^2 \frac{n_{m+1}}{n_0} \tag{13a}$$

Similarly, the reflectance is:

$$R \equiv \frac{I_r}{I_0} = \frac{|\, e_0^{-} \,|^2}{e_0{}^{+} \,|^2} = |\, r^{+} \,|^2 \tag{13b}$$

3. Formulae for the transmittance and reflectance

In cases *a)* and *b)* there is a single layer with two boundaries in the system, so its **C** matrix is [from (9), (5) and (8)]:

$$\mathbf{C} = \mathbf{A}_{01}\,\mathbf{B}_1\,\mathbf{A}_{12} = \frac{1}{t_{01}\,t_{12}} \begin{bmatrix} e^{i\delta 1} + r_{01}\,r_{12}\,e^{-i\delta 1}, & e^{i\delta 1}\,r_{12} + e^{-i\delta 1}\,r_{01} \\ e^{i\delta 1}\,r_{01} + e^{-i\delta 1}\,r_{12}, & e^{i\delta 1}\,r_{01}\,r_{12} + e^{-i\delta 1} \end{bmatrix} \tag{14}$$

By (14) and (11), the transmission and reflection coefficients are:

$$t^{+} = \frac{1}{c_{11}} = \frac{t_{01}\, t_{12}}{e^{i\delta 1} + r_{01}\, r_{12}\, e^{-i\delta 1}} \qquad r^{+} = \frac{c_{21}}{c_{11}} = \frac{r_{01}\, e^{i\delta 1} + r_{12}\, e^{-i\delta 1}}{e^{i\delta 1} + r_{01}\, r_{12}\, e^{-i\delta 1}} \tag{15}$$

Since the refractive index of a transparent material is a real quantity, so $t_{j-1,j}$, δ_j and $r_{j-1,j}$ are real, too, and the transmittance and reflectance are:

$$T = \frac{(t_{01}\, t_{12})^2\, n_2}{(1 + r_{01}^2\, r_{12}^2 + 2\, r_{01}\, r_{12} \cos 2\, \delta_1)\, n_0}$$

$$R = \frac{r_{01}^2 + r_{12}^{+} + 2\, r_{01}\, r_{12} \cos 2\, \delta_1}{1 + r_{01}^2\, r_{12}^2 + 2\, r_{01}\, r_{12} \cos 2\, \delta_1} \tag{16}$$

In case *c)* there are two layers with three boundaries in the system. As a media "0" and "3" are the same (air) the indices "3" are replaced by "0". The **C** matrix of the system is

$$\mathbf{C} = \mathbf{A}_{01}\, \mathbf{B}_1\, \mathbf{A}_{12}\, \mathbf{B}_2\, \mathbf{A}_{20}$$

and the transmission coefficient:

$$t^{+} = \frac{t_{01}\, t_{12}\, t_{20}}{e^{i\delta 2}\, (e^{i\delta 1} + r_{01}\, r_{12}\, e^{-i\delta 1}) + r_{20}\, e^{-i\delta 2}\, (r_{12}\, e^{i\delta 1} + r_{01}\, e^{-i\delta 1})} \tag{17}$$

Introducing notations A, B, φ_1, φ_2,

$$A e^{i\varphi 1} \equiv e^{i\delta 1} + r_{01}\, r_{12}\, e^{-i\delta 1}$$

$$B e^{i\varphi 2} \equiv e^{i\delta 1}\, r_{12} + e^{-i\delta 1}\, r_{01} \tag{18}$$

(17) simplifies into

$$t^{+} = \frac{t_{01}\, t_{12}\, t_{20}}{A\, e^{i\delta 2} + B\, r_{20} e^{-i\delta 2}}$$

and the expression of the transmittance is:

$$T = |t^{+}|^2 = \frac{(t_{01}\, t_{12}\, t_{20})^2}{A^2 + B^2 + 2\, A\, B\, r_{20} \cos(\varphi_1 - \varphi_2 + 2\, \delta_2)} \tag{19}$$

