Estimating the number of layers required and other properties of blocker and dichroic optical thin films

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Empirically derived formulas are given that allow the thin-film designer to estimate in advance the number of layers needed to meet various thin-film optical performance requirements. The estimation of peak optical density and width of higher-order blocker bands and their suppression are also discussed.

Key words: Thin-film properties, thin-film design, estimating thin films, higher-order reflectance bands.

1. Introduction

Before a coating is designed, it is helpful to have some idea of whether the goal of the design is achievable. The ability to estimate performance limits can avoid fruitless design efforts and avoid the neglect of potential performance gains or simplifications. In the case of antireflection coatings, a broad range of empirical data has been collected and reported[1] on optimized designs to provide a formula to estimate what can be expected in typical cases. Dobrowolski *et al.*[2] have recently reported an extension of Ref. 1. The thrust of this paper is to aid in the estimation of the number of layers and other properties of dichroic, bandpass, and blocking filters.

2. Bandpass and Blocker Coatings

Bandpass, long-wave pass, and short-wave pass, filters can be made by the proper positioning of stacks of layers that have a quarter-wave optical thickness (QWOT) to block or reflect the unwanted wavelengths. Thelen[3] appears to have been the first to discuss minus filters, and he references related work by Young,[4] wherein the blocked band is in the middle of two passbands, one on each side. Dobrowolski[5] applied them in detail, and Thelen discusses them in his book.[6] It is helpful when working with any of these designs to be able to estimate how many layers will be required for attaining the desired reflection or blocking and how wide the blocked band will be. The optical density [OD = log(1/transmittance)] increases almost linearly with the number of layers in a stack. The width of the blocking band increases with the ratio of the indices of the high- and low-index materials in the stack. The relative width of the blocking band is less with higher orders of the reflection-band central wavelength. We can use all these facts to estimate how many pairs of a given material combination will be required for achieving a given result.

A. Estimating the Width of a Blocking Band

Macleod[7] gives Eq. (1) and its derivation for the estimated half-width [$2\Delta g$ from Eq. (1)] of the blocking band in the frequency-related units of g, which equals λ_0/λ, where λ_0 is the wavelength at which the layers of the stack are of one QWOT:

$$\Delta g = \frac{2}{\pi} \arcsin\left(\frac{n_H - n_L}{n_H + n_L}\right) \quad (1)$$

For materials such as TiO_2 and SiO_2, this gives a half-width of 0.138 for $n_H = 2.26$ and $n_L = 1.46$. If such a stack were centered at 539 nm, the edges of the reflecting band would be at approximately 474 and 626 nm. In the infrared, where Ge and ThF_4 can be used with $n_H = 4.0$ and $n_L = 1.35$, one might get $\Delta g = 0.330$. With a stack centered at 10 μm, this would imply band edges at approximately 6.7 and 13.3 μm.

The spectral distributions tend to be symmetrical

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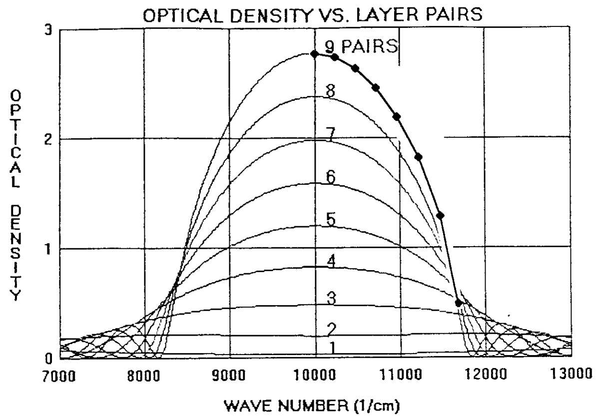

Fig. 1. Example with different numbers of layer pairs with indices of 2.3 and 1.46 plotted on a linear frequency scale that also illustrates that the peak OD increases almost linearly with additional layer pairs after the first few pairs. The values calculated from the approximation, $\cos^{0.5}(1.315\delta g/\Delta g)$ are plotted on the right-hand side of the 9 PAIRS curve.

