Further guidance for broadband antireflection coating design

Ronald R. Willey

Willey Optical Consultants, 13039 Cedar Street, Charlevoix, Michigan 49720, USA (ron@willeyoptical.com)

Received 9 August 2010; revised 16 October 2010; accepted 29 November 2010;
posted 3 December 2010 (Doc. ID 133106); published 13 January 2011

Recent investigations have added to and refined the understanding of the behavior of broadband antireflection coating designs and provided further guidance for achieving more nearly optimal designs. The ability to optimize designs wherein the overall optical thickness of the design is constrained to a specific value has allowed this investigation. A broader bandwidth than previously reported has been studied and statistically fit more precisely by a polynomial equation, and also two linear equations for routine approximations have been derived. It has also been found that the optimal number of layers in the design can be predicted as a function of the bandwidth. © 2011 Optical Society of America

OCIS codes: 310.0310, 310.5696, 310.6805, 310.4165, 310.1210, 310.1620.

1. Introduction

The earlier report [1] of estimating procedures for broadband antireflection (BBAR) coatings as a function of bandwidth (B), index of the last layer (L), overall coating optical thickness (C), and difference (D) between the high and low index (except the last layer) was in 1991. This was later expanded [2–4] by extended studies. These reports have now been consolidated into one publication [5]. Design techniques which draw upon these observations have been described in more detail recently [6–8].

The ability to constrain the overall optical thickness (or physical thickness, if desired) of a given design while it is being optimized by *FilmStar* [9] thin film design software has been a key factor in the recent studies. Other applications of constrained optimization have also been reported by Tikhonravov *et al.* [10]. The earlier work (Ref. [5], pp. 141–158 and Ref. [7]) showed that the minimum achievable average reflectance (Rave) in the antireflection (AR) band tends to be at overall coating thicknesses that are quantized ($C = 1$, 2, 3, etc.), and only lesser performance can be obtained between these thicknesses. Dobrowolski *et al.* [11] alluded to this in their report. This present work deals primarily with designs of the first and minimal thickness ($C = 1$) for achieving the lowest Rave, and it particularly focuses on variations of Rave with B and overall thickness, where D and L are kept constant.

The bandwidth B is defined as the longest wavelength in the band divided by the shortest, or the highest frequency divided by the lowest, if plotted on a wavenumber (cm^{-1}) scale. The overall thickness of the AR coating is described here in terms of a multiple of a quarter-wave optical thickness (QWOT) at the longest wavelength (or the lowest frequency) in the AR band. An example of this would be that an AR coating from 440 to 660 nm would have a B value of 1.5 and the overall thickness would be expressed in QWOTs at 660 nm.

2. Design Procedures

The results shown here are all for substrates of index 1.52 in a medium of index 1.0 where dispersion is ignored, since the results can be easily adjusted when dispersion is considered. The issue of the variation of the results with different substrate indices appear to be small over the range of substrates that transmit in the visible spectrum, but these have been somewhat addressed in the recent related report [8]. Dobrowolski *et al.* [11] showed results for substrates of index 4.0 that do show some influence of substrate index. However, their results were probably limited by the index (2.2) of the lowest index layers.

0003-6935/11/09C274-05$15.00/0

Amotchkina [12] gives an expression for the influence of substrate index. However, this function is unclear in that it seems to imply that lower Rave in a band is possible for substrates of higher index than it is for substrates of lower index. Further studies with substrate index as a variable seem to be in order.

AR designs of various overall thicknesses were optimized using the constrained optimization to confine the overall optical thickness of the design to specific values. Targets of equal magnitude were evenly spaced in wavenumbers over the full AR band, and the number of layers for the design was specified. A minimum of four targets per ripple in the AR band were used to insure that any uncontrolled rises in reflectance between the targets were suppressed. All of the layers were used as design variables. Rave has been computed as the average of the reflectance at many more intervals than the optimization targets, equally spaced in wavenumbers. The "workbook" function of *FilmStar* was set up to minimize the Rave in the band *and* to constrain the overall optical thickness of the design to whatever value had been set. The program then optimized the design until no further improvement could be made and the thickness constraint was as specified. Without the constraint, designs have tended to seek some "optimal" thickness, which seems to minimize Rave, but the previous studies have shown that the "optimum" designs reached may not be the best possible design, which might be found in the adjacent regions of thickness. The constrained optimization in the workbook has allowed the investigation of the minimum Rave versus thickness.

