INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF OPTICS A: PURE AND APPLIED OPTICS

J. Opt. A: Pure Appl. Opt. 4 (2002) 400–403 PII: S1464-4258(02)34255-7

Complex refractive index of a slab from reflectance and transmittance: analytical solution

Enrico Nichelatti

ENEA - CR Casaccia, FIS-OTT, Via Anguillarese, 301–00060 S Maria di Galeria, Rome, Italy

E-mail: nichelatti@casaccia.enea.it

Received 26 February 2002, in final form 19 April 2002
Published 23 May 2002
Online at stacks.iop.org/JOptA/4/400

Abstract
Analytical expressions are derived that allow one to calculate the complex refractive index of a planar slab from normal-incidence intensity reflectance and transmittance.

Keywords: Complex refractive index, slab, reflectance, transmittance, extinction coefficient, inverse problem, optical constants, substrate

1. Introduction

For the reliable optical characterization of a thin film, knowing the optical constants of the substrate on which the film lies is very important. If the substrate is a partially absorbing slab with plane-parallel faces, measuring its intensity reflectance and transmittance spectra, $R(\lambda)$ and $T(\lambda)$, with a spectrophotometer—where λ is the wavelength of light in vacuum—before the film deposition is a method, commonly adopted for its experimental simplicity, of deducing the complex refractive-index dispersion of the substrate material.

To the author's knowledge, explicit formulae for calculating *analytically* the complex refractive index, $n(\lambda) - ik(\lambda)$, of a substrate from $R(\lambda)$ and $T(\lambda)$ have been never reported in the literature. In some papers about thin-film optical characterization, where the problem of finding the optical constants of the substrate is explicitly discussed, the solution is found by resorting to numerical means [1, 2]. In other papers, more focused on deriving the optical constants of a slab from spectrophotometric measurements, an iterative numerical procedure is adopted as a preliminary step to solving the problem [3, 4].

The aim of this paper is to derive the fully analytical solution to the inverse problem, indicated as $(R, T) \to (n, k)$, consisting of finding n and k from R and T for a slab with plane-parallel faces. The proposed analytical solution represents a simpler way, as compared to numerical methods, for calculating $n(\lambda)$ and $k(\lambda)$: in principle, by using the analytical solution this task can be accomplished at any chosen wavelength even with the help of a common pocket calculator.

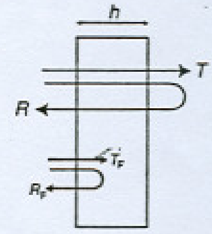

Figure 1. Partially absorbing slab with plane-parallel faces: h, geometrical thickness of the slab: R and T, intensity reflectance and transmittance overall coefficients of the slab; R_F and T_F, intensity reflectance and transmittance coefficients of a single face.

2. Reflectance and transmittance of a slab (direct problem)

Before tackling the inverse problem, $(R, T) \to (n, k)$, it is useful to first recall the equations of the direct problem, $(n, k) \to (R, T)$, that consists of calculating the intensity reflectance and transmittance coefficients once the optical constants of the slab are known.

Therefore, let us consider a partially absorbing slab with plane-parallel faces immersed in air (figure 1) and assume normal incidence of light. Let $n(\lambda) - ik(\lambda)$ be the complex refractive index of the slab. The intensity reflectance and transmittance coefficients of each slab face, $R_F(\lambda)$ and $T_F(\lambda)$, are[1] (the explicit dependence on λ is omitted for the sake of

[1] Note that in [3] and [4] an expression different from equation (2) is utilized for the intensity transmittance of the slab face. As one can verify, that expression [3, 4] leads to $R_F + T_F > 1$ for $k > 0$, and this is clearly unrealistic.

brevity) [5, 6]

$$R_F = \left|\frac{n - ik - 1}{n - ik + 1}\right|^2 \tag{1}$$

$$T_F = \frac{4n}{|n - ik + 1|^2}. \tag{2}$$

The above equations keep true both for light incidence from air and from inside the substrate, and their sum gives $R_F + T_F = 1$, as one can verify, which represents energy conservation at the slab face. However, the validity of this energy-conservation rule and the definability of the intensity reflectance R_F itself for the incidence of light from inside the slab would deserve a discussion of its own, because the reflected wave couples with the incident one for incidence from inside an absorbing medium [6]. For this reason, the use of R_F (for incidence of light from inside the slab) in any theory should be limited to slab materials which are only partially absorbing (e.g. dielectric materials): by explicitly writing the expression for $R_F + T_F$ given in reference [6], it can be demonstrated that the above energy-conservation law is approximately true when $k^2 \ll n$. Hence defining R_F in such cases is commonly accepted.

