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Design of hybrid coatings composed of homogeneous layers and refractive index gradients

Vesna Janicki[a,b], Robert Leitel[c], Steffen Wilbrandt[c], Olaf Stenzel[a], Dieter Gäbler[a], Norbert Kaiser[a]
[a] Fraunhofer Institut für Angewandte Optik und Feinmechanik, Optical Coatings Department, Albert-Einstein-Str. 7, 07745 Jena, Germany
[b] Ruđer Bošković Institute, Division of Laser and Atomic Research and Development, Bijenička cesta 54, 10000 Zagreb, Croatia
[c] Friedrich-Schiller-Universität Jena, Institut für Angewandte Physik, Max-Wien-Platz 1, 07743 Jena, Germany

ABSTRACT

Inhomogeneous coatings are promising for superior optical properties, e.g. broadband antireflection, in comparison to conventional HL-stack designs. Although a lot of excellent theoretical work on optical behaviour of rugates and gradient index films has been done during the last decades, there is no real breakthrough in industrial fabrication. The realization of such coatings leads to an extensive and time-consuming computer-aided control, because of complicated layer designs with continuously changing refractive index gradients. We describe the design and optical performance of an omnidirectional antireflection coating that essentially represents a hybrid coating composed from homogeneous layers and linear refractive index gradient layers.

Keywords: antireflection, gradient index, mixing layers, omnidirectional

1. INTRODUCTION

Antireflective films are among the most frequently used coatings. They are applied in almost each optical system to improve intensity of transmitted light and prevent appearance of ghost images due to multiple reflections on intrinsic surfaces. The requirements are set on the spectral region and range of incidence angles where a low reflectivity is expected. Typically, two material based HL-systems are used, but if performance at oblique incidence or, especially, broad angular range is necessary, the implementation of at least one additional material of intermediate refractive index is favourable. However, traditional dielectric multilayer antireflection stacks remain limited for this purposes by the choice of available materials having both, good mechanical and optical properties at the same time. In this case, the application of gradient index layers is preferable.

The ideal antireflective coating for a given spectral and angular range would be a gradient index structure having refractive index varying from the value of substrate, at substrate side, to the value of incidence medium towards the surface[1-3]. This means that in the case of substrate/air interface, the coating should end with a refractive index of air or at least close to it. The problem is how to achieve such low values, since there are no suitable low index materials. Potential approaches to obtain gradients of low refractive index are moth's eye structures[4] or increased porosity of the film towards the incidence medium[5]. However, the main drawback is the mechanical resistance and cleaning of such surfaces.

This paper presents an alternative approach for antireflection designs, combining homogeneous and linear graded index layers. The introduced hybrid coatings[6] are optimised for the visible spectral region and for omnidirectional incidence up to 50 degrees. This method merges the advantages of gradient index layers, e.g. reduced scatter losses due to the absence of abrupt changes of refractive indices at interfaces, and the capability of fabrication inhomogeneous coatings on industrial deposition plants. Additional profits that can be expected from inhomogeneous coatings are their good mechanical properties, like low stress and better tribological resistance[7-9] than classical multilayer stacks. Fig.1. represents a general refractive index profile of a hybrid coating.

