2011 2nd International Conference on Chemical Engineering and Applications
IPCBEE vol. 23 (2011) © (2011) IACSIT Press, Singapore

Optical Properties of Multilayers with Rough Boundaries

František Vižďa

Department of Mathematics and Physics, Faculty of Military Technology,
University of Defence, Kounicova 65, 662 10 Brno, Czech Republic
e-mail: frantisekvizda@seznam.cz

Abstract. A method of the optical analysis of thin films is presented. This method is based on measuring and interpreting the spectral dependences of the reflectance or transmittance. The thin films are used in chemical and optical industry. The formulae expressing the reflectance and transmittance of the rough thin films are derived within the scalar theory of diffraction. Possibilities and limitations of the method are illustrated by means of the selected samples of thin films.

Keywords: thin films, optical properties, interference coatings

1. Introduction

In this paper the differences between the spectral dependences of the coherent reflectance of multilayers (thin films) with smooth boundaries on the one hand and the multilayers with rough boundaries on the other hand are studied. Using a numerical analysis for the spectral dependences of the coherent reflectance and coherent transmittance the influence of the roughness of the boundaries of multilayers is discussed. Conclusions implied by this numerical analysis are important for practice in chemical and optical industry.

The multilayers are frequently used in chemical and optical industry. There are many reasons of originating random roughness of the boundaries of multilayers. One of the important reasons of the existence of this defect is residual roughness of substrates on which the multilayer systems are deposited (see [1-5]).

2. Theory

The following assumptions specify a physical model of the multilayers under consideration (see [1]):

1. Boundaries are locally smooth, i.e. the tangent plane to the boundary in its arbitrary point deviates only slightly from this boundary over the region the linear dimensions of which are much larger than a wavelength of incident light.

2. Slopes of the irregularities of the boundaries are very small that the shadowing and multiple reflections among these irregularities can be neglected (the rms value of angles corresponding to the slopes is much smaller than unity).

3. A stationary isotropic normal stochastic process generates roughness of the boundaries. The mean values of random functions describing all the rough boundaries are equal zero.

4. The mean levels of all the boundaries are formed by mutually parallel planes.

5. The rms values σ of the height of the irregularities of all the boundaries are smaller than the wavelength λ ($\sigma << \lambda$ or $\sigma < \lambda$).

6. The dimensions of the illuminated parts of the boundaries are much larger than the wavelength λ (it is assumed that the illuminated parts of the boundaries are formed by rectangles in their mean planes with the dimensions $2X$ and $2Y$, $2X$, $2Y >> \lambda$).

7. Materials forming the multilayer system are homogeneous and isotropic from the optical point of view.

Normal incidence of light (λ is the wavelength of the incident light) on the mean planes of the boundaries of the systems is supposed. We shall only deal with light waves coherently reflected and transmitted by the rough multilayers. These waves will be described by the coherent reflectance and coherent transmittance.

It is assumed that all the boundaries are the identical and randomly rough. The quantity η is a random function describing all the boundaries of the multilayer system, σ are the rms value of the height of the irregularities of all the boundaries (see Fig. 1). N denotes the number of layers, n_k represents the refractive index of the k-th layer, n_0 is the refractive index of the ambient (for air $n_0 = 1$), $n = n_{N+1}$ is the refractive index of the substrate, the symbol $\overline{d}_k$ denotes the mean thickness of the k-th layer.

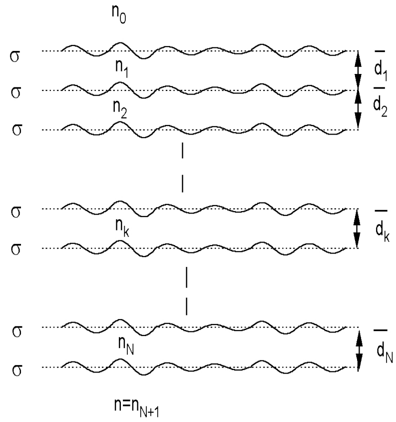

Fig. 1: Multilayer system with identical randomly rough boundaries.

One can use the scalar theory of diffraction of light for deriving the formulae for the coherent reflectance and coherent transmittance of the rough multilayer system. If the conditions of the Fraunhofer approximation are fulfilled at detecting the light flux reflected or transmitted by the rough identical multilayer system the coherent reflectance R_c and the coherent transmittance T_c of this system can be expressed as follows (see e.g. [1,2]):

$$R_c = R_0 \exp\left(-\frac{16\pi^2 n_0^2 \sigma^2}{\lambda^2} \right), \tag{1}$$

$$T_c = T_0 \exp\left(-\frac{4\pi^2 (n - n_0)^2 \sigma^2}{\lambda^2} \right), \tag{2}$$

Where R_0 and/or T_0 is the coherent reflectance and/or coherent transmittance of the ideally smooth multilayer system (see e.g. [1,2]).

3. Numerical analysis

In this section the numerical analysis of the formulae presented in the foregoing section (Eqs. (1-2)) will be introduced. This analysis enables us to discuss the influence of the boundary roughness on the coherent reflectance and coherent transmittance of the multilayer systems in a quantitative way.

