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Estimation of the average residual reflectance of broadband antireflection coatings

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We deal with optimal two-material antireflection (AR) coatings for the visible and adjacent spectral regions. It has been shown before that, for a given set of input parameters (refractive indices of the substrate, ambient medium and high- and low-index coating materials, and for a given spectral width of the AR coating), such designs consist of one or more clusters of layers of approximately constant optical thickness and number of layers. We show that, through the analysis of many different optimal coatings, it is possible to derive two parameters for a simple empirical expression that relates the residual average reflectance in the AR region to the number of clusters. These parameters are given for all possible combinations of relative spectral bandwidth equal to 2, 3, and 4; low-index to ambient-medium index ratio equal to 1.38 and 1.45; and high-to-low index ratio equal to 1.4, 1.5, and 1.7. The agreement between the numerically and the empirically calculated values of residual average reflectance is excellent. From the information presented the optical thin-film designer can quickly calculate the required number of layers and the overall optical thickness of an AR coating having the desired achievable residual average reflectance.

OCIS codes: 310.1210, 310.6805.

1. Introduction

Antireflection (AR) coatings make up more than 50% of the total optical thin-film market [1]. It is not surprising, therefore, that a great number of publications are devoted to this topic. The first book on thin-film optics, published in 1946 [2], was devoted almost entirely to AR coatings. There are at least several thousands of papers that deal with the design, fabrication, and applications of various types of AR coating. Multiple references to the most essential publications in this area can be found in Refs. [3–8].

During the past two decades researchers have focused their efforts mainly around two-component AR coatings that consist of alternating layers of high-and low-index materials [3,7,8]. This was triggered by the tremendous progress in thin-film technology that made possible the accurate production of two-component AR designs that consist of non-quarter-wave layer optical thicknesses. Currently quite complicated AR coatings of this type with several dozens of layers can be successfully manufactured [7]. The thin-film maximum principle [9] shows that, at normal angle of incidence, two-component AR designs with the highest and lowest available refractive indices form an optimal class of AR designs. This result has also been confirmed numerically [10]. However, it should be mentioned that, for an oblique angle of incidence, especially for AR coatings operating over wide angular ranges, other types of design might be preferable [4–6].

The ability to predict the achievable residual reflectance level in AR coatings designed to operate in given spectral bands would be a great asset to thin-film designers. This average residual reflectance depends on many design parameters. It is known from thin-film theory (Ref. [14], pages 17–20) that spectral

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properties of any coating depend on the ratios of refractive indices of all the layer materials and surrounding media. For two-component designs we should consider the ratio of high and low refractive indices, the ratio of substrate and ambient medium refractive indices, and the ratio of low refractive index and ambient medium refractive index. For all the coatings, in particular for AR coatings, the design total optical thickness is an extremely important design parameter [15,16]. The computational experiments of many authors [3,17,18] show that the average residual reflectance depends strongly on the width of the AR spectral region. It is evident that it is extremely difficult to obtain an analytical expression for the average residual reflectance because so many essential parameters are involved and because their dependencies are interconnected.

An attempt to predict the achievable performance of broadband AR coatings that was based on numerical and statistical analyses was presented in Ref. [17], in which an empirical formula predicting the average residual reflectance of broadband AR coatings depending on the most essential parameters was given. According to this formula the average value of residual reflectance tends to zero with a growing total optical thickness of AR designs. Another version of such a formula is presented in Ref. [19].

Here we attempt to obtain a formula for estimation of the achievable average residual reflectance of broadband AR coatings. Because it is difficult to obtain such a formula entirely on the basis of rigorous theoretical considerations, we use an empirical approach based on well-established specific properties of AR designs and also exploit some of our previous theoretical results. It is well known that spectral reflectance curves of optimal AR designs exhibit specific Chebyshev-like oscillations around average residual reflectance levels [3,17,18]. With a growing design total optical thickness, specific layer clusters are formed in optimal AR designs [18]. Designs with a large number of layers have quasi-periodic groups of layer clusters whose origin was theoretically explained with the help of the Fourier-transform theory [18]. In Section 2 we consider and compare the results of multiple computational experiments for designing AR coatings with various spectral widths and various input design parameters. These results obviously demonstrate cluster structures in optimal AR designs and empirically indicate the existence of limits on average residual reflectances of AR designs for all the combinations of design parameters considered.

