

# Resolution of two problems in the Fourier analysis of thin films

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The most common approaches to the application of the Fourier transform method to the synthesis of thin films suffer from two difficulties. The function of reflectance or transmittance to be transformed has been variously approximated, but none of the approximations has been recognized as giving accurate results for all cases. The transformed results for high-reflectance cases have what appear to be distortions in the frequency and in the amplitude scales. These problems and their solutions are the subjects of this paper. It is shown that the reflectance amplitude is the function that should be transformed and that the inclusion of multiple reflections eliminates the distortions in frequency and amplitude.

*Key words:* Thin films, Fourier analysis,  $Q$  functions.

## Introduction

It has been recognized for some decades that it is possible to synthesize an index-versus-optical-thickness profile in a thin film, which will generate a required reflection-versus-wave-number (frequency) profile when appropriate Fourier transform methodology is applied. This would obviate the need for iterative design processes for the required result to be achieved. Dobrowolski and Lowe<sup>1</sup> have documented the history of the research up to recent times. Dobrowolski and colleagues have also been instrumental in advancing the understanding and application of the technique as it has been understood thus far. As a result of my collaboration with Dobrowolski and Verly,<sup>2</sup> where we compared Fourier results with those arrived at by a different approach, I became interested in two of the apparently unresolved questions of the Fourier technique, which are the principal subjects of this paper. They are the  $Q$  function (defined below) and reflection band distortions in frequency and amplitude, which have been addressed also by Bovard.<sup>3</sup>

Much of the published research to date has been restricted to small reflections in nonabsorbing and nondispersive media. I also observe the same restrictions except for the small reflections. This limitation and its removal is the major subject of this paper.

Verly *et al.*<sup>4</sup> described ways to overcome this limitation in practice with the use of iterative procedures incorporated with the synthesis of the Fourier method. Bovard<sup>3</sup> presented another approach. Some of my efforts to gain an understanding of how to remove this small-reflection limitation are addressed here.

## Problems

The first problem is finding a universal  $Q$  function that will apply to all cases. The  $Q$  function is described in detail by Verly *et al.*<sup>4</sup> with references to earlier research. I will define the  $Q$  function as that function of reflectance (or transmittance) versus frequency ( $1/\text{wavelength}$ ) that can be Fourier transformed to define a proper index of refraction profile versus thickness, which produces the required spectral reflectance. Verly implies that none of the  $Q$  functions as they are used with their current Fourier transform methods will give an exact result for all cases. Some functions work well for low reflectors, some work fairly well for high reflectors, but most require some iterative postsynthesis optimization. I have found that one of Verly's  $Q$  functions is the universal function when properly applied, and I discuss how I arrived at this conclusion.

The second problem is that the simpler applications of the Fourier method to high-reflection stacks, such as many quarter-wave optical thicknesses (QWOT's) of high and low-index materials like titania and silica, will generate reflection bands that have the correct form but are calculated to be narrower and more reflective than reality. This indicates that the approximations used have not been adequate for the

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Received 16 June 1992.

0003-6935/93/162963-06\$06.00/0.

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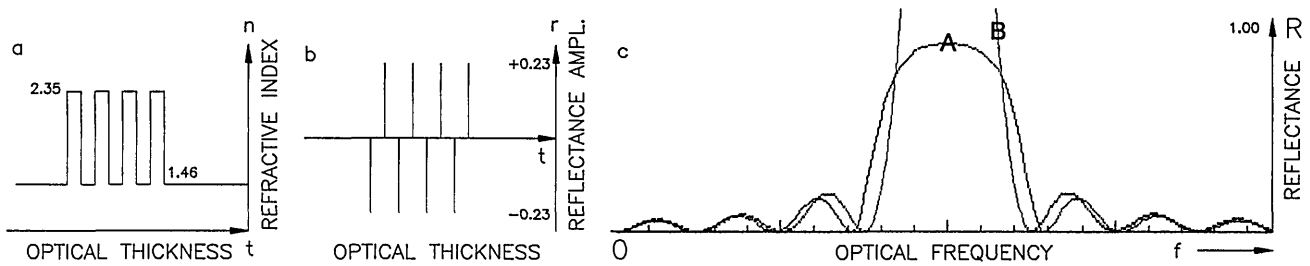


