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Reflectance and transmittance model for multilayer optical coatings with roughness at oblique incidence

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ABSTRACT

Surface roughness is really important to the ultra-low loss of multilayer optical coatings. Reflectance and transmittance model for multilayer optical coatings with surface roughness has been established at normal incidence by A. V. Tikhonravov et al. in 2003. However, under the condition of oblique incidence, no further model which is based on the model of Tikhonravov has ever been reported. In this paper, an approximate reflectance and transmittance model is established for the thin film system with roughness at oblique incidence by analogy and usage of the concept of equivalent refractive index. The small-scale roughness model's effectiveness has been theoretically demonstrated according to the effective medium theory. However, the large-scale roughness model's effectiveness needs other methods to be proved, as the scattering effect of different scale roughness is different. This model might play a significant role to research the scattering loss of oblique incident thin film systems, such as mirrors in ring lasers, deep ultraviolet lasers and interferometers with ultra long cavity length.

1. Introduction

In the optics of thin film, it is generally assumed in layer system analysis that the interfaces and surfaces of layers are ideally flat surfaces. However, actually any thin film has certain surface roughness. In some applications, this roughness has a very important influence on its optical characteristics, such as deep-ultraviolet sculpture [1], ring lasers [2], gravitational wave detectors [3], etc. Therefore, it is important to establish a theoretical analysis model of multilayer optical characteristics when considering surface roughness.

Roughness surface is usually described by root mean square (RMS) roughness and power spectral density function [4–8]. The former ignores the characteristic of surface spatial wavelength, and the latter is difficult for recurrent computation to be expanded to multilayer system. Considering these, based on the different scattering effect mechanism between surface roughness of different spatial wavelength, Tikhonravov [9] proposed the concept of large and small scale RMS roughness, expanded rough surface single-layer optical characteristics calculation model to multilayer system, and had the model embedded in Optilayer software. There is a possibility in Optilayer software to use “interlayers” instead of interface roughness. However, it is only verified to be suitable for the situation of normal incidence, and the equivalent thickness and refractive index of interlayers might change for different angle of incidence, which has not been verified by Tikhonravov. Moreover, Tikhonravov et al. only numerically prove the effectiveness of the model, and there has no strict theoretical verification of the model.

This paper is divided into five sections. In Section 2, based on the concept of large and small scale RMS roughness, the oblique incidence multilayer reflectance and transmittance theoretical model is obtained by analogy and transfer matrix method, when considering surface roughness. In Section 3, the convergence of the model under extreme conditions is proved from two aspects, incidence angle and surface roughness. Finally, adopting multilayer approximate method which is based on effective medium theory, Section 4 makes strict theoretical verification to prove the effectiveness of the small-scale roughness model proposed in this paper, with the conclusions given in Section 5.

2. Model description

2.1. The concept of transfer matrix

After years of experimental test and theoretical work, the approximation calculation formula of single-layer's optical characteristics has been established, when considering surface roughness. However, the formula of multilayer's optical characteristics has seldom been researched. Therefore, how to transfer single-layer's optical characteristics to multilayer's optical characteristics appears particularly important. Because transfer matrix method [10] can easily expand single-layer's optical characteristics to multilayer's optical characteristics, which is very suitable for the strict deduction of multilayer calculation model when there is surface imperfection, we adopt transfer matrix method to deduce the formula in this paper. Generally only the condition of normal incidence is considered

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in the analysis of thin film system, but in the actual application, not all conditions are ideally normal incidence. Therefore, we need to establish a model of the thin film system under the condition of oblique incidence. Essentially, transfer matrix method transfers single-layer's optical characteristics to entire multilayer's optical characteristics by step-by-step transitive relation between layers and interfaces. The specific model is described as follows:

The multilayer structure is shown in Fig. 1.

Where r_j, $t_j (j = 1, 2, \ldots, m, s)$ are amplitude reflection and transmission coefficients of jth layer's upper surface, respectively, and m is the multilayer system's number of layers, n_j, $d_j (j = 1, 2, \ldots, m, a, s)$ are refractive indexes and thicknesses of jth layer. Here subscript a and s represent ambient environment and substrate, respectively. Furthermore, $\delta_j (j = 1, 2, \cdots, m, a, s)$ are optical admittances of jth layer, and according to effective refractive index concept, we know that:

$$\delta_j = \begin{cases} n_j \cos\theta_j, S\text{—polarization} \\ {}^{n_j}/_{\cos\theta_j}, P\text{—polarization} \end{cases}. \quad (1)$$

Here θ_j are transfer angles of jth layer.

In this multilayer structure, the roughness on surfaces and interfaces might not only change the specular properties of layers, such as reflectance and transmittance, but also produce diffuse scattering [11–13]. Therefore, we must also consider the possible influence of scattering to multilayer system, and this will be discussed in Section 2.2.