The overall reflectance and transmittance coefficients of the slab, $R(\lambda)$ and $T(\lambda)$, can be calculated from equations (1) and (2) with infinite summations over the multi-reflected contributions of the faces. The slab is assumed to be optically thick, i.e. its geometrical thickness, h, is much larger than the coherence length of light, so that optical interference among multi-reflections is averaged out [7] and *incoherent* summations of the multi-reflected intensities can be considered [6]. Setting $\alpha(\lambda) = 4\pi k(\lambda)/\lambda$ as the absorption coefficient of the slab material, it ensues that

$$R = R_F + R_F T_F^2 \exp(-2\alpha h) \sum_{m=0}^{\infty} [R_F \exp(-\alpha h)]^{2m} \tag{3}$$

$$T = T_F^2 \exp(-\alpha h) \sum_{m=0}^{\infty} [R_F \exp(-\alpha h)]^{2m} \tag{4}$$

from which, recalling that

$$\sum_{m=0}^{\infty} q^m = \frac{1}{1 - q} \tag{5}$$

for $|q| < 1$, one gets [7]

$$R = R_F + \frac{R_F T_F^2 \exp(-2\alpha h)}{1 - R_F^2 \exp(-2\alpha h)} \tag{6}$$

$$T = \frac{T_F^2 \exp(-\alpha h)}{1 - R_F^2 \exp(-2\alpha h)}. \tag{7}$$

The above equations (6) and (7), through equations (1) and (2), represent the solution to the direct problem $(n, k) \to (R, T)$.

3. Complex refractive index of a slab (inverse problem)

3.1. Step 1: deduction of R_F and αh from R and T

To find the solution to the inverse problem, $(R, T) \to (n, k)$, which consists of calculating n and k from R and T, let us first derive R_F and αh from R and T. Therefore, let us rearrange equation (6) as follows:

$$R - R_F = \frac{R_F T_F^2 \exp(-2\alpha h)}{1 - R_F^2 \exp(-2\alpha h)}. \tag{8}$$

Now, by dividing equation (8) by equation (7), and then taking the natural logarithm of the result, one gets

$$\alpha h = \ln\left(\frac{R_F T}{R - R_F}\right). \tag{9}$$

By substituting equation (9) into equation (7) and using $T_F = 1 - R_F$, the following second-degree algebraic equation in the unknown R_F is obtained:

$$(2 - R)R_F^2 - [2 + T^2 - (1 - R)^2]R_F + R = 0 \tag{10}$$

whose only acceptable solution is

$$R_F = (2 + T^2 - (1 - R)^2 - \{[2 + T^2 - (1 - R)^2]^2 - 4R(2 - R)\}^{1/2})(2(2 - R))^{-1}. \tag{11}$$

The other mathematical solution to equation (10), which differs from equation (11) in the opposite sign in front of the square root, cannot be accepted because, as one can verify, it would lead to R_F values such that $R_F \geqslant R$, and this would contradict equation (3).

Note that, in equation (11), R_F is expressed in terms of R and T only, and one can show this fact by writing $R_F = R_F(R, T)$, where the wavelength dependence through $R(\lambda)$ and $T(\lambda)$ is understood. Once R_F has been found by means of equation (11), its value can be substituted into equation (9) to find αh as a function of R and T (however, we do not report here the fully explicit expression of αh for the sake of brevity).

3.2. Some useful relationships for n and k

Now, it is useful deriving some relationships for the real and imaginary parts of the complex refractive index, n and k.