Fig. 1. Refractive index and Fresnel reflectance amplitude versus optical thickness and the resulting reflectance intensity versus optical frequency for a seven-layer (eight-interface) QWOT stack of silica and titania. Curve A is the true reflectance of the stack, and curve B is the simple Fourier transform of b without multiple reflections being accounted for.

cases in question. I will describe what I mean by the simple Fourier analysis approach. Given an index-of-refraction-versus-thickness profile as in Fig. 1a, the reflectance amplitude at each interface between homogeneous layers is calculated by the Fresnel equation:

$$r = (n_0 - n_1)/(n_0 + n_1). \quad (1)$$

Note that this is the same as the  $n'/2n$  used by the referenced authors to represent the change in index divided by twice the average index. The latter form is useful in dealing with continuously varying index profiles (inhomogeneous), which I avoid here for simplicity in illustrating the points of this paper. These delta functions, which are positive and negative, are spaced along an optical thickness axis as shown in Fig. 1b. The spacing in the optical thickness determines the phase relationships of each of these reflections in the usual way. Since the reflectance amplitude as a function of thickness  $r(t)$  has both a magnitude and phase, it is actually a complex function. The function in Fig. 1b is Fourier transformed to give curve B in Fig. 1c. This is the reflectance intensity or the magnitude of the complex reflectance amplitude squared, which is what can be measured in a spectrophotometer. Curve A in Fig. 1c shows the true reflection of a QWOT stack of seven layers (eight interfaces). Note that the scale of the simple Fourier result gives a peak reflection of 349%, which is clearly impossible in reality. Note also that the Fourier result has all the same structural features, but the width of the reflection band and the sidelobe positions appear to have a frequency scale distortion. This was a thrust of Bovard's<sup>3</sup> study.

Dobrowolski and Lowe,<sup>1</sup> Bovard,<sup>3</sup> Verly *et al.*,<sup>4</sup> and Southwell<sup>5</sup> have found ways to overcome these prob-

lems approximately and arrive at useful results in many applications. I believe that I have come to an additional understanding of the solution to the two problems mentioned that is not readily gained from the published literature.

### Investigations

In my earlier empirical research,<sup>6</sup> to understand the natural basis for the ideal broadband antireflection coating, I examined the admittance versus optical thickness for such coatings. These functions have a periodicity and form that suggested that there was possibly a Fourier relationship that might add some understanding to that investigation. This led me to the collaboration with Dobrowolski and Verly.<sup>2</sup> This then led me to ponder the question of the universal  $Q$  function. As a result of my concurrent research in the admittance domain, I spent some time seeking answers in the admittance realm. However, this did not prove fruitful. I have concluded that the ultimate answer can probably be expressed in the admittance form but that it would tend to obscure rather than clarify the understanding.

I then investigated the realm of optical density because of the logarithmic nature of some of the functions used by Dobrowolski and Lowe,<sup>1</sup> Bovard,<sup>3</sup> Verly *et al.*,<sup>4</sup> and Southwell.<sup>5</sup> This seemed promising initially because the high-reflection cases came onto a more tractable scale. I examined example cases such as a thin slab of germanium in air. Here a simple Fourier method would indicate two reflections of equal and opposite amplitude separated by the optical thickness of the slab as seen in Fig. 2. This would transform to a simple sine-squared function of reflectance intensity as a function of frequency.

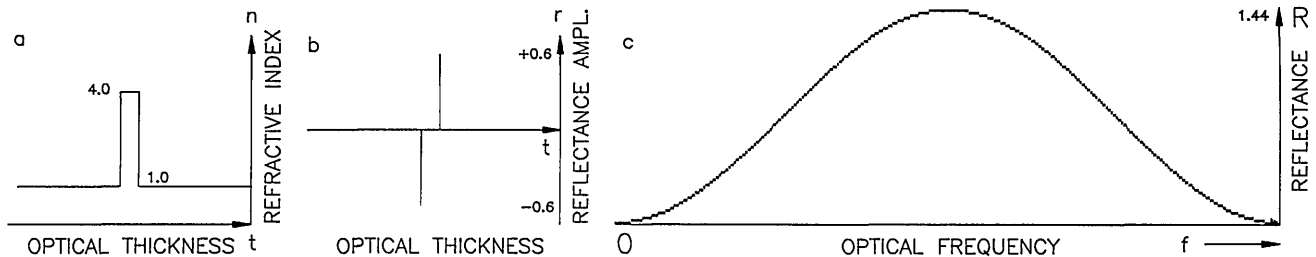


Fig. 2. Properties of a two-interface thin germanium slab in air in the same format as in Fig. 1, but the effects of multiple internal reflections are neglected.

