

Limits to the Average Reflectance in a Broadband AR Coating Design and Avoiding Local Minima in the Design Process

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Abstract

When attempting to optimize an optical coating, such as minimizing the reflection from a glass surface, the optimization process often stops at a design which is indicated to be the minimum (best), but is only a "local minimum," since there exists another lower "real minimum" for those conditions. A procedure using constrained optimization has been employed here to continue the optimization process past the local minimum and ultimately find the real minimum for any given overall thickness of the coating design. This procedure has been used to map the lower limits of the average reflectance (%Rave) in a given bandwidth versus the overall thickness of the coating design. To yield a low %Rave, a minimum thickness has been found necessary, and three times that overall thickness is judged to be a practical limit for a working broad band antireflection (BBAR) coating. The results of this mapping are explained from various viewpoints, and a formula is provided to estimate the minimum %Rave which can be achieved for a given bandwidth, thickness, and material choice.

Introduction

Figure 1 shows an example BBAR which is the subject of this work. The bandwidth, B , is here defined as the longest wavelength in the AR band divided by the shortest. For the visible spectrum from 380 to 780 nm, this would be $B = 2.053$. In this case of Fig. 1, $B = 2.4$. The goal is to minimize the %Rave in the antireflection (AR) band.

The problem of encountering a "local minima," but not the lowest possible minimum in the %Rave of the coating design optimization, has been recognized for many decades. Figure 2, reproduced from our earlier report[1], shows examples of designs where the minimum %Rave achieved by the automatic design optimization process would terminate at different "local minima" levels other than the lowest possible real minimum for that overall thickness coating. The usual optimization of the merit function of the AR design, or the reduction of the %Rave by varying the thickness of the layers of the design, finds a point where the %Rave cannot be further reduced by small perturbations of the layer thickness varia-

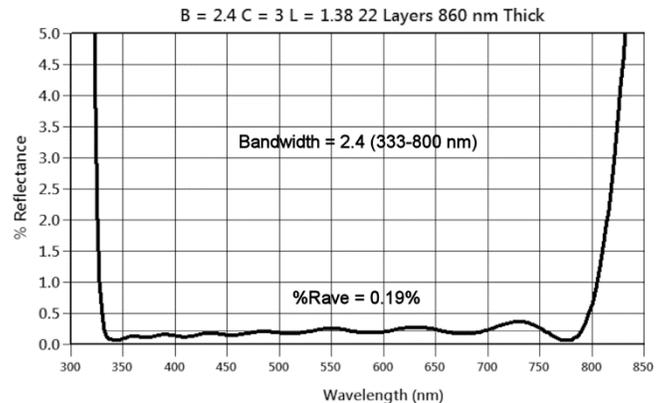


Figure 1: Example BBAR coating with a bandwidth of 2.4 and an %Rave of 0.19%.

bles, and the optimization terminates at that local minimum. Figure 2 shows two things: one is that many optimizations may terminate at an %Rave which is not the lowest minimum which could be obtained, and the second is that the best designs appear to cluster at certain discrete or "quantized" thicknesses and not usually in between such thicknesses. This present study has used a technique to avoid these local minima and identify the design with the lowest %Rave for a given overall coating thickness.

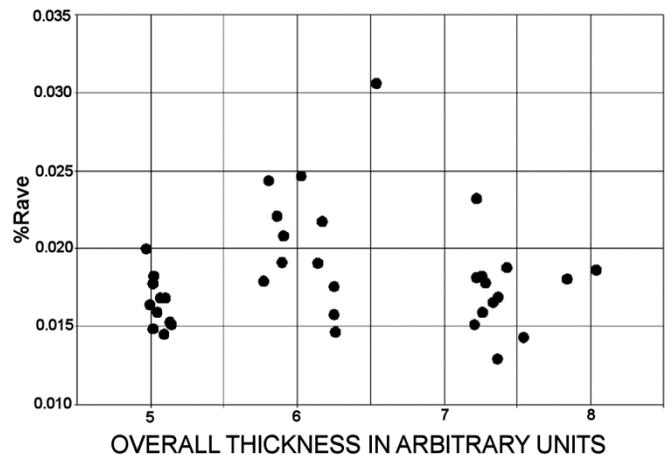


Figure 2: %Rave versus thickness results after optimization from a variety of starting designs.

