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**COMPUTATIONAL EXPERIMENTS ON THE DESIGN OF ANTIREFLECTION  
COATINGS AND AN EMPIRICAL EXPRESSION FOR THE MINIMUM  
RESIDUAL REFLECTANCE**

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A simple empirical expression for the minimum residual reflectance of antireflection coatings is proposed. The expression relates the minimum residual reflectance in the antireflection spectral range to the basic design parameters. The numerically and empirically calculated values of residual reflectance are in good agreement. An accurate qualitative analysis of the expression is given.

**1. Introduction.** Antireflection (AR) coatings are the most widely used optical coatings. Their production makes up more than 50% of the total thin film coating market [1]. It is not surprising that there are several hundreds of papers devoted to the design and fabrication of AR coatings. A tremendous progress in the thin-film technology has made possible an accurate production of complicated AR designs consisting of several dozens of layers [2]. The ability to predict an average residual reflectance of AR coatings in the antireflection spectral ranges is very important for thin-film designers. This average residual reflectance depends on many design parameters. From the thin-film theory [3] it is well known that the reflectance of any coating depends on the ratios of the refractive indices of all layer materials and ambient media. It was shown by many authors that the total optical thickness and the width of the AR spectral range are extremely important design parameters (see, for example, [4]). It is natural that an analytical expression for the average residual reflectance would be probably quite complicated, since such an expression involves many essential parameters and since these parameters are interrelated. On the other hand, an adequate empirical expression for the average residual reflectance would be extremely useful from the practical point of view. The idea to obtain an empirical expression for the average residual reflectance of AR coatings is not new. In [5] R. Willey proposed an empirical formula estimating the average residual reflectance of AR coatings. This formula was obtained on the basis of numerical and statistical analysis. According to this formula, the average value of residual reflectance tends to zero with increasing total optical thickness of AR designs. In [1, 6] it is shown that, on the contrary, the average residual reflectance value tends to its nonzero minimum with infinitely increasing total optical thickness.

In this paper we discuss some results of about 2000 computational experiments on the design of AR coatings with various design parameters. In our computational experiments, we applied the needle optimization technique [7–9], which is the most powerful modern tool for the design of multilayer optical coatings. We used the latest design software, which made it possible to synthesize the AR coatings with different total optical thicknesses and different numbers of layers. Due to this fact, we obtained the AR designs with various combinations of refractive indices and various widths of AR spectral ranges. Based on the results of these multiple computational experiments, we derived an empirical expression for the minimum achievable residual reflectance. In Section 2 of this paper, the consistency between our computational experiments and our empirical expression is demonstrated. In Section 3 a qualitative analysis of the empirical expression is given. Our final conclusions are presented in Section 4.

**2. An empirical expression for the minimum residual reflectance and some results of computational experiments.** The maximum principle in thin-film optics [10] shows that, at the normal incidence, two-component AR designs, i.e. the designs consisting of alternating layers with high- and low-index materials, form an optimal class of AR designs. Because of this, we consider only two-component AR coatings. Let  $n_H$  and  $n_L$  be the refractive indices of high- and low-index materials,  $n_s$  and  $n_a$  be refractive indices of the substrate and the ambient medium, and  $\lambda_l$  and  $\lambda_u$  be the lower and upper limits of the AR spectral range, respectively. It is well known [3] that the spectral characteristics of multilayer coatings depend not on the absolute values of  $n_H$ ,  $n_L$ ,  $n_s$ , and  $n_a$  but on the ratios  $\rho_{HL} = n_H/n_L$ ,  $\rho_{La} = n_L/n_a$ , and  $\rho_{sa} = n_s/n_a$ . The average residual reflectance of each AR design is defined as

$$R_{av} = \frac{1}{\lambda_u - \lambda_l} \int_{\lambda_l}^{\lambda_u} R(\lambda) d\lambda,$$

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where  $R(\lambda)$  is the reflectance of the design under study.

It is also known [1, 11] that the AR designs have a specific structure: they consist of quasiperiodic groups of layers, the so-called clusters. The number of clusters grows when the design total optical thickness increases. In [6] it is shown that the average residual reflectance  $R_{av}$  can be represented in the form

$$R_{av} = R_{\infty} b^{1/M},$$

where  $M$  is the number of AR design clusters. It is obvious that the parameter  $R_{\infty}$  represents the minimum achievable average residual reflectance. The parameter  $R_{\infty}$  depends on the ratios  $\rho_{HL}$ ,  $\rho_{La}$ , and  $\rho_{sa}$  and on the width of the AR spectral range  $\lambda_u/\lambda_l$ . The parameter  $R_{\infty}$  was found by the least-squares method for 175 sets of input design parameters. In Figs. 1 and 2 we present the values of  $R_{\infty}$  calculated for the AR spectral ranges 400–1200 nm ( $\lambda_u/\lambda_l = 3$ ) and 400–1600 nm ( $\lambda_u/\lambda_l = 4$ ). In the design process, seven values of  $\rho_{HL}$  and five values of  $\rho_{La}$  were taken. These experimental values of  $R_{\infty}$  are marked in Figs. 1 and 2 by circles.