In case *d)* there are three layers with four boundaries, and the "0" medium is the same as the "4" one, and the "1" as the "3" one. The matrix **C** for this system

$$\mathbf{C} = \mathbf{A}_{01}\,\mathbf{B}_1\,\mathbf{A}_{12}\,\mathbf{B}_2\,\mathbf{A}_{21}\,\mathbf{B}_1\,\mathbf{A}_{10}$$

Using the relations

$$r_{j-1,j} = -r_{j,j-1}; \quad t_{j-1,j}\,t_{j,j-1} = 1 - r^2_{j-1,j} \tag{20}$$

we get for t^+

$$t^+ = \frac{(1-r_{12}^2)(1-r_{01}^2)}{e^{i\delta 2}\,(e^{i\delta 1} + r_{01}\,r_{12}\,e^{-i\delta 1})^2 - e^{-i\delta 2}\,(r_{12}\,e^{i\delta 1} + r_{01}\,e^{-i\delta 1})}$$

and for the transmittance, with the notations in (18):

$$T = \frac{(1-r_{01}^2)^2\,(1-r_{12}^2)^2}{A^4 + B^4 - 2\,A^2\,B^2 \cos(2\,\varphi_1 - 2\,\varphi_2 + 2\,\delta_2)} \tag{21}$$

4. Formulae for the extremes of intensity

The transmittance and reflectance depend on wavenumber through the refractive indices and through the phase changes in the layers. Since the refractive index is a slowly varying function of wavenumber in the region of normal dispersion, and the phases, δ_j-s, are proportional to the wavenumber, the positions of intensity extremes can be assumed to be determined mainly by terms containing the phases. In this case, the intensity has its extremes at the wavenumbers where

$$\cos 2\,\delta_j = \pm 1$$

In the following, the values of transmittance or reflectance belonging to $\cos 2\,\delta_1 = 1$ will be denoted by T_1 and R_1 and the ones belonging to $\cos 2\,\delta_1 = -1$, by T_2 and R_2, respectively; T_1, R_1, T_2 and R_2 can be either minima or maxima of the spectrum, according to the values of the refractive indices.

a) *A single thin layer*

The expressions for the extremes of transmittance are get from (16), using (20):

$$T_1 = \left(\frac{t_{01}\,t_{12}}{1 + r_{01}\,r_{10}}\right)^2 \equiv 1\,; \qquad T_2 = \frac{(t_{01}\,t_{10})^2}{(1 - r_{01}\,r_{10})} = \left(\frac{2\,n_0\,n_1}{n_0^2 + n_1^2}\right)^2 \tag{22}$$

directly implying that T_2 is always a minimum in the spectrum. (The transmittance has its minimum at $\cos 2\,\delta_1 = -1$ for every value of n_1.)

b) *A thin layer on an infinitely thick substrate*

We get from (16):

$$R_1 = \left(\frac{r_{01} + r_{12}}{1 + r_{01} r_{12}}\right)^2 = \left(\frac{n_0 - n_2}{n_0 + n_2}\right)^2; \qquad R_2 = \left(\frac{r_{01} - r_{12}}{1 - r_{01} r_{12}}\right)^2 = \left(\frac{n_0 n_2 - n_1^2}{n_0 n_2 + n_1^2}\right)^2 \tag{23}$$

Since

$$R_1 - R_2 = \frac{4 r_{01} r_{12} (1 - r_{01}^2)(1 - r_{12})^2}{1 - r_{01}^2 r_{12}^2}$$

R_2 is a minimum and R_1 a maximum if

$$\text{sign}\,(r_{12}) = \text{sign}\, r_{01} \quad \text{that is} \quad \text{sign}\,(n_0 - n_1) = \text{sign}\,(n_1 - n_2) \tag{24}$$

c) *and* d) *Thin layer on a thick substrate*

Cases *c)* and *d)* involve two interference terms in the expressions of transmittance (19), (21). On account of the interference term arising from the substrate (it is the term containing δ_2) the transmittance can greatly vary within the spectral slit width. Because of the finite slit width, the measured spectrum $\overline{T}(\tilde{\nu})$ will differ from $T(\tilde{\nu})$, the true one.

