Refined criteria for estimating limits of broad-band AR coatings.

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ABSTRACT

A decade ago we introduced empirically derived formulas which allowed one to estimate the performance which can be achieved in the design of broad-band antireflection (AR) coatings based upon the indices of refraction of the materials to used, the bandwidth required, and the overall thickness of the coating. This has proved to be a useful tool to avoid attempting impossible designs and to guide the designer toward an optimal result. It can also be helpful to non-designers who need to know what can and cannot be done before specifying a system AR coating requirement. In the new work reported here, formulas with additional accuracy have been developed by further data generation and the application of modern statistical analysis tools. The overall thickness parameter used in the equations has also been better defined and understood, and the tendency of overall thicknesses to have quantization has been studied further. These findings are discussed in conventional thin film design terms and also from the Fourier synthesis/analysis viewpoint.

Keywords: broad-band antireflection coatings, optical coating design, estimating limitations, design guidance

1. INTRODUCTION

We previously provided[1,2] empirically derived formulas which allow one to estimate the minimum average reflectance that can be achieved in the design of broad-band (AR) coatings. As an illustration, the percent reflection versus wavenumber (cm^{-1}) of typical broad band antireflection (BBAR) coating design is shown in Fig. 1. This has an Rave of 0.87195% from 10000 to 35000 cm^{-1} (1000 to 285.7 nm). This, incidentally, might be scaled to cover 400-1400 nm or 440-1540 nm. The bandwidth (B) is defined as the ratio of the highest frequency to the lowest (or the longest wavelength to the shortest). In this case, B equals 3.5. We use the wavenumber (linear in frequency) scale here in preference to a wavelength scale because the relations are more linear in frequency. Figure 2 shows the same design over a broader spectral range from 1-40001 cm^{-1}. It can be seen that there are high reflection bands on either side of the AR band. One might say that the reflection which would have been in the AR band without the coating, has been redirected to the regions outside of the AR band. We will later refer to the information available from the spectra to the left (low frequency or long wavelength) side of the AR band. Another useful tool for the designer is the reflectance versus coating thickness plot at the lowest frequency (longest wavelength) in the band. Figure 3 shows this for the same coating as in Figs. 1 and 2.

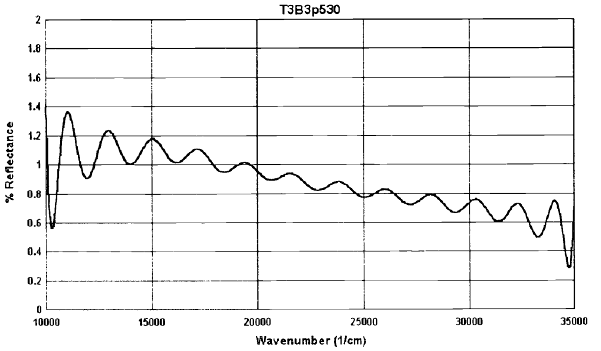

Fig. 1. Typical broadband AR design for 10000 to 35000 cm^{-1} where B = 3.5.

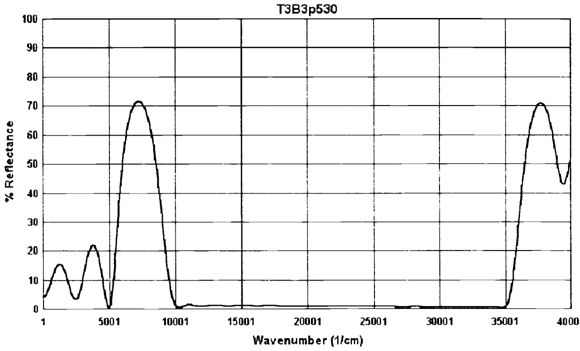

Fig. 2. Same design as in Fig. 2, but shown on expanded scale.