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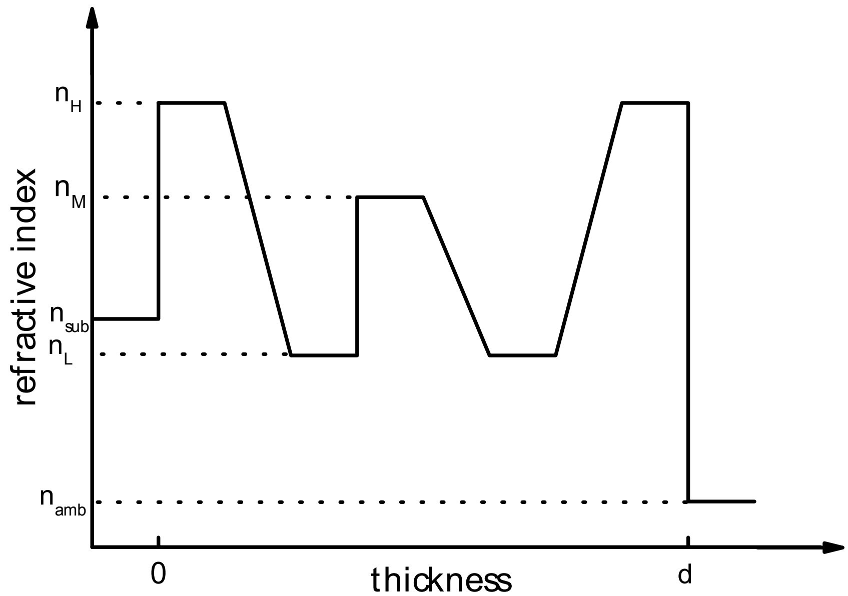

Figure 1. General refractive index profile of a hybrid coating of thickness *d*. Here, n_H and n_L are the refractive indices given by the pure materials and n_M stands for any achievable intermediate refractive index in the profile. Substrate's refractive index is denoted by n_{sub}, while n_{amb} is the ambient one.

The design of the antireflection coating was synthesized utilizing the numerical optimisation software recently developed by Tikhonravov et al[14-15]. The hybrid coating was optimised for BK7 glass substrate and commonly applied thin film materials Nb_2O_5 and SiO_2, keeping in mind the constraints due to limitations of available deposition technology (Sec. 2). Two designs differing in their number of layers and thus total thickness were generated and compared with a classical design obtained for the same purpose. Error analyses concerning thickness and refractive indices have been performed for the thinner design. In addition, the most sensitive layer parameters have been detected (Sec. 3).

2. METHODOLOGY

2.1. Specifications and design constraints

The required antireflection coating had to minimise reflectance *R* in the range 480-680 nm and for angles of incidence 0°-50°. Here *R* is an average of the reflectance at *s*-polarization R_s and *p*-polarization R_p. The additional requirement in synthesis was that at the same time the difference between R_s and R_p should be as low as possible for angle of incidence of 50° in the specified spectral region. As mentioned before, BK7 glass was the substrate, SiO_2 the low index material and Nb_2O_5 the high one. The intermediate refractive indices were calculated using the pure materials indices and their filling factors in the mixture.

The obtained coating is intended to be produced by co-evaporation of the two materials by electron beam guns in a Leybold Syrus Pro 1100 deposition plant, where such successful co-depositions have already been done[10]. The maximal and minimal refractive index of linear gradient layers of the design were limited by the technique of deposition. Since it is very difficult to control precisely low rates of deposition, the highest achievable (and still well reproducible) refractive index mixture is 2.1 and the lowest 1.6 at a wavelength of 570 nm. Besides this it is not possible to obtain arbitrarily steep gradient of the mixture due to the technical reasons. Thus, the change in refractive index of 0.5 in 25 nm of thickness was the maximal allowed steepness of refractive index gradient in the design.

2.2. Optimisation method

The most common approach to synthesis of rugate filters (i.e. coatings having continuous variation of refractive index with thickness) is based on the inverse Fourier transform relation between spectral function $Q(\lambda)$ and refractive index profile. One of the method's problems is that *Q*-function is not known exactly, but only its approximate values[11-13]. An

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alternative method in synthesis of rugate designs was followed using software specially developed for rugate systems[14,15] based on numerical optimisation technique. Here, spectral performance of the refractive index profile is calculated without approximation. The deviation of the performance of the model from the desired target values is optimised through the minimisation of the merit function.