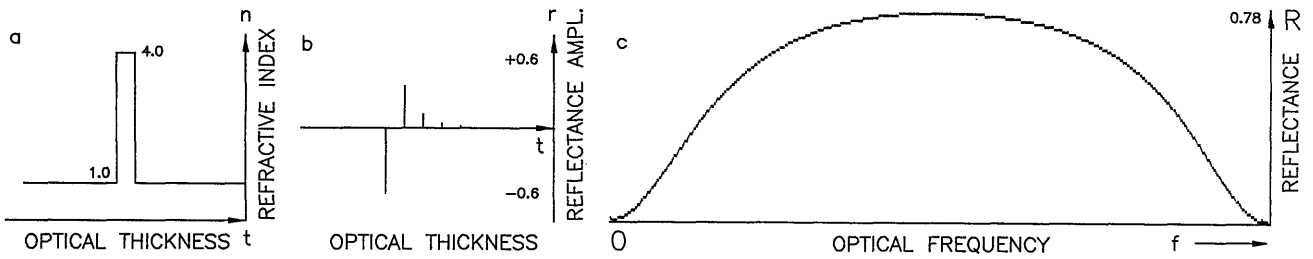


Fig. 3. Same as Fig. 2 with the multiple reflections properly taken into account.

However, it is known from experience and the physically correct matrix solutions of reflectance that the reflectance peaks are broader and flatter at the tops than a simple sine-squared function. I digitized the true matrix solution to this and other examples and

transformed them to see what function would generate such a result. This pointed to what has since become more clear: the multiple internal reflections are what causes the nonsinusoidal shape of the reflectance. This led to a rethinking of the problem