when plotted versus frequency or g values. Figure 1 is an example with different numbers of layer pairs of 2.3 and 1.46 indices plotted in linear frequency or wave numbers. The Δg predicted by Eq. (1) would be 0.1434, but the measured width is wider than this for small numbers of layer pairs. Equation (1) predicts a number for the width based on a high number of pairs. There is an approximation of a pivot point at approximately the OD = 0.7 or 80% reflectance level. As the number of layer pairs is increased, this point does not change very much, but the slope at the point gets progressively steeper. Figure 1 also illustrates how linearly the peak OD increases with additional layer pairs after the first few pairs.

Also note that the shape of the OD curve is approximately $\cos^{0.5}(\pi\delta g/2\Delta g)$, where δg is the distance from the QWOT central wavelength in g units. Points calculated with this formula are plotted on the right-hand side in Fig. 1. However, note that the $\pi/2$ is not precise and for the example of 9 pairs is actually 1.315 for best fit. This approximation is also valid only up to $\delta g = \Delta g$, of course. The integrated area under this curve from $-\Delta g$ to $+\Delta g$ is approximately $1.57\Delta g$. This times the OD added at the peak by each new pair will give an estimate of the OD times bandwidth contribution of each pair.

B. Estimating the Optical Density of a Blocking Band

The optical density at the maximum point of the QWOT stack is given in approximation (2), where p is the number of layer pairs in the stack. This will depend on whether the stack starts with a high- or a low-index layer, but as long as p is more than a few pairs, it gives a good approximation of the average OD_P at the peak:

$$\mathrm{OD}_P \approx 2\log^{1/2}\left[\left(\frac{n_\mathrm{H}}{n_\mathrm{L}}\right)^p + \left(\frac{n_\mathrm{L}}{n_\mathrm{H}}\right)^p\right]. \tag{2}$$

In the typical case, using the high index as the first layer gives a lower OD than starting with the low index first does. Actually, it is because the last layer of the stack is of low index and acts as an antireflection coating. The first layer of low index next to the substrate can usually be eliminated if it is not much different from the substrate index. Therefore the greatest OD_P for the fewest layers comes from starting and finishing the stack with the high-index material.

The change in OD with the addition of each new pair given in approximation (3) can be derived from approximation (2):

$$\Delta\mathrm{OD} \approx 2\log\left(\frac{n_\mathrm{H}}{n_\mathrm{L}}\right). \tag{3}$$

This is sufficiently correct as long as there are more than a few layers.

Approximation (3) combined with the integral over the bandwidth given above allows us to estimate the OD bandwidth product (ODBWP) of each additional pair. This is approximated by

$$\begin{aligned}\mathrm{ODBWP} &\approx 1.57\Delta g\Delta\mathrm{OD}\\ &\approx 2\log\left(\frac{n_\mathrm{H}}{n_\mathrm{L}}\right)\arcsin\left(\frac{n_\mathrm{H}-n_\mathrm{L}}{n_\mathrm{H}+n_\mathrm{L}}\right).\end{aligned} \tag{4}$$

As far as I am aware, the ODBWP has not been proposed before as an estimating tool.

