Predicting achievable design performance of broadband antireflection coatings

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An empirically derived formula, which can be used to predict the average residual reflection that can be expected from an antireflection (AR) coating design as a function of bandwidth, overall thickness, available indices of the coating materials, number of layers, etc., is presented. This formula can be a useful tool not only for the thin-film designer but also for the nondesigner or system engineer to estimate the performance limits of an AR coating for a given application before the design is accomplished. The general predictions are also found to be consistent with the results of two recent AR design competitions involving many independent investigators. Some insight with respect to the basic underlying principles of AR coatings can also be gleaned from the results and the process by which they are found.

Key words: Thin-film design, broadband AR coatings, performance estimation.

Introduction

The problems of understanding,[1] designing,[2,3] and producing[4] very broadband antireflection (VBBAR) coatings have been previously addressed. Here I draw on those results and further investigations to provide a tool for the engineer or designer to estimate the performance that can be expected from a VBBAR design before the design process is started. To this end, I have fit my cumulative results to an equation for the average reflectance in the antireflection (AR) band as a function of four major variables. These variables are bandwidth (B), index of refraction of the last layer (L), overall optical thickness of the coating (T), and the difference (D) between the highest and the lowest indices used (except for the last layer). It was also found that the minimum number of homogeneous layers required can be predicted. I show how these formulas were developed, what their limitations are, how to apply them, and what factors are of major and minor importance.

An AR design problem was posed by Thelen and Langfeld[5] for the thin-film conference in Berlin in September of 1992. The problem was to design an AR coating from 400 to 900 nm that had less than 1% reflectance at 0° and 30° angles of incidence for random polarization over the band. The maximum physical thickness allowed for the film stack was 2000

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nm, and the choice of indices was limited to given values that approximate the real materials of magnesium fluoride, silica, alumina, tantala, and titania. The maximum physical thickness of titania allowed was 150 nm. The contest was to achieve the lowest average reflectance over the band, within the 1% constraint, in which the square of the reflectance at 30° in s polarization was weighted half as much as the square of the reflectance at 0°. Thelen and Langfeld[5] reported the results of the many designs submitted. The results correlate well with earlier work and have added additional breadth and insight, as discussed below.

Procedure

To gain empirical design data for a general estimating formula, series of designs were optimized over fixed bandwidths to give the lowest average reflectance in the band while each of the major factors was varied. These empirical results were used to determine the reflectance as a function of these variables. Figure 1 shows such a series for finding average reflectance R as a function of bandwidth B, where L, T, and D are held constant. In effect, this is taking the partial derivative of R with respect to B at specific values of L, T, and D. Here the bandwidth is defined as the longest wavelength in the band divided by the shortest wavelength. Figure 2 shows the change in R with respect to overall optical thickness T, while B, L, and D are fixed. I have found it most convenient to use T in units of one wavelength of the optical thickness at the wavelength that is the geometric mean of the wavelengths at the ends of the AR band,
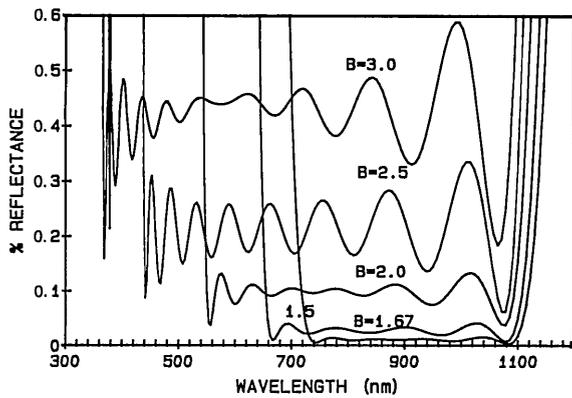
Fig. 1. Variation of the percentage of reflectance versus wavelength with bandwidth, while $T = 3.0$, $L = 1.38$, and $D = 0.89$. This illustrates how the minimum average reflectance decreases with bandwidth.