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2. LOCAL MINIMA AND QUANTIZATION

It has been our experience that the optimization of a starting design for a BBAR coating, other than one of only a few layers, tends to reach a conclusion at a local minimum which is not always the best that can be done in the general region of available variable parameters. The variables are generally: the indices of the materials, the layer thicknesses, the total coating thickness, and the number of layers. Ordinarily, the materials and therefore the indices of refraction are fixed by choice prior to optimization; the number of layers are specified; and the optimization is only on the thicknesses of the layers. The Rave and overall thickness of the coating results from these choices and the optimization process. We have written and used programs to constrain the results to a specific overall thickness, but this generally turns out to be unnecessary to achieve a desired result. Figure 4 shows the Rave results versus overall coating thickness at the end of optimization runs for a number of starting designs. Note that these seem to cluster at certain thickness intervals leading to the "true" minimum in a given thickness region. Figure 5 is a similar illustration for many optimized designs of a BBAR where B is 1.5 and the overall thickness varies over a range of more than 5 to 1. This illustrates the observation that optimized designs that are truly the minimum Rave for a given overall thickness region seem to be at quantized thickness intervals. Further evidence of this quantization is seen in Verly's plot from our paper[3] on the Fourier viewpoint of AR coatings which is reproduced as Fig. 6.

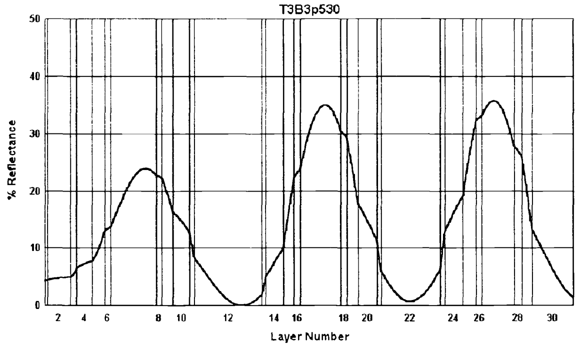

Fig. 3. Reflectance versus coating thickness for same design as in Figs. 1 and 2. Will be shown useful for design purposes below.

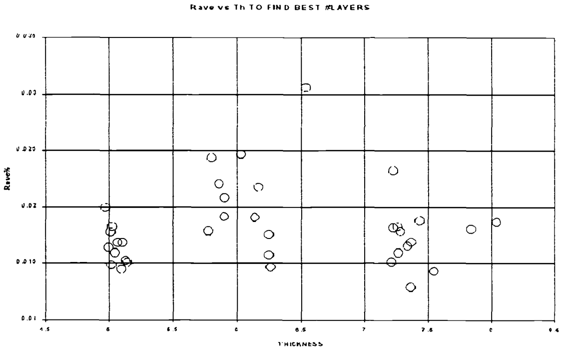

Fig. 4. %Rave results after optimization versus thickness from a variety of starting designs.

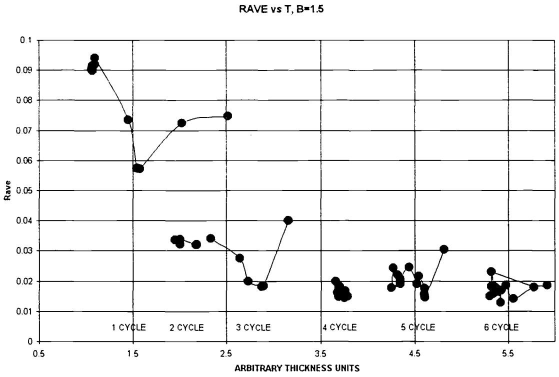

Fig. 5. Many optimized designs from different starting points as in Fig. 4. B for this AR series versus thickness is 1.5.

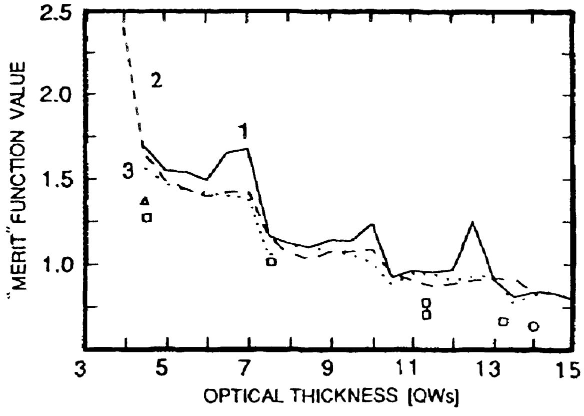

Fig. 6. Rave related results from Verly's Fourier synthesis technique. Note similarities to Figs. 5 and 7.