The optimization procedure which was used here was the Numerical Optimization Library Gradient Method, which allows the use of constrained parameters such as a target thickness and other functions that can be calculated from the design results in a spreadsheet. The optimization engine used in *FilmStar* is from the DSNL Library [13]; it maximizes (or minimizes) a function (such as the Rave over a band of wavelengths), and it constrains some parameter(s) to be either equal to some specified value, and/or some other parameter(s) to be greater than or less than some specified value. Insufficient detail is available with respect to Ref. [13] to allow the reader to reproduce the exact algorithm used here; however, any thin film design software such as that used in Ref. [10], which allows optimization while constraining one or more variables to specific values will allow the reader to reproduce the results shown here.

Figure 1 shows the results of three series of designs at various bandwidths and constrained thicknesses. It can be seen that the Rave in each series passes through a minimum as the target overall thickness is changed in the search for the minimum. The detail designs, with physical thickness in nanometers, are listed here from one design in each of the bandwidth groupings of Fig. 1 that is *not* the optimal overall optical thickness and one that is close to optimal. For $B = 5.0$ with an Rave of 1.563% and an optical thickness (OT) of 2.662 QWOTs at the longest wavelength in the band, a design that is *not* quite optimal is substrate (sub.), 2.4458H, 33.474L, 1.1484H, 21.6454L, 9.6783H, 48.1029L, 20.297H, 32.0422L, 32.4915H, 13.4054L, 137.9588H, 12.0765L, 32.9633H, 33.532L, 16.503H, 99.6046L, air. The *best* design found had an Rave of 1.527% and an OT of 2.670. This design is sub., 2.4818H, 34.1517L, 1.1811H, 22.3309L, 9.7111H, 48.7225L, 20.3723H, 32.3402L, 32.7848H, 13.4608L, 138.0571H, 12.2452L, 33.2942H, 33.6269L, 17.304H, 96.4009L, air.

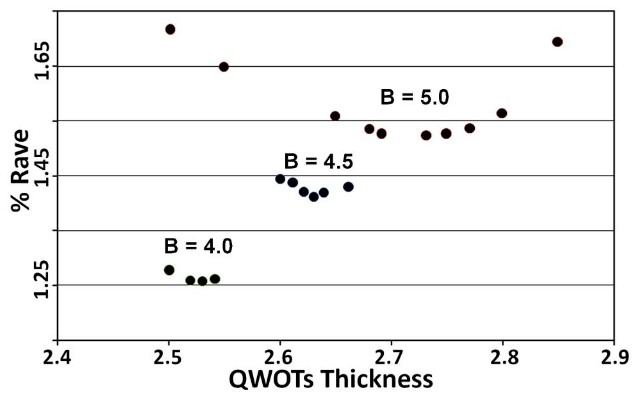

Fig. 1. Patterns of the minimum Rave in the AR band versus the overall OT of designs for B values of 4.0, 4.5, and 5.0, where the QWOT thicknesses were each constrained. This illustrates that the best Rave depends on the specific thickness of the design.

For $B = 4.5$ with an Rave of 1.439% and an OT of 2.611 QWOTs at the longest wavelength in the band, a design that is *not* quite optimal is sub., 5.5616H, 57.1022L, 2.6948H, 3.3408L, 13.8721H, 46.1965L, 29.9376H, 25.1048L, 47.0107H, 7.0877L, 87.485H, 10.795L, 39.7749H, 34.2281L, 19.645H, 108.625L. The *best* design found had an Rave of 1.412% and an OT of 2.630. This design is sub., 5.6779H, 58.157L, 2.644H, 4.7673L, 13.6198H, 47.7311L, 29.1185H, 25.4371L, 47.3973H, 7.1958L, 89.2788H, 9.9249L, 41.1231H, 32.9361L, 20.6803H, 105.6455L.

For $B = 4.0$ with an Rave of 1.274% and an OT of 2.515 QWOTs at the longest wavelength in the band, a design that is *not* quite optimal is sub., 8.1384H, 59.3936L, 1.8266H, 1.7877L, 21.3634H, 40.4167L, 41.1902H, 14.7344L, 0.0213H, 0.6882L, 94.0393H, 7.2142L, 50.6228H, 32.8306L, 23.8027H, 118.1649L. The *best* design found had an Rave of 1.258% and an OT of 2.530. This design is sub., 8.489H, 59.9869L, 1.8151H, 2.3942L, 21.3487H, 40.9361L, 41.223H, 14.468L, 1.0206H, 1.1681L, 94.5144H, 6.8767L, 50.8424H, 32.8122L, 24.1237H, 116.8043L.