which define B. However, T correlates even better with the number of periods in a plot of reflectance versus thickness at the longest wavelength in the band (as is discussed below and shown in Fig. 8). The four factors B, L, T, and D were found to be the major variables affecting the minimum average reflectance that can be achieved. It was found that the substrate index has no major effect on the minimum reflectance possible in the ranges examined as long as T was greater than 1/2. The most major influence on the minimum average reflectance, and the most restricted in practice, is the index of the last layer, which needs to be as low as practical. The reason for this has been extensively discussed in previous work.[1–4] This is why magnesium fluoride is mostly used as the last layer. It would also be desirable from the design point of view to use the lowest index in the stack in order to have index differences D as large as possible. However, it has been found[4] that the process that uses magnesium fluoride and titania stacks of more than a few layers has excessive scattering and therefore silica is used instead of magnesium fluoride for the inner layers.
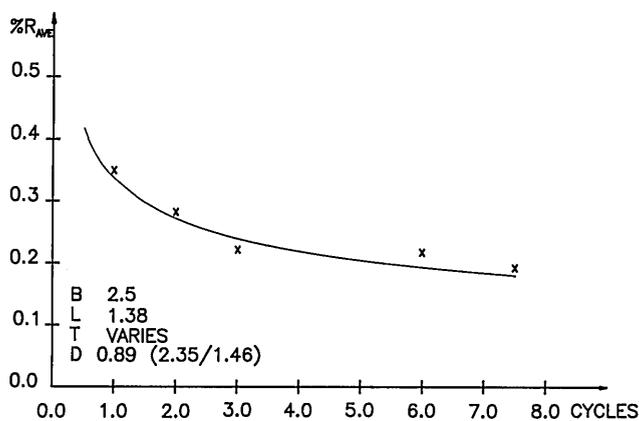

Fig. 2. Average reflectance in the band versus optical thickness in cycles (or waves at the geometric mean wavelength of the band). The curve is from the formula, while the X's are from empirical data.

Another minor observation is that the number of minima in the residual ripple of the AR band is proportional to bandwidth B and overall optical thickness T and is independent of the indices and number of layers in the design. The number of minima in the band is approximately equal to $8B/3 + 2T - 4$.

Formula

The collection of data of R versus B, L, T, and D was empirically fit to functions over the range of the investigation to arrive at Eq. (1):

$$R_{\text{AVE}}(B, L, T, D)\%$$
$$= (4.378/D)(1/T)^{0.31}[\exp(B - 1.4) - 1](L - 1)^{3.5}. \quad (1)$$

The difference in index between the layers of the stack (D) is divided into a constant. One divided by overall optical thickness T is taken to the 0.31 power. The bandwidth has the constant 1.4 substracted from it and then it raises exponentially to that power. The index of the last layer minus one is raised to the 3.5 power. The product of these four factors is the estimated minimum average reflectance in percentage that can be expected in designs within the applicable limits. The ranges over which these variables have been thus far shown to give reasonable estimates are as follows:

B from 1.4 to 5.0,
L from 1.1 to 2.2,
T from 1.0 to 9.0,
D from 0.4 to 2.8.

To set these in perspective, these studies were originally done for the visible and near-infrared spectral range. B, for example, was tested from a 400–600-nm (1.5) bandwidth to a 400–1200-nm (3.0) bandwidth. The lowest real index (L) that we use is ~1.38, but I have studied (in design) the use of imaginary materials below 1.1 and real materials, such as silica, up to 1.46. The D values come from the differences between high-index titania at as much as 2.58 and down to the low index of magnesium fluoride at 1.38 and combinations of intermediate materials. The overall optical thickness of the stack (T) is given in waves of the geometric mean wavelength of the band, which have previously been referred to as cycles.[2,3] In coatings on high-index substrates like germanium, where there are several lower and intermediate indices between the substrate and an index of 1.0, I have shown[1] that half-cycle or step-down coatings seem most advantageous. In the case of visible band materials, there is no significant choice of lower-index materials to make the step-down approach practical. The simplest broadband solutions in the visible are of the classic three-layer type, which is, in effect, a one-cycle design (see Refs. 1 and 2). Macleod[6] contributed an interesting design study to the Thelen–Langfeld problem,[5] which he evolved toward an optimal one-cycle design before it was even submitted to an optimization process.
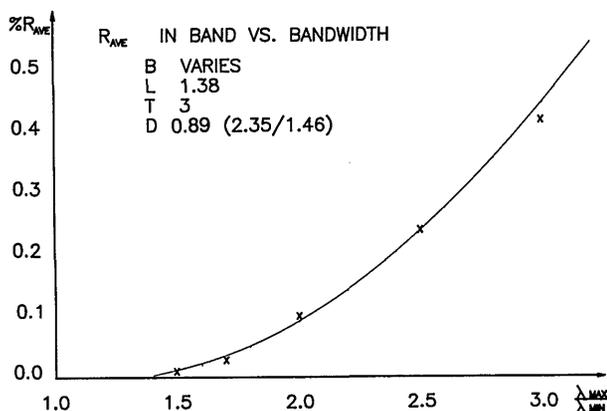
Fig. 3. Average reflectance in the band versus bandwidth as seen in Fig. 1. The curve is from the formula, while the X's are from empirical data.