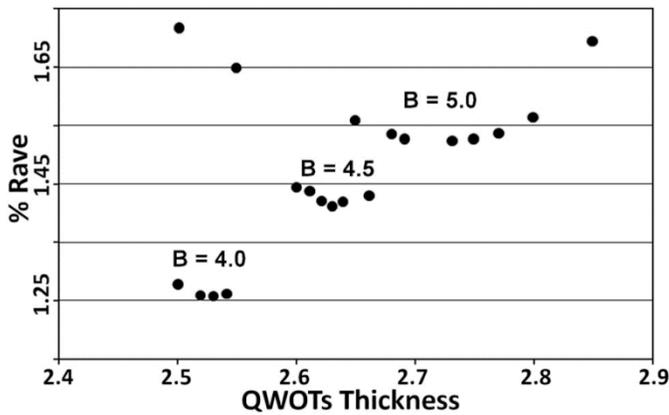


Figure 3: Patterns of the minimum %Rave in the AR band versus the overall OT of designs for B values of 4.0, 4.5, and 5.0, where the QWOT thicknesses were each constrained.

It was further shown in Ref. 1 that some minimum number of layers are required for the minimum %Rave over a given bandwidth and overall thickness. It was also shown in Ref. 1 that more layers than the minimum required can be detrimental, in that each layer interface causes a reflection which must be dealt with to reduce the %Rave of the overall design.

FilmStar[2] software, which has been used here, has an option to employ **constrained design** optimization, wherein a constraint, such as the overall thickness of a design, can be maintained during the optimization process. This has been used in this study to find %Rave minima at **specific** thicknesses. Figure 3 reproduced from Ref. 3 shows how the lowest %Rave tends to change with the constrained overall thickness. However, Fig. 4, reproduced from Ref. 4, shows another critical characteristic for the results of this study.

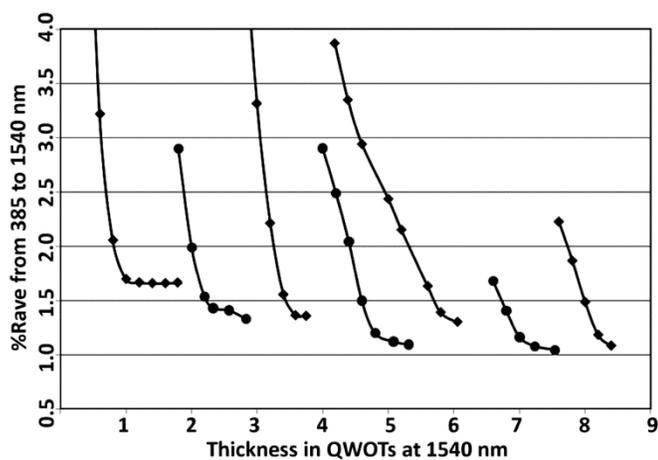


Figure 4: %Rave for the best designs at controlled thickness designs on 1.52 (dots) and 2.35 (diamonds) substrates.

Once a minimum %Rave has been found, additional thickness may be added (unwittingly) by the optimization program in

such a way that the minimum %Rave does not change significantly, as seen most clearly in the left case of Fig. 4, as the overall thickness increases. Note that Fig. 3 does not show this special case behavior. The reason for Fig. 4 is explained on page 129 of Ref. 5 and further below. The natural process of optimization seems to take excess thickness and place it in a part of the design thickness in a way that does not increase the %Rave. Figure 5 shows a minimum thickness design of 7 layers **overlaid** on a design just like it that has 16 layers with excess thickness added next to the substrate in a way in which it does not increase the %Rave. This is occurring in each of the cases shown in Fig. 4. Note that %R versus thickness in Fig. 5 is nearly identical for layers 1-7 of the thin design as compared to layers 7-16 of the thick design.