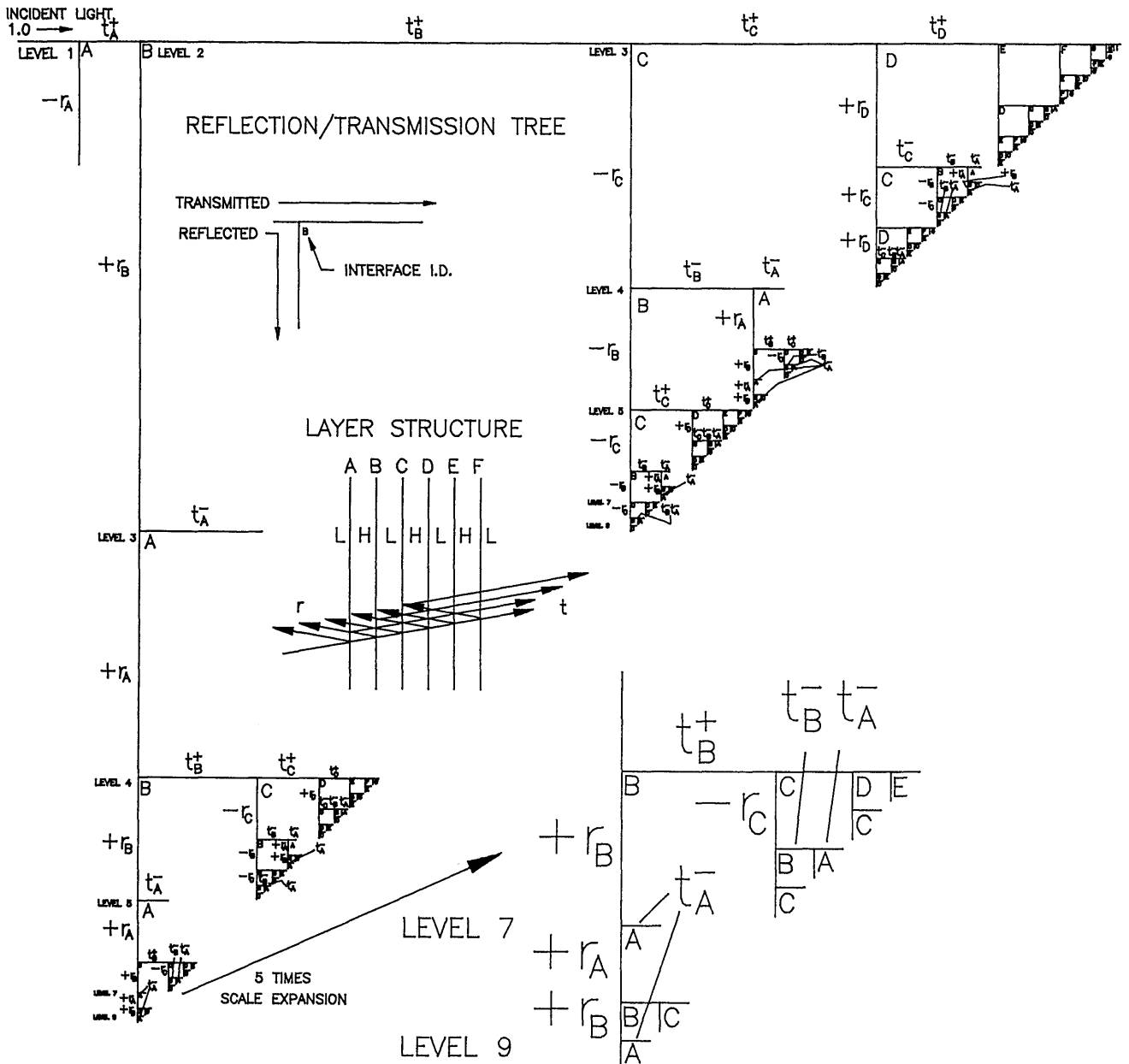


Fig. 4. Reflectance/transmittance tree used to account for multiple-reflection components. See Table 1 for the resultant data.

Table 1. Power and Sign of Each Component  $r$  and  $t$  of Emerging Reflected Rays Illustrated in Fig. 4

Component	$r_A$	$r_B$	$r_C$	$r_D$	$t_A^+$	$t_A^-$	$t_B^+$	$t_B^-$	$t_C^+$	$t_C^-$	Level
1	-1										1
2		1			1	1					3
3	1	2			1	1					5
4	2	3			1	1					7
5	3	4			1	1					9
6			-1		1	1	1	1			5
7	1	1	-1		1	1	1	1			7
8		-1	2		1	1	1	1			7
9	1		2		1	1	2	2			9
10	2	2	-1		1	1	1	1			9
11	1	-2	2		1	1	1	1			9
12	2	2	-1		1	1	1	1			9
13		2	-3		1	1	1	1			9
14	1	-2	2		1	1	1	1			9
15	2	2	-1		1	1	1	1			9
16	1	1	-1		1	1	1	1			7
17				1	1	1	1	1	1	1	7
18	1	1		1	1	1	1	1	1	1	9
19		-1	-1	1	1	1	1	1	1	1	9
20			1	2	1	1	1	1	1	1	9
21		-1	-1	1	1	1	1	1	1	1	9
22	1	1		1	1	1	1	1	1	1	9

and what I now believe is the simplest and correct view of the situation. I calculated the phase and magnitude of each multiple reflection for the germanium slab and also two other interface examples. I then transformed the reflectance amplitude versus optical thickness and found the reflectance amplitude versus frequency and its square, the reflectance intensity. This agreed in detail with the matrix solution and experimental results as shown in Fig. 3 for the germanium case of Fig. 2. This confirmed my hypothesis of the effect of multiple reflections.

**Results**

The above investigations into several points of view led, albeit indirectly, to a viewpoint that makes the understanding relatively simple. This viewpoint is in effect that all thin-film coatings control reflectance (neglecting absorption and scattering). The transmittance is the residual after reflectance has been accounted for. When the amplitudes and phases of all the reflectances (including multiples) as viewed from the side of the incident beam are known, the Fourier transform of this function of reflectance versus thickness gives the correct reflectance versus frequency. This is then squared to give the reflectance intensity

that can be measured. Hodgkinson<sup>7</sup> and Hodgkinson and Stuart<sup>8</sup> described approaches to obtaining the amplitudes and phases.