Fig. 5. Average reflectance in the band versus the number of layers. This implies that the minimum number of layers for best results equals 6T + 2. The X's are empirical results.

More recently I was motivated by the work of Rastello and Premoli[7] to expand the study to cover the infrared band that was the subject of their study and the competition reported by Aguilera et al.[8] This gave further refinement and range to the applicability of the estimation formula. The agreement with the referenced results was also satisfactory in the infrared.

Results

I now compare the empirical results with the values that would be estimated by Eq. (1). Figure 2 shows reflectance R versus optical thickness, and Fig. 3 shows the variation of R with bandwidth while other factors are held constant. The X's are the empirical results, and the curves are the prediction of the formula. The fits show the prediction of Eq. (1) to be a reasonable approximation of the results obtained by exhaustive design.

Figure 4 shows R versus L, which points out the advantage of lower indices if they could be found or simulated. Figure 5 shows many test cases in which the number of layers in the designs were progres-

sively reduced until the results passed through a minimum R. It was counterintuitive to find that the performance improved slightly as the number of layers was reduced down to some minimum while T was kept constant. The minimum number of layers is approximately equal to $6T + 2$ in the visible studies shown in Fig. 5, where $B = 2.5$, $L = 1.38$, and $D = 0.89$. With the infrared examples,[7,8] where $B = 1.597$, $L = 2.2$, and $D = 2.0$, the minimum number is more of the order of $4T + 2$. Further reduction in the number of layers below some minimum then causes the achievable results to degrade rapidly, which is also observed in the collected results of Thelen and Langfeld.[5]

Figure 6 shows the influence of the index difference between the high and low indices in the stack. This difference is separated from the last layer index, which is a special case. Another empirical but counterintuitive result was that using a greater variety of indices (more than two) in the body of the coating was actually a design disadvantage in these cases with a finite number of homogeneous layers. The results of the Thelen–Langfeld problem[5] point to the same thing. Two indices with the largest practical difference give the lowest R; we use three only because of
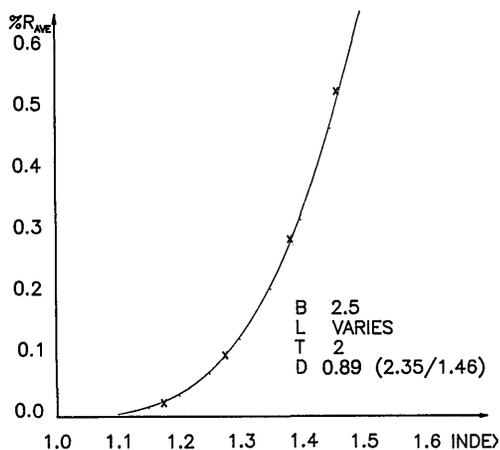

Fig. 4. Average reflectance in the band versus index of refraction of the last layer. The curve is from the formula, while the X's are from empirical data.
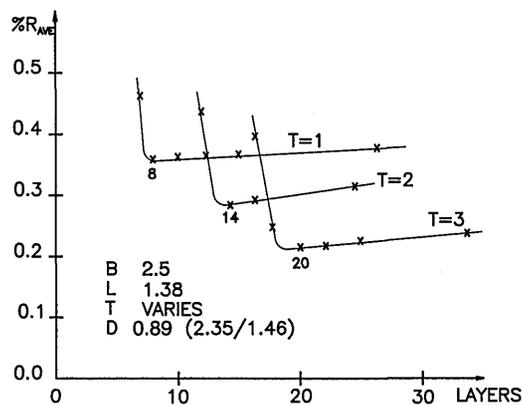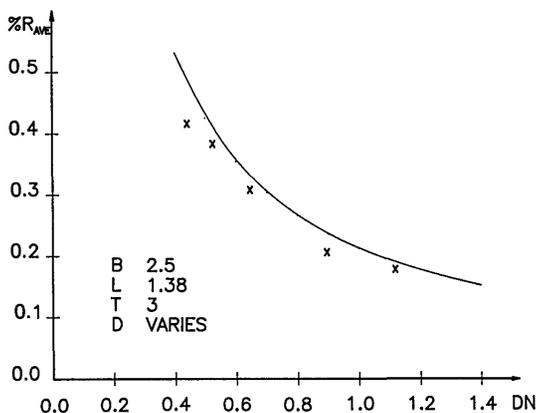