$$\overline{T}(\tilde{\nu}) = \int_{-\infty}^{\infty} T(\tilde{\nu}')\, s(\tilde{\nu}' - \tilde{\nu})\, d\tilde{\nu}' \tag{25}$$

$s(\tilde{\nu}' - \tilde{\nu})$ being the spectral slit function. For triangular slit function

$$s(\tilde{\nu}' - \tilde{\nu}) \equiv 1 - \left(\frac{|\tilde{\nu} - \tilde{\nu}'|}{\Delta\tilde{\nu}}\right)\frac{1}{\Delta\tilde{\nu}} \qquad \text{for} \quad \tilde{\nu} - \Delta\tilde{\nu} \leq \tilde{\nu}' \leq \tilde{\nu} + \Delta\tilde{\nu}$$

$$s(\tilde{\nu}' - \tilde{\nu}) \equiv 0 \qquad \text{for} \quad |\tilde{\nu} - \Delta\tilde{\nu}| > \Delta\tilde{\nu}$$

(where $\Delta\tilde{\nu}$ is the spectral slit width) the measured transmittance will be:

$$\overline{T}(\tilde{\nu}) = \frac{1}{\Delta\tilde{\nu}} \int_{\tilde{\nu}-\Delta\tilde{\nu}}^{\tilde{\nu}+\Delta\tilde{\nu}} T(\tilde{\nu}') \left[1 - \frac{|\tilde{\nu}' - \tilde{\nu}|}{\Delta\tilde{\nu}}\right] d\tilde{\nu}' \tag{26}$$

In cases *c)* and *d)* $T(\tilde{\nu})$ is of the form

$$T(\tilde{\nu}) = \frac{c}{a^2 + b^2 - 2\,ab\cos\psi(\tilde{\nu})} \equiv \tau_{\tilde{\nu}}(\psi) \tag{27}$$

where $\psi(\tilde{\nu}) = \varphi_1 - \varphi_2 + 2\delta_2$ in case *c)*
$\psi(\tilde{\nu}) = 2\varphi_1 - 2\varphi_2 + 2\delta_2$ in case *d)*
while a, b, c depend on the wavenumber through the refractive indices only. As the refractive index is a slowly varying function of wavenumber in the region of normal dispersion, it can be assumed to be constant at least for a few periods of the term containing $\cos\psi$, and so can be a, b and c. Then $\tau_{\tilde{\nu}}(\psi)$ is a periodic function of ψ, of a period 2π and can be expanded into Fourier series. (The Fourier coefficients will be functions of the wavenumber.) $\tau_{\tilde{\nu}}(\psi)$ being an even function, its Fourier series contains only cosine terms:

$$\tau_{\tilde{\nu}}(\psi) = \sum_{n=0}^{\infty} a_n^{(\tilde{\nu})} \cos(n\psi) \tag{29}$$

The measured transmittance can be expressed as

$$\overline{T}(\tilde{\nu}) = \frac{1}{\Delta\tilde{\nu}} \int_{\tilde{\nu}-\Delta\tilde{\nu}}^{\tilde{\nu}+\Delta\tilde{\nu}} \tau_{\tilde{\nu}'}(\psi(\tilde{\nu}')) \left[1 - \frac{|\tilde{\nu}' - \tilde{\nu}|}{\Delta\tilde{\nu}}\right] d\tilde{\nu}' \tag{30}$$

Considering ψ as the independent variable in the integral (30):

$$\overline{T}(\tilde{\nu}) \equiv \bar{\tau}_{(\tilde{\nu})}(\psi(\tilde{\nu})) = \frac{1}{\Delta\psi} \int_{\psi-\Delta\psi}^{\psi+\Delta\psi} \tau(\psi') \left[1 - \frac{|\psi' - \psi|}{\Delta\psi}\right] d\psi' \tag{31}$$

where $$\Delta\psi = 4\pi n_2 d_2 \Delta\tilde{\nu}$$

and substituting the Fourier series (29) for $\tau\tilde{\nu}(\psi)$ and integrating by terms, we get

$$\bar{\tau}_{\tilde{\nu}}(\psi) = \frac{1}{\Delta\psi} \int_{\psi-\Delta\psi}^{\psi+\Delta\psi} \sum_{n=0}^{\infty} a_n \cos(n\psi') \left[1 - \frac{|\psi' - \psi|}{\Delta\psi}\right] d\psi' =$$

$$= \sum_{n=0}^{\infty} \left(\frac{\sin\frac{n\Delta\psi}{2}}{\frac{n\Delta\psi}{2}} \right)^2 a_n \cos(n\psi) \tag{32}$$