C. Estimating the Number of Layers and Thickness Needed

As an example of the application of approximation (4), let us take the case of a requirement for a 99% reflector from 400 to 700 nm with $n_\mathrm{H} = 2.25$ and $n_\mathrm{L} = 1.45$. How many pairs would we estimate are required for such a design? Such a design would probably consist of gradually increasing or decreasing the layer thicknesses in the stack to give smooth coverage over the reflection band. The real issue is how much reflection needs to be generated by the layer pairs to cover the band. We can work out that this band has a Δg of 0.273 about a λ_0 of 509 nm, and the OD over the band must be 2.0 (1% transmittance). This gives a total ODBWP of $2 \times 0.273 \times 2.0$ or 1.092 required. By using approximation (4), we find that the ODBWP per layer pair would be ~0.0832. Dividing this into the 1.092 required gives us the estimate that 13.125 pairs would be required, or ~26 layers. We also know that each of these layers would average approximately one QWOT at 509 nm. Dividing the optical thicknesses for a QWOT of 0.12725 μm by the indices of the high and low layers and multiplying by 13 layers of each index, we get an estimated physical thickness of 1.876 μm. Note that estimation of the physical thickness required is expected to be applicable only when the designs are nearly quarter-wave stacks. The estimation of the number of layers to produce a given ODBWP as de-

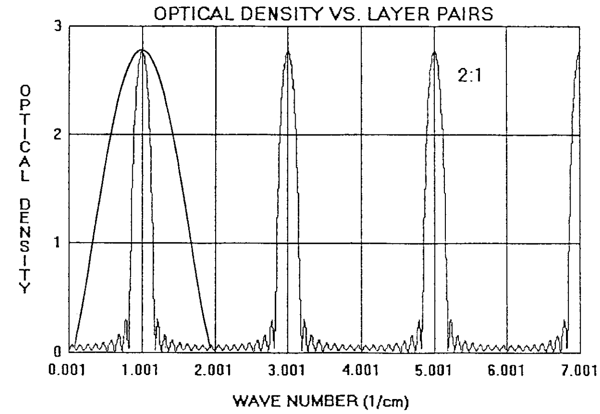

Fig. 2. Higher-order reflectance bands for one QWOT each of high- and low-index material per pair (equal thicknesses) showing that the block band repeats at each odd multiple of a QWOT and has an equal width of the band in Δg. The first cycle of the curve generated by approximation (5) for this case is superimposed on the plot.

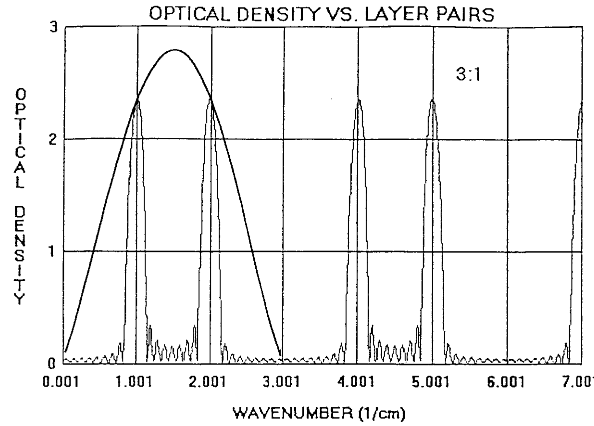

Fig. 3. Reflectance bands with a 3:1 ratio between the overall thickness of the layer pairs to the thinnest layer of the pair, which adds the second and fourth harmonics but suppresses the third and multiples of it, such as the sixth, etc. The first cycle of the curve generated by approximation (5) for this case is superimposed on the plot.

scribed above, on the other hand, is not particularly dependent on the thickness of the layers involved.

D. Estimating More Complex Coatings

If the higher-order reflection bands do not come into play, it may be practical to divide the spectral band to be covered into subsections and just consider the sum of the layers needed to meet the ODBWP of each subsection. This has been found to be practical for estimation purposes before a design is started. Angles other than normal incidence will probably add to the number of layers required.

There may be more complex coatings to be estimated when there are multiple bands to be blocked. In such cases, it would be logical to look first to see if higher-order reflectances of the QWOT stack can be useful to the requirements.