Let us write the complex refractive index of the slab material in polar form, i.e.

$$n - ik = \rho \exp(i\phi) \tag{12}$$

where ρ and ϕ are univocally determined real-valued functions of λ. By using this polar form, from equations (1) and (2), after some mathematical rearrangements, one has

$$|\rho \exp(i\phi) + 1|^2 = \rho^2 + 2\rho\cos\phi + 1 = \frac{4n}{T_F} \tag{13}$$

$$|\rho \exp(i\phi) - 1|^2 = \rho^2 - 2\rho\cos\phi + 1 = \frac{4nR_F}{T_F}. \tag{14}$$

By adding and subtracting the above two expressions, one gets the following equations:

$$\rho^2 = 2n\frac{1 + R_F}{1 - R_F} - 1 \tag{15}$$

$$\cos\phi = \frac{n}{\rho} \tag{16}$$

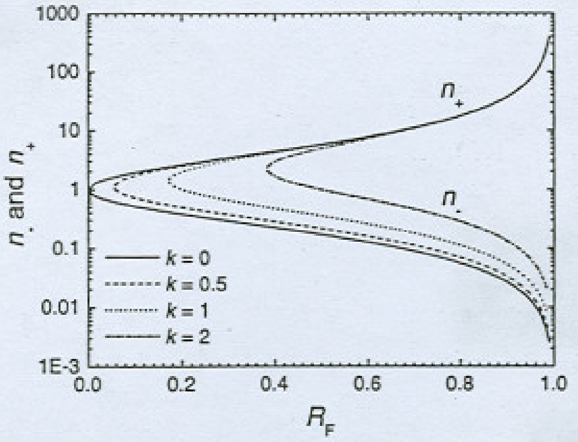

Figure 2. Dependence of n_+ (branches with $dn/dR_F > 0$) and n_- (branches with $dn/dR_F < 0$) on the reflectance R_F of a single face of the slab for some values of the extinction coefficient k. The loci where the two branch families meet are described by the formula $n_\pm = (1 + R_F)/(1 - R_F)$.

where $T_F = 1 - R_F$ has been utilized. By comparing equations (15) and (16), the following result for $\cos\phi$ can be written:

$$\cos\phi = \frac{n}{(2n\frac{1+R_F}{1-R_F} - 1)^{1/2}}. \quad (17)$$

Because ϕ is real-valued, $|\cos\phi| \leqslant 1$. Hence the following bounds can be established for n from equation (17) after some mathematical manipulations:

$$\frac{1 - R_F^{1/2}}{1 + R_F^{1/2}} \leqslant n \leqslant \frac{1 + R_F^{1/2}}{1 - R_F^{1/2}}. \quad (18)$$

Since $\rho^2 = n^2 + k^2$, one gets from equation (15) the following expressions for n and k (we retain, for k, only the positive square root for physical reasons):

$$n = n_\pm = \frac{1 + R_F}{1 - R_F} \pm \left[\frac{4R_F}{(1 - R_F)^2} - k^2\right]^{1/2} \quad (19)$$

$$k = \left[2n\frac{1 + R_F}{1 - R_F} - (n^2 + 1)\right]^{1/2}. \quad (20)$$

In principle, both the solutions reported in equation (19), n_+ and n_-, are mathematically acceptable, and the proper solution has to be selected on physical grounds. One can notice that the solution n_+ is usually the best candidate for dielectric materials ($k \ll n, n > 1$) because

$$n_+ \simeq \frac{1 + R_F^{1/2}}{1 - R_F^{1/2}} > 1 \qquad n_- \simeq \frac{1 - R_F^{1/2}}{1 + R_F^{1/2}} < 1 \quad (21)$$

when $k^2 \ll 4R_F/(1 - R_F)^2$. On the other hand, if $k^2 = 4R_F/(1 - R_F)^2$, the two solutions coincide and are $n_+ \equiv n_- = (1 + R_F)/(1 - R_F)$.

Figure 2 shows the dependence of n_+ and n_- on the face reflectance R_F, for some representative values of k, as calculated by equation (19). In this figure, the n_+ branches can be distinguished from the n_- branches because the former ones monotonically grow with R_F, while the latter ones monotonically decrease with R_F. By a close inspection of figure 2, one concludes that selecting the proper solution for n (i.e. n_+ or n_-) on physical grounds should be relatively straightforward in most cases.