The question then arises as to what constitutes one "quanta" of overall thickness (T). Several possible definitions were examined, and the simplest was chosen to be "one half wave of optical thickness at the lowest frequency (or longest wavelength) in the AR band." In our first report on this type of work[1], the thickness unit was chosen as the wavelength that was the geometric mean of the shortest and longest wavelengths in the AR band. The new definition would give the same result as the old when B is equal to 4, but would differ for other B-values. It appears that the high frequency (or short wavelength) end of the AR band has little or no influence on the behavior associated with the overall thickness

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value. Verly, et al.[3] used the equivalent of our new definition in the work seen in Fig. 6.

Note the similarity in the shapes of Figs. 5 and 6. The minimum Rave (and "merit" function value) decreases with increasing thickness, rapidly at first and then with decreasing impact as the overall thickness increases. A further correlation and confirmation of this comes from a totally independent result by Thelen and Langfeld[4]. Figure 7 shows the results from their AR design contest with 44 competitive designs. The best of these are found to have the same decreasing Rave with thickness after some minimum thickness optimized design. The minimum overall thickness for the lower left design point in Fig. 7 works out to be 1.125 times a half wavelength at the longest wavelength. In this figure, minima can also be seen near 2, 3, and 5 times this thickness, further supporting the quantization observation.

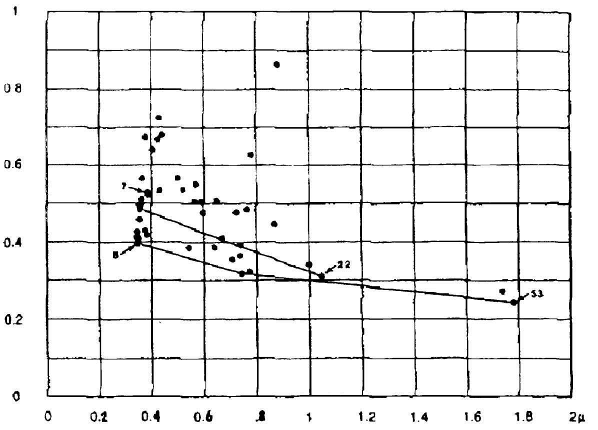

Fig. 7. Results from Thelen-Langfeld[4] AR design contest of 44 entries. The vertical scale is "Merit" but equivalent to %Rave.

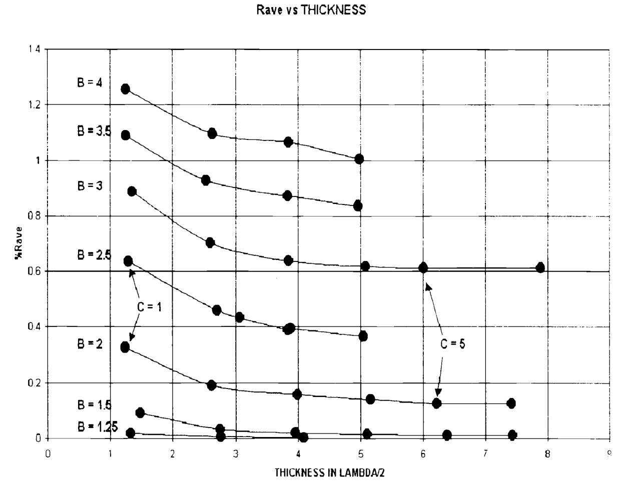

Fig. 8. %Rave for "true" minima designs over range of B =1.25 to 4 and C = 1 to 7.