Macleod[7] also illustrates, as in Fig. 2, that, for one QWOT each of high- and low-index materials per pair (equal thicknesses), the reflectance or block band repeats at each odd multiple of a QWOT. The width of each of these block bands is the same in Δg. This then leads to the fact that the third-harmonic frequency will have 1/3 the relative width at that wavelength as at the fundamental QWOT wavelength. Similarly, the fifth harmonic will be 1/5 as wide. This then allows the creation of narrower bands when needed, but it is at the expense of 3 or 5 times as thick a stack for a given block band wavelength. Using high- and low-index materials that are closer to each other can accomplish the same thing with thinner stacks if the appropriate materials are usable. The free width between block bands also needs to be considered.

If any of these higher-order reflection bands contribute to the reflection needed, they do not add to the layer count because they already exist from some other part of the coating. If, however, a high-order reflection band is in a place where transmission is needed, the design would have to be changed to suppress that band. Baumeister[8] showed how different bands can be suppressed by using something other than a unity ratio between the thicknesses of the high- and low-index layers. For example, a 3:1 ratio between the overall thickness of the pair to the thinnest layer will add the second and fourth harmonics but suppress the third, sixth, etc., as seen in Fig. 3. A 4:1 ratio will add the second but not the fourth, etc., as seen in Fig. 4.

If we call the ratio A:1, it can be seen that the Ath harmonic of g_0 has a zero value and that the peaks of the harmonics have an envelope that is approximately a sine function of g from 0 to π. An empirical fit to the data yields

$$\mathrm{OD}_N \approx \left|\mathrm{OD}_E \sin^{1.2}\!\left(\frac{\pi N g}{A}\right)\right|, \qquad N = 1, 2, \ldots . \quad (5)$$

Here OD_N is the OD of the peak of the Nth harmonic block band, and OD_E is the OD of the peak achieved

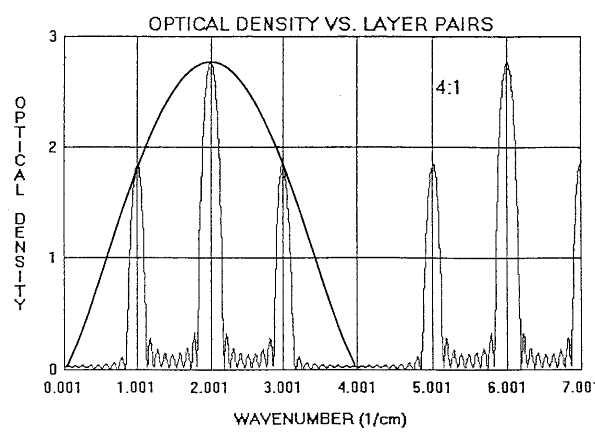

Fig. 4. Reflectance bands as seen in Fig. 3 but with a 4:1 ratio, which also adds the second harmonic but suppresses the fourth, eighth, etc. The first cycle of the curve generated by approximation (5) for this case is superimposed on the plot.

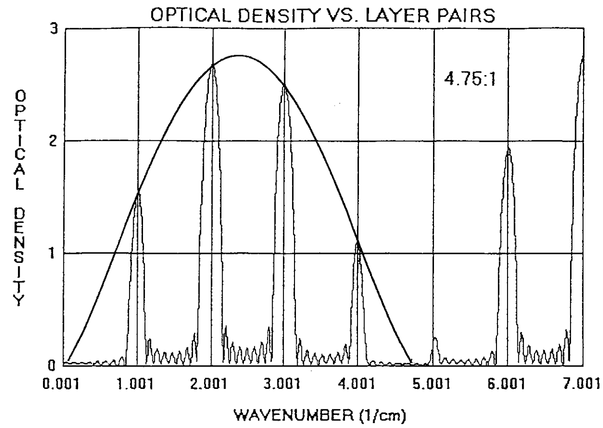

Fig. 5. Illustration that shows that approximation (5) gives the correct results for an A of 4.75, where the reflectance goes to zero at $g = 4.75$. The first cycle of the curve generated by approximation (5) for this case is superimposed on the plot.

by an equal-thickness pair stack. This is illustrated in Figs. 2–6.

It is interesting to note that approximation (5) gives the correct results even for noninteger values of A, such as 4.75 and even 1.5, as seen in Figs. 5 and 6.