It can be seen from (32) that the Fourier coefficients of the measured spectrum differ from the original ones by the factors

$$\left(\frac{\sin\frac{n\Delta\psi}{2}}{\frac{n\Delta\psi}{2}} \right)^2$$

The Fourier coefficients of higher order decrease at least as $1/n^2$, so the spectrometer "smoothes" the rapid changes of the spectrum. If

$$n_2 d_2 > \frac{5}{\pi} \frac{1}{\Delta\tilde{\nu}}$$

holds for the optical density of the substrate, even the first Fourier coefficient is less than 0.01. In the following this is assumed to hold and the measured spectrum is approached by its zeroth-order Fourier component, that is, by

$$\bar{T}(\tilde{\nu}) \approx \frac{1}{2\pi} \int_{-\pi}^{\pi} \tau_{\tilde{\nu}}(\psi)\, d\psi \tag{33}$$

The expressions for the measured transmittance (33) can be treated like the ones for cases *a)* and *b)*. It can be assumed that the extremes of $\bar{T}$ lie at the wavenumbers where $\cos 2\delta_1 = \pm 1$, the extremes of transmittance will be denoted again by T_1 and T_2, respectively.

After substituting (27) for (33) and integrating, we get

$$\bar{T}(\tilde{\nu}) = \frac{c}{|a^2 - b^2|} \tag{34}$$

c) *A thin layer on a much thicker substrate*

From (34) and (19) one gets

$$\bar{T}(\tilde{\nu}) = \frac{t_{01}^2 t_{12}^2 t_{20}^2}{A^2 - B^2 r_{20}^2} \tag{35}$$

After having replaced (18) for A and B, the extremes of (35) are:

$$T_1 = \frac{t_{01}^2 t_{12}^2 t_{20}^2}{(1 + r_{01} r_{12})^2 - r_{20}^2 (r_{01} + r_{12})^2} = \frac{2 n_0 n_2}{n_0^2 + n_2^2}$$

$$T_2 = \frac{t_{01}^2 t_{12}^2 t_{20}^2}{(1 - r_{01} r_{12})^2 - r_{20} (r_{01} - r_{12})^2} = \frac{4 n_0 n_1^2 n_2}{(n_1 + n_2)^2 (n_1^2 + n_0^2)} \tag{36}$$

Since

$$\frac{1}{T_1} - \frac{1}{T_2} = \frac{4 r_{01} r_{12} (1 - r_{20}^2)}{t_{01}^2 t_{12}^2 t_{20}^2}$$

T_1 is minimum and T_2 maximum if

$$\operatorname{sign}(r_{01}) = \operatorname{sign}(r_{12})$$

d) *Thin layers on both sides of a thick substrate*

From (34) and (21):

$$\bar{T}(\tilde{\nu})\ \frac{(1-r_{12}^2)^2\,(1-r_{01}^2)^2}{A^4-B^4} = \frac{(1-r_{01}^2)^2\,(1-r_{12}^2)^2}{(1+r_{12}^2)\,(1+r_{01}^2)+4\,r_{01}\,r_{12}\cos 2\,\delta_1}$$

The extreme values are

$$T_1 = \frac{(1-r_{01}^2)\,(1-r_{12}^2)}{(1+r_{12}^2)\,(1+r_{01}^2)+4\,r_{01}\,r_{12}} = \frac{2\,n_0\,n_2}{n_0^2+n_2^2}$$

$$T_2 = \frac{(1-r_{01}^2)\,(1-r_{12}^2)}{(1+r_{12}^2)\,(1+r_{01}^2)-4\,r_{01}\,r_{12}} = \frac{2\,n_0\,n_1^2\,n_2}{n_1^4+n_0^2\,n_2^2} \tag{37}$$