The bulk of the work reported in this paper was a new and fairly exhaustive set of designs in search of "true" minima in Rave over a broad range of B and overall thickness. Unless otherwise noted, all designs were with a low index of 1.46 and a high index of 2.35. Dispersion was not included in this work as it would not be expected to change the nature of the conclusions. The last layer of the lowest practical index available (1.38 in this region) as discussed extensively in the earlier works[1,2] was also not used here for the same reasons. However, if we were designing a real system such as these for the visible and near IR region, we would in fact include a last layer of MgF_2 in a design which was otherwise TiO_2 and SiO_2 in order to achieve even lower Rave per refs. 1 and 2. The reasons for not using just MgF_2 and TiO_2 is discussed in an earlier paper[5].

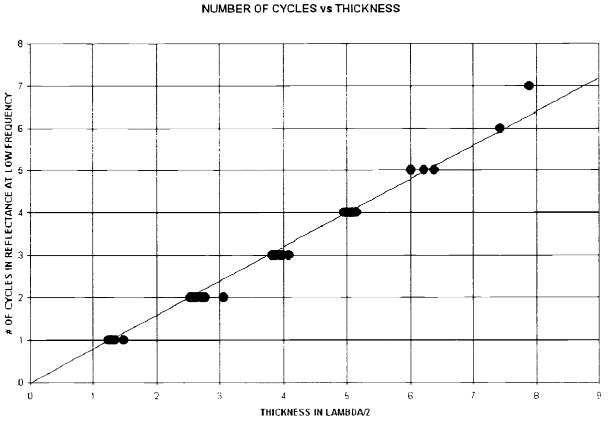

Fig. 9. Number of cycles (C) versus thickness (T) for all the cases seen in Fig. 8. The line is the fit for C = T/1.25.

Figure 8 shows the results of "true" minima in Rave found in the range of B from 1.25 to 4 and T from 1 to 8. The same behavior as in Figs. 6 and 7 is again observed. The quantization as a function of thickness seems to occur at about a half wavelength at the longest wavelength multiplied by 1.25. We will inject here that examination of Fig. 6 by Verly et al. points to minima that seem to occur in intervals of a half wavelength at the longest wavelength multiplied by 1.33. Henceforth, a thickness cycle (C) will be referred to as a half wavelength at the longest wavelength multiplied 1.25. Figure 9 shows a summary plot of C versus T for all of the cases from Fig. 8 and a line of C equal to T/1.25, where the fit is adequate for the work at hand.

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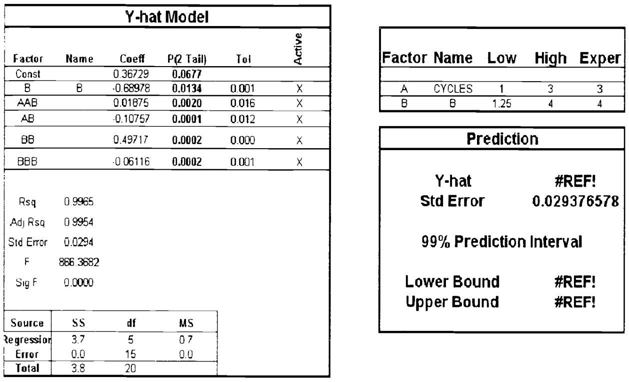
3. PREDICTION EQUATIONS

It can be seen in Fig. 8 that Rave is a strong function of B and C up to C equal 3.0, but is a much weaker function of T after that. Therefore, it was decided to treat the region where C<3 separately from the region where C>3. Design of Experiments (DOE) statistical techniques[6] and software[7] were used to find a best fit of the data and equation for Rave as a function of B and C. Figures 10 and 11 show the statistical results and a plot of the fitted curve for C<3 while Figs. 12 and 13 show the same for C>3. Because Rave improves so little with increasing C after C = 3, we do not recommend such designs as practical solutions to real problems. However, we did make a fit-check between the two models for the two regions where they meet at C = 3.0. Figure 14 shows the predicted points from the first and second models as compared to the actual points for C = 3.0. The greatest departures here are less than 1/20th% in Rave, not a matter of any concern to us. The worst case errors in fit over both regions are of this same order and the Standard Errors seen in Figs. 10 and 12 are 0.029% and 0.039% respectively.