The above findings correspond to the second  $Q$  function used by Verly, *et al.*<sup>4</sup> which is

$$Q(f) = [1 - T(f)]^{1/2}, \tag{2}$$

where  $T(f)$  is the transmittance intensity versus frequency  $f$  or

$$T(f) = [1 - R(f)] = [1 - r(f)r(f)^*], \tag{3}$$

and  $r(f)$  is the reflectance amplitude and  $r(f)^*$  is its complex conjugate. Therefore

$$Q(f) = r(f), \tag{4}$$

where  $r(f)$  has a magnitude and phase or is a complex function. When  $r$  is small and the number of reflection interfaces are small, the multiple reflections are sufficiently small to be neglected. This is the basis of most of the research reported in the literature. This, however, is not true for either large  $r$ 's as found between germanium and air or for silica and titania QWOT stacks of more than a few layers. It can be

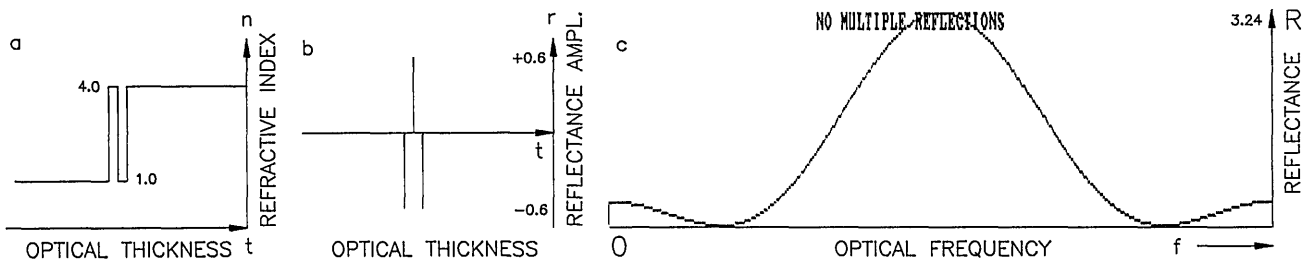


Fig. 5. Properties of three interfaces between germanium and air without proper consideration of the multiple reflections.

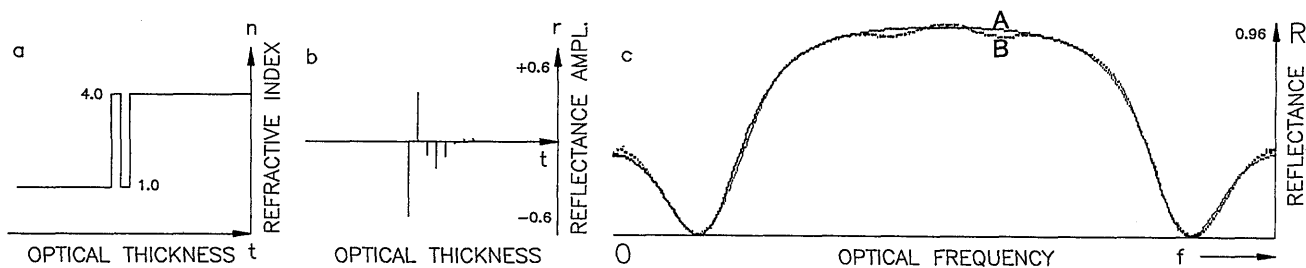


Fig. 6. Same as Fig. 5 with the multiple reflections included. Curve A is the correct matrix result. Curve B is the Fourier result when reflections to the 15th order only are used. More reflections need to be included for better agreement.

shown that they require the inclusion of detailed  $r$  factors to high orders of multiple reflections to yield a correct reflectance spectrum. Otherwise one would find the same distortions described by Bovard<sup>3</sup> and others.

