Antireflection design concepts with equivalent layers

Uwe B. Schallenberg

Some novel concepts of designing antireflection (AR) coatings with equivalent layers are presented. As an introduction, essential papers concerning thin-film optics and AR designs are cited, and the AR problem and a previously introduced AR-hard design type are discussed. Based on the known matrix formalism, a potential AR region, an equivalent stack index, and an equivalent substrate index are defined to use the theory of stop-band suppression as a starting point for the design of broadband AR coatings. The known multicycle AR design type is identified as a typical solution to the AR problem if the presented approach is used. © 2006 Optical Society of America

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1. Introduction

A. Brief Chronological Review

Antireflection (AR) coatings are essential parts of any optical arrangement. Although an AR coating consists generally of only one to four layers and standard AR designs have been used for more than 60 years, there are permanently increasing requirements for the optical and nonoptical parameters of an AR coating. Before starting a discussion about new AR concepts, the old and the known ones have to be remembered and studied. Two groups of concepts and theories can be distinguished over the years. The first group spans the time from the beginning of practical thin-film optics in 1936 to the middle of the 1980s. It is characterized by the introduction of basic theories of thin-film optics (Table 1).

The application of a single-layer AR coating was published for the first time by Strong in 1936. Only a few years later, in 1940, in Jena, Germany, Geffken applied for a patent for a three-layer coating. Equivalent layers were introduced into optics for the first time by Herpin in 1947. Early in the 1950s, Abelès and Epstein published basic papers concerning fundamental matrix formalism and the application of equivalent layers.

The synthesis of optical multilayers using Fourier synthesis was started in 1952 by Pohlack and was fundamentally discussed by Delano in 1967. In 1960 an essential connection between thin-film optics and microwave network theory was established by Young and Seely and helped to synthesize multilayer AR designs over a prescribed frequency band. The use of equivalent layers in AR coatings was basically discussed by Berning for the first time in 1962. In 1964 the standard quarter-half-quarter design was modified by Rock by means of substitution of the first quarter-wave layer.

A substantial discussion about multilayer AR coatings was provided by Musset and Thelen in 1970. The research of Alfred Thelen is particularly connected with the theory of stop-band suppression as a basic design principle using multiple periods in thin-film filters and mirrors, published in 1973, with a first part issued already by 1963. Ohmer published the essential formulas to design three-layer equivalent films in 1978. Finally, still as part of this first group, in 1985 Southwell took the flip-flop approach to substitute a layer with an unavailable refractive index.

A second group is characterized both by the discussion of inhomogeneous layers as a general AR solution, including their substitution by homogeneous multilayers, and by AR designs generated by the intense use of thin-film software and optimization techniques (Table 2).

In general there are solutions for any AR problem that entail application of inhomogeneous layers. Already in the 60s, efforts were made to realize technical solutions for producing inhomogeneous index profiles, published for the first time by Jacobsson and Martensson. But since about 20 years ago, it has been known that good solutions for AR designs are also achievable if the inhomogeneous layer is divided
into steps of layers with homogeneous indices. Two design contests in 1988 and 1992 essentially drove the discussion about broadband AR coatings,21,22 and different methods have been applied to synthesize an inhomogeneous index profile.23,24 In this context so-called multicycle AR designs were introduced.25,26 However, it has to be considered now that any improvement in the performance of an AR coating inevitably involves an increase of the total thickness of the coating.27

At present, the progress in thin-film optics is essentially driven by commercially available thin-film design software, particularly by the application of the needle optimization technique.28 Besides using computer-aided design methods, researchers are making efforts to design AR coatings analytically.29,30 In this context it seems possible to design AR coatings for any angle of incidence that points to a "perfect" AR coating for the future.31 Recently, AR coatings for plastic optics were presented, and it was shown that an AR design generated by an optimization procedure with the needle technique can be synthesized analytically as well.32,33

B. Antireflection Problem

Besides concepts and theories, a characterization of the AR problem itself helps to introduce some terms and definitions. There is an optical substrate, transparent in a given spectral region, that gives a residual reflectance \( R_S \) in this spectral region if an incoming light beam falls upon the boundary between the substrate and the incident medium. \( R_S \) depends directly on the refractive indices of the substrate \( n_S \) and the incident medium \( n_0 \), whereby in most of the cases the incident medium is air. The residual reflectance is undesired and has to be decreased to less than a given reflectance \( R_{\text{min}} \) within a given spectral region from a lower wavelength \( \lambda_1 \) to an upper wavelength \( \lambda_2 \). This AR region is characterized by an AR bandwidth \( BW_{AR} \) given by the ratio of these two wavelengths:

\[
BW_{AR} = \frac{\lambda_2}{\lambda_1}.
\] (1)