The refractive index profile of the design is considered and represented in the software as polyline (Fig.2.). The polyline is defined by a set of corner points (z_i, n_i) connected by straight lines representing segments of linear change of refractive index. Here n_i is the refractive index of the layer with corresponding thickness z_i, at the reference wavelength λ_0 that is defined as

$$\lambda_0 = \sqrt{\lambda_m \lambda_M} \ . \qquad (1)$$

λ_M and λ_m are the upper and the lower boundary of the spectral range where the target is defined. Thus, any continuous refractive index profile can be well approximated by increasing the number of corner points. In the optimisation process the segments are divided into a number of subsegments represented by homogeneous sublayers all having equal thickness and refractive indices equal to the mean values of the individual subsegment (Fig.3.). The number of sublayers should be adequate for a reasonably good approximation of the gradient layers.

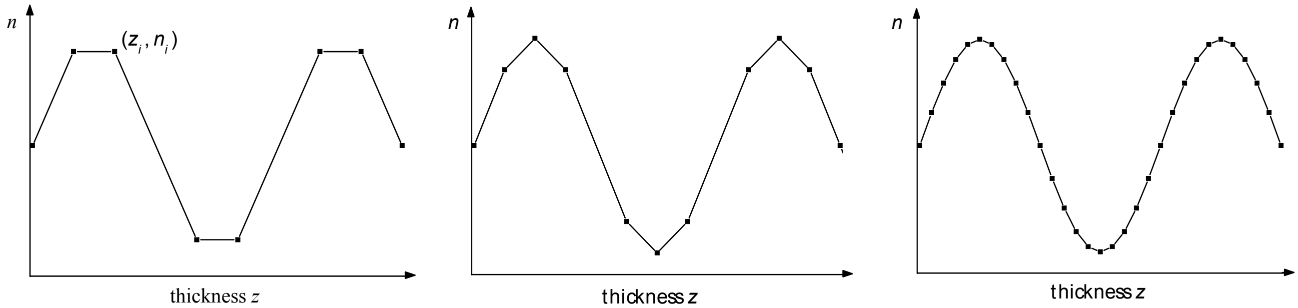

Figure 2. A sinusoidal shaped refractive index profile, represented by polylines, can be well approximated by increasing the number of corner points (z_i, n_i) (black rectangles).

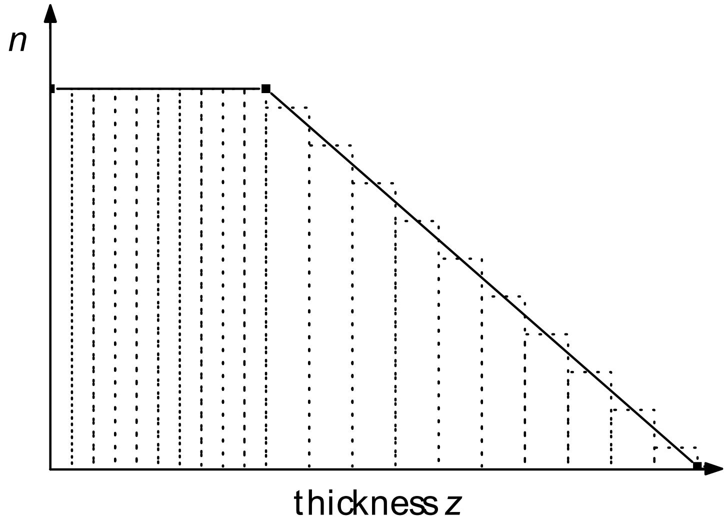

Figure 3. Division of segments into homogeneous sublayers of equal thickness and refractive indices equal to the mean values of the individual sublayer.

