ANNALS OF FACULTY ENGINEERING HUNEDOARA
- INTERNATIONAL JOURNAL OF ENGINEERING
Tome IX (Year 2011). Fascicule 3. (ISSN 1584 - 2673)

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OBTAINING THE ABSORPTION SPECTRA OF SILICON FROM THE IR REFLECTANCE SPECTRA RECORDED AT TWO ANGLES

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ABSTRACT: This paper presents an analytical method for obtaining optical constants $\bar{n}$ and $\bar{k}$, which define the complex refractive index $\tilde{n} = \bar{n} - i\bar{k}$ of solid absorbent materials. From specular reflectance, IR spectra recorded at two different incidence angles φ01 and φ02 the reflectances R are measured, using unpolarized radiation. We present an analytical method, using some approximations, to obtain reflectance spectra $\bar{k} = f(\tilde{\nu})$ and $\bar{n} = f(\tilde{\nu})$ from the reflectance spectra $R = f(\tilde{\nu})$ recorded at two different incidence angles, using non-polarized radiation. To illustrate this method silicon was chosen. In order to obtain the optical constants $\bar{n}$ and $\bar{k}$ of silicon we used specular reflectance IR spectra. The spectra were recorded with a UR20 spectrograph, using non-polarized radiation. The specular external reflection spectra recorded at two or more different incidence angles can be used to determine the refractive index and absorption index spectra corresponding to solid materials.
KEYWORDS: optical constants, two angles IR reflectance spectra, refractive index spectra

INTRODUCTION

The reflection of a plane polarized monochromatic radiation on the boundary of two different optical media is expressed by the Fresnel complex reflection coefficient $\tilde{r} = r \cdot \exp(i\delta)$. Two reflection coefficients $\tilde{r}_s$ and $\tilde{r}_p$ are defined for two components of plane polarized radiation with the electric field vector located perpendicular and parallel to the plane of incidence, respectively.

The square modulus of the complex reflection coefficient is the reflectance (or the reflectivity) $R_s = \tilde{r}_s \cdot \tilde{r}_s^*$ or $R_p = \tilde{r}_p \cdot \tilde{r}_p^*$. In the first approximation we can consider the reflectance for natural radiation to be the arithmetic mean of the two components R_s and R_p:

$$R = \frac{R_s + R_p}{2} \tag{1}$$

If we consider that the two components in incident radiation do not have equal weight, we can introduce a parameter S whose value is between S = 0 for the radiation polarized parallel to the incidence plane ($R = R_p$) and S = ∞ for the radiation polarized perpendicular to the incidence plane ($R = R_s$) [2]. S is defined as the ratio between the intensity of light polarized perpendicular to the plane of incidence and the parallel polarized one reaching the detector:

$$S = \frac{R_s^0}{R_p^0} \tag{2}$$

where: R_s^0 and R_p^0 are the perpendicular and parallel components that were measured.

The reflectance can be expressed by:

$$R = \frac{S}{S+1} R_s + \frac{1}{S+1} R_p \tag{3}$$

The reflection coefficients $\tilde{r}$ and the reflectance R depend on the relative complex refractive index of refractive and incidence medium, respectively:

$$\tilde{n} = \frac{\tilde{n}_1}{n_0} = \bar{n} - i\bar{k} \tag{4}$$

according to relations:

$$\tilde{r}_s = |\tilde{r}_s| \exp(i\theta_s) = \frac{\cos\varphi_0 - \tilde{n}\cos\tilde{\varphi}}{\cos\varphi_0 + \tilde{n}\cos\tilde{\varphi}} \tag{5}$$

$$\tilde{r}_p = |\tilde{r}_p| \exp(i\theta_p) = \frac{\tilde{n}\cos\varphi_0 - \cos\tilde{\varphi}}{\tilde{n}\cos\varphi_0 + \cos\tilde{\varphi}} = -\tilde{r}_s \frac{\tilde{n}\cos\tilde{\varphi} - \sin\varphi_0 \tan^2\varphi_0}{\tilde{n}\cos\tilde{\varphi} + \sin\varphi_0 \tan^2\varphi_0} \quad (6)$$

where $\tilde{\varphi}$ is the complex refractive angle, from Snell refraction law:

$$\sin\varphi_0 = \tilde{n}\sin\tilde{\varphi} \quad (7)$$

A single measurement of the reflectance at a certain frequency is insufficient to determine the two optical constants $\bar{n}$ and $\bar{k}$. Several methods that use at least two experimental values of measurable physical quantities corresponding to reflection [3] are known. Usually, they use graphical methods since the optical constants $\bar{n}$ and $\bar{k}$ can not be explicitly expressed from the reflectance expressions [4].