The minimum Rave has been systematically evaluated as a function of bandwidth (B), number of layers, and overall thickness (QWOTs). This was done primarily with $D = 0.89$ ($n_H = 2.35$ minus $n_L = 1.46$) and $L = 1.46$, but it was also evaluated with $L = 1.38$. The points in Fig. 2 show some of the design results. This extends the previous work and that of others [10–12,14] from $B = 4.0$ to $B = 6.0$. The data with $D = 0.89$ and $L = 1.46$ were

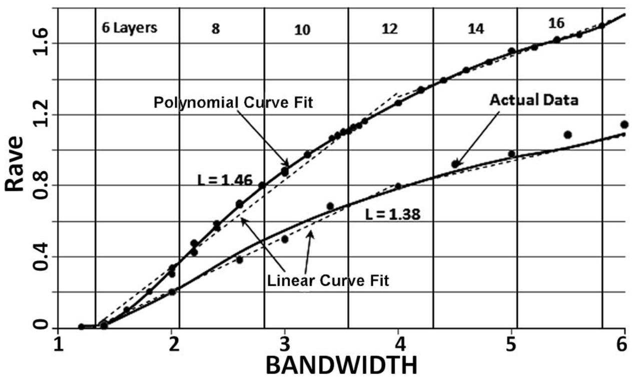

Fig. 2. Rave versus B for $L = 1.46$ and 1.38 ($C = 1$). The dots are actual designs, solid lines are from statistical polynomial curve fits to these results, and dashed lines are from linear fit equations.

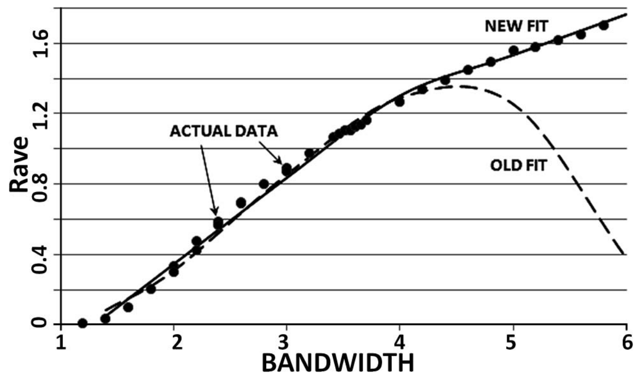

Fig. 3. Comparison of previous estimation equation (OLD FIT) with the actual data and the statistical polynomial equation (NEW FIT).

statistically fitted to a sixth-order polynomial using DOEKISS [15] regression analysis software to the following equation, and it is plotted as the upper solid curve in Fig. 2:

$$\text{Rave} = 3.99569 - 8.95463 \times B + 7.40513 \times B^2 - 2.89893 \times B^3 + 0.60833 \times B^4 - 0.06582 \times B^5 + 0.00288 \times B^6.$$

In order to account for other D and L values, the above equation needs to be multiplied by

$$(6.447/D) \times (L - 1)^{2.55},$$

which was derived from the report of earlier work [2].

For $D = 0.89$ and $L = 1.38$, this produces the lower solid line in Fig. 2. This equation is easily calculated in a program such as Excel, and a linear approximation is also provided below to be easier to use with a hand calculator. The linear data fit (two straight lines) would be found by

$$\text{Rave} = (6.447/D) \times (a \times B + c) \times (L - 1)^{2.55},$$

where $a = 0.491$ and $c = -0.638$ when $1.3 < B < 4.0$. If $4.0 < B < 6.0$, then $a = 0.231$ and $c = 0.377$. These results are plotted in Fig. 2 as dashed lines.

The previous best estimate equation from p. 151 of Ref. [5] for bandwidths up to 4.0 is plotted as the dashed line in Fig. 3 for comparison with the new linear fit. These new equations should be adequate for estimating what is practical with respect to Rave for a given bandwidth.

Tikhonravov *et al.* [14] and Amotchkina [12] have done similar investigations to this using somewhat different approaches, and their estimation equations give almost identical results over the ranges which they have investigated (B only up to 4.0).

3. Number of Layers in a Design

The other parameter that has come into focus in this study has been the minimum number of layers in a given optimal design. Dobrowolski *et al.* [11] and Tikhonravov *et al.* [14] have also mentioned the number of layers in their design studies. A layer is defined here as the space between two index of refraction interfaces that is occupied by a single homogeneous index, independent of any relationship to its physical or optical thickness. Figure 4 shows how the optimal Rave varies with thickness, number of layers, and bandwidth (which is shown to the right of each point). Most striking are the results for six-layer (6) designs, where it can be seen that the performance improves significantly from a design which is too thin at 2.22 QWOTs to one at 3.06 QWOTs. This confirms earlier observations [1–6] that a minimum thickness is required to achieve the best results (this is what is currently called a $C = 1$ design). Designs of eight layers (8) show a similar linear progression, and designs of more layers follow the same pattern.