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In the case of layers prepared by co-deposition of Nb_2O_5 and SiO_2 it is experimentally proven[16] that the refractive index $n(\lambda)$ of the mixture may be approximated by

$$n(\lambda) = \mu n_H(\lambda) + (1-\mu) n_L(\lambda)\,. \qquad (2)$$

Here n_H and n_L stand for indices of pure materials, i.e. Nb_2O_5 and SiO_2, and μ is the fraction of the high index material, that can take value between 0 and 1. It is assumed that the same relation holds for the case of complex refractive indices if extinction coefficient k is much smaller than refractive index n , ($k \ll n$). Eq. (2) relates the dispersion of refractive index of pure materials to the dispersion of their mixture. In this way both, dispersion and absorption are included into the calculation of the spectral performance of the model.

3. RESULTS AND DISCUSSION

3.1. Hybrid designs

As the result of the calculations two different designs have been obtained consisting of 9 and 13 corner points. Their refractive index profiles at the wavelength of 570 nm and the corresponding reflectance for different angles of incidence together with that for uncoated substrate are shown in Fig.4. and Fig.5., respectively. The last four points (F, G and H, I) represent homogeneous layers of pure high and low index materials. The search in the literature shows similarity of the profiles to DeBell´s classical multilayer designs[1]. Corresponding total thickness of the hybrid designs are 526 nm (9 corner points) and 839 nm (13 corner points), respectively. The discrepancy from the specifications as expressed in terms of the function of merit (FOM) has 40% lower value in the case of the thicker design. However, both designs fit the target specifications well. Besides the quality of the optical performance, additional thickness and more corner points in the thicker one have to be taken into consideration. Because of the limitations defined in Sec.2.1., a smooth transition between points D and F, i.e. continuous linear refractive index gradient, is not feasible. The approximation with an additional segment by inserting the point E does not spoil the quality of the performance (FOM) significantly.

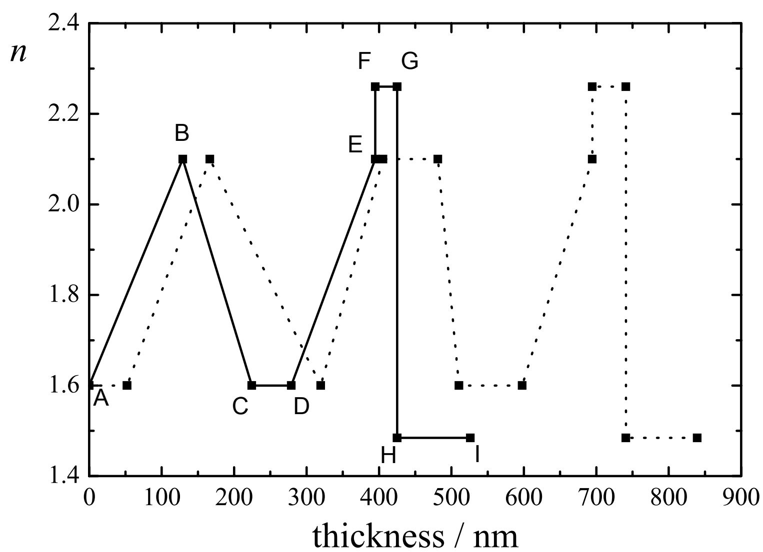

Figure 4. Refractive index profiles for the two hybrid designs at 570 nm, capital letters stand for corner points.

