New viewpoint on the synthesis of thin films using Fourier transforms

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ABSTRACT

Previously published works on the use of Fourier transforms to synthesize thin film designs have mentioned two problems. One has been a lack of a relational function of reflectance to the index profile, or "Q-function", which gives satisfactory results for both high and low reflectance cases. The other is that the reflectance versus frequency profiles of well know results, from the matrix approach, showed a significant distortion for high reflectors. Our investigations have concluded that the tranform of the simple reflectance amplitude versus optical thickness gives correct results in reflectance versus frequency for all cases when multiple reflections are properly taken into account. The limitation of using only non-dispersive and non-absorbing media still applies to this work. The challenging antireflection coating problem posed for this meeting (a 400 to 900 nm bandwidth and less than 1% reflectance from 0 to 30 degrees) is used as an example to see what insight may be gained by the use of Fourier and related viewpoints.

1. INTRODUCTION

It has been recognized for some decades that there should be a possibility to synthesize an index versus optical thickness profile in a thin film which will generate a desired reflection versus wavenumber (frequency) profile by the use of appropriate Fourier transform methodology. This would eliminate the need for iterative design processes to achieve the required result. Dobrowolski, et al.(1) have described the history of the work 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 our collaboration with Dobrowolski and Verly (2) where we compared Fourier results with those arrived at by our empirical approach, we became interested in two of the apparently unresolved questions of the Fourier technique which are the principal subjects of this paper. These are the "Q-function" (to be defined below) and reflection band distortions in frequency and amplitude which have been addressed also by Bovard (3).

Published work to date has been mostly restricted to small reflections in non-absorbing and non-dispersive media. We 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.(4) descibed ways to overcome this limitation in practice with the use of iterative procedures incorporated with the synthesis of the Fourier method. Bovard (3) presented another approach. We address here some of our efforts to gain an understanding of how to remove this small reflection limitation.

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The thin film design challenge posed by Thelen and Langfeld for the September 1992 EurOpto meeting in Berlin was examined from the Fourier viewpoint. That problem requires that the coating on a 1.52 index substrate in air have less than 1% reflectance from 400 to 900nm in randomly polarized light at 0 and 30 degrees. This turns out to be a difficult design problem when limited to practical materials and no more that 2 micrometers of physical thickness. The viewpoints resulting from the general Fourier technique gave us some confidence that our solution was one in the neighborhood of a unique and optimal solution. We will be surprised if and when radically different solutions are found.

2.PREVIOUS DIFFICULTIES

The first difficulty has been to find a Q-function which will apply to all cases. The Q-function is described in detail by Verly (4) with references to earlier work. We here define the Q-function as that function of reflectance (or transmittance) versus frequency (1/wavelength) which 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 post-synthesis optimization. We have found that one of Dobrowolski and Verly's Q-functions is the "universal" function when properly applied, and we discuss how we arrived at this solution.

Another difficulty is that the simpler applications of the Fourier method to very high reflection stacks, such as many 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 cases in question. We will describe what we 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,

$$r = (n0-n1)/(n0+n1). \qquad (1)$$

These delta functions, which are positive and negative, are spaced along an optical thickness axis as seen in Fig. 1b. The function in Fig. 1b is Fourier transformed to give Curve B in Fig. 1c. Curve A in Fig. 1c shows the true reflection of a QWOT stack of seven layers (8 interfaces). Note that the scale of the simple Fourier result gives a peak reflection of 349% which is clearly not possible in reality. Note also that the Fourier result has all of the same structural features, but the width of the reflection band and the side lobe positions appear to have a frequency scale distortion. This was discussed extensively in Bovard's (3) work.

Papers by Dobrowolski (1), Bovard (3), Verly (4), and Southwell (5) have found ways to approximately overcome these problems and arrive at useful results in many applications. We believe that we have come to an additional understanding of the solution to the two problems mentioned which are not readily discernible from the published literature.

3.EMPIRICAL STUDIES

We examined the admittance versus optical thickness for broadband antireflection coatings (6) in an effort to understand the natural basis for "ideal" antireflection coatings. The admittance versus thickness functions had a periodicity and form that suggested that there was possibly a Fourier relationship which might add some understanding to that investigation. This led us to the collaboration with Dobrowolski and Verly (2). This then led us to ponder the question of the "universal" Q-function. As a result of our concurrent work in the admittance domain, we spent some time seeking answers in the admittance realm. However, this did not prove fruitful. We 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.

The realm of optical density appeared promising because of the logarithmic nature of some of the functions used by Dobrowolski (1), Bovard (3), Verly (4), and Southwell(5). This seemed promising initially because the high reflection cases came onto a more tractable scale. We 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. 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. We 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 non-sinusoidal shape of the reflectance. This led to a rethinking of the problem and what we now believe is the simplest and correct view of the situation. We calculated the phase and magnitude of each of the multiple reflections for the Germanium slab and also other two interface examples. We 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 our hypothesis of the effect of multiple reflections.

4.RESULTS

The above investigations into several points of view led, albeit indirectly, to a viewpoint which 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 of 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 which can be measured. Hodgkinson, et al. (7,8) described approaches to obtaining the amplitudes and phases.

The above findings correspond to the second Q-function used by Verly (4) which is

$$Q(f) = SQR(1-T(f)); \tag{2}$$

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

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

and r(f) is the reflectance amplitude. Therefore

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

When r is small and the number of reflection interfaces is small, the multiple reflections are sufficiently small to be neglected. This is the basis of most of the work 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 shown that these require the inclusion of detailed r's to high orders of multiple reflections to yield a correct reflectance spectrum. Otherwise, we would find the same distortions described by Bovard (3) 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. We discussed this in a brief tutorial paper (9) 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, we expanded our empirical investigations to deal with multiple reflections from three and four interfaces. We have not yet found a simple relation to allow us to calculate these from a recursive formula, although it seems likely that such "simple" relationships exist. The early work of Pegis (10) and Hodgkinson and Stuart (8) may prove helpful in this pursuit. We resorted to a straightforward but somewhat tedious method to find the amplitude and phase of each reflection which is reported in some detail in a recently submitted paper (11).

Figures 4 and 5 compare the cases where the multiple reflections are excluded and included in the calculations for a hypothetical stack of three interfaces between air and germanium. This data was taken to the 15th order. The residual ripples in the spectrum still indicate that higher orders are needed to give a more precise result in this case of a very high reflectance at each interface.

5.SUMMARY OF THE SOLUTION

The conclusion with respect to the first question of the "universal" Q-function is that it is simply the reflectance amplitude. This is the second Q-function described by Verly (4) when 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 transformation from the reflectance versus optical thickness profile to the reflection versus optical frequency profile if all of the multiple reflections are properly taken into account.

We 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.

6.AN EXAMPLE

We first attacked the broad band and broad angle antireflection coating challenge mentioned above by the application of the techniques of design and performance estimation which we previously described (12). That work was done considering only normal incidence, but it did provide a reasonable starting point for a design. The design was optimized with respect to the required performance by a typical iterative procedure. The number of layers which could be simultaneously varied in the process was 40 and the number of specified optimization target points was limited to 50. We concluded that somewhat more layers and target points would have been helpful at the intermediate design stages. The target points had to be somewhat further spaced from each other than desired to cover the bandwidth and angles. Once the design had converged to a minimum, it was examined with various thin film analysis and display tools to study the nature of what might be the basic principles of such a design.

In our earlier works (6,2), we pointed out the undulatory nature of the index, admittance, and reflectance versus thickness of most AR coatings which pointed to the Fourier connection. This was also found to be the case here. Figure 6 shows the admittance amplitude and phase versus optical thickness for the final design submitted to the competition. We believe, on the basis of the earlier observations of this paper, that the reflectance amplitude versus thickness would be even more useful than Fig. 6, but we do not yet have that software available. The derivative of that should closely resemble that which can be transformed to give the spectral reflectance. Figure 7 shows the actual interface reflectance amplitudes of one version of the design versus optical thickness; note the relationship to Fig. 6. Figure 8 shows the the Fourier transform of Fig. 7 and Fig. 9 shows the actual reflectance versus frequency found by the matrix method. Since the effects of multiple reflections hava not been taken into account in Fig. 8, there are some obvious distortions, but the general similarity of Figs. 8 and 9 can be seen. Figure 10 shows a spline curve fit to the reflectance amplitude points of Fig. 7. This seems to show a frequency modulation of the curve versus optical thickness. This is perhaps to be expected since the reflectance amplitudes at each interface are limited to a few specific values and therefore frequency modulation is more fitting than the amplitude modulation which is more apparent in Fig. 6.

With respect to the polarization aspects of the problem, it is interesting to note that the admittance of the s- and p-polarizations at 30 degrees and the normal incidence admittance shown in Fig. 6 all have the same shape but differing amplitudes and produce much the same reflectance versus frequency in Fig. 9 except for small frequency shifts. We show the data from Fig. 6 plotted in the complex plane in Fig. 11 for the normal incidence and Fig. 12 for the 30 degree s-polarization. These spirals are consistent with the earlier reports (6,2) where the admittance spirals smoothly from the admittance of the substrate to the admittance of the media. Both Figs. 11 and 12 are very similar in form and differ only in scale. Again, we expect that reflectance amplitude "circle diagrams" might be even more revealing as in the case of Fig. 6 above, but we don't readily have this capability at the moment.

Our experience suggests that more optical thickness in the design would add more cycles to these spirals and further smooth and reduce the reflectance in the AR band. From our empirical work reported with Verly and Dobrowolski (2), we hypothesize that the best results would be obtained at certain integral numbers of cycles in the optical thickness and lesser portions of a cycle might even be detrimental.

Having examined the AR results from the Fourier and other viewpoints, we see a consistency and "smoothness" in the results. This would lead us to be surprised if there turn out to be other solutions to this problem that are significantly different from the one described. We would, however, expect the solutions using inhomogeneous "layer" structures to show a small advantage in achieving a smoother AR band.

7.CONCLUSION

We have thus far demonstrated what relationships correctly transform from index profiles to spectral profiles or the analysis of a thin film. This is, of course, now more easily done by the matrix approach in common use. The ultimate goal is the use 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 work which 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. Further investigations are planned in this area. In the mean time, the techniques represented in references 1, 3, 4, and 5 are practical tools to help solve classes of problems where the approximations implied are not a serious limitation. The example given here shows a little of the potential for the Fourier and other points of view to give additional insight into the underlying nature of given systems of "layers".

The possibility of using the Fourier technique in general to directly solve difficult problems still seems to be great enough to justify further investigations to overcome the present limitations and find a way to properly account for the multiple reflections in the transform process or at least postprocessing.

8.REFERENCES

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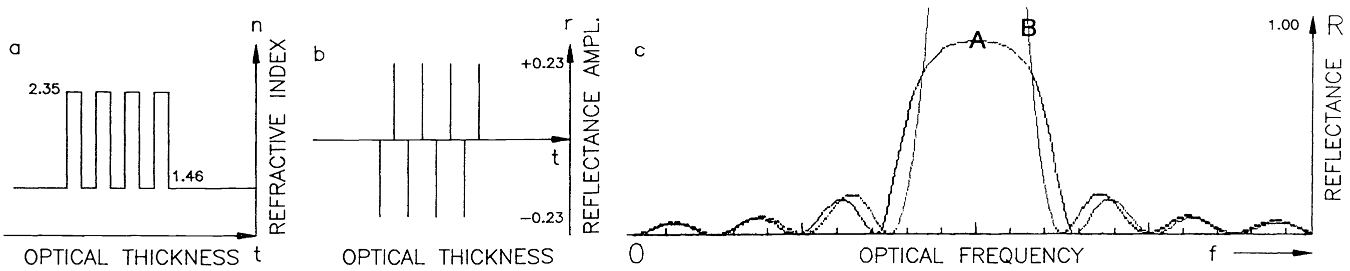


Fig. 1 Seven (7) layer or eight (8) interface QWOT stack of silica and titania. Curve A is true reflectance. Curve B and subfigure b is reflectance without considering multiple reflections.

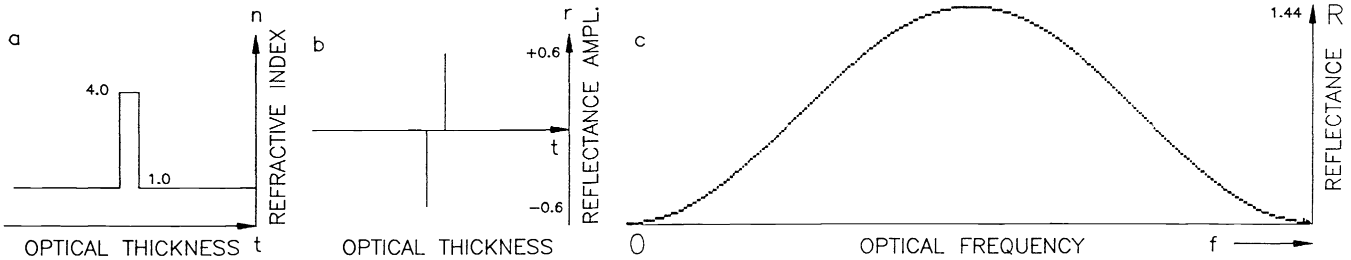


Fig. 2 Two interface Germanium slab (thin) in air, seen in index profile, reflectance amplitude profile, and reflectance intensity versus frequency (1/wavelength).

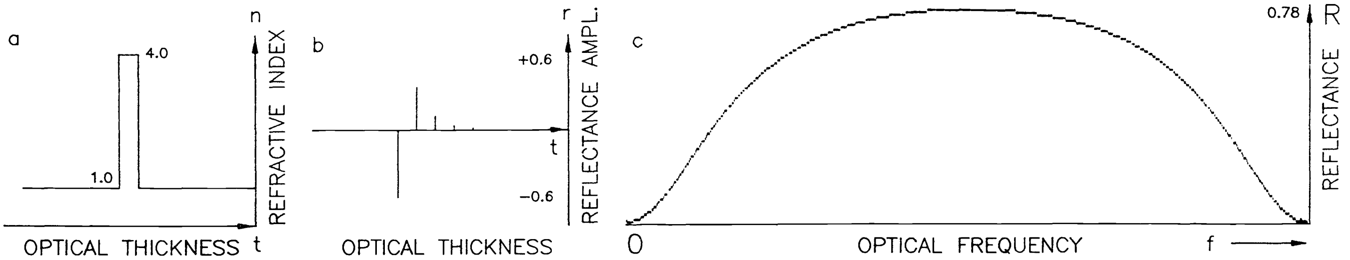


Fig. 3 Germanium slab in air with multiple reflections properly taken into account. This agrees in detail with matrix calculation results.

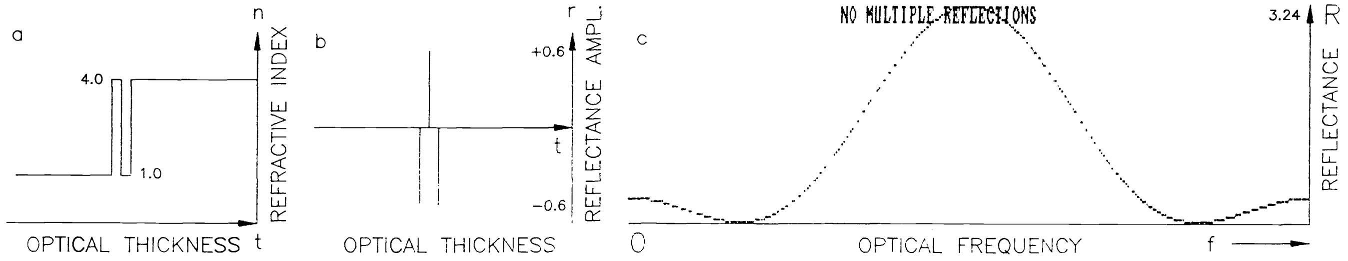


Fig. 4 Three (3) interfaces between Germanium and air excluding multiple reflection considerations.

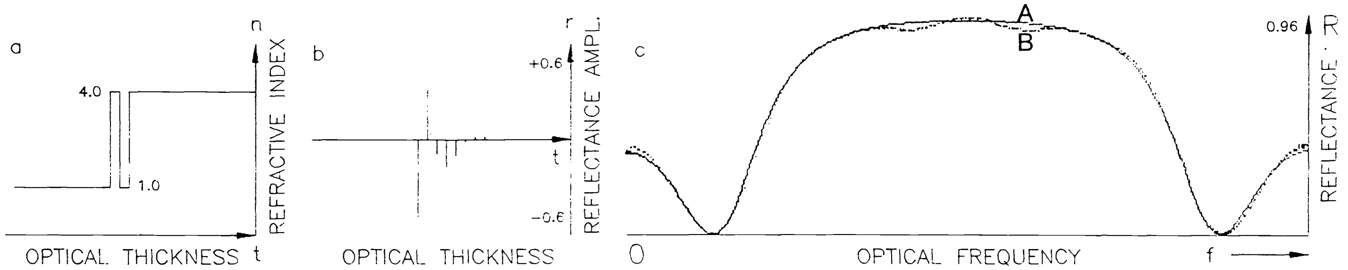
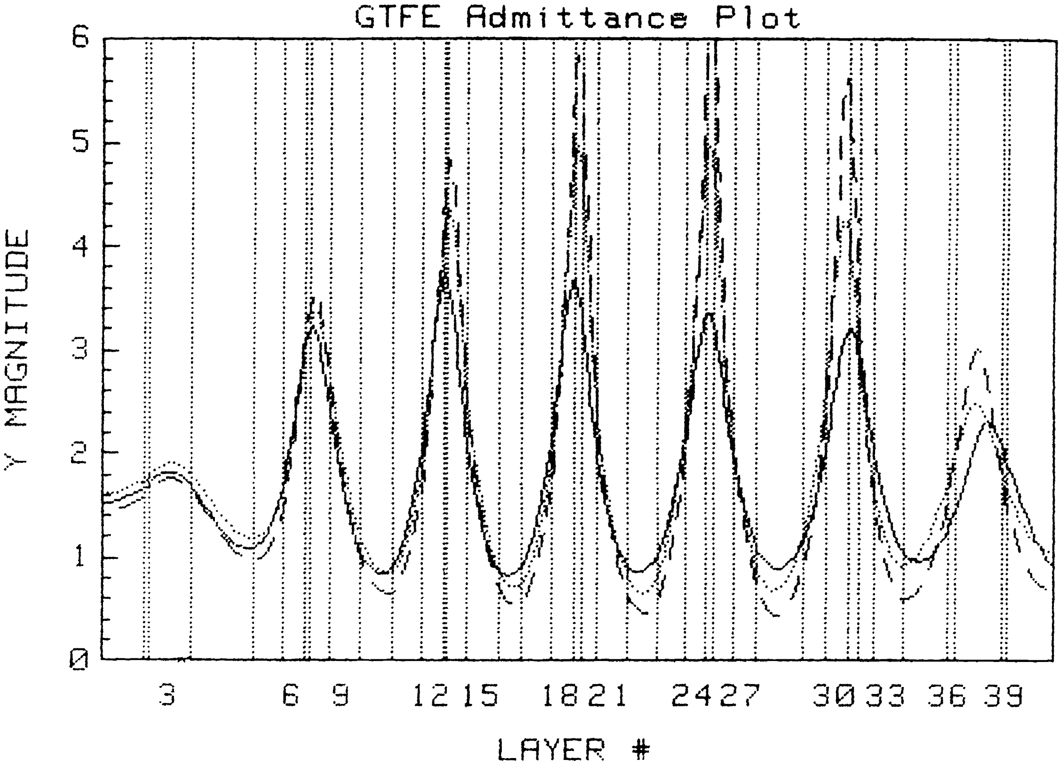


Fig. 5 Same as Fig. 4 with multiple reflections included. Curve A is correct matrix result. Curve B is Fourier result using reflections to the 15th order only.



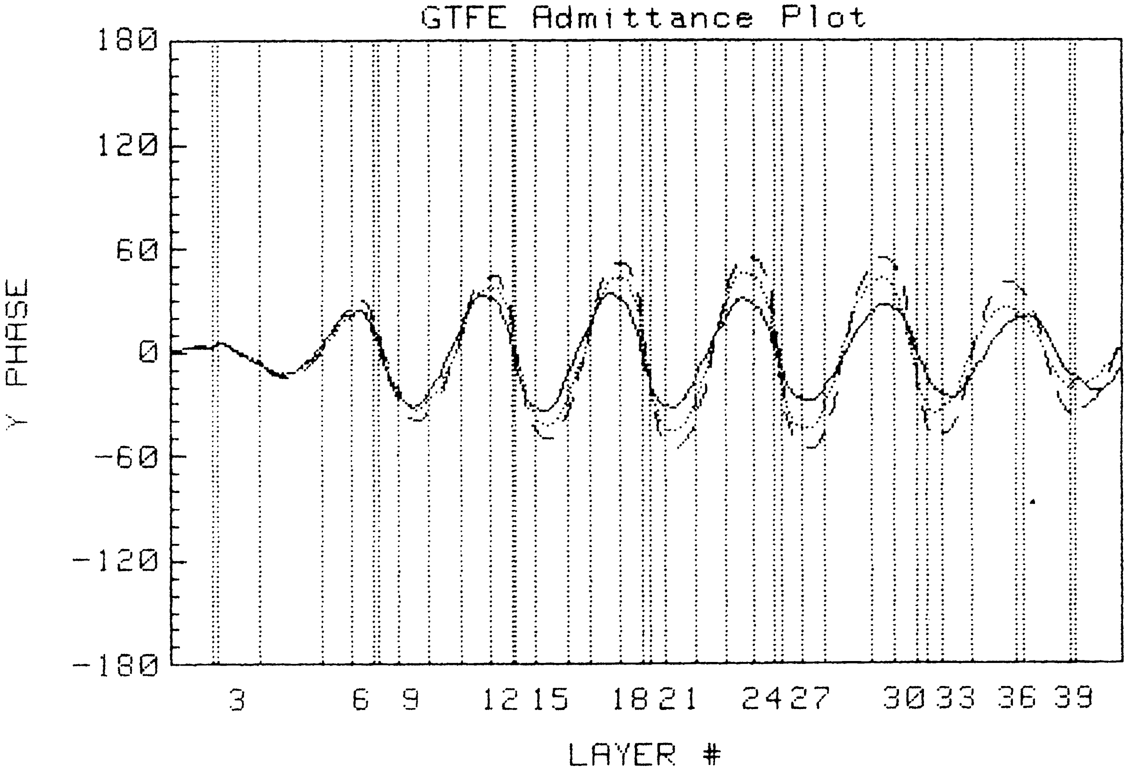


FIG. 6. ADMITTANCE AMPLITUDE AND PHASE VERSUS OPTICAL THICKNESS FOR THE BERLIN CONFERENCE THIN FILM AR DESIGN PROBLEM. SOLID LINE AT 0 DEGREES, DOTTED LINE 30 DEGREES P-POLARIZATION, DASHED LINE 30 DEGREES S-POL.

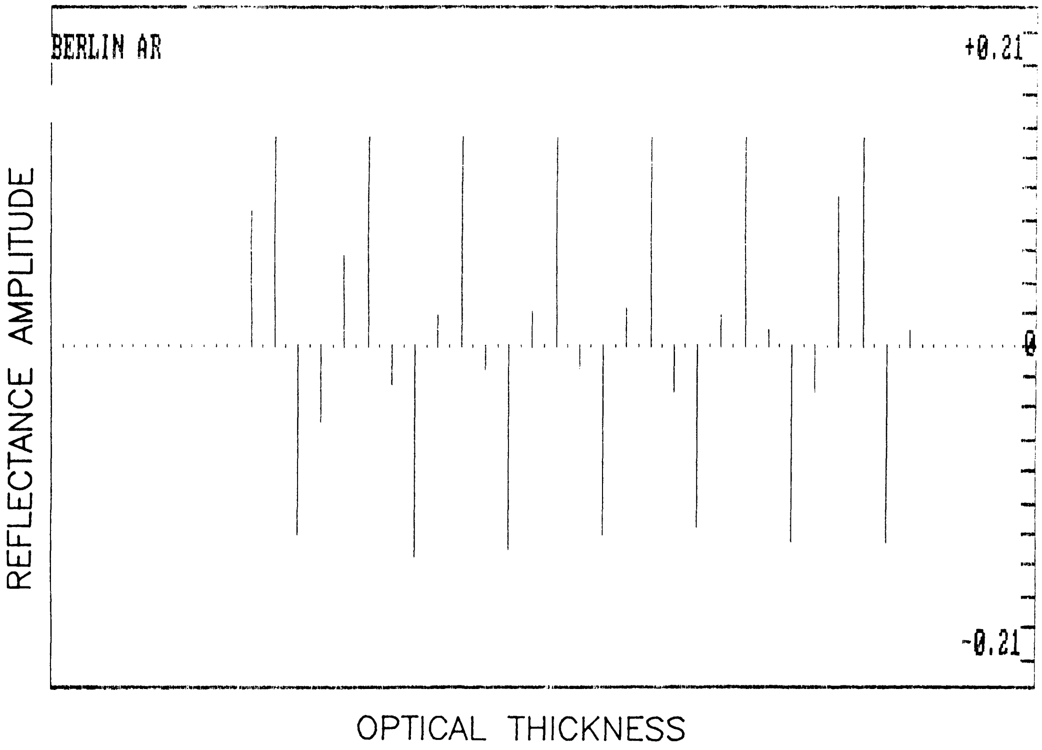


FIG. 7. REFLECTANCE AMPLITUDE VERSUS OPTICAL THICKNESS OF A SIMILAR DESIGN TO THAT FOR THE BERLIN PROBLEM.

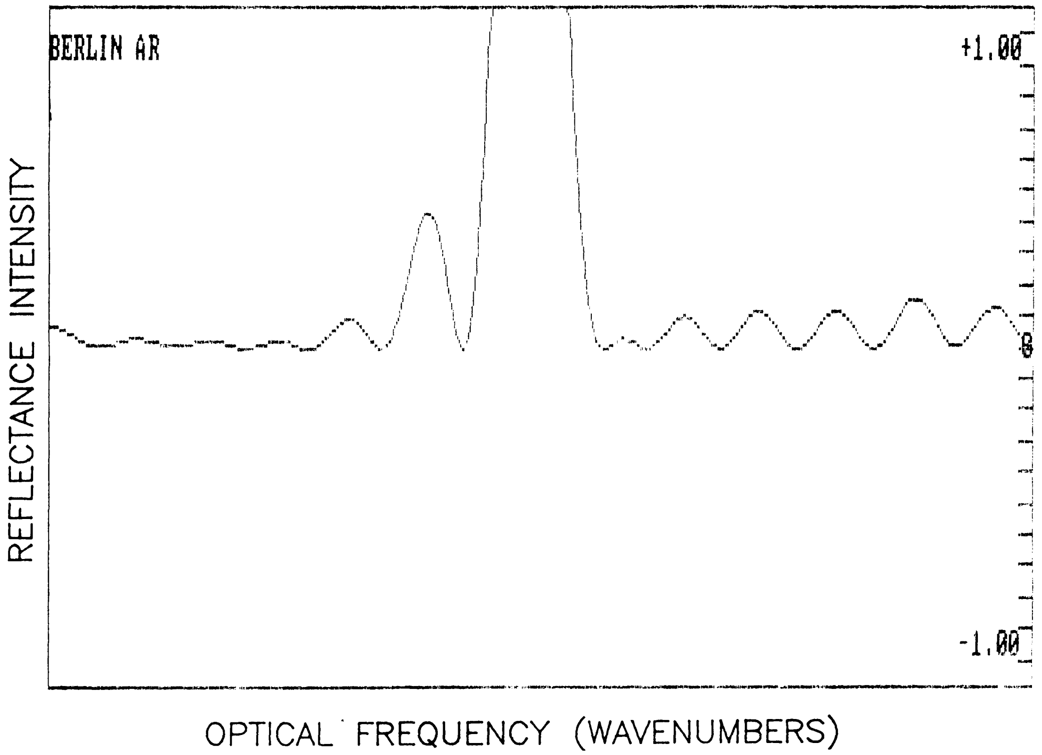
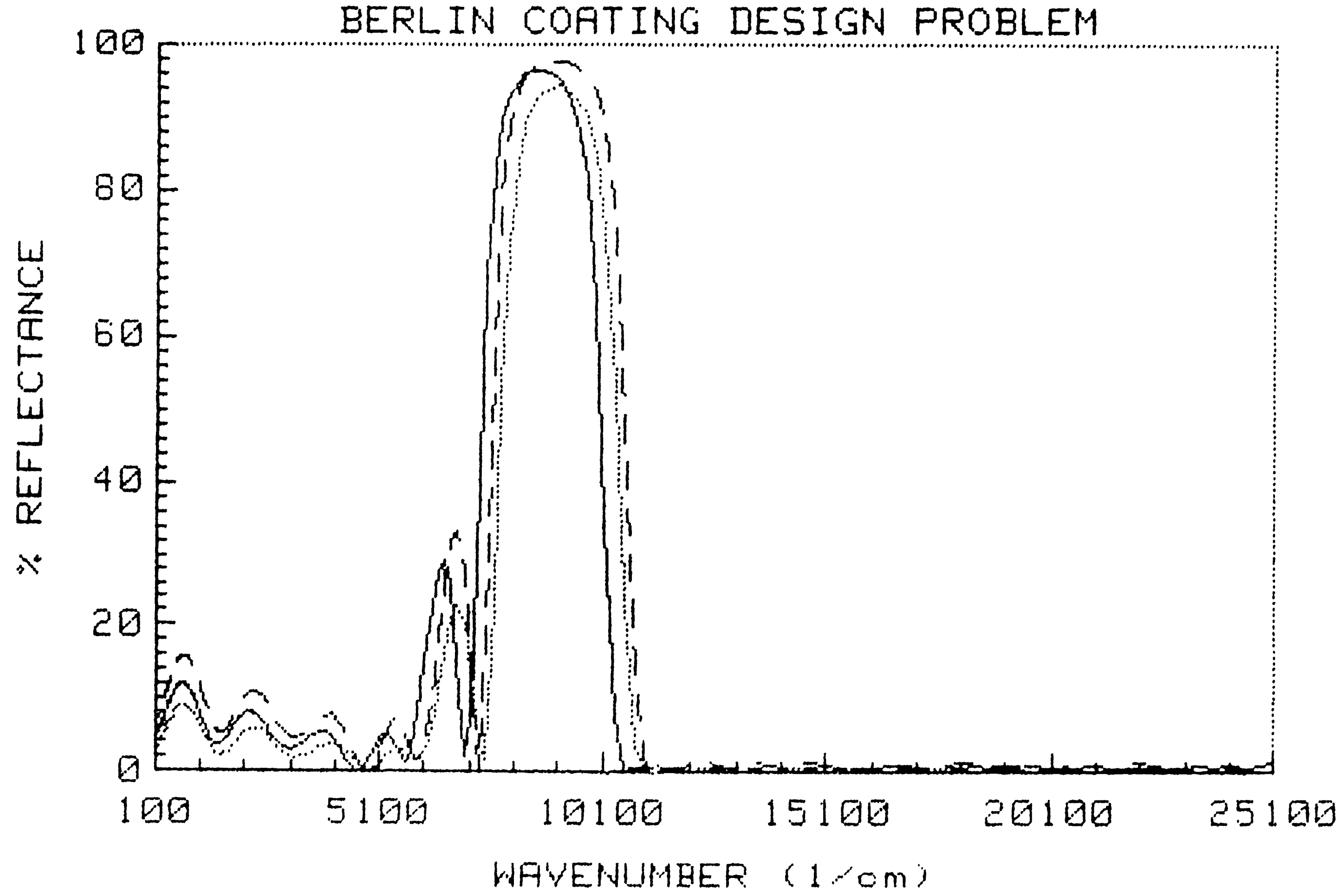


FIG. 8. FOURIER TRANSFORM OF FIG. 7 TO THE REFLECTANCE VERSUS FREQUENCY DOMAIN. REFLECTANCE AMPLITUDE HAS BEEN SQUARED TO GIVE THE REFLECTANCE INTENSITY WHICH CAN BE READILY MEASURED.



FI9. 9. REFLECTANCE INTENSITY VERSUS FREQUENCY BY THE MATRIX METHOD FOR THE ACTUAL DESIGN SUBMITTED FOR THE BERLIN AR PROBLEM. THE CODES FOR THE ANGLES AND POLARIZATIONS ARE THE SAME AS IN FIG. 6.

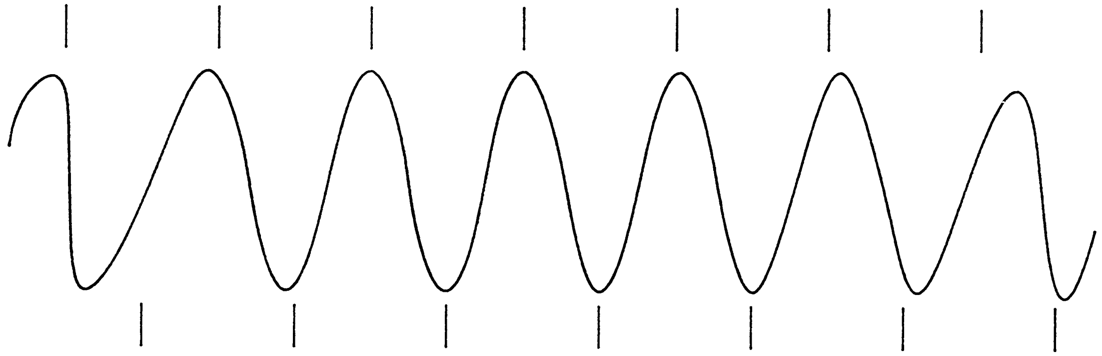


FIG. 10 SPLINE CURVE FIT TO THE REFLECTANCE AMPLITUDE POINTS FROM FIG. 7. SEEMS TO SHOW SOME FREQUENCY MODULATION.