In Section 3 we propose a simple two-parameter formula that expresses with high accuracy the average residual reflectance of optimal AR designs as a function of the number of clusters. Our previous theoretical results enable us to relate the number of clusters to the total optical thickness of a design and to other design parameters. From this formula we can derive an expression that permits one to estimate the relative decrease in the residual AR design reflectance resulting from a further elaboration of the design structure. We believe that these expressions and the two-dimensional plots for the lowest possible average residual reflectances presented in Section 3 will be useful for the design and manufacture of practical broadband AR coatings. Final conclusions are presented in Section 4.

2. Numerical Study of Sequences of Optimal Antireflection Designs

As mentioned above, we consider single band normal incidence two-material AR coatings. Throughout this paper, the ambient medium is assumed to be air with $n_a = 1$ and the substrate is assumed to be glass with $n_s = 1.52$. Refractive indices of low- and high-index materials n_L and n_H can have different values that are specified later. The lower and upper limits of the AR spectral region are denoted by λ_l and λ_u, respectively.

It was shown in Ref. [11] that the optimization of AR designs with respect to the thicknesses of design layers is an optimization problem that is close to the optimization of convex functions. This is an important fact because any convex function has a single minimum that can be reliably found using various optimization methods. Thus, from a computational point of view, designing AR coatings is usually simpler than the design of optical coatings of other types. In our computational experiments we applied modern versions of the needle optimization technique [13] that enable one to obtain not a single AR design but a series of optimal AR designs with various combinations of design total optical thicknesses and numbers of layers. These two design parameters are denoted below as TOT and N, respectively.

Modern design software makes possible the generation of a whole series of AR designs with different TOT and N values in a short period of time. Because of this fact we were able to perform a numerical investigation of multiple AR designs with various combinations of refractive indices n_H and n_L and various widths of AR spectral bands. From a theoretical point of view, ratios of refractive indices are more important than their absolute values [14]. In what follows we therefore choose to work with the ratios of high and low refractive indices $\rho_{HL} = n_H/n_L$ and low and ambient medium refractive indices $\rho_{La} = n_L/n_a$. Along with the above parameters, each AR design is also characterized by its average residual reflectance R_{av}, which is defined by the equation

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

where $R(\lambda)$ is the reflectance of the design. The main goal of our computational experiments was to study the dependence of the average residual reflectance values R_{av} on the design total optical thickness TOT and other design parameters. To achieve this goal we constructed several hundred AR designs with differ-

Table 1. Parameters of the AR Designs for the 400–1200 nm Spectral Region

Design	Total Optical Thickness (nm)	Number of Layers	Average Residual Reflectance
D1	807	10	0.855
D2	1546	18	0.662
D3	2280	26	0.596
D4	3002	34	0.565
D5	3711	42	0.546
D6	4437	50	0.533
D7	5178	56	0.525
D8	5757	62	0.516
D9	6468	72	0.514
D10	7209	78	0.510
D11	7803	86	0.507
D12	8495	94	0.505
D13	9213	102	0.503
D14	9817	108	0.501
D15	10563	116	0.500
D16	11268	124	0.498
D17	11848	130	0.497
D18	12536	138	0.497
D19	13191	142	0.496
D20	13883	152	0.495

ent combinations of design parameters. It is obviously impossible to present detailed information about all these designs here, but luckily the presentation of all the results is not necessary because there are some basic structural properties that are typical for all sets of optimal AR coatings with fixed ρ_{HL}, ρ_{La} and λ_u/λ_l values. These structural properties are presented in detail for one set of optimal AR designs.