Fig. 6. Average reflectance in the band versus the index of refraction difference in all layers except the last. The curve is from the formula, while the X's are from empirical data.

scattering considerations that are due to the physical properties resulting from our processes, as mentioned above. I should point out, however, that earlier work[1-3] with unlimited choices of index would imply that a smooth variation of index from the substrate to the medium should be the best, but as that opportunity is not available, only two materials seem to give the best results.

The influence of the substrate index was found to be almost negligible in the cases studied. This is not true for $T < 0.5$, but for $T > 1$ the previous studies[1] show that the index profiles first rise to a level higher than that of the substrate before falling toward 1.0. Therefore the starting index has little or no influence on the final results.

As mentioned above, Fig. 2 shows the effect of overall optical thickness. This has also been studied from other points of view[2,3] in which the effects of extra thickness seemed to have little advantage when any hypothetical indices could be used. The advantage of extra thickness may be in the ability to compensate partially for the lack of the desired very-low-index last layer.

Figure 7 was graciously provided by Thelen and Langfeld from their report on the Berlin AR design problem results.[5] The problem's requirement for including the 30° performance in merit function F introduces some small difference in the results from those of Eq. (1), which is for only near-normal angles of incidence. However, the nature of the results are very consistent with Eq. (1). Because the problem dealt with a low-index (1.52) substrate and a limited selection of real materials, no solutions were offered with less than $T = 1$ of optical thickness. Figure 7 is shown in physical thickness, but 350–400 nm approximates $T = 1$ in these cases. Merit function F is slightly more complex than just the average reflectance in the band used in Eq. (1) because of the 30° factor, but is similar to it to within a scale factor. The similarities of the results shown in Fig. 7 with
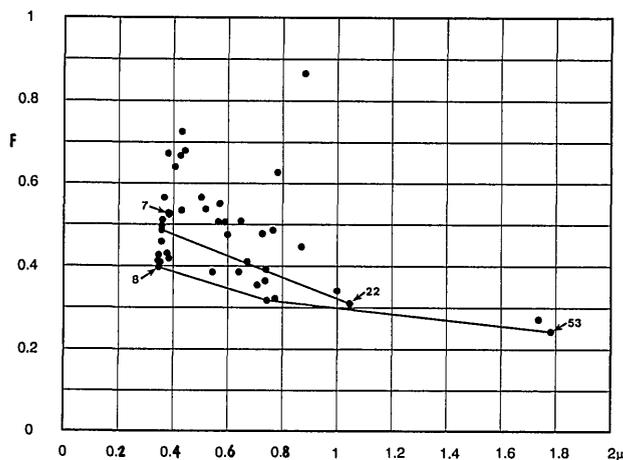
those shown in Figs. 2 and 5 are what I wish to point out. All three figures show the need for a T of at least one cycle and some improvement with optical thickness, but with less and less effect beyond $T = 3$. I have taken the liberty of adding the number of layers to a few of the key design results in Fig. 7. These are consistent with the $6T + 2$ estimate for the minimum number of layers. The best result at the thinnest end of the designs had 8 layers and $T = 1$. The best design with a physical thickness of ~1050 nm or a T of ~3 had 22 layers. However, I was able to optimize that design further to be slightly better with 20 layers, which is $6T + 2$. The best design of the contest at ~1780 nm of physical thickness and $T = 5$ had 53 layers. Preliminary work on reducing the number from 53 layers also points to the fact that
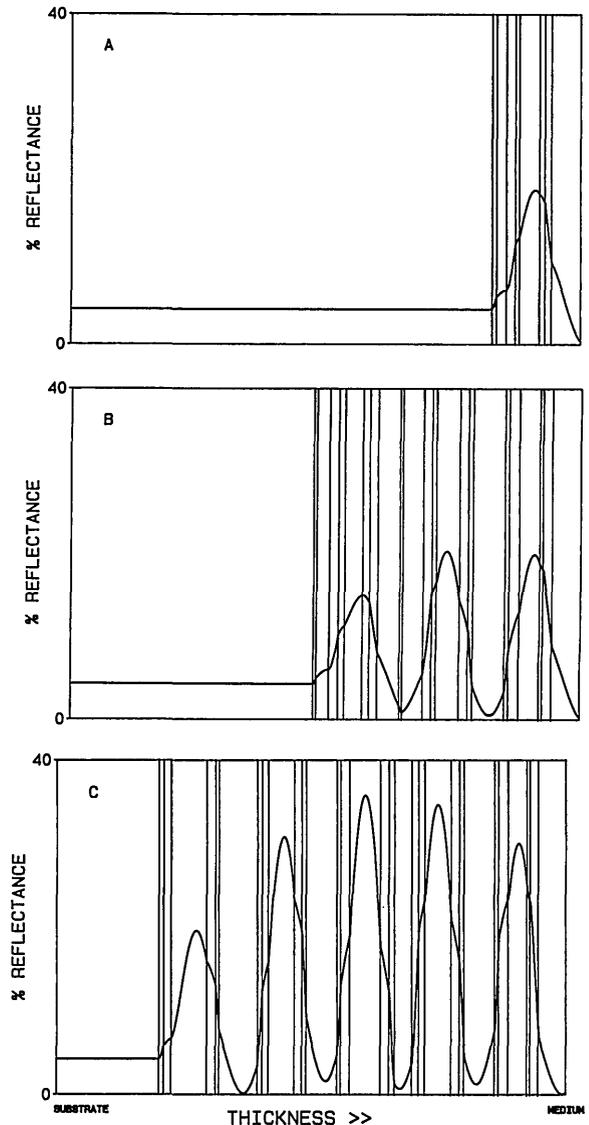