❖ MODEL DETAILS

We present an analytical method, using some approximations, to obtain reflectance spectra $\bar{k} = f(\tilde{v})$ and $\bar{n} = f(\tilde{v})$ from the reflectance spectra $R = f(\tilde{v})$ recorded at two different incidence angles, using non-polarized radiation [5,6].

For two different incidence angles φ_{01} and φ_{02} the refraction law is written:

$$\sin\varphi_{01} = \tilde{n}\sin\tilde{\varphi}_1 \text{ and}$$

$$\sin\varphi_{02} = \tilde{n}\sin\tilde{\varphi}_2 \quad (8)$$

By writing equation (3) for the two angles of incidence, we obtain the system of equations:

$$S \cdot R_{s1} + R_{p1} - (S+1) \cdot R_1 = 0 \quad (9)$$

$$S \cdot R_{s2} + R_{p2} - (S+1) \cdot R_2 = 0 \quad (10)$$

If in relations (5) and (6) we introduce the notations:

$$\tilde{n}\cos\tilde{\varphi}_1 = X - i \cdot Y \text{ and}$$

$$\tilde{n}\cos\tilde{\varphi}_2 = U - i \cdot Z \quad (11)$$

then the reflectances for two polarization states corresponding to the two different incidence angles, are:

$$R_{s1} = \frac{(X - \cos\varphi_{01})^2 + Y^2}{(X + \cos\varphi_{02})^2 + Y^2} \text{ and}$$

$$R_{s2} = \frac{(U - \cos\varphi_{02})^2 + Z^2}{(U + \cos\varphi_{02})^2 + Z^2} \quad (12)$$

respectively:

$$R_{p1} = R_{s1} \frac{(X - \sin\varphi_{01}\tan\varphi_{01})^2 + Y^2}{(X + \sin\varphi_{01}\tan\varphi_{01})^2 + Y^2} \text{ and}$$

$$R_{p2} = R_{s2} \frac{(U - \sin\varphi_{02}\tan\varphi_{02})^2 + Z^2}{(U + \sin\varphi_{02}\tan\varphi_{02})^2 + Z^2} \quad (13)$$

X, Y, U and Z depend on the complex refractive index according to the relations:

$$\tilde{n}^2 = (X - i \cdot Y)^2 + \sin^2\varphi_{01} \quad ;$$

$$\tilde{n}^2 = (U - i \cdot Z)^2 + \sin^2\varphi_{02} \quad (14)$$

By equating the right side of each relationship (12) we get:

$$XY - UZ = 0 \quad (15)$$

$$X^2 + Z^2 - Y^2 - U^2 + \sin^2\varphi_{01} - \sin^2\varphi_{02} = 0 \quad (16)$$

The nonlinear system of equations (9), (10), (15) & (16) leads to optical constants $\bar{n}$ and $\bar{k}$.

❖ RESULTS AND DISCUSSION

To illustrate this method silicon was chosen. The refractive index values for this material are well known and stressed in the reference literature [9,10,11].

In order to obtain the optical constants $\bar{n}$ and $\bar{k}$ of silicon we used specular reflectance IR spectra. The spectra were recorded with a UR20 spectrograph, using non-polarized radiation. For IR radiation incident on the sample, the proportion of the plane polarized component, perpendicular to the plane of incidence, is 63% which corresponds to the parameter of equation (3) S = 1.7.

Figure 1 presents the IR reflectance specular spectra of silicon recorded at two incidence angles 20 and 55 degrees respectively.