In equation (20), the positiveness of the expression under the square root is assured by equation (18). On the other hand, imposing the positiveness of the expression under the square root in equation (19) and the positiveness (for physical reasons) of k leads to the following bounds for k:

$$0 \leqslant k \leqslant \frac{2R_F^{1/2}}{1 - R_F}. \quad (22)$$

Incidentally, the right-hand member of this last condition also sets a mathematical lower limit to the slab thickness. As a matter of fact, considering that $k = \lambda\alpha/(4\pi)$ and equation (9), one gets

$$h \geqslant \frac{\lambda}{4\pi}\frac{1 - R_F}{2R_F^{1/2}} \ln\left(\frac{R_F T}{R - R_F}\right). \quad (23)$$

However, in most cases this lower limit represents a very small thickness value, i.e. of the same order of magnitude as λ.

3.3. *Step 2: deduction of n and k from R_F and αh*

The final expression for the extinction coefficient of the slab, $k = k(R, T)$, can be simply obtained from equation (9) by considering that $\alpha = 4\pi k/\lambda$. The slab geometrical thickness, h, is assumed as known. One gets

$$k(R, T) = \frac{\lambda}{4\pi h} \ln\left[\frac{R_F(R, T)T}{R - R_F(R, T)}\right]. \quad (24)$$

Here, too, the wavelength dependence through $R(\lambda)$ and $T(\lambda)$ is understood besides the explicit dependence through the factor $\lambda/(4\pi h)$. In the above equation, k is calculated from R and T (also through equation (11)), h and λ being considered as parameters; this fact has been shown by writing $k = k(R, T)$.

Now, equation (24) can be substituted into equation (19) to also deduce the real part, n, of the complex refractive index. Therefore, the final expression for $n = n(R, T)$ is

$$n_\pm(R, T) = \frac{1 + R_F(R, T)}{1 - R_F(R, T)} \pm \left\{\frac{4R_F(R, T)}{[1 - R_F(R, T)]^2} - \left(\frac{\lambda}{4\pi h}\right)^2 \ln^2\left[\frac{R_F(R, T)T}{R - R_F(R, T)}\right]\right\}^{1/2}. \quad (25)$$

Equations (24) and (25), together with equation (11), represent the searched analytical solution to the inverse problem $(R, T) \rightarrow (n, k)$. The proper refractive-index solution, n_+ or n_-, has to be selected by referring to physical considerations, as previously discussed.

4. Application to a real case

As an example application, a real slightly absorbing sample was characterized with the proposed method. The sample was a grey glass for architectural applications having geometrical thickness $h = (4.9 \pm 0.1)$ mm. The intensity reflectance and transmittance spectra of the sample, $R(\lambda)$ and $T(\lambda)$, are shown in figure 3 and were measured with a Perkin-Elmer Lambda 19 spectrophotometer. The wavelength resolution (bandwidth)

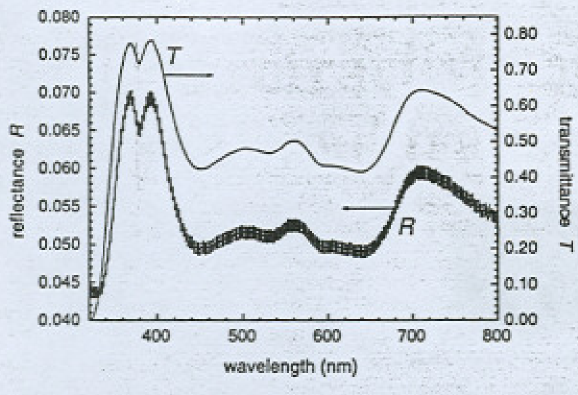

Figure 3. Measured intensity reflectance (left scale), $R(\lambda)$, and transmittance (right scale), $T(\lambda)$, of a grey glass for architectural applications. The error bars represent measurement uncertainties.

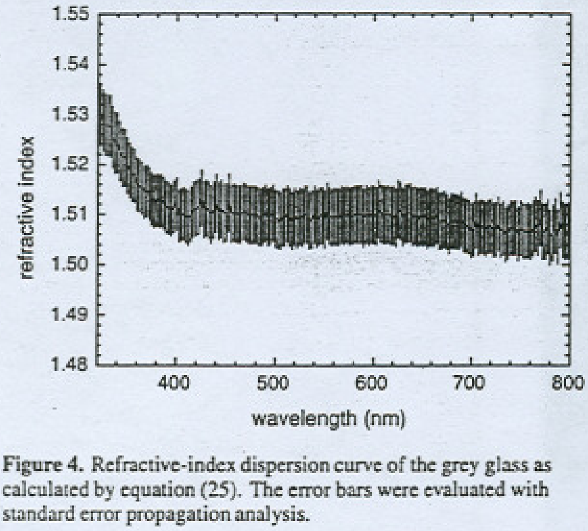

Figure 4. Refractive-index dispersion curve of the grey glass as calculated by equation (25). The error bars were evaluated with standard error propagation analysis.

was $\Delta\lambda = 1$ nm over all the examined spectral range, for which a maximum coherence length of light of about 640 μm was estimated. This ensures that the glass can be considered as optically thick.