The reflectance amplitude is therefore the sought-after  $Q$  function. The fact that reflectance versus optical thickness transforms to reflectance versus optical frequency is similar to the fact that voltage versus time transforms to voltage versus (temporal) frequency. I discussed this in a brief tutorial paper<sup>9</sup> on the concepts of the Fourier transform method.

The solution to the distortion problem is to include the multiple reflections in detail. To confirm this and add the weight of further example cases, I expanded my empirical investigations to deal with multiple reflections from three and four interfaces. I have not yet found a simple relation that allows me to calculate these from a recursive formula, although it seems likely that such simple relationships exist. The early research of Pegis<sup>10</sup> and Hodgkinson and Stuart<sup>8</sup> may prove helpful in this pursuit. I resorted to a straightforward but somewhat tedious method to find the amplitude and phase of each reflection. To keep the phase relations simple, I worked only with QWOT layers, but this method could be extended for general optical thicknesses. Figure 4 shows a portion of a reflectance/transmittance tree that can be used to find the  $r$  and  $t$  factors that make up each multiple reflection. The chart represents rays that are transmitted through an interface as horizontal lines and those that are reflected as vertical lines. The nomenclature is taken from MacLeod,<sup>11</sup> where the  $r$  factors are reflectance amplitude and the  $t$  factors are transmittance amplitude. The superscript plus signs on the  $t$  factors indicate a ray continuing through the stack in its original direction, the minus signs are for transmittance through an interface while the ray is traveling in reverse. The minus signs on the  $r$  factors indicate the phase change at a low- to high-index interface. This binary tree permits one to account for all the reflections and transmissions until they emerge from the film stack as a final reflection ( $t_A^-$ ) or transmission ( $t_B^+$  in the case of only two interfaces, A and B). That is, each  $t_A^-$  is the terminus of a ray path, which results in a multiple reflection to be added (with phase) to the other reflections from the film. The factors defining the amplitude of such a reflection are found by

starting at the  $t_A^-$  and multiplying it by each  $r$  or  $t$  encountered as one moves back down (up) the branches of the tree to the trunk at the incident light. This can be used to generate a truth table such as that shown in Table 1. These factors can be used in a spread sheet program to calculate the total reflections at successive phase levels. These then can be used as the  $r$  input data for the Fourier transform, which yield the correct reflectance spectra. In Figs. 5 and 6 are compared the cases where the multiple reflections are excluded and included in the calculations for a hypothetical stack of three interfaces between air and germanium. These data were taken to the 15th order. The residual ripples in the spectrum in Fig. 6 still indicate that we need higher orders to give a more precise result in this case of a high reflectance at each interface.

### Conclusions

The conclusion with respect to the first question of the universal  $Q$  function is that it is simply the reflectance amplitude as seen by an observer, wherein all the multiple reflections are included. This has its basis in the second  $Q$  function described by Verly<sup>4</sup> when it is rewritten in terms of  $r(f)$  instead of  $T(f)$ .

The second conclusion is closely related and is that there are no distortions in the Fourier transformation from the reflectance-versus-optical-thickness profile to the reflection-versus-optical-frequency profile if all the multiple reflections are properly taken into account.

I have suggested that it is most illuminating to view all optical thin films as reflection-controlling devices. The resulting transmittance or optical density (neglecting losses) is a by-product of the reflectance.

I have concentrated thus far on what relationships correctly transform from index profiles to spectral profiles or the analysis of a thin film. This is now more easily done by the matrix approach in common use. The ultimate goal is the use of the Fourier technique to transform a spectral profile to the index profile or to synthesize a thin-film design. The reversibility of the transform makes this feasible and has been the motivation for most of the historic research that has been done. It appears that the general direct synthesis without iterative refinement will require a technique to partition the multiple reflections when translating the reflectance-versus-thickness profile from the transform to an index-

versus-thickness profile. It is not yet clear how this may be done. Kaiser and Kaiser<sup>12,13</sup> have addressed some aspects of the problem in ways that may also prove helpful. Further investigations are planned in this area. In the mean time the techniques represented in Refs. 1, 3, 4, and 5 are practical tools to help solve classes of problems where the approximations implied are not a serious limitation.

The potential of the Fourier technique in general for solving difficult problems directly still seems to be great enough to warrant further investigations to overcome the present limitations.

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