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Diffuse Reflectance of Thin Films with Defects

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Abstract

This paper presents the method of the optical analysis of thin films with defects. The attention is devoted to the defects consisting in boundary roughness. This method is based on interpreting the spectral dependences of the diffuse reflectance of light [1-5]. Thin films are used in the optical and military industries and in military applications, for example for the creation of anti-reflective layers or laser mirrors [6]. The numerical analysis confirms the fundamental influence of the parameters of the defects of thin films on the diffuse reflectance.

KEY WORDS: *diffuse reflectance; thin films; rough boundaries; optical quantities; optical analysis*

1. Introduction

In this paper the spectral dependences of the diffuse reflectance of single TiO2 layer on glass with identical rough boundaries are studied. Using a numerical analysis for the spectral dependences of the diffuse reflectance the influence of the roughness of the boundaries of single layer on substrate is described. Conclusions implied by this numerical analysis are important for practice in chemical and optical industry.

The rms value of the heights of the irregularities σ of the boundary roughness of thin films exhibiting this defect is usually in the range from several nanometres to several tens of nanometres [7-11].

There are many reasons of originating random roughness of the boundaries of thin films. One of the important reasons of the existence of this defect is residual roughness of substrates on which the systems of thin films are deposited [12-15].

The diffuse reflectance of thin films with smooth boundaries (σ = 0 nm) is equal to zero. In this case the total reflectance is given only by the coherent part of reflectance. The optical parameters of thin films and the parameters that described boundary roughness can be found by various experimental methods. One of these methods described in this paper is based on interpreting the spectral dependences of diffuse reflectance. Often used methods are also spectroscopic ellipsometry [16-21] or atomic force microscopy (AFM) [22-26]. When several methods are combined [27-30] the uncertainties of searched optical parameters of thin films (e.g. using least squares method) are smaller.

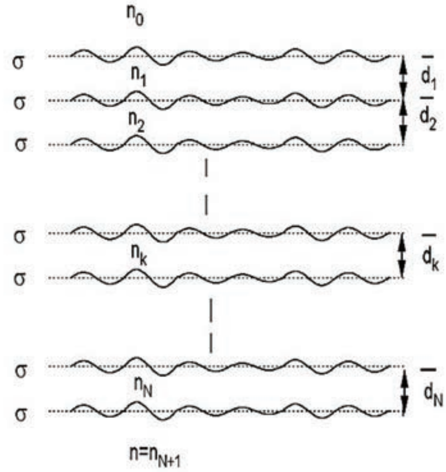

Fig. 1. The system of thin films with identically rough boundaries

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In Fig. 1 the system of thin films with identically rough boundaries is described. All the boundaries have the same profile of the heights of the irregularities. It means that the rms values of the heights of the irregularities σ are the same for all boundaries. *N* denotes the number of layers, nk represents the refractive index of the *k*-th layer, n_0 is the refractive index of the ambient, $n = n_{N+1}$ is the refractive index of the substrate and denotes the mean thickness of the *k*-th layer.

2. Theory

The following assumptions of a physical model of thin films must be fulfilled [6]:

– Boundaries are locally smooth, the shadowing and multiple reflections among the irregularities of thin films can be neglected,

– the stationary isotropic normal stochastic process generates roughness of the boundaries and the mean values of random functions describing all the rough boundaries are equal to zero,

– the mean levels of all the boundaries are formed by mutually parallel planes,

– the rms values of the height of the irregularities of all the boundaries are smaller than the wavelength λ of the incident light,

– the dimensions of the illuminated parts of the boundaries are much larger than the wavelength, materials forming the system of thin films are homogeneous and isotropic from the optical point of view,

– the normal incidence of light on the mean planes of the boundaries of thin films is assumed.

Using the scalar theory of diffraction of light, Fraunhofer approximation and Helmholtz-Kirchhoff integral (e.g. [2-4]) one can derive the following formula for the diffuse reflectance of the rough system of thin films [4]:

$$R_D = R_0\left[1-\exp\left(-\frac{16\pi^2\sigma^2}{\lambda^2}\right)\right]\left[1-\exp\left(-\frac{\pi^2\alpha_0^2T^2}{\lambda^2}\right)\right], \qquad (1)$$

where R_D denotes the diffuse reflectance, R_0 is the reflectance of ideally smooth thin films, n_0 is the refractive index of the ambient, *T* represents the correlation length of the rough boundary and α_0 is the half acceptance angle of detector.

3. Numerical analysis

The numerical analysis of the dependence of diffuse reflectance on the wavelength of incident light for identical TiO_2 layer on glass is introduced. In this analysis it is assumed that the refractive index of the ambient is $n_0 = 1$ (air) and the refractive index of the substrate (glass) is 1.52.

The value of the mean thickness of TiO_2 layer is 300 nm and the refractive index of TiO_2 layer is represented by the spectral dependence $n_1 = A + B/\lambda^2$, where $A = 2.16$ and $B = 62000$ nm^2.