The new results also confirm that fewer layers are better, down to some minimum number of layers. For example, it can be seen in Fig. 4 that an eight-layer design at about 3.02 QWOTs gives the same Rave (~0.34%) as a six-layer design at 2.47 QWOTs. Therefore, there are a minimum number of layers for any desired bandwidth; more layers than that will add unnecessary thickness to the design. For example,

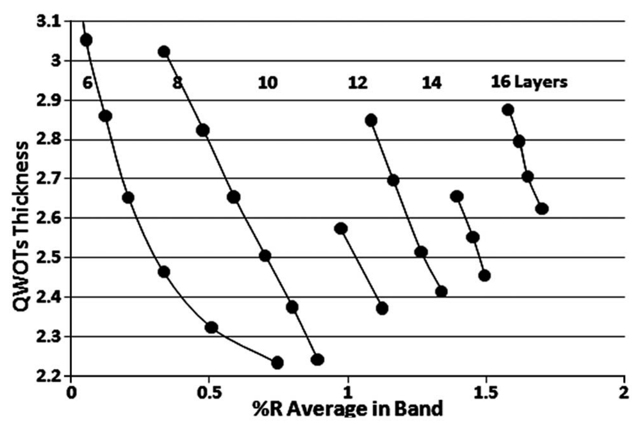

Fig. 4. Overall OT of various optimal designs versus Rave in band as a function of number of layers. The bandwidth is shown to the right of each associated point.

a coating for $B = 1$ (V coat) needs only two layers, and more layers would be wasteful (purely for design purposes). The results can be fitted to linear equations to provide estimates of the minimum and maximum number of layers needed for an optimal design as a function of bandwidth (B); they are as follows:

$$\text{minimum \# layers needed} = 0.3725 \times B - 0.907$$

$$\text{maximum \# layers needed} = 0.3725 \times B - 0.162$$

These limits are plotted vertically on Fig. 2 for guidance in designing BBARs.

Figure 5 shows the thickness of optimal designs as a function of bandwidth and number of layers. Because the Rave has been seen in Fig. 2 to be generally linear with bandwidth, it is not shown in Fig. 5 to preserve clarity in the figure. It can also be seen from Fig. 5 along with Figs. 2 and 4 that there are usually two or more optimal designs for a given bandwidth that have thicknesses that differ in accordance with the number of layers.

4. Reflectance Minima in the AR Band

It has been found that the number of minima in the AR band (ripples) is generally one half of the number of layers for an optimal design. Figure 6 shows an example of a 30 layer design with 15 ripples in the AR band. This particular design happens to be a $C = 3$ design as opposed to those in the rest of this report, which are $C = 1$. Although the number of layers divided by 2 seems to hold true in general, it has been observed that the ripple pattern becomes distorted and even nearly flat when the bandwidth and overall thickness are near the boundary where more or fewer layers are required for better performance.

The C value of an unknown coating can be estimated from the measured spectrum in the bandpass and the number of ripples. The AR bandwidth is measured, Fig. 2 is used to find the likely number of layers for that bandwidth when $C = 1$, and that number of layers is divided into the observed number of minima to give the estimated value of C. Figure 6 has a bandwidth of 4.0 and 15 minima. This B would give an estimate of 12 layers from Fig. 2, and therefore C is estimated at 2.5. In this case, the actual design was 30 layers and $C = 3$, so this implies that there might be some room for improvement in the coating by adding or subtracting up to six layers. This is because it has previously been determined [1–6] that $C = 2.0$ or 3.0 might be better than $C = 2.5$ due to quantization effects.

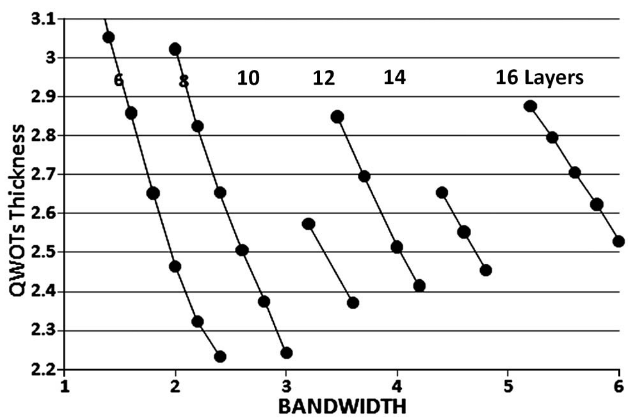

Fig. 5. Thickness of various optimal designs versus bandwidth and number of layers.