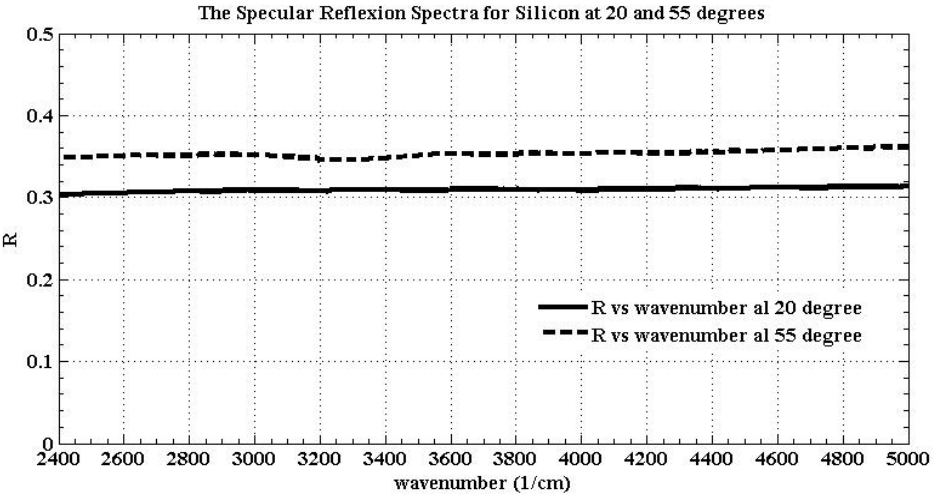

Fig. 1. The reflectance specular spectra of silicon recorded at two incidence angles, using non-polarized light

To obtain optical constants $\overline{n}$ and $\overline{k}$ from reflectance spectra we used our own computer program in MATLAB language, calling a routine for solving systems of nonlinear equations. To do this, first we wrote the nonlinear system of equations (9), (10) (15) and (16) to canonical form.

To find the solution of the nonlinear equations system it is very important to choose the correct test-solution to resolve the routine. For this, we started from the value X = U = 3.4 and Y = Z = 0 since it is known from reference literature that in the spectral range examined $n \cong 3.4$ and k=0 for silicon [9, 10, 11]. In (14) the contribution of the second term on the right is small, so X = U = n = 3.4 and Y = Z = k = 0.

The refractive index $\tilde{n}$ and optical constants $\overline{n}$ and $\overline{k}$ respectively are calculated from equation (14) based on X and Y values obtained by solving the nonlinear equations system.

Figure 2 shows the refractive index spectrum of silicon obtained from specular reflectance spectra recorded at two incidence angles 20 and 55 degrees.

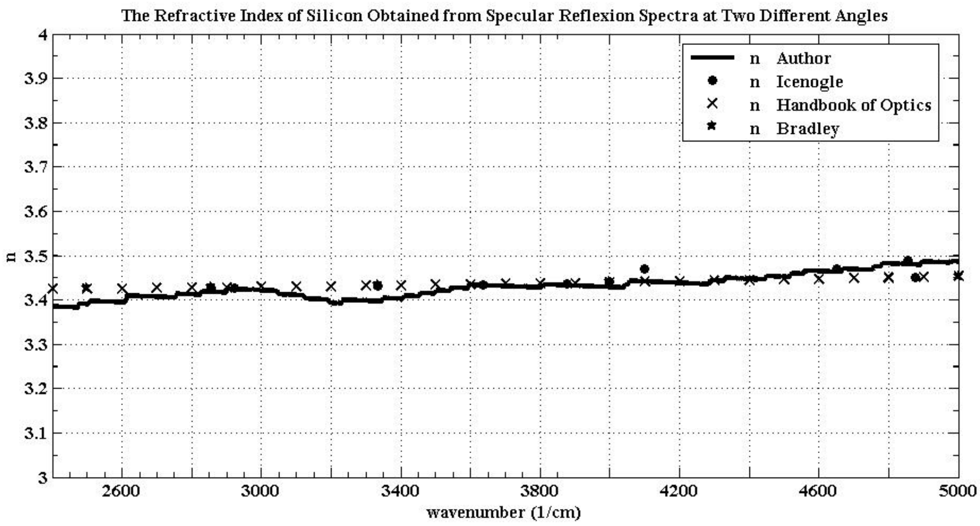

Fig. 2. The refractive index of silicon obtained from the specular reflectance spectra at two different incidence angles: 20^0 and 55^0

The refractive index spectrum obtained by processing the silicon specular reflectance spectra are in very good agreement with the corresponding data from the reference literature, as can be noticed in Figure 2. The absorption index $\overline{k}$ values are equal to zero over the whole spectral range analyzed, in agreement with literature data.

❖ CONCLUSIONS

The specular external reflection spectra recorded at two or more different incidence angles can be used to determine the refractive index and absorption index spectra corresponding to solid materials.

When the radiation used to record the spectra is non-polarized or partially polarized it is important to know the contribution of the two components Rs and Rp in the incident radiation.

It is important to choose the correct initial solutions to start the routine for solving nonlinear equations system. The start solutions of the program for solving nonlinear equations system can be based on values of X and U close to $\overline{n}$ =3.4. The initial values of Y and Z should be close to $\overline{k}$ =0.

The values of the optical constants $\overline{n}$ and $\overline{k}$ obtained by the method are in agreement with the corresponding values reported in the reference literature.

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