Within this AR region there is a reference wavelength \( \lambda_0 \) given by

### Table 2. Selection of Essential Papers Concerning AR Designs and Thin-Film Software

<table>
<thead>
<tr>
<th>Year</th>
<th>Author(s)</th>
<th>Subject</th>
<th>Reference Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>1965</td>
<td>Anders and Eichinger</td>
<td>Inhomogeneous thin films</td>
<td>17</td>
</tr>
<tr>
<td>1968</td>
<td>Jacobsson and Martensson</td>
<td>Evaporated inhomogeneous thin films</td>
<td>18</td>
</tr>
<tr>
<td>1992</td>
<td>Thelen and Langfeld</td>
<td>Design contest: AR coatings for lenses</td>
<td>20</td>
</tr>
<tr>
<td>1992</td>
<td>Verly et al.</td>
<td>Synthesis of inhomogeneous coatings</td>
<td>21, 22</td>
</tr>
<tr>
<td>1993</td>
<td>Willey</td>
<td>Predicting AR design performance</td>
<td>25</td>
</tr>
<tr>
<td>1996</td>
<td>Tikhonravov et al.</td>
<td>Needle optimization technique</td>
<td>26</td>
</tr>
<tr>
<td>1999</td>
<td>Schallenberg et al.</td>
<td>Analytical design of AR coatings</td>
<td>27, 28</td>
</tr>
<tr>
<td>2002</td>
<td>Dobrowolski et al.</td>
<td>Toward perfect AR coatings</td>
<td>29</td>
</tr>
<tr>
<td>2002</td>
<td>Schulz et al.</td>
<td>AR coatings for plastic optics</td>
<td>30, 31</td>
</tr>
</tbody>
</table>
\[ \lambda_0 = 2\lambda_1\lambda_2 / (\lambda_1 + \lambda_2). \]  

(2)

Thus the uncoated substrate causes an AR problem, and this problem can be solved by applying at least one thin film onto the substrate. Those methods that do not use thin interference films to solve the AR problem are not discussed here. We also confine ourselves to the discussion of normal incidence and AR design solutions for low-index substrates.

For a single wavelength or a small AR region, the AR problem is perfectly solved if the single thin film has a refractive index \( n = (n_s n_0)^{1/2} \) and if it has a physical thickness \( d \) so that the optical thickness \( nd = \lambda_0 / 4 \). Usually, a single MgF\(_2\) layer is used for this purpose, and most of the simple optical lenses are coated in this way as a very cheap solution to the AR problem.

C. Antireflection-Hard Design Type

However, often the straightforward single-layer AR coating does not answer the AR problem, and a multilayer has to be designed. As one of the latest solutions, we innovated a so-called AR-hard design type, which was developed to realize scratch-resistant and antireflective coatings for plastic optics but that could also be applied as an AR coating onto any other type of optics.\(^{30,32}\) The AR-hard design can be characterized as follows. A step-down index profile is set to match the refractive index of the substrate to the refractive index of the incident medium. Each equivalent layer index \( E \) of this step-index profile is less than \( n_s \) [Fig. 1(a)], and, usually, also less than the given lowest refractive index \( n_L \). However, it can be synthesized by a symmetrical sequence of three quarter-wave (QW) layers given by the term LAL, where L and A stand for QW layers with refractive indices \( n_L \) and \( n_A \), respectively. The refractive index of the middle A layer is given by the transformation

\[ n_{AI} = n_L^2 / E, \]  

(3)

with \( i = 1 \) to 5 in this AR-hard example. This refractive index is also unavailable, but it can be substituted by using the known Herpin index because it is in the interval of the two given refractive indices \( n_L \) and \( n_{AI} \), which finally results in a design consisting of thick L-index and thin H-index layers. The thickness profile gives a typical arrangement with thin layers of the high-index material and thick layers of the low-index material [Fig. 1(b)].

The spectral performance of this AR-hard example shows a low residual reflectance within a bandwidth \( BW_{AR} = 1.6 \) [Fig. 1(c)]. The thickness characteristic as reflectance versus the thickness plot at the upper-wavelength end of the AR region shows a multicycle behavior, in this case with 4.5 cycles. The first half-cycle is given by a single L layer. Each of the following four cycles is composed of an LHL layer sequence of a different thickness [Fig. 1(d)].