Table 1 presents the characteristics of twenty AR designs with various TOT values obtained for refractive indices $n_H = 2.35$, $n_L = 1.45$ and for the 400–1200 nm AR wavelength region. The design total optical thicknesses TOT, number of layers, and the average values of the residual reflectances R_{av} are listed in columns 2–4. As one would expect, R_{av} values decrease with an increase in design total optical thicknesses. The dependence of R_{av} on the design parameters will be discussed later in more detail.

It is necessary to stress that, for any combination of refractive indices and AR spectral bandwidths, a set of optimal AR designs is always arranged in such a way that total optical thicknesses and number of layers of optimal designs are increased monotonically by nearly equal increments. This property is clearly seen in Table 1. It was discussed in detail in our previous paper [3], where the quantization of optimal AR designs was explained by the formation of special clusters of layers in optimal designs.

According to the third column of Table 1, the number of layers of AR designs usually increases by eight from one optimal design to the next, because, for this particular AR problem, layer clusters are formed that consist of eight layers. The formation of new layer clusters is illustrated in Fig. 1, where the refractive-index profiles of the first five designs from Table 1

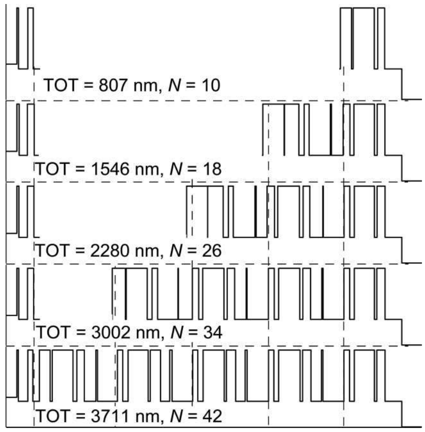

Fig. 1. Refractive-index profiles of the first five designs from Table 1 .

are shown. The refractive-index profiles of designs D1–D4 are presented in Fig. 1 in a discontinuous form to illustrate clearly the formation of layer clusters. One can see that there are groups of four layers at the substrate side and groups of six layers at the ambient medium side that were formed in the D1 design and then are repeated from one design to another with only small variations. Eight-layer clusters with nearly the same layers are formed inside the designs between these two groups of initial and final layers. The D2 design has one such cluster, D3 has two clusters, and so on.

In Ref. [3] the following equation for estimating the optical thickness T_c of layer clusters was obtained:

$$T_c = \frac{\lambda_u}{2}\left[1 + \frac{2}{\pi}\arcsin\left(\frac{\rho_{HL} - 1}{\rho_{HL} + 1}\right)\right]. \qquad (2)$$

Note that λ_u here is the upper wavelength boundary of the AR spectral band and ρ_{HL} is the ratio of the high and low refractive indices. For our current values of these parameters, Eq. (2) results in a value for T_c that is equal to 691 nm, which is in excellent agreement with the average increment of 688 nm in the optical thicknesses of AR designs in the second column of Table 1.

Reflectances of the D1–D5 designs are shown in Fig. 2 by use of wavenumber spectral units. In Fig. 2 the wavenumber is defined by the expression $2\pi/\lambda$, where λ is the wavelength of the incident light in vacuum. The spectral region from 400 to 1200 nm thus corresponds to from 52360 to 157080 cm^{-1} in the wavenumber scale. One can see that the spectral reflectance curves have specific oscillations inside the AR spectral band. The origin of these oscillations is explained in Ref. [20] on the basis of the general analytical properties of the spectral characteristics of optical coatings [21]. Because this topic has no direct bearing on the main goal of our paper, we do not discuss it here and refer the interested reader to Ref. [20]. In all other computational experiments with AR coatings analogous structural properties and cluster

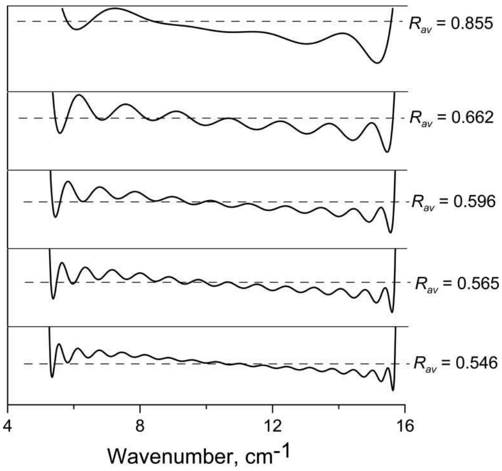

Fig. 2. Reflectances of the first five designs from Table 1.