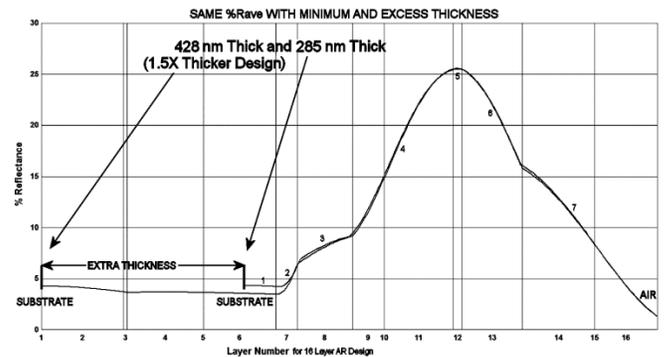


Figure 5: %Reflectance versus thickness, evaluated at 800 nm, of two designs with similar %Rave performance, but the minimum thickness case has 285 nm overall thickness and 7 layers, and the 1.5x thicker design has 428 nm thickness and 16 layers.

Figures 6 and 7 show another viewpoint on how this happens. Figure 6 shows the Reflectance Amplitude (RA) diagram (see Ref. 5, Sec. 1.3) of a minimum thickness optimal design (285 nm thick) where there are 7 layers from the substrate to the medium (air or vacuum) spiraling clockwise in reflectance amplitude toward the zero-reflection point at the origin of the RA diagram. When additional thickness is added to the sub-

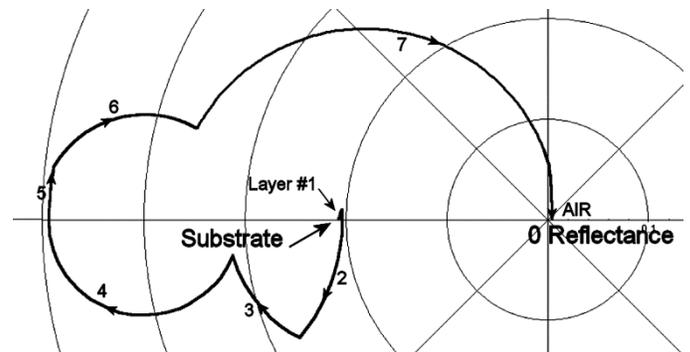


Figure 6: The Reflectance Amplitude (RA) diagram (see Ref. 5, Sec. 1.3) of the minimum thickness optimal design of Fig. 5 (285 nm thick)(evaluated at 800 nm) where there are 7 layers from the substrate to the medium (air or vacuum) spiraling clockwise in reflectance amplitude from the substrate toward the zero-reflection point at the origin of the RA diagram.

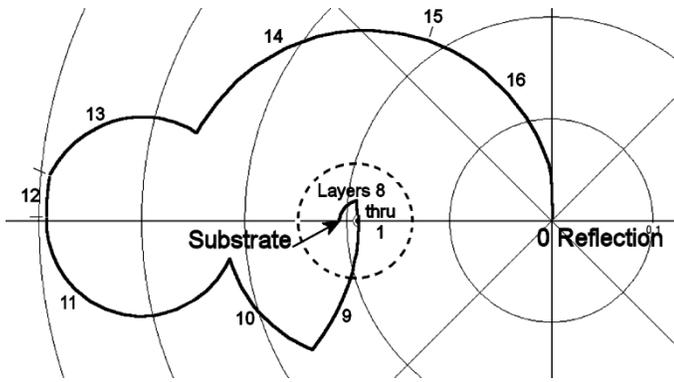


Figure 7: The RA diagram of the $1.5\times$ thickness optimal design of Fig. 4 (428 nm thick) where there are 16 layers from the substrate to the medium. However, the RA of layers 1 through 8 remains near the substrate on this diagram, showing that the effect is not significantly different from that in Fig. 6.

strate before the regular AR coating as seen in Fig. 5, it tends to keep the RA near the substrate point in Fig. 5 and within the dotted circle of Fig. 7 on the RA diagram. This implies from Fig. 7 that the effect of layers 1 through 8 does not notably change the reflectance of the coating because it is acting much like it has an index similar to the substrate. This effect tends to happen automatically by the action of the optimization process acting to reduce the %Rave while adding thickness to the coating.