In order to approximate the experimental dependence of  $R_{\infty}$  on the parameters  $\rho_{HL}$ ,  $\rho_{La}$ ,  $\rho_{sa}$ , and  $\lambda_u/\lambda_l$ , the following empirical expression was derived:

$$R_{\infty} \approx f_1(\rho_{La}, \rho_{sa}) \left[ \frac{\pi}{4} \left( \frac{\pi}{120} \right)^{1/(\lambda_u/\lambda_l - 1)} \right]^{(1 - 1/\rho_{HL}^2)/\sqrt{\rho_{La} - 1}}. \quad (1)$$

Here

$$f_1 = \frac{\rho_{sL}^2 (1 - \rho_{La}^2)^2 + \rho_{La}^2 (1 - \rho_{sL}^2)^2}{(\rho_{La} + \rho_{sL})^2 (1 + \rho_{La} \rho_{sL})^2}, \quad \rho_{sL} = \frac{\rho_{sa}}{\rho_{La}}.$$

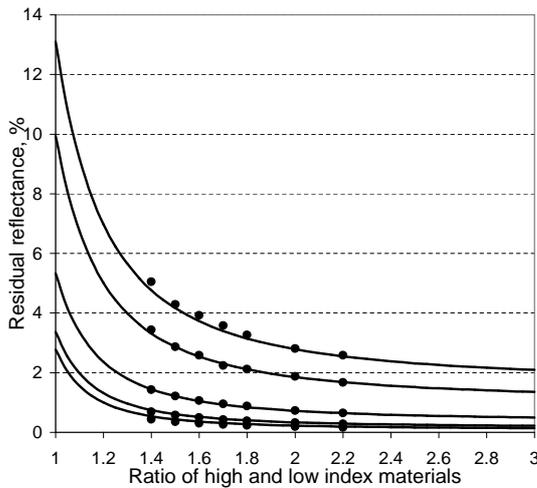


Fig. 1.

Minimum achievable reflectance values of  $R_{\infty}$  calculated for the AR spectral range from 400 to 1200 nm with different values of  $\rho_{HL}$  and  $\rho_{La}$ . The curves are calculated from expression (1), depending on various values of  $\rho_{La}$ .

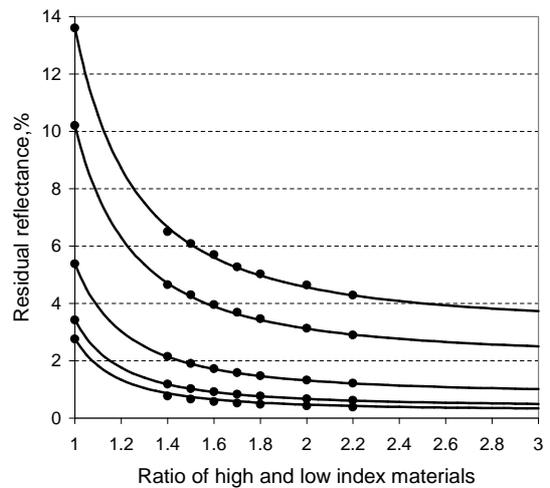


Fig. 2.

Minimum achievable reflectance values of  $R_{\infty}$  calculated for the AR spectral range from 400 to 1600 nm with different values of  $\rho_{HL}$  and  $\rho_{La}$ . The curves are calculated from expression (1), depending on various values of  $\rho_{La}$ .

It can be clearly observed from Figs. 1 and 2 that the experimental values of  $R_{\infty}$  and its values obtained from the empirical expression (1) are in good agreement.

**3. Qualitative analysis of the empirical expression for  $R_{\infty}$ .** It is obvious that the agreement between the experimentally obtained values of  $R_{\infty}$  and the empirical expression does not guarantee that expression (1) is physically meaningful. The formula we obtained must be adequate from the standpoint of the basic theoretical facts of thin film optics. First, it is well known that an increase of the ratio  $\rho_{HL}$  leads to decreasing  $R_{\infty}$  and to tending  $R_{\infty}$  to a nonzero lower limit. On the other hand, it is obvious that, if  $\rho_{HL}$  tends to 1, a two-component coating converges to a single layer. Passing to the limits in expression (1), we obtain

$$\lim_{\rho_{HL} \rightarrow +\infty} R_{\infty} = C(\rho_{La}, \rho_{sa}, \lambda_u/\lambda_l), \quad \lim_{\rho_{HL} \rightarrow 1} R_{\infty} = f_1(\rho_{La}, \rho_{sa}),$$

where the function  $C$  is a nonzero constant with respect to  $\rho_{HL}$  and the function  $f_1$  is the average reflectance of a single layer with the refractive index equal to  $n_L$ .

Second, it is also known that an increase of the ratio  $\rho_{La}$  leads to increasing residual reflectance. On the other hand, if  $\rho_{La}$  converges to 1, the residual reflectance tends to zero. It can be clearly seen from expression (1) that

$$\lim_{\rho_{La} \rightarrow \infty} R_{\infty} = D(\rho_{HL}, \rho_{sa}, \lambda_u/\lambda_l), \quad \lim_{\rho_{La} \rightarrow 1} R_{\infty} = 0,$$

where the function  $D$  is a nonzero constant with respect to  $\rho_{La}$ .

Third, an extension of the AR spectral range leads to an increase of the AR residual reflectance. On the other hand, when  $\lambda_u/\lambda_l$  tends to 1, this means that the spectral range converges to a single spectral point. The AR designs for a single spectral point are well known, and there exists an analytical two-layer design whose residual reflectance is equal to zero. Indeed,

$$\lim_{\lambda_u/\lambda_l \rightarrow \infty} R_{\infty} = E(\rho_{HL}, \rho_{La}, \rho_{sa}), \quad \lim_{\lambda_u/\lambda_l \rightarrow 1} R_{\infty} = 0,$$

where the function  $E$  is a nonzero constant with respect to  $\lambda_u/\lambda_l$ .

Our study of qualitative behavior shows that the above-proposed empirical expression is physically meaningful.

**4. Conclusion.** In this paper we propose an empirical expression for the estimation of the minimum achievable residual reflectance. The expression is in good agreement with our experimental results and is physically meaningful. Using this expression, a specialist dealing with design and manufacture of AR optical coatings will be able to predict the minimum achievable residual reflectance.

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