Y-hat Model

Factor	Name	Coeff	P(2 Tail)	Tol	Active
Const		0.36729	**0.0677**		
B	B	-0.68978	**0.0134**	0.001	X
AAB		0.01875	**0.0020**	0.016	X
AB		-0.10757	**0.0001**	0.012	X
BB		0.49717	**0.0002**	0.000	X
BBB		-0.06116	**0.0002**	0.001	X

Rsq	0.9965
Adj Rsq	0.9954
Std Error	0.0294
F	866.3682
Sig F	0.0000

Source	SS	df	MS
Regression	3.7	5	0.7
Error	0.0	15	0.0
Total	3.8	20	

Factor	Name	Low	High	Exper
A	CYCLES	1	3	3
B	B	1.25	4	4

Prediction

Y-hat	#REF!
Std Error	0.029376578

99% Prediction Interval

Lower Bound	#REF!
Upper Bound	#REF!

Fig. 10. Results of multiple regression analysis on data represented in Fig. 8 over all cases where C < 3.0

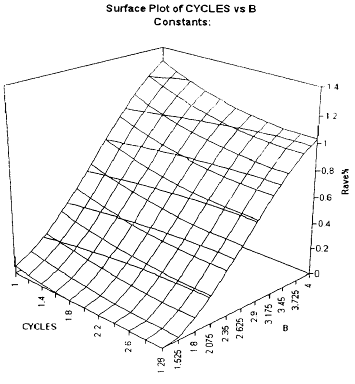
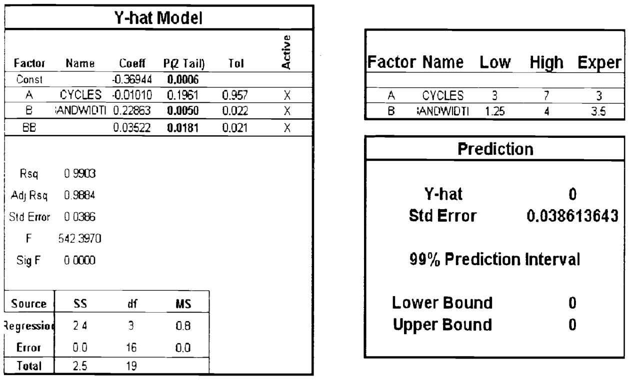


Fig. 11. Surface plot of %Rave versus B and C from the results of Fig. 10.



Y-hat Model

Factor	Name	Coeff	P(2 Tail)	Tol	Active
Const		-0.36944	**0.0006**		
A	CYCLES	-0.01010	0.1961	0.957	X
B	ANDWIDTI	0.22863	**0.0050**	0.022	X
BB		0.03522	**0.0181**	0.021	X

Rsq	0.9903
Adj Rsq	0.9884
Std Error	0.0386
F	542.3970
Sig F	0.0000

Source	SS	df	MS
Regression	2.4	3	0.8
Error	0.0	16	0.0
Total	2.5	19	

Factor	Name	Low	High	Exper
A	CYCLES	3	7	3
B	ANDWIDTI	1.25	4	3.5

Prediction

Y-hat	0
Std Error	0.038613643

99% Prediction Interval

Lower Bound	0
Upper Bound	0

Fig. 12 Results of multiple regression analysis on data represented in Fig. 8 over all cases where C >3.0

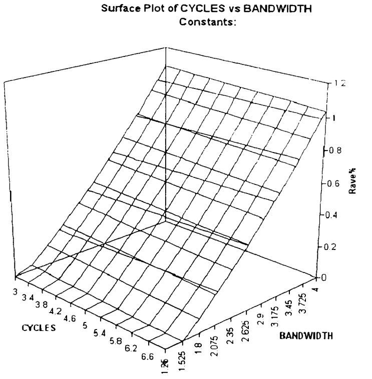


Fig. 13 Surface plot of %Rave versus B and C from the results of Fig. 12.