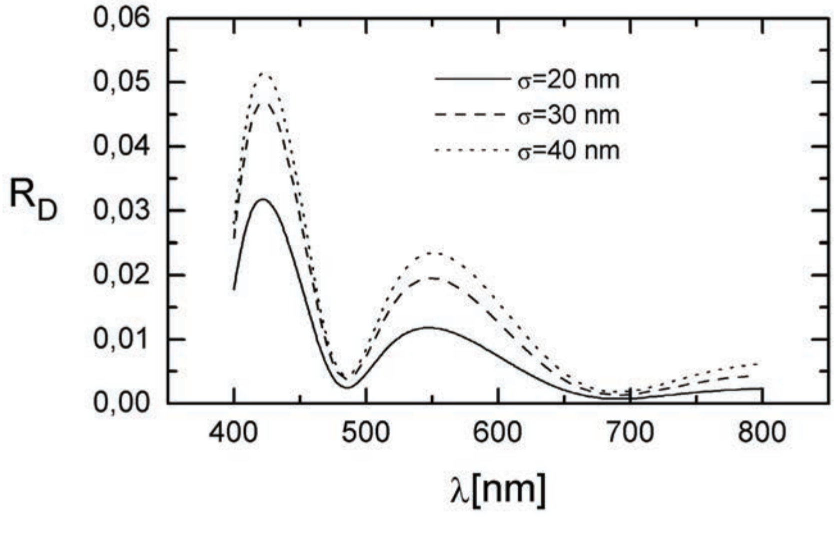

Fig. 2. Spectral dependences of the diffuse reflectance of the single TiO_2 layer on glass for various values of σ.

In Fig. 2 it is shown that the diffuse reflectance increases if the rms value of the heights of irregularities σ increases. This dependence is calculated for correlation length *T* = 3000 nm and for the half acceptance angle of detector α_0 = 0.03 rad.

The differences between curves are much greater than usual experimental uncertainty and therefore it is possible to determine the parameters describing the roughness of thin films.

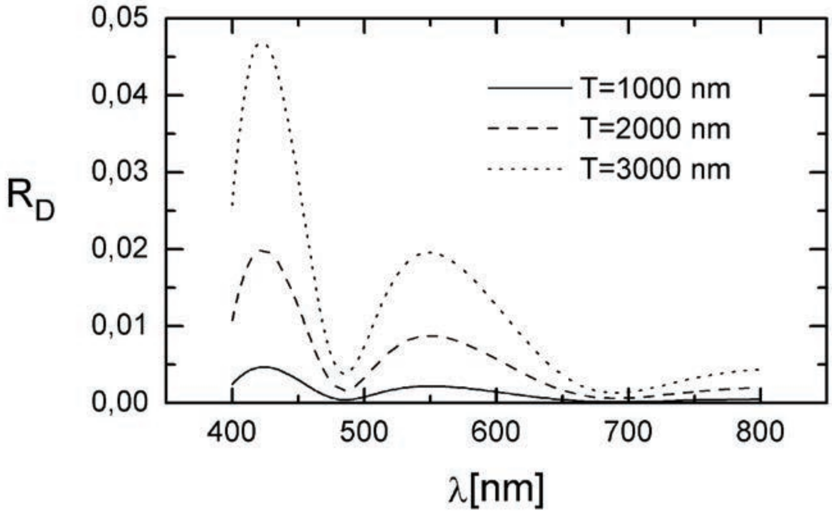

Fig. 3. Spectral dependences of the diffuse reflectance of the single TiO_2 layer on glass for various values of *T*.

In Fig. 3 it is shown that the diffuse reflectance increases if the value of correlation length *T* increases. This dependence is calculated for the rms value of the heights of irregularities σ = 30 nm and for the half acceptance angle of detector α_0 = 0.03 rad.

If the correlation length is close to zero the diffuse reflectance decreases to zero.

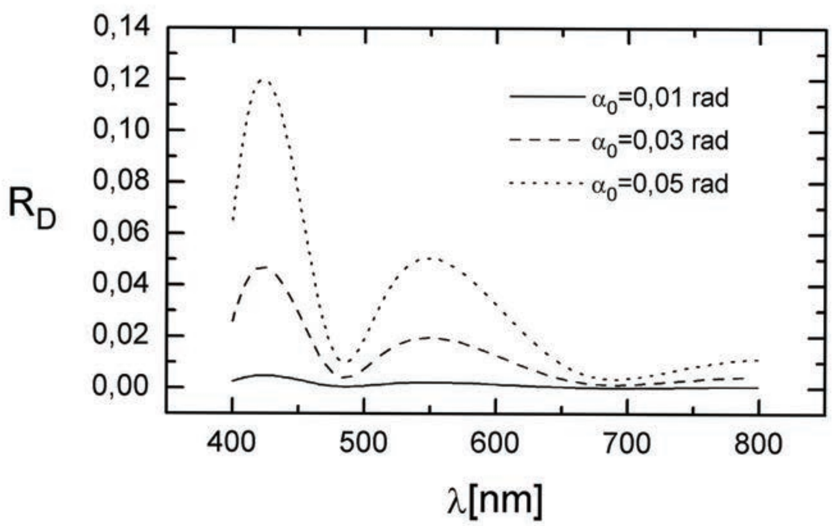

Fig. 4. Spectral dependences of the diffuse reflectance of the single TiO_2 layer on glass for various values of α_0.

In Fig. 4 it is shown that the diffuse reflectance increases if the value of the half acceptance angle of detector α_0 increases. This dependence is calculated for the rms value of the heights of irregularities σ = 30 nm and for the correlation length *T* = 3000 nm.

The difference between curves calculated for various values of the half acceptance angle of detector is greater than usual experimental uncertainty.

4. Conclusions

In this paper it is shown that the diffuse reflectance of thin films depends especially on the rms value of the heights of irregularities σ and on the correlation length *T* of randomly rough boundaries. Moreover, it is shown that the eq. (1) can be used for interpreting the spectral dependences of the diffuse reflectance of thin films with rough boundaries. The influence of the defects of thin films on the diffuse reflectance is relatively great compared with the usual experimental uncertainty. It is shown that the influence of the correlation length and the rms value of the heights of irregularities cannot be neglected. This procedure enables us to find parameters describing the optical parameters of thin films (e.g. the mean values of thicknesses and the spectral dependences of refractive indices). The diffuse reflectance depends on the half acceptance angle of the detector and therefore it is necessary to pay attention to the exact determination of this experimental parameter.

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