Getting Out of a Local Minimum

It has been the author's experience that BBAR design optimizations almost always stop at a local minimum. The author primarily uses four optimization engines available in FilmStar[2]: Damped Least Squares (DLS), Levinberg-Marquart (LM), Simplex, and NOL Gradient. The latter is the engine with the option to apply constraints. It has been found that, when DLS stops at an "optimum", a continued attempt to use DLS to improve the result is futile. However, when LM is used, LM may provide some design improvement (albeit asymptotic) by its continued reapplication. Simplex seems to asymptotically improve designs and seldom terminates itself until it has tried 32768 iterations (which it does rapidly).

The constrained thickness optimization using the NOL Gradient engine will find a minimum which it cannot improve without some change in the design parameters. The present approach has been to change the constrained thickness goal by a small amount (typically one nm, occasionally 5 nm) and re-optimize. The thickness is then changed back to its original value and re-optimized. This cycle usually provides some improvement in the design. The effect is like shaking a container of granular material to cause it to settle (by gravity) into its lowest level. This might also seem to be similar to the falling of a leaf or feather where it travels horizontally back and forth as it flutters downward to the Earth. Software has been written using FilmStar Basic[2] to automate this "falling leaf" procedure for a specified number of iterations to

converge on the real (rather than local) minimum for that overall thickness design. In many cases, the convergence of this is slow and asymptotic.

This tool has been used to seek the real minimum design of BBAR coatings as a function of overall thickness. This was initially done for a bandwidth B of 2.0, similar to the visible spectrum. The designs used 1.46 for the low index layers and 2.35 for high index. The number of layers was taken to be at least as large as had been learned from previous experiences[1,5]. The investigations started at a thickness of 200 nm and extended to 1200 nm in some cases.

Figure 8 shows the "real" minima of %Rave, for these designs in the 400-800 nm band, which were found versus overall thicknesses from 240-1200 nm. There are a few features in Fig. 8 which confirm things that have been suspected in the past from more random observations. One is that there is a strong barrier to low AR performance if the overall thickness of the design is not greater than some minimum thickness, such as about 250 nm in this case. Another thing is that there is a nearly constant %Rave over a range of thicknesses greater than where the minimum is first found, and this has been explained above. This "flat" can be observed in Fig. 8 from about 250-340, 540-640, 850-940, and 1070-1140 nm.

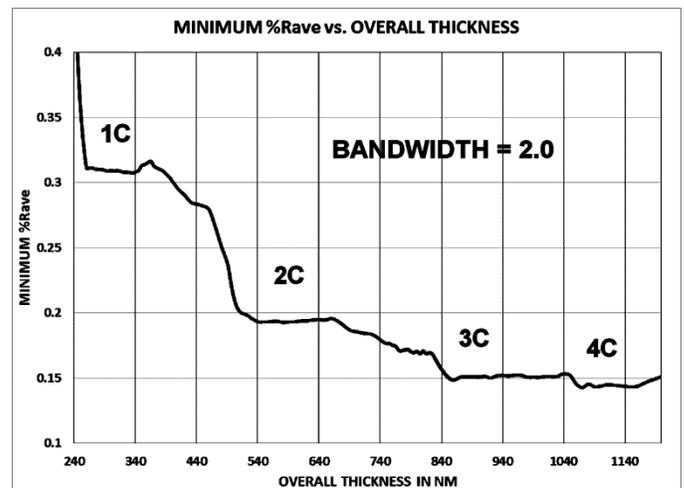


Figure 8: The "real" minima of %Rave for a BBAR which is achievable for a design of $B = 2.0$, $L = 1.46$, $H = 2.35$, and the minimum necessary number of layers.