We can draw some conclusions concerning the AR-hard application:

(i) It is known that a step-down index profile that matches the refractive index of the substrate to the
refractive index of the incident medium acts as an AR design.

(ii) It is possible to substitute an unavailable refractive index that is less than a given low refractive index $n_1$, by using a symmetrical Lal sequence of three QW layers. The synthesized middle refractive index $n_a$ of such a QW sequence can be substituted by using the known Herpin-index formalism.

(iii) The unavailable refractive indices of the step-down index profile can be substituted by using different sequences of LAL-QW layers.

(iv) The spectral performance of the presented AR-hard application is determined by the number of steps within the step-down index profile, but the AR bandwidth is limited to a value of $\sim 1.6$.

Because multicycle AR designs with $BW_{AR} \geq 2$ are known, the question was how to broaden the bandwidth by using the experience of the AR-hard design type. Some approaches concerning this problem were presented at the Society of Photo-Optical Instrumentation Engineers (SPIE) conference held in St. Etienne, France, in 2003. Following this context, we present some new concepts in Section 2 that use both equivalent layers and stop-band suppression to broaden the AR bandwidth to a prescribed value.

2. Antireflection Design Concepts

A. Definition of an Equivalent Stack Index

If we want to discuss the AR problem theoretically, we have to make some considerations and definitions. We define a multilayer consisting of $p$ layers of different refractive indices $n_1, n_2, n_3, \ldots, n_p$, but of the same optical thickness equal to a quarter of the reference wavelength $\lambda_0$:

$$n_1 d_1 = n_2 d_2 = n_3 d_3 = \cdots = n_p d_p = \lambda_0 / 4,$$  \hspace{1cm} (4)

i.e., we have QW layers, and the multilayer is a QW stack (QWS). Using Eq. (4), we determine that the phase thickness $\phi$ of a QW layer depends only on the wavelength $\lambda$ given by

$$\phi = 2\pi / \lambda \times n d = \pi / 2 \times \lambda_0 / \lambda.$$

Using the known matrix formalism that shows this QWS has a characteristic matrix given by the characteristic matrices of the individual layers:

$$\begin{pmatrix} M_{11} & iM_{12} \\ iM_{21} & M_{22} \end{pmatrix} = \prod_{i=1}^{p} \begin{pmatrix} \cos \phi & i \sin \phi / n_i \\ i \sin \phi & \cos \phi \end{pmatrix}.$$  \hspace{1cm} (6)

Using the elements of the characteristic matrix yields the reflectance of a QWS given by

$$R = \frac{(n_0 M_{11} - n M_{22})^2 + (n_0 n_3 M_{12} - M_{21})^2}{(n_0 M_{11} + n M_{22})^2 + (n_0 n_3 M_{12} + M_{21})^2}.$$  \hspace{1cm} (7)

Similar to the known definition of the index of an equivalent layer, there is an equivalent stack index (ESI) $E$ of the QWS, given by

$$E(\phi) = \left( \frac{M_{11}}{M_{12}} \right)^{1/2} = \left( \frac{(a_1 \cos^{n_1-1} \phi + a_2 \cos^{n_2-3} \phi + a_3 \cos^{n_3-5} \phi + \cdots)^{1/2}}{b_1 \cos^{n_1-1} \phi + b_2 \cos^{n_2-3} \phi + b_3 \cos^{n_3-5} \phi + \cdots} \right)^{1/2},$$  \hspace{1cm} (8)

where $M_{12}$ and $M_{21}$ are the secondary diagonal elements of the characteristic matrix according to Eq. (6) and the coefficients $a_1, a_2, a_3, \ldots, b_1, b_2, b_3, \ldots$ are only functions of the refractive indices of the single layers determined by the matrix elements themselves. $E(\phi)$ is a symmetrical function, and it is completely defined in the phase range $0 \leq \phi \leq \pi$ based on the symmetry of the cosine function. In contrast to the known equivalent layer index, which is defined for symmetrical multilayers only, the ESI is defined independently of the symmetry of the QWS. Because it is impossible to define an equivalent phase thickness of an asymmetrical QWS, only an ESI can be linked to such a QWS (Fig. 2).