The equation which results to predict Rave in the region which we recommend, C<=3.0 is:

$$\mathbf{Rave = 0.36729 - 0.68978B + 0.49717BB - 0.06116BBB - 0.10757BC + 0.01875BCC} \qquad (1).$$

The equation for the region which we do not recommend, C>3.0 is:

$$\mathbf{Rave = -0.36944 + 0.22863B + 0.03522BB - 0.01010C} \qquad (2).$$

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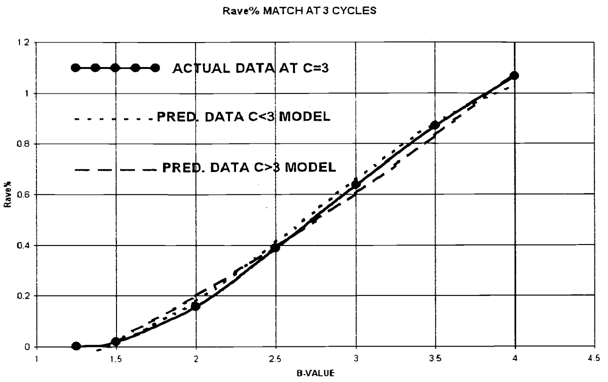

Fig. 14. Predicted points at C = 3.0 from both models and the actual data points from the Fig. 8 results.

4. NUMBER OF LAYERS

In our earlier work[1,2] it became apparent that there was a definite minimum for the number of layers required for an optimal AR of a given overall thickness. It was also found that any more than the minimum number of layers slightly increased Rave as seen in Fig. 15. We conjecture that this is because each layer adds to the overall reflectance of the coating in a way which needs to be further dealt with; therefore there is an advantage to using the minimum number of layers required by the circumstances. It is our practice to attempt to remove the thinnest layer in any design and reoptimize in hopes of further decreasing the Rave. Often, the automatic optimization will reduce one or more layers to a vanishingly small thickness without human intervention. In these cases, the layers can be removed from the design without any effect on the resulting Rave. An aid to understanding where layers can best be removed is a plot of reflectance versus thickness as shown in Figs. 3 and 16. Each of these figures represent cases where the minimum number of layers has been reached; but if there were an unneeded layer, it might show up as a very thin layer in either of these plots. These plots are made for the lowest frequency in the AR band (or the longest wavelength). Figures 3 and 16 are both for cases where C = 3.0; this can be determined by number of cycles in reflectance seen from zero to maximum overall thickness in these figures. The same information is available as in Fig. 2 by counting the number of reflectance maxima between zero and the lowest frequency in the AR band. Figure 2, however, gives no information as to the number of layers in the coating. Figure 3 is for a design where B = 3.5 whereas Fig. 16 is for a case where B = 1.5.

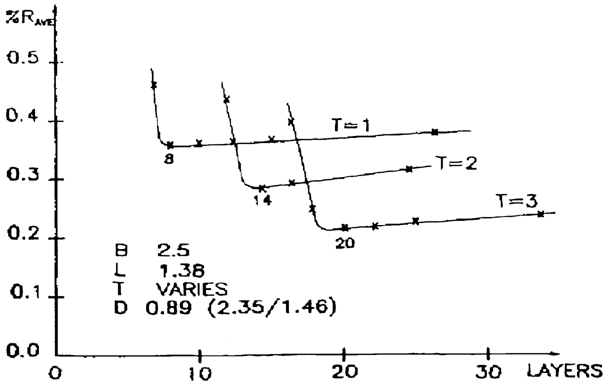

Fig. 15. Results from our earlier work[1,2] where the number of layers was reduced until the least %Rave was found.