From the formulae for T_1 and T_2, it can be shown easily that T_1 is a minimum and T_2 a maximum if

$$\text{sign}\ (r_{01}) = \text{sign}\ (r_{12}).$$

5. Determination of the refractive index of the thin layer from the extreme values of intensity

The refractive index of the thin layer (n_1) appears in, hence can be computed from the formulae for T_2 (or R_2) from among (22), (23), (35), (36). Let us introduce the following notations:

$$x = n_1^2/n_0 n_2 \ \text{(for case } a)\text{: } x = n_1/n_0)$$

$$Y = \text{ch}\,(\ln x)\ \text{(for case } a),\ c),\ d))$$

$$Y = \left|\frac{1-X}{1+X}\right| \qquad \text{(for the case } b)) \tag{38}$$

Y and the intensities are related as:

$$a)\ \ Y = 1/\sqrt{T_2}$$

$$b)\ \ Y = \sqrt{R_2}$$

$$c)\ \ Y = 2/T_2 - \text{ch}(\ln(n_2/n_0))$$

$$d)\ \ Y = 1/T_2 \tag{39}$$

The solution of (38) for x is:

$$X = Y \pm \sqrt{Y^2 - 1} \quad \text{(in cases } a), c), d)) \tag{40a}$$

$$X = \frac{1 \mp Y}{1 \pm Y} \quad \text{(in case } b)) \tag{40b}$$

Since the functions ch (ln x) and $|1 - x|/|1 + x|$ have their extremes at $x = 1$, for a given value of T_2 or R_2, the smaller value of x must be taken in (40) if $x < 1$ and the greater one if $x > 1$, that is, the minus sign is taken in (40a) if $x < 1$ and the plus one, if $x > 1$; and in (40b), the minus sign is in the numerator if $x < 1$, and in the denominator, if $x > 1$.

6. Discussion

Formulae (40) yield the refractive index of a thin transparent layer from the transmittance or reflectance measured at wavenumbers where the optical thickness of the layer is an odd multiple of the half wavelength. But that extreme can be either a maximum or a minimum in the spectrum depending on the refractive index of the substrate, so the value

$$[\text{sign}\,(n_0 - n_1)]\,[\text{sign}\,(n_1 - n_2)]$$

is needed for selecting the suitable interference peak. That means, it has to be known whether the refractive index of the layer is smaller or greater than that of the substrate.

The other uncertainty comes from the fact that the formulae (40) give two solutions for x, according to the two signs. For the selection of the right sign, it has to be known whether the refractive index of the layer is smaller or greater than the square root of that of the substrate. [See (38).]

As a final result, the refractive index of the thin layer can be determined by the method described if one knows its range:

$$\begin{aligned} \text{I:}\ & n_1 < \sqrt{n_2} < n_2 \\ \text{II:}\ & \sqrt{n_2} < n_1 < n_2 \\ \text{III:}\ & n_1 > n_2 > \sqrt{n_2} \end{aligned} \tag{41}$$

7. Application of the method

In order to show the applicability of the described method, the refractive indices of thermally grown silica layers on silicon slices (with impurity concentration of 10^{15} atoms/cm^3) were determined in the infrared region and compared with published refractive index data for silica glass [3]. (The optical properties of the thermal SiO_2 films are very similar to those of silica glass [4].) The thicknesses of the substrate slices were about 0.2 mm, those of the oxide layers were 400 to 700 nm. The transmission spectra were recorded by a Zeiss UR-10 spectrophotometer in the region 1800 to 5000 cm^{-1}. In this region, both the silicon and the silica films are transparent; the refractive index of the silicon is 3.42, that of the silica being about 1.4, the condition

$$n_1 < \sqrt{n_2} < n_2$$

holds.