Fig. 8. Reflectance versus thickness at 900 nm, which illustrates the undulatory nature of the results and that various designs can be described in terms of these cycles of thickness T. Curves A and B are one- and three-cycle designs from the best of the Berlin design problem contributions.[5] Curve C is an adaptation and refinement of the best of the contributions.

Fig. 7. Thelen–Langfeld[5] results of merit function versus physical thickness from the contributions to the Berlin 1992 design problem. The number of layers is shown for selected designs. The upper line connects the best designs that used no tantala while the lower line connects those that did use tantala.

32 layers ($6T + 2$) may be enough to get the same results. Note that the best seven-layer design in Fig. 7 is not as good as the best 8-layer design. This is also consistent with Fig. 5.

The upper line in Fig. 7 connects points of designs that used no titania in the design. These cases with the lower resultant D value do not achieve as good a result as those that use near the maximum amount of titania for a higher D.

To emphasize the characteristics of T further, I have plotted in Fig. 8 the reflectance versus thickness at the longest design wavelength in the band (900 nm) of some of the best designs from the Thelen–Langfeld problem. These are consistent with the periodic nature pointed out in earlier works.[1-3] The general shape of the periods is similar when plotted as admittance versus thickness, and the earlier works show the characteristic curves on the admittance amplitude versus phase plots. All these appear to point to a natural periodic shape or function that would be the ideal AR design if there were no restrictions on the indices that could be used in an inhomogeneous structure of a given optical thickness.

Summary

The empirically derived formula permits the estimation of the minimum average reflectance of VBBAR coatings in the visible and the infrared regions. The variables with major effects on the results are the lowest available index, bandwidth, index difference from high to low, overall optical thickness, and the number of layers into which the overall thickness is divided. Substrate index is not a significant factor, and intermediate indices between the highest and lowest indices available can be a disadvantage. This latter finding was somewhat unexpected.

The general results are somewhat independently confirmed by being consistent with results of the design contributions of many experienced coating designers, from around the world to the Berlin AR design problem[5] and to that reported by Aguilera et al.[8]

The formula can be used to predict reasonably the best performance that can be expected of a design of homogeneous layers for a given set of materials. The ideal number of layers in a design for a given thickness and the number of ripple minima in the band can also be predicted. These estimating formulas are expected to be useful tools for engineers and designers.

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