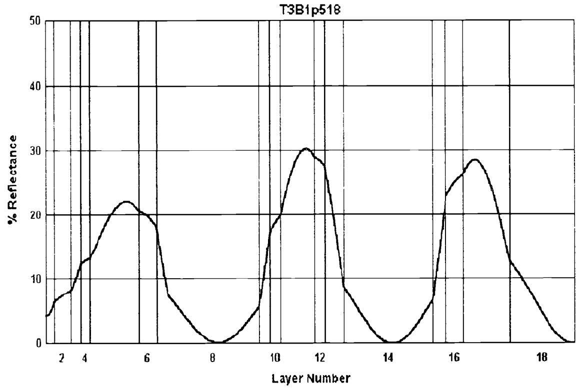

Fig. 16. Reflectance versus thickness where C = 3.0 and B = 1.5. B is small enough to require only 6 layers per cycle.

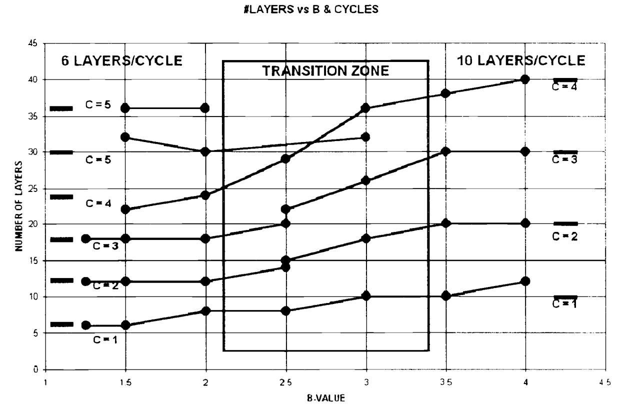

Fig. 17. Number of layers in "true" optimal designs from Fig. 8 as a function of B and C.

It has been discovered that, for low B-values, these designs, to be optimal, tend to require a number of layers equal to 6×C. Whereas 10×C layers are needed for large B-values. Figure 16 illustrates the 6× case with 18 layers. In the central cycle of this plot, we observe a central high index layer which is flanked by a low/high layer pair on each side

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that leads to low index layers on each side of those between each maxima in reflection. It has been observed that the first and last cycles tend to be slightly different from any intervening cycles. The intervening cycles, which have been examined (up to C = 7) tend to be very similar and have either 6 or 10 layers as mentioned above. The cycle next to the substrate (first cycle) usually needs two extra layers at the substrate to provide an optimal design. The last cycle on the other end of the stack often performs better with two less layers. The result, with two more on the one end and two less on the other, is that the number for the overall thickness is still either 6 or 10 per cycle for small or large values of B respectively. Figure 3 shows this for the 10×C case and Fig. 16 for the 6×C case.

These reflectance versus thickness plots are closely related to effective index versus thickness plots which might result from a Fourier synthesis design as discussed in ref. 3. We interpret the need for 10 layers per cycle for high B-values to be due to a need to have smoother effective index transitions which more closely match the ideal index versus thickness profile and admittance plots as discussed in Chap. 1 of ref. 2. When the B-value is smaller, 6 layers per cycle are adequate because the need to match the ideal profile is less stringent.

It was found that there is a region between B = 2 and B = 3.5 where the optimal designs have layers per cycle which are intermediate between 6 and 10. These results are shown in Fig. 17 where this region is referred to as the Transition Zone. The advice to the designer for cases such as these is to start with too many layers for a given B and C, and reoptimize the design removing thinner layers as possible until a minimum Rave is achieved. It can be seen that the design of BBAR coatings is not strictly a matter of submitting a starting design to optimization software, because local minima are found more often that might have been expected. Evidence of this is seen in the Thelen-Langfeld contest results^4 shown in Fig. 7. Only four (4) of the designs submitted had minimal Rave for their overall thickness out of the 44 designs submitted! Knowing the number of layers which will lead to a minimal Rave for a given B and C, and what that Rave should be, should be helpful to the BBAR designer.