B. Potential Antireflection Region

We know that an equivalent layer has stop bands and passbands that depend on the equivalent index whether it is an imaginary value or a real one, respectively. If we use a QWS whose ESI shows a passband at $E > 0$, then this QWS can be used as an AR coating within the passband, provided the ESI is additionally in the interval $1 < E(\phi) < n_3$. Accordingly, any QWS has a potential AR region where $1 < E < n_3$. In this region the reflectance is less than or equal to the reflectance of the uncoated substrate, and hence the required AR region between $\lambda_1$ and $\lambda_2$ is always part of this potential AR region and the potential AR region itself is always part of a passband. Figure 3 illustrates this definition of a potential AR region.

C. Stop-Band Suppression

Now we can make the following consideration: The general condition to use a QWS as an AR design is the
existence of a passband around the reference wavelength, and the special condition is the width of the passband; that is, the potential AR region has to be greater than the required AR region. One way to broaden the passband is to suppress higher-order stop bands. Since the first application in 1955, stopband suppression has been used mainly to design heat-reflecting mirrors, with a band of high reflectance in the near infrared and a broad passband down to the visible.\(^\text{13,14,34}\) Figure 4 shows an example of such a heat reflector.

To achieve a high reflectance, we use a basic period consisting of \( p \) layers of different refractive indices repeated \( q \) times, whereby suppression of higher-order stop bands is determined exclusively by the layer sequence within this basic period. In this sense, the design of broadband AR coatings seems to be an application of the theory of stop-band suppression. If we deal with AR coatings, we do not need a periodic arrangement of a basic layer sequence, but we use the corresponding layer sequence of the basic period to suppress higher-order stop bands to achieve a broad passband and a broad potential AR region.

To suppress higher-order stop bands, we need to use more than two different refractive indices in a periodic QW sequence.\(^\text{13,34}\) Thelen already made the required calculations and worked out some tables that list possible refractive indices to suppress higher-order stop bands.\(^\text{35}\) Figure 5 shows some examples of QWSs with different orders of stop-band suppression, and we can choose these QWSs as starting designs for broadband AR coatings.

D. Definition of an Equivalent Stack Substrate

However, stop-band suppression works only with symmetrical layer sequences as a basic assumption. It is known that a symmetrical QWS acts as an absentee layer at wavelengths where its phase thickness is an even multiple of \( 2\pi.\) As an example, second- and third-order suppression occurs with a five-layer QWS (Fig. 6). This symmetrical QWS has a phase value \( \phi_0 \) of an even multiple of \( 2\pi \) at spectral points at which the normalized wave number reaches a value of 0.8 and 1.2. At these spectral points, the ESI has a limit with a value of 1.245. This is approximately the value of the root of the refractive index of the substrate, but the \( M_{12} \) element of the characteristic matrix is zero, which results in \( R(\phi_0) = R_s. \) There is a broad potential AR region with \( 1 < E < n_s, \) but in its symmetrical form this QWS is not suitable for an AR design.

To overcome this problem, we also define an equivalent index \( S \) of a QWS given by

\[
S = \frac{n_s M_{22}}{M_{11}} = \frac{n_s (c_1 \cos^p \phi + c_2 \cos^{p-2} \phi + c_3 \cos^{p-4} \phi + \cdots)}{d_1 \cos^p \phi + d_2 \cos^{p-2} \phi + d_3 \cos^{p-4} \phi + \cdots},
\]

where \( M_{11} \) and \( M_{22} \) are the principal diagonal elements of the characteristic matrix of the QWS according Eq. (6) and the coefficients \( c_1, c_2, c_3, \ldots \) and \( d_1, d_2, d_3, \ldots \) are again functions of the refractive indices of the single layers and are determined by the matrix elements themselves. The equivalent index \( S \) is called the equivalent stack substrate (ESS), which is similar to an ESI, with stop bands and passbands that depend on its imaginary or real value, respectively (Fig. 7).

Using Eqs. (4)–(9) allows us to write the reflectance of any QWS as

\[
R = \frac{M_{11}^2 (n_0 - S)^2 + M_{12}^2 (n_0 n_s - E^2)^2}{M_{11}^2 (n_0 + S)^2 + M_{12}^2 (n_0 n_s + E^2)^2},
\]

which is similar to the reflectance formula of a single layer. Because the \( M_{11} \) and \( M_{12} \) elements are zero under different conditions, the reflectance of the QWS is enveloped by

\[
R = \frac{(n_0 - S)^2}{(n_0 + S)^2} \quad \text{at} \quad M_{12} = 0, \quad \text{Eq. (11a)}
\]

\[
R = \frac{(n_0 n_s - E^2)^2}{(n_0 n_s + E^2)^2} \quad \text{at} \quad M_{11} = 0. \quad \text{Eq. (11b)}
\]
This is the reason why the terms $E$ and $S$ have been called ESI and ESS, respectively. At phase values at which the $M_{12}$ element is zero, the reflectance is determined by the ESS. Conversely, at phase values at which the $M_{11}$ element is zero, the reflectance is determined by the ESI, assuming that the limits of ESS and ESI in fact exist at these phase values. In this sense we still agree with the theory of stop-band suppression, but we have to expand the theory by the application of the ESI.