As seen here and in Refs. 1 and 3, the best designs seem to be "quantized" in more or less discrete overall thicknesses which have previously[3] been referred to as cycles of C1, C2, C3, etc. The reasons for this quantization are planned to be the subject of a future paper. It was concluded some time ago that two or even three times the minimum overall thickness of C1 offers some significant benefit in %Rave beyond the minimum thickness, but thicker than C3 was considered a point of diminishing returns. It can be seen from Fig. 8 that a C2 design can provide a %Rave of about 60% of a C1 design, and a C3 design can provide better than 50% of the C1 designs. However, C4 has a smaller improvement which is not considered worth the additional cost.

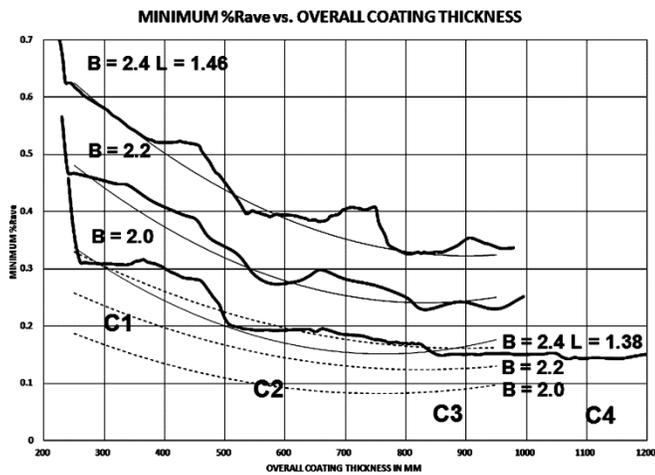


Figure 9: Expanded version of Fig. 8 to show bandwidths of 2.2 and 2.4, and last layer indices of 1.46 and 1.38, versus overall thickness. The smooth curves are from fits to the data for $L = 1.46$ (solid) and $L = 1.38$ (dotted).

The work reported in Fig. 8 was extended in Fig. 9 to include B-values of 2.2 and 2.4. This was then further expanded to include last layers of index 1.38. This last layer was shown in Refs. 3 and 5 to be a major factor in what %Rave can be achieved. The benefits of this 1.38 index last layer is shown by the dotted lines of Fig. 8. References 1 and 3 provided equations to estimate the %Rave which can be achieved based on the bandwidth, B; the last index, L; the overall thickness in C; and the difference in indices, D. Here, similar results have been found for B, C, and L; where D has been held fixed to $D = 2.35 - 1.46 = 0.89$ for TiO_2 and SiO_2 , but the last layer was evaluated at 1.46 and 1.38.

The formula to estimate the %Rave in the band (B) is:

$$\%Rave = 7.321 - 1.16E-4*t(nm) - 4.34*B - 5.766*L + 5.86E-07*t^2 - 3.843E-04*B*t(nm) + 3.499*B*L$$

The formula to estimate the number of layers needed, from page 367 of Ref. 5, is:

$$\#Layers = 2*B*C + 0.5*C^3 - 1.1*C + 4.5$$

Conclusions

Local minima are found to be common results of the BBAR coating design process. An approach has been implemented in the coating design program to continually perturb the design from its local minimum at which it has terminated the optimization, until no lower minimum can be found by this perturbed optimization. The real minima have been mapped and shown in Fig. 7 for such coatings with a bandwidth of $B = 2.0$ or 400-800nm and which are composed of 1.46 and 2.35 index materials of an appropriate number of layers on 1.52 index substrates. It has been found that thickness may be added to a nearly optimized BBAR design by an optimization

program without significantly changing the %Rave. The mechanism and reason for this has been explained from the point of view of the %R versus thickness of the design and also by using the Reflectance Amplitude Diagram point of view. It is generally practical to estimate in advance what the limitations and possibilities of the %Rave for a BBAR design will be.

References

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