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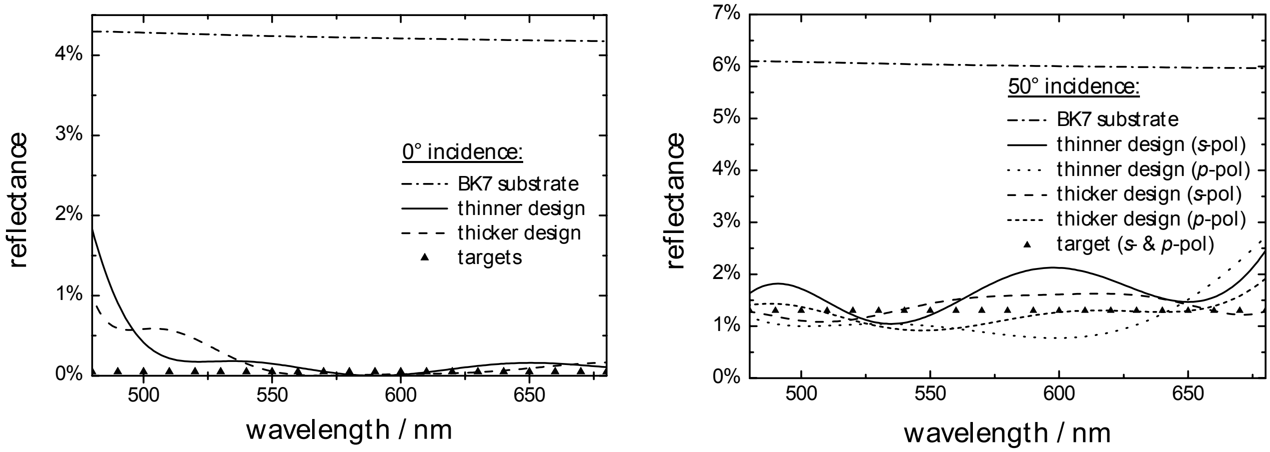

Figure 5. Optical performance of the thinner and thicker hybrid design for semi-infinite substrate (no back-side reflectance). Triangles represent target reflectance at 0° incidence (left) and for *s* and *p* polarisation at the incidence angle of 50° (right).

Besides good optical performance and small physical thickness, the quality of these designs is in their simplicity due to the small number of corner points forming the refractive index profile. The starting and the finishing points of the segments represent always the minimal and maximal allowed refractive indices of the mixtures. Thus, only the *n* values of the two mixtures have to be well controlled and repeatable. This minimizes possibility of error in refractive indices at the corner points.

3.2. Comparison with a classical HL design

Defining the same specifications, substrate and materials, a classical high-low (HL) multilayer stack has been obtained. It consists of 7 layers having the total thickness of 553 nm. The refractive index profile and the spectral performance compared with the thinner of the two hybrid designs, that is also thinner than the classical one, is shown in Fig.6. and Fig.7. The HL stack has 19% better FOM compared to the thinner hybrid. Its drawback is the first H layer which is only 4.6 nm thick (the similar HL design without so thin layers gives 10% worse FOM than the hybrid).

The hybrid coatings predict a very good reflection suppression and satisfy the specifications defined for 0° and 50° well. In Fig. 8. the average reflectance is depicted in the specified spectral region as a function of angle of incidence. Even for angles up to 60° the reflectance of the coated substrate is expected to be lower than that of the uncoated BK7 substrate at 0°. The hybrid coatings have equally good spectral and angular performance as the classical HL design.

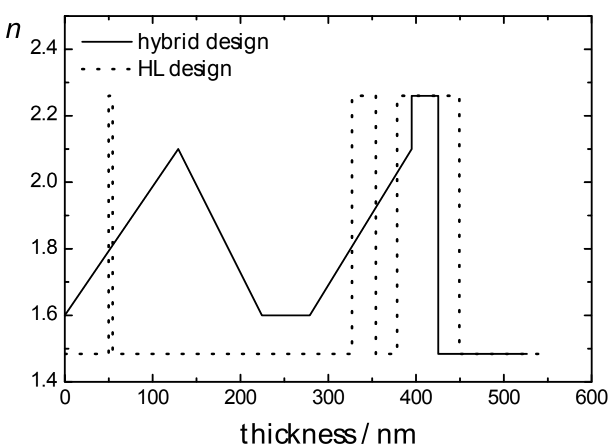

Figure 6. Comparison of refractive index profiles of the thinner hybrid design and the classical HL design.