Using the data of Fig. 6 and setting, for example, a required $S(\phi_S) = 1.08$ to obtain $R(\phi_S) = 0.15\%$ according Eq. (11a), Eq. (9) makes it possible to calculate the unknown refractive indices. Figure 8 shows the AR region of such an asymmetrical five-layer QWS derived from the symmetrical QWS example given in Fig. 6.

Fig. 5. Spectral performance of QW stacks with different orders of stop-band suppression: (a) second-order suppression (ABBA)$^4$ with $n_A = 1.45$, $n_B = 1.95$; (b) second- and third-order suppression (ABCBA)$^3$ with $n_A = 1.45$, $n_B = 1.85$, $n_C = 2.35$; (c) second-fourth-order suppression (ABCCBA)$^2$ with $n_A = 1.45$, $n_B = 1.72$, $n_C = 2.12$, $n_D = 2.35$ (Thelen, Ref. 35).

Fig. 6. ESI and reflectance $R$ versus the normalized wave number, the symmetrical five-layer ABCBA QWS, with refractive indices $n_S = 1.52$, $n_0 = 1$, $n_A = 1.46$, $n_B = 1.954$, and $n_C = 2.35$.

Fig. 7. ESS versus the normalized wave number, the asymmetrical five-layer ABCDA QWS with refractive indices $n_A = 1.46$, $n_B = 1.65$, $n_C = 2.35$, and $n_D = 2.273$. 

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and profile steps. The theory of stop-band suppres-
sion serves as a basis of broadband AR design, but it
can give only a starting point for realizing potential
AR designs because asymmetrical QWS have to be
used. ESI and ESS have to be used to synthesize the
needed refractive indices. It seems possible to derive
a straightforward algorithm to design broadband AR
coatings analytically. As for the required formulas,
this has to undergo further investigation. However,
numerical calculations that use a short algorithm to
determine the ESI and the ESS of any QWS provide
a quick overview of possible refractive indices, a topic
that we will follow up-on and present the results for
in a future paper.

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3. Conclusions
We have discussed some novel concepts of designing
broadband AR coatings, and the progress in this mat-
ter can be concluded as follows: It is possible to sub-
stitute theoretically each refractive index of a step-
index profile, regardless of whether it is less than the
given lowest refractive index, by using a stack of at
least three QW layers. The QW stacks of each step of
the step-index concept can be identified by the cy-
cles of the known multicycle AR coatings. The re-
quired AR bandwidth can be directly connected with
the number of layers within the QWS approach. The
performance of the residual reflectance within the AR
bandwidth is determined by the number of the QWSs

E. Multicycle Antireflection Design
As a result of this approach, we have to use asym-
metrical QWSs, fundamentally, except we have the
LAL trilayers as with the AR-hard design. QWSs of
four layers suppress the second-order stop band
themselves, QWSs with five layers are capable of
suppressing the second- and third-order stop bands,
and QWSs with six layers suppress the second, third,
and fourth orders, and so on. If we are able to syn-
thetize a QWS with given ESS and ESI, we repeat
this procedure to synthesize further QWSs with dif-
ferent equivalent indices according to a given step-
index profile. Thus the final AR design approach
consists of q QWSs, each consisting of p QW layers,
and we have another analogy to the theory of stop-
band suppression. In contrast to this theory, we do
not have a periodical arrangement of a basic layer
sequence if we apply the presented AR design ap-
proach, but we have a sequence of different QWSs;
that is, we have a multicycle AR design. The thick-
ness of the cycles is directly connected with the re-
quired bandwidth of the AR region and the number of
QW layers within the stack. The number of cycles
determines the performance of the residual reflect-
ance within the AR region. Practical results for
broadband AR coatings using our approach are
presented in another paper on optical interference coat-
ings.

Fig. 8. ESI, ESS, and reflectance R versus the normalized wave
number, the asymmetrical five-layer ABCDA QWS with refractive
indices n_x = 1.52, n_0 = 1, n_A = 1.46, n_B = 1.68, n_c = 2.35, n_D = 
2.73.


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