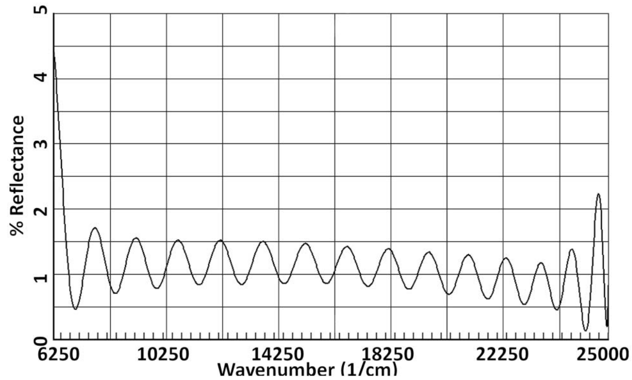

Fig. 6. Fifteen minima (ripples) in the AR band of a $B = 4.0$ ($C = 3$) design with 30 layers. The 61 targets at a value of 0.1%T are shown on the bottom of the plot. Rave was calculated for approximately 400 equally spaced values over the band.

5. Conclusions

It has been shown that the optimum design for the minimum Rave in a very BBAR coating depends on the bandwidth, specific overall thickness of the coating, and the number of layers. Variations from that optimal thickness cause departures from the optimum Rave. Results which have been fitted to new equations extend the range of validity of the estimating and also provide for estimation with a hand calculator in addition to a more detailed spreadsheet formula. The number of layers needed can be estimated. Also, the number of minima in the AR band can be used to estimate the design properties of an unknown coating from its measured spectral curve.

References

1. R. R. Willey, "Broadband antireflection coating design performance estimation," *Society of Vacuum Coaters Annual Technical Conference Proceedings* (1991), Vol. 34, pp. 205–208.
2. R. R. Willey, "Predicting achievable design performance of broadband antireflection coatings," Appl. Opt. **32**, 5447–5451 (1993).
3. R. R. Willey, "Refined criteria for estimating limits of broadband AR coatings," Proc. SPIE **5250**, 393–399 (2004).
4. R. R. Willey, "Broadband antireflection coating design recommendations," *Society of Vacuum Coaters Annual Technical Conference Proceedings* (2004), Vol. 47, pp. 16–21.
5. R. R. Willey, *Practical Design of Optical Thin Films*, 2nd ed. (Willey Optical, 2007), pp. 139–158.
6. R. R. Willey, *Practical Design of Optical Thin Films*, 2nd ed. (Willey Optical, 2007), Appendix C.
7. R. R. Willey, "Looking outside the box for broadband AR coating designs," in *Optical Interference Coatings (OIC)* (Optical Society of America, June 2010).
8. R. R. Willey, "Expanded viewpoint for broadband AR coating designs," Appl. Opt. **50**, C86–C89 (2011).

9. F. T. Goldstein, FilmStar, FTG Software Associates, P.O. Box 579, Princeton, N.J. 08542.
10. A. Tikhonravov, M. Trubetskov, and T. Amotchkina, "Application of constrained optimization to the design of quasi-rugate optical coatings," Appl. Opt. **47**, 5103–5109 (2008).
11. J. A. Dobrowolski, A. V. Tikhonravov, M. K. Trubetskov, Brian T. Sullivan, and P. G. Verly, "Optimal single-band normal-incidence antireflection coatings," Appl. Opt. **35**, 644–658 (1996).
12. T. Amotchkina, "Empirical expression for the minimum residual reflectance of normal- and oblique-incidence antireflection coatings," Appl. Opt. **47**, 3109–3113 (2008).
13. Numerical Optimization Library, DSNL Version 2.0, Technologix Corporation, 12020 113th Avenue NE, Kirkland, Wash. 98034-6938.
14. A. Tikhonravov, M. Trubetskov, T. Amotchkina, and J. Dobrowolski, "Estimation of the average residual reflectance of broadband antireflection coatings," Appl. Opt. **47**, C124–C130 (2008).
15. DOE KISS 2007 Software, SigmaZone.com and Air Academy Associates, LLC, 1650 Telstar Drive, Suite 110, Colorado Springs, Colo. 80920.