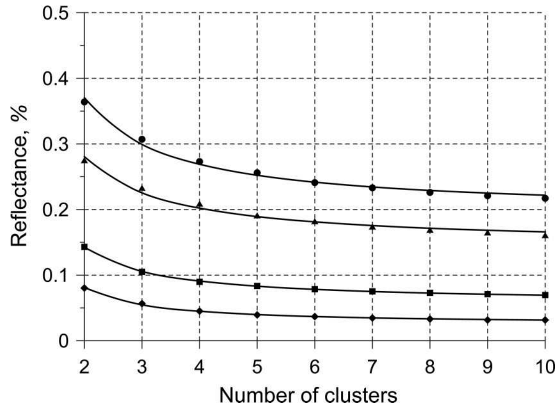

Fig. 3. Average residual reflectances R_{av} of AR coatings designed for the AR spectral band from 400 to 800 nm with different refractive-index ratios: $\rho_{HL} = 1.4$, $\rho_{La} = 1.45$ (circles), $\rho_{HL} = 1.5$, $\rho_{La} = 1.45$ (triangles), $\rho_{HL} = 1.7$, $\rho_{La} = 1.45$ (squares), $\rho_{HL} = 1.7$, $\rho_{La} = 1.38$ (diamonds). The solid curves, calculated from Eq. (3), are in excellent agreement with the experimental data.

formations were observed. For each combination of refractive indices and AR spectral bandwidths we designed sets of AR coatings with as many as several hundred layers. In Table 2 we present only the integrated results of our computational experiments.

In the fourth and fifth columns of Table 2 we compare the theoretical and the experimental optical thicknesses of the layer clusters. Good agreement between these values is always observed. The number of layers in the cluster is listed in the sixth column of Table 2. One can see that the cluster thicknesses and the number of layers within them in general increase with an increase of the relative width of the AR spectral band. It is also seen from Table 2 that optical thicknesses of layer clusters are mainly dependent on the width of the AR spectral band and are much less dependent on the refractive indices.

Because the cluster structure is a basic property of optimal AR designs, it is reasonable to depict the dependence of R_{av} not on design total optical thickness or on the number of layers in a design, but on the number of clusters in a design. In Figs. 3–5 we present the experimental dependence of R_{av} on the number of design clusters for different AR spectral bands. Different markers are used to plot the results for different combinations of refractive indices. All the experimental data presented in Figs. 3–5 suggest that there are lower limits for the average residual reflectances R_{av}. These limits, of course, depend on the refractive indices used in the AR designs as well as on the width of the AR spectral band.

Table 2. Integrated Results for a Series of Optimal AR Designs for Different Combinations of Refractive Indices and AR Spectral Bandwidths

Spectral Range (nm)	λ_u/λ_l	Refractive Indices n_H, n_L	Optical Thickness of Clusters, Obtained Experimentally (nm)	Optical Thickness of Clusters Predicted by the Theory (nm)	Number of Layers in One Cluster
400–600	1.5	1.45, 2.35	372	346	4
400–700	1.75	1.45, 2.35	420	403	4
400–800	2.0	1.45, 2.03	465	443	6
400–800	2.0	1.45, 2.175	452	451	6
400–800	2.0	1.45, 2.466	478	467	6
400–800	2.0	1.38, 2.346	459	467	6
400–900	2.25	1.45, 2.35	520	518	6
400–1000	2.5	1.45, 2.35	590	576	6
400–1100	2.75	1.45, 2.35	640	642	8
400–1200	3.0	1.45, 2.03	687	664	8
400–1200	3.0	1.45, 2.175	698	677	8
400–1200	3.0	1.45, 2.465	709	700	8
400–1200	3.0	1.38, 2.346	720	700	8
400–1500	3.75	1.45, 2.35	900	864	10
400–1600	4.0	1.45, 2.03	919	885	10
400–1600	4.0	1.45, 2.175	930	903	10
400–1600	4.0	1.45, 2.465	955	934	10
400–1600	4.0	1.38, 2.346	949	934	10

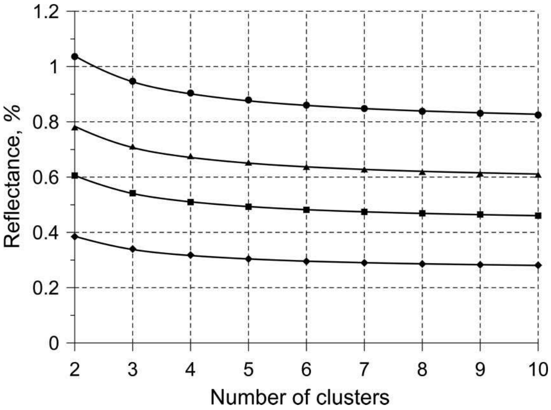

Fig. 4. Average reflectances R_{av} of AR coatings designed for the AR spectral band from 400 to 1200 nm with different refractive-index ratios: $\rho_{HL} = 1.4$, $\rho_{La} = 1.45$ (circles), $\rho_{HL} = 1.5$, $\rho_{La} = 1.45$ (triangles), $\rho_{HL} = 1.7$, $\rho_{La} = 1.45$ (squares), $\rho_{HL} = 1.7$, $\rho_{La} = 1.38$ (diamonds). The solid curves, calculated from Eq. (3), are in excellent agreement with the experimental data.

Table 3. Parameters R_∞ and b Found by the Least-Squares Method for the Twelve Sets of R_{av} Values Presented in Figs. 3–5

λ_u/λ_l	ρ_{HL}	ρ_{La}	R_∞	b	ln b
2	1.4	1.45	0.195	3.604	1.28
2	1.5	1.45	0.145	3.720	1.31
2	1.7	1.45	0.058	6.042	1.80
2	1.7	1.38	0.025	10.659	2.37
3	1.4	1.45	0.691	1.822	0.60
3	1.5	1.45	0.575	1.862	0.62
3	1.7	1.45	0.430	1.985	0.69
3	1.7	1.38	0.259	2.219	0.80
4	1.4	1.45	1.154	1.356	0.30
4	1.5	1.45	1.011	1.375	0.32
4	1.7	1.45	0.813	1.441	0.37
4	1.7	1.38	0.522	1.562	0.45

3. Empirical Equation for the Average Residual Reflectance of AR Designs

The results in Section 2 show that it is reasonable to relate the average residual reflectances of AR designs to the number of design clusters M. To approximate the experimentally obtained dependence of the average residual reflectance R_{av} on the number of clusters M we use the following two-parameter equation:

$$R_{av} = R_\infty b^{1/M}. \tag{3}$$

The parameter R_∞ represents the minimum achievable average residual reflectance for a given set of input design parameters. Both R_∞ and b depend on the refractive-index values as well as on the width of the AR spectral band. The parameters R_∞ and b can be found by the least-squares method and are given in Table 3 for the twelve sets of input parameters corresponding to Figs. 3–5. Analytical dependencies presented by Eq. (3) with continuous M values are represented by the solid curves in Figs. 3–5. Clearly there is excellent agreement between the experimental R_{av} values and the values obtained from the empirical Eq. (3).

Parameters R_∞ and b depend on the ratios of refractive indices ρ_{HL} and ρ_{La} as well as on the ratio of the boundary wavelengths of the AR spectral band. Table 3 shows that, for λ_u/λ_l equal to 3 and 4, R_∞ exhibits a stronger dependence on these input parameters than on b. We performed a great number of additional computational experiments to obtain more detailed information about the dependence of R_∞ on the input design parameters. Results of these experiments are summarized in Figs. 6–8 in which we present R_∞ values for the three ratios of boundary wavelengths of the AR spectral bands and for the different refractive index ratios ρ_{HL} and ρ_{La}. For the sake of convenience R_∞ values are presented as level curves. Equation (3) can be used to derive an expression for the gain in optical performance when another

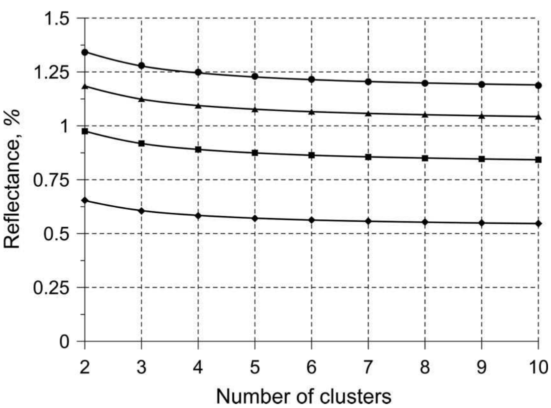

Fig. 5. Average values of residual reflectances R_{av} of AR coatings designed for the AR spectral band from 400 to 1600 nm with different refractive-index ratios: $\rho_{HL} = 1.4$, $\rho_{La} = 1.45$ (circles), $\rho_{HL} = 1.5$, $\rho_{La} = 1.45$ (triangles), $\rho_{HL} = 1.7$, $\rho_{La} = 1.45$ (squares), $\rho_{HL} = 1.7$, $\rho_{La} = 1.38$ (diamonds). The solid curves, calculated from Eq. (3), are in excellent agreement with the experimental data.

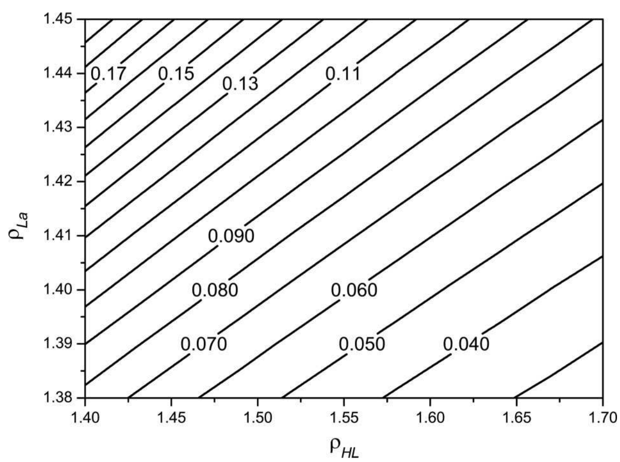

Fig. 6. Minimum achievable values of the average residual reflectance R_{av} for the relative widths of the AR spectral band $\lambda_u/\lambda_l = 2$ and for different refractive-index ratios ρ_{HL} and ρ_{La}.

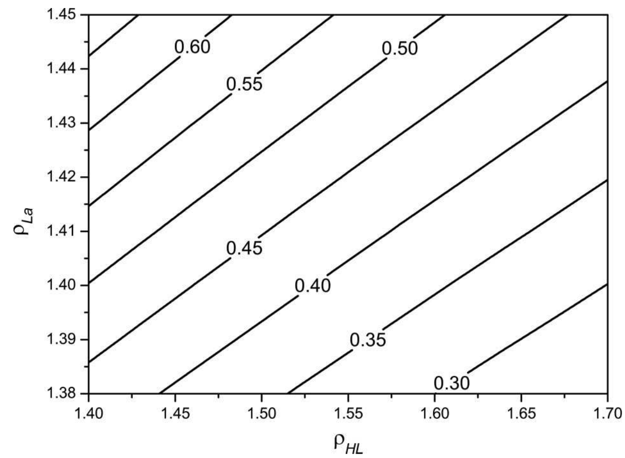

Fig. 7. Minimum achievable values of the average residual reflectance R_{av} for the relative widths of the AR spectral band $\lambda_u/\lambda_l = 3$ and for different refractive-index ratios ρ_{HL} and ρ_{La}.

cluster is added to a particular AR coating design:

$$\Delta R_{av} \approx R_\infty \cdot \frac{\ln b}{M^2}. \tag{4}$$

The sixth column of Table 3 presents ln b values for several sets of input parameters. One can see that only for $\lambda_u/\lambda_l = 2$ do these values exceed 1. To illustrate an application of Eq. (4), let us replace ln b in Eq. (4) by 1. Consider the relative decrease of the residual reflectance when the number of clusters in the AR design is increased from 3 to 4. With $M = 3$, Eq. (4) estimates this decrease to be 11% of the previous value. If $M = 5$ the further addition of a cluster to the AR design will result only in a 4% reduction in the residual reflectance. It will be up to the optical coating engineer to decide whether such an increase in the complexity of the design structure is warranted by such a small improvement in the performance of the AR coating.

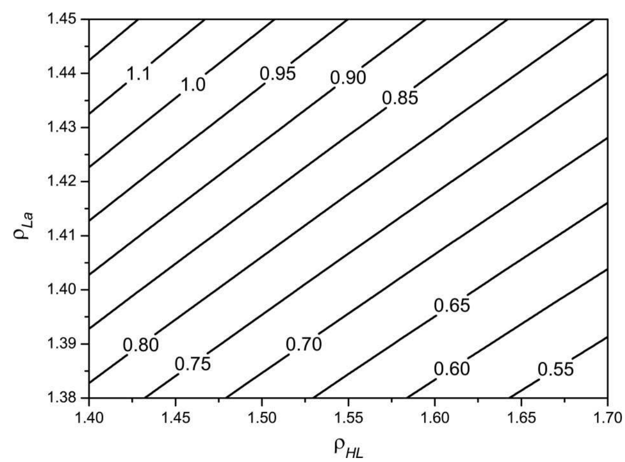

Fig. 8. Minimum achievable values of the average residual reflectance R_{av} for the relative widths of the AR spectral band $\lambda_u/\lambda_l = 4$ and for different refractive-index ratios ρ_{HL} and ρ_{La}.

4. Conclusions

The empirical Eqs. (2)–(4), the data in Tables 2 and 3, and the data contained in Figs. 3–8 provide the thin-film designer with all the information required to assist him in the design of wideband antireflection coatings for the visible and adjacent spectral regions. To design an AR coating for glass with a refractive index of 1.52 immersed in air, with a spectral width of $\lambda_u/\lambda_l = 2$, 3, or 4; with $\rho_{La} = 1.38$ or 1.45; and with $\rho_{HL} = 1.4$, 1.5, or 1.7, it is sufficient to look up the number of clusters required to achieve the desired residual reflectance in Figs. 3–5, and the optical thickness and number of layers in the cluster from Table 2. From this it is a simple matter to calculate the approximate overall thickness and the number of layers required in the AR coating. With this information one can obtain a satisfactory solution with most commercial thin-film design programs using materials that take into account the dispersion of the optical constants. For other values of ρ_{La} and ρ_{HL}, the parameter R_∞ can be estimated from Figs. 6–8 and the value of parameter b interpolated from the values listed in Table 3. The residual reflectance in the AR region can then be evaluated with the aid of Eq. (3) for a reasonable value of the number of clusters M. Equation (4) serves to investigate the effect on R_{av} of adding additional clusters. The optical thickness of the clusters can be obtained from Eq. (2). For other widths λ_u/λ_l of the AR spectral region, interpolated values of R_∞ and b should also serve as a good starting point for numerical calculations.

It should be noted that refractive indices of coating materials exhibit a significant dispersion in wide spectral regions. In many publications on AR coatings nondispersive material indices are used and we also follow this tradition. Most of the calculations were performed with a low refractive index that was equal to 1.45. This refractive index was chosen because most optical coating engineers use silica as the low-index material. In this research the wide spectral regions usually extended into the IR part of the spectrum and a refractive index of 1.45 was deemed to be a reasonable average value for the refractive index of silica for such a broad spectral region. It is obvious that the same approach could be used to produce corresponding information for the design of wideband AR coatings in the infrared spectral region for semiconducting substrate materials. A shortened version of this paper was first presented at the 2007 Optical Interference Coatings Topical Meeting [18].

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