5. MINIMA AND SHAPES

As can be seen in Fig. 1, there are small minima in the AR band or ripples. These can be used to determine the overall thickness (T via C) of a sample AR coating of unknown details. In the case of a V-coating such as a laser AR, there is one minimum in its narrow band. Three and four layer AR coatings usually have two minima in the band. With the much broader band AR coatings, we have found that the number of minima is predicted by: B(C+1)-1. This even fits the V-coat and 3 and 4-layer AR cases. Figure 18 shows the results of the optimal cases reported here, and this could be used as a look-up chart to determine C when B and the number of the minima in the band are measured on a spectrophotometer.

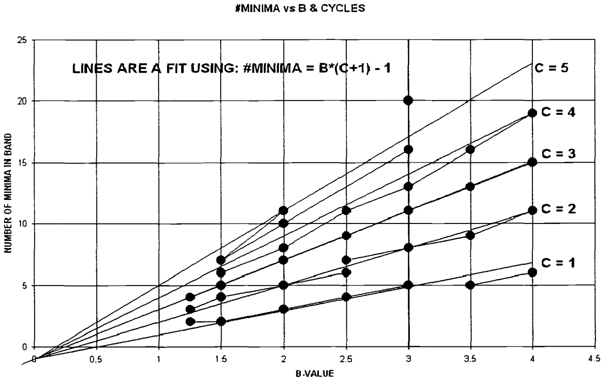

Fig. 18. Number of minima in the AR band versus B and C. This can be used to estimate T(C) from a spectral trace.

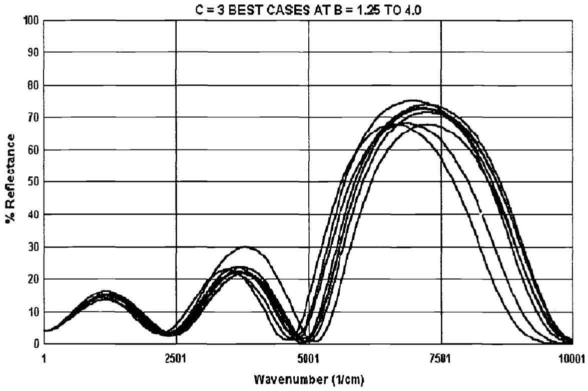

Fig. 19. Low wavenumber or long wavelength end of spectra beyond the AR band. Shows that C = 3 and gives other insight.

Observation of the low frequency spectra beyond the AR band of a design, as seen on the left of Fig. 2, can be a useful guide in the design of a BBAR. Figure 19 is a plot of that region for all of the C = 3 optimal designs found in this study, where B ranges from 1.25 to 4. It can be seen that the reflectance spectra are all very similar. It has been observed that less-than-optimal designs can have significant distortions from this shape. For example, the lobes can tend to merge or distort if the thickness is smaller or larger than the ideal T for a given C, and the shape can be distorted if an optimum

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has not been reached by the design. In examining Fig. 19, the trace that is slightly out of line with the others could be an indication of a potential for improvement in that particular design.

There is a somewhat similar behavior in the shape of the passband trace as seen in Fig. 1. Most optimal designs reach a regular rippled trace like that of Fig. 1. The slope of that trace can often be changed and leveled by adjustment of the optimization targets, although the Rave tends to remain the same. When less than the minimum number of layers for a given B and C are used, this mono-frequency ripple can become highly distorted by the appearance of additional frequency components. This can also be an indication of a potential for improvement in a design.

6. CONCLUSIONS

Earlier work on the general nature and behavior of broadband AR coatings has been expanded here. Equations with additional accuracy to predict the average reflectance in the AR band have been developed with the aid of modern statistical analysis tools (DOE). The overall thickness parameter used in the equations has also been better defined and understood, and the tendency of overall thicknesses to have quantization has been demonstrated. The use of overall thicknesses greater than three cycles is proscribed because of their almost negligible benefit. Design guides as to overall thickness, number of layers, and visual aids as to shape have been provided.

ACKNOWLEDGMENT

All of the design and optimization work here has been done using FTG Software[8]. We would like to thank Dr. Fred Goldstein for his various stimulating discussions and contributions to this work.

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