Oxide layers were grown on both sides of the silicon slices; and owing to the condition of growth, both oxide layers were of the same thickness. So the samples corresponded to model *d)*. Since $n_1 < n_2$; T_2 is a maximum and since $x = n_1^2/n_0 n_2 < 1$, the minus sign has to be taken before the square root sign in (40a). Taking into account the conditions above, the refractive index of the oxide layer becomes:

$$n_1 = \sqrt{n_2 \left(\frac{1}{T_2} - \sqrt{\frac{1}{T_2^2} - 1} \right)} \tag{42}$$

But (42) can be applied only if the boundary surfaces of the sample are perfect planes, that is, if the roughness of the surfaces is much below the wavelength. Otherwise, the intensity decreases because of light scattering, and its value cannot be used for the determination of the refractive index. The suitable polish of the substrate was checked by measuring the transmittance of the pure Si slice and comparing to the theoretical one. From (16), the transmittance of a single layer is

$$\frac{(1 - r_{02}^2)^2}{1 + r_{02}^4 - 2\, r_{02}^2 \cos 2\, \delta_2}$$

and the averaged transmittance

$$\bar{T}(\tilde{\nu}) = \frac{1 - r_{02}^2}{1 + r_{02}^2}$$

Replacing the refractive index $n_2 = 3.42$ of Si yields the value $\bar{T}(\tilde{\nu}) = 0.54$, in agreement with the measured one within the reading error of the spectrometer. In the spectra of a few samples, dense interference fringes, arising from the substrate, were seen. In these cases, we calculated the refractive index from the arithmetic mean of the transmittance at the peaks [assuming the amplitude of the second harmonic to be negligible in (29) because of (32)].

The results have been compiled in Table I, containing the measured transmittance extremes T_{max}, the wavenumbers of the interference peaks $\tilde{\nu}_{max}$, the calculated refractive indices n and refractive indices published for silica glass n_i.

Fig. 2 shows the accuracy of the refractive index measurements as a function of T_{max}, ΔT being the accuracy of transmittance measurement.

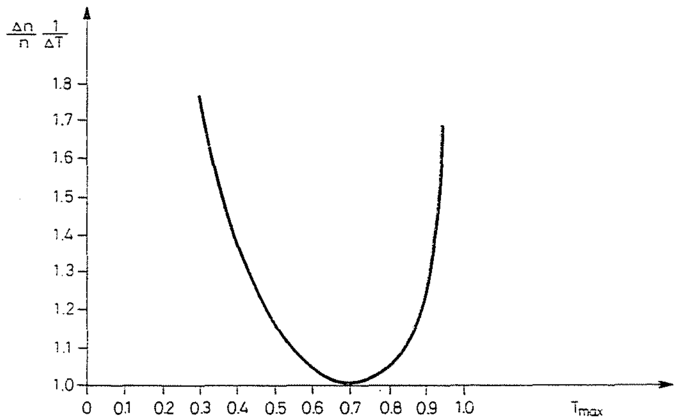

Fig. 2. Relative accuracy of the refractive index ($\Delta n/n$) versus maximum transmittance T_{max}. (ΔT is the accuracy of transmittance measurement.)

Table I

Refractive indices of silica layers on silicon slices determined by infrared interference method, compared to the refractive indices published in [3] for silica glass

Sample	$\tilde{\nu}_{max}$ (cm^{-1})	T_{max}	n	n_i
1	2250	0.840	1.365	1.371
2	2450	0.845	1.373	1.387
3	2600	0.850	1.389	1.395
4	2900	0.855	1.399	1.408
5	3200	0.870	1.414	1.417
6	3330	0.870	1.414	1.419
7	3420	0.875	1.423	1.421
8	3800	0.880	1.431	1.427

($\tilde{\nu}_{max}$ is the wavenumber of maximum transmittance, T_{max} is the maximum value of transmittance, n is the calculated refractive index and n_i is the published refractive index at $\tilde{\nu}_{max}$.)

Summary

The thickness of a thin transparent layer on a transparent substrate can be determined from the wavenumber of an interference peak and the refractive index of the layer at the same wavenumber. A method is presented for determining the refractive index of a thin transparent layer from the transmittance or reflectance measured at the wavenumber of an interference peak. The following systems are considered:

a) a single thin layer
b) a thin layer on an infinitely thick substrate
c) a thin layer on a thick substrate
d) two thin layers of the same thickness and material on both sides of a thick substrate.

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