These properties can be useful in designing blockers for laser lines with doubled, tripled, quadrupled, etc., harmonics. These series of figures suggest ways to adjust the relative blocking in the harmonics by the choice of the A value. Other applications for these harmonics may appear in the future in areas such as fiber-optic communications filtering, etc.

3. Dichroic Reflection Coatings

The estimation of general coating spectral shapes such as color correction filters may be reasonably approximated by the above methods in most cases. In the case of dichroic filters for color separation, etc.,

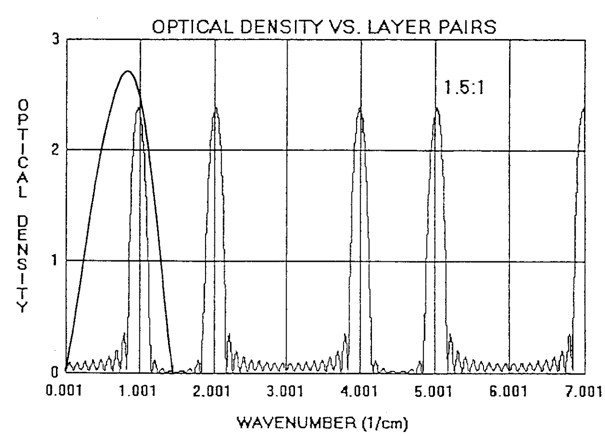

Fig. 6. Illustration that shows that approximation (5) gives the correct results even for a smaller value of A such as 1.5, where the reflectance goes to zero at $g = 1.5$. The first cycle of the curve generated by approximation (5) for this case is superimposed on the plot.

the above approach should be satisfactory. However, it is also of great interest to know how many layers are needed to achieve a certain edge slope between the pass and block bands. This is often the determining factor, rather than the OD, in such filters.

The steepness of the side of an edge filter is in inverse proportion to the number of layers or pairs. The spectral distance from the high to the low transmittance region is usually the important factor for the designer. This might be from 80% to 20% T (approximately 0.1 to 0.7 OD) or some other choice of limits. If we call the spectral distance dg and the peak density at the QWOT wavelength OD_P, the effect of steepness may be approximated by the empirically developed approximation (6):

$$dg \approx \frac{2}{3}\left(\frac{\Delta g}{{OD_P}^{1.74}}\right). \tag{6}$$

We know the Δg from Eq. (1) and the OD_P from approximation (2). The 2/3 factor would need to be changed if the specific OD range from high to low transmittance or reflectance were changed from the 80% to 20% T used above. Because we know that the peak OD is directly proportional to the number of layers in the stack, the dg will be inversely proportional to the number of layers (to some power). This shows how adding layers for steepness has a strong effect at a low total number of layers, but a weak effect if there are already many layers.

4. Summary

It has been shown that the ODBWP can be a useful tool for estimating the number of layers required, and a formula [approximation (4)] has been given for its application. A formula [approximation (5)] has been developed to estimate the peak OD of higher-order reflection bands of layer stacks of any constant and repetitive ratio between the thickness of high- and low-index layers. An empirical formula [approximation (6)] has been given for the estimation of the edge steepness between the passbands and block bands of a dichroic filter. A new notation, A, different from what has been used by Baumeister[8] and others up to this time, has been employed for the ratio of total thickness of a high- and low-index pair of layers to the thickness of the thinnest layer of the pair. This is somewhat more convenient for the application of approximation (5) and indicates where the nodes of the harmonic reflectance bands will be, at integral multiples of A.

It has been shown that there is quite a bit that can be estimated about most coating designs even before the design is started. The estimating process also provides guidance for the design process. It might be said that the estimating process is the first-order design as in lens design, and computer optimization is the rigorous completion of the design process. The new material presented here has been empirically derived for the aid of optical thin-film engineers. More rigorous mathematical derivations and proofs are left for future investigators.

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