Define the transfer matrix of the jth layer's upper surface as follows [9]:

$$B_j = \begin{bmatrix} 1/t_j & r_j/t_j \\ r_j/t_j & 1/t_j \end{bmatrix}. \quad (2)$$

Define the transfer matrix of the jth layer's internal part as follows [10]:

$$C_j = \begin{bmatrix} e^{i\varphi_j} & 0 \\ 0 & e^{-i\varphi_j} \end{bmatrix} = \begin{bmatrix} e^{ikn_j d_j \cos\theta_j} & 0 \\ 0 & e^{-ikn_j d_j \cos\theta_j} \end{bmatrix}. \quad (3)$$

Here $\varphi_j = kn_j d_j \cos\theta_j$ are phase thicknesses of jth layer, $k = \frac{2\pi}{\lambda}$.

Define the transfer matrix of the total multilayer system as follows [10]:

$$C = \begin{bmatrix} 1/t & r^*/t^* \\ r/t & 1/t^* \end{bmatrix}. \quad (4)$$

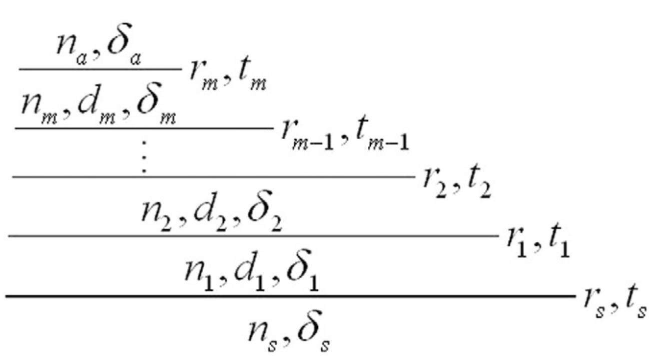

Fig. 1. Schematic representation of m-layer structure with amplitude reflection and transmission coefficients r_m and t_m, ambient environment and substrate refractive indexes n_a and n_s, layer thickness d_m, and optical admittance δ_m.

Here r, t are total amplitude reflection and transmission coefficients of multilayer surface, respectively, and r^*, t^* represent complex conjugate of r, t.

Especially, define the transfer matrix of substrate's upper surface as follows:

$$B_s = \begin{bmatrix} 1/t_s & r_s/t_s \\ r_s/t_s & 1/t_s \end{bmatrix}. \quad (5)$$

In a general case, as for the single-layer system, we know the expression $C = B_1 C_1 B_s$, which represents the transfer relation between substrate's upper surface, layer's internal part and layer's upper surface. We can expand it to the situation of multilayer system by mathematical induction, according to transfer relation between layers, we obtain the expression as follows [9]:

$$C = B_m C_m B_{m-1} C_{m-1} \cdots B_2 C_2 B_1 C_1 B_s. \quad (6)$$

In order to calculate C, we need to know values of $\cos\theta_j$ according to Eq. (3). We know from Snell's law of refraction that:

$$n_a \sin\theta_a = n_m \sin\theta_m = n_{m-1} \sin\theta_{m-1} = \cdots = n_2 \sin\theta_2 = n_1 \sin\theta_1 = n_s \sin\theta_s. \quad (7)$$

Then we can obtain values of $\cos\theta_j$ from Eq. (7) that:

$$\cos\theta_j = \sqrt{1\text{-}\left(\frac{n_a \sin\theta_a}{n_j}\right)^2} \quad (j = 1, 2, \ldots, m). \quad (8)$$

Especially, $\cos\theta_s = \sqrt{1\text{-}\left(\frac{n_a \sin\theta_a}{n_s}\right)^2}$, $\cos\theta_a = \sqrt{1\text{-}\sin^2\theta_a}$.

Generally, n_j, d_j, λ, θ_a, n_s, n_a $(j = 1, 2, \ldots, m)$ are all known, therefore, according to Eqs. (1)–(8), if we want to calculate r, t, we only need to obtain values of r_j, t_j, r_s, t_s $(j = 1, 2, \ldots, m)$. Based on these, then we analyze the calculation of r_j, t_j, r_s, t_s.

2.2. Single-layer's optical characteristics with large-scale and small-scale roughness

From the transfer matrix model, we can see that if we want to calculate the total reflectance and transmittance of multilayer system, we must deduce the calculation formula of r_j, t_j, r_s, t_s, which is also the biggest difference between the model in this paper and Tikhonravov's normal incidence model. Then we deduce the calculation formula of r_j, t_j, r_s, t_s as follows:

First of all, we want to introduce the definition of large-scale and small-scale roughness. According to the relationship between surface spatial wavelength and incident light wavelength, surface roughness can be divided into large-scale roughness and small-scale roughness [9]. When surface spatial wavelength is bigger than incident light wavelength, we define surface roughness as large-scale roughness; when surface spatial wavelength is smaller than incident light wavelength, we define it as small-scale roughness. The scattering caused by large-scale roughness will induce the loss of light energy; however, the scattering caused by small-scale roughness will not induce the loss of light energy [9]. Due to the difference of light energy's propagation characteristic, the effect caused by large-scale and small-scale roughness is different.

As we know, when we look at a surface with roughness from a large incidence angle, the surface seems smoother than the normal incidence situation, and with the increasing incidence angle, it is getting smoother. In other words, the equivalent RMS roughness value becomes smaller. However, this does not change the relationship between surface spatial wavelength and incident light wavelength. Therefore, in this paper, we assume that the incidence angle does not influence the change of propagation modes.