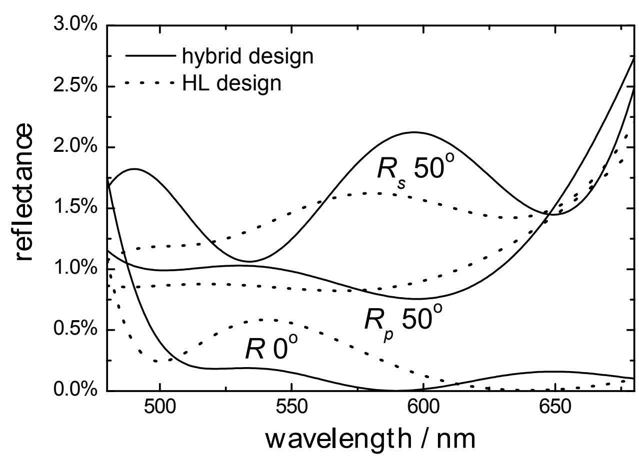

Figure 7. Comparison of reflectance spectra of the two designs.

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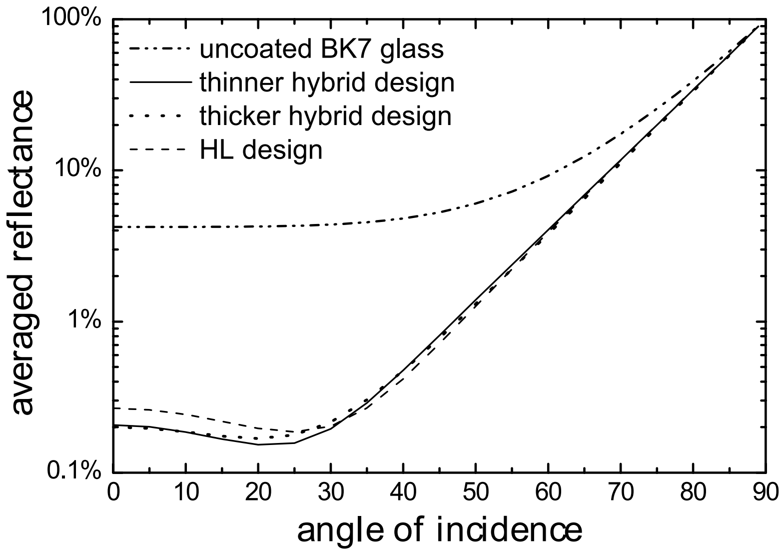

Figure 8. Reflectance averaged over the spectral range of interest and polarization as a function of angle of incidence.

3.3. Sensitivity and error analysis

The sensitivity to fabrication errors and the knowledge where are the most critical corner points is very important for manufacturing of the proposed coatings. In order to detect which points are the most sensitive to errors, the coordinates (z_i , n_i) of each corner point of the thinner design have been varied individually by ±1% and the function of merit has been checked. The corresponding relative changes in FOM are presented in Tab.1. The worst performance of the coating was obtained in the case of increased refractive index at point D, decreased thickness of the last layer (point I) and decreased refractive index at point E.

Table1. Sensitivity of FOM of thinner hybrid design to errors in individual corner points defined in Fig.4.

corner point	relative change in FOM / %			
	change in refractive index +1%	change in refractive index -1%	change in thickness +1%	change in thickness -1%
A	**2.7**	2.4	-	-
B	0.3	0.5	0.5	0.5
C	**4.3**	1.0	0.8	0.3
D	**7.4**	1.7	0.8	0.5
E	3.6	**6.7**	2.0	0.3
F	-	-	**2.0**	0.3
G	-	-	0.1	0.1
H	-	-	0.1	0.1
I	-	-	2.7	**7.0**

The models of hybrid coatings, where each gradient index segment was divided into ten sublayers of constant refractive indices, was imported into Optilayer® software and the implemented error simulation procedure has been performed. A variation of 1% was permitted in both, thickness and refractive index. For the homogeneous layers of pure materials no error in refractive index was allowed. The corridor probability has been set to the value of 68.27%. The results of the calculations for the two hybrid systems are presented in Fig.9 and for the HL-design in Fig.10. One can see that the corridor is broader for the thicker systems, which results from the higher number of parameters. The corridor of the thinner design is about as small as that of the HL-stack, although the last mentioned varies more along the wavelength scale. At 50° the HL-stack is clearly better.