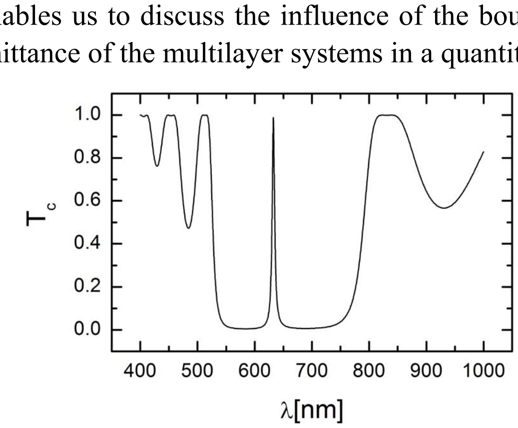

Fig. 2: Spectral dependence of the coherent transmittance of smooth monochromatizing system $G(HL)^4 2H(LH)^4 G$.

The eleven-layer system $1(HL)^5HG$ and seventeen-layer $G(HL)^4 2H(LH)^4 G$ system are chosen for the numerical analysis, i.e. the spectral dependences of the reflectance R_c and transmittance T_c of these systems are presented. Within this analysis it is assumed that the H-film and/or L-film is formed by a TiO_2 and/or SiO_2 film. The spectral dependences of their refractive indices n_H and n_L are represented by the following formulae: $n_j(\lambda) = A_j + B_j / \lambda^2$ (j=H,L). The values of A_j and B_j are chosen as follows: $A_H = 2.16$, $B_H = 62000$ nm^2, $A_L = 1.46$ and $B_L = 5000$ nm^2 (see e.g. [2]). The values of refractive indices of the ambient n_0 and the substrate n are chosen as follows: $n_0 = 1$ (air) for $1(HL)^5HG$, $n_0 = 1.52$ for $G(HL)^4 2H(LH)^4 G$ and $n = 1.52$ (for both multilayers, G - the substrate is glass). The values of the mean thicknesses of eleven-layer system $1(HL)^5HG$ and seventeen-layer $G(HL)^4 2H(LH)^4 G$ are given by the following values: $d_H = \lambda_0 / (4 n_H (\lambda = \lambda_0))$, $d_L = \lambda_0 / (4 n_L (\lambda = \lambda_0))$ and $\lambda_0 = 632.8$ nm.

In Fig. 2 the spectral dependence of the coherent transmittance of the multilayer of $G(HL)^4 2H(LH)^4 G$ is presented. This multilayer enables us to transmit the light with the wavelength closed to $\lambda_0 = 632.8$ nm. All the boundaries of $G(HL)^4 2H(LH)^4 G$ (seventeen-layer system) monochromatizing system are smooth.

In Fig. 3 the spectral dependence of the coherent reflectance of the reflective multilayer of $1(HL)^5HG$ (eleven-layer system) with identically rough boundaries is shown. In Fig. 3 we can see that if the roughness of the boundaries increases the coherent reflectance decreases.

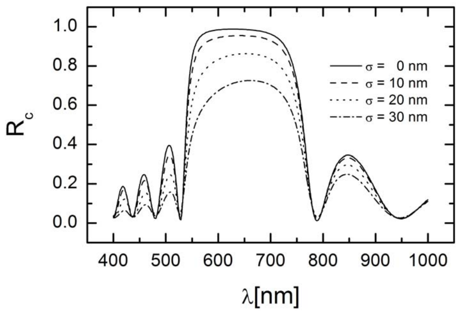

Fig. 3: Spectral dependence of the reflectance of reflective system $1(HL)^5HG$ for various boundary roughness.

4. Conclusion

In this paper formulae expressing the coherent reflectance and coherent transmittance of multilayer systems with identical randomly rough boundaries are used for describing the spectral dependences of the coherent reflectance and coherent transmittance of a rough eleven-layer system and smooth seventeen-layer system of TiO_2/SiO_2 on glass.

It is shown that the differences between the spectral dependences are so considerable that one must use this fact for the optical analysis of these systems.

5. Acknowledgements

The research described in this paper was supported by the Organization Development Project (the project of the Department of Mathematics and Physics) awarded by the Ministry of Defence of the Czech Republic.

6. References

[1] I. Ohlídal, and F. Vižďa. Optical quantities of multilayer systems with correlated randomly rough boundaries. *J. Mod. Opt.* 1999, **46**: 2043-2062.

[2] I. Ohlídal, F. Vižďa, and M. Ohlídal. Optical analysis by means of spectroscopic reflectometry of single and double layers with correlated randomly rough boundaries. *Opt. Eng.* 1995, **34**: 1761-1768.

[3] D. Franta, I. Ohlídal, D. Nečas, F. Vižďa, O. Caha, M. Hasoň, and P. Pokorný. Optical Characterization of HfO_2 thin film. *Thin Solid Films* 2011, **519**: 6085-6091.

[4] D. Franta, I. Ohlídal, P. Klapetek, and M. Ohlídal. Characterization of thin oxide films on GaAs substrates by optical methods and atomic force microscopy. *Surf. Interface Anal.* 2004, **36**: 1203-1206.

[5] D. Nečas, D. Franta, V. Buršíková, and I. Ohlídal. Ellipsometric characterisation of thin films non-uniform in thickness. *Thin Solid Films* 2011, **519**: 2715-2717.