The refractive-index and extinction-coefficient dispersion curves of the sample, shown in figures 4 and 5, were calculated by using equations (25) and (24), respectively. Between the two solutions available for the refractive index, the $n_+(\lambda)$ solution was selected as the physically correct one over all the considered spectral range because $n_-(\lambda) < 1$, which is unrealistic for a glass. The curves shown in figures 4 and 5 were checked for correctness by calculating from them the overall intensity reflectance and transmittance spectra with equations (6) and (7), and then comparing these calculated spectra with the measured ones. The reproduction of the measured spectra was completely successful.

5. Conclusions

The analytical solution found in this paper represents a useful alternative to numerical methods to deduce the complex refractive index of a slab from reflectance and transmittance

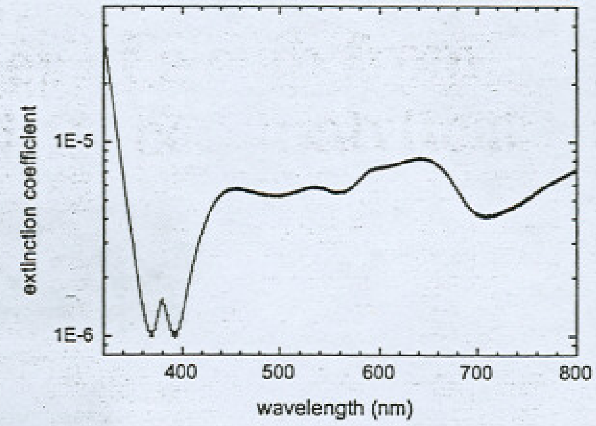

Figure 5. Extinction-coefficient dispersion curve of the grey glass as calculated with equation (24). The error bars were evaluated with standard error propagation analysis.

measurements. Besides the obvious advantages of using an analytical solution with respect to a numerical one, it has been shown that the inverse problem, $(R, T) \rightarrow (n, k)$, admits two sets of mathematical solutions, i.e. (n_+, k) and (n_-, k); the proper set has to be selected according to physical considerations. Moreover, the intervals mathematically and physically available to n and k have been deduced (equations (18) and (22)). Considering the bounds of these intervals could become useful when trying at least to state acceptable ranges for n and k in difficult cases, such as for the analysis of almost opaque substrates for which T is comparable with the instrumental sensitivity.

Acknowledgment

Useful discussions with M Montecchi are gratefully acknowledged.

References

[1] Stenzel O, Hopfe V and Klobes P 1991 Determination of optical parameters for amorphous thin film materials on semi-transparent substrates from transmittance and reflectance measurements *J. Phys. D: Appl. Phys.* **24** 2088–94

[2] Seredenko M M and Murashko M P 1993 Determining of optical constants by the spectrophotometric method *Sov. J. Opt. Technol.* **60** 534–6

[3] Khashan M A and El-Naggar A Y 2000 A new method of finding the optical constants of a solid from the reflectance and transmittance spectrograms of its slab *Opt. Commun.* **174** 445–53 Nassif

[4] Khashan M A and El-Naggar A Y 2001 Dispersion of the optical constants of quartz and polymethyl methacrylate glasses in a wide spectral range: 0.2–3 μm *Opt. Commun.* **188** 129–39

[5] Born M and Wolf E 1987 *Principles of Optics* (Oxford: Pergamon) ch 13

[6] Macleod H A 1986 *Thin-Film Optical Filters* 2nd edn (Bristol: Adam Hilger) ch 2

[7] Potter R F 1985 *Handbook of Optical Constants of Solids* Basic parameters for measuring optical properties ed E D Palik (London: Academic) ch 2

حاول الحصول على مقالات الدكتور
خشان ودراساته في
Opt. Comm.