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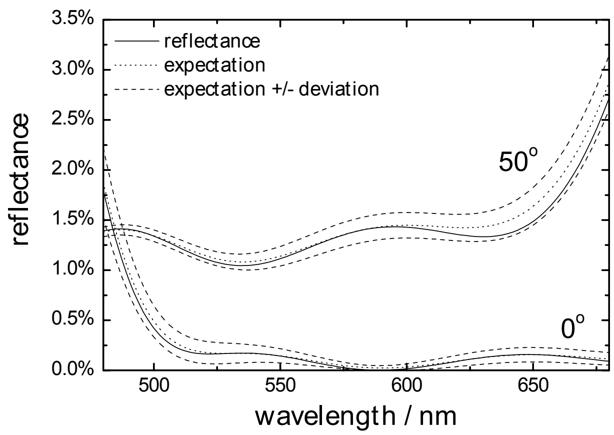

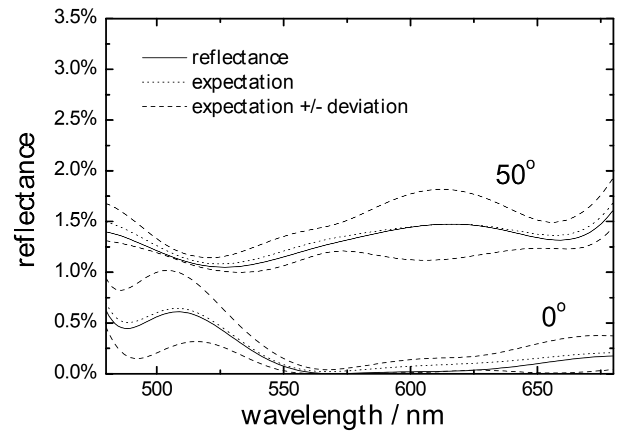

Figure 9. Reflectance variations of the thinner (left) and thicker (right) hybrid design caused by 1% random errors of thickness and refractive indices.

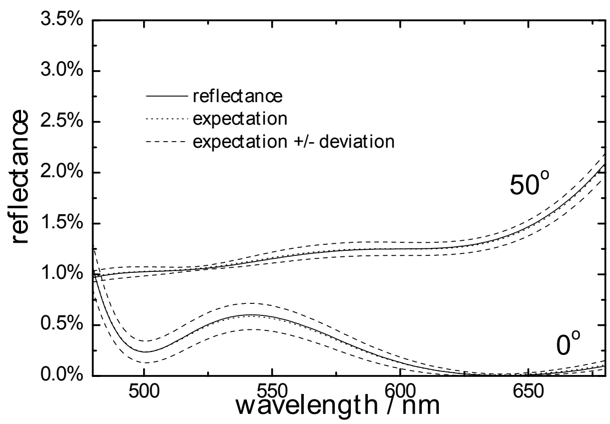

Figure 10. Reflectance variations of the HL-design caused by 1% random errors of thickness and refractive indices

4. CONCLUSIONS

Antireflective hybrid optical coatings presented in this paper are a synthesis of dielectric homogeneous and gradient index layers. It is demonstrated that such designs show excellent optical performance in broad angular range. These designs may be practically produced by co-evaporation of a high and a low index coating materials. Small physical thickness, low number of corner points, segments starting and finishing only in maximal and minimal allowed refractive indices of the mixtures and absence of refractive index values close to that of ambient (air) make these designs feasible and affordable as broad angular range antireflective coatings. Mechanical stability and low scattering due to the reduced number of interfaces are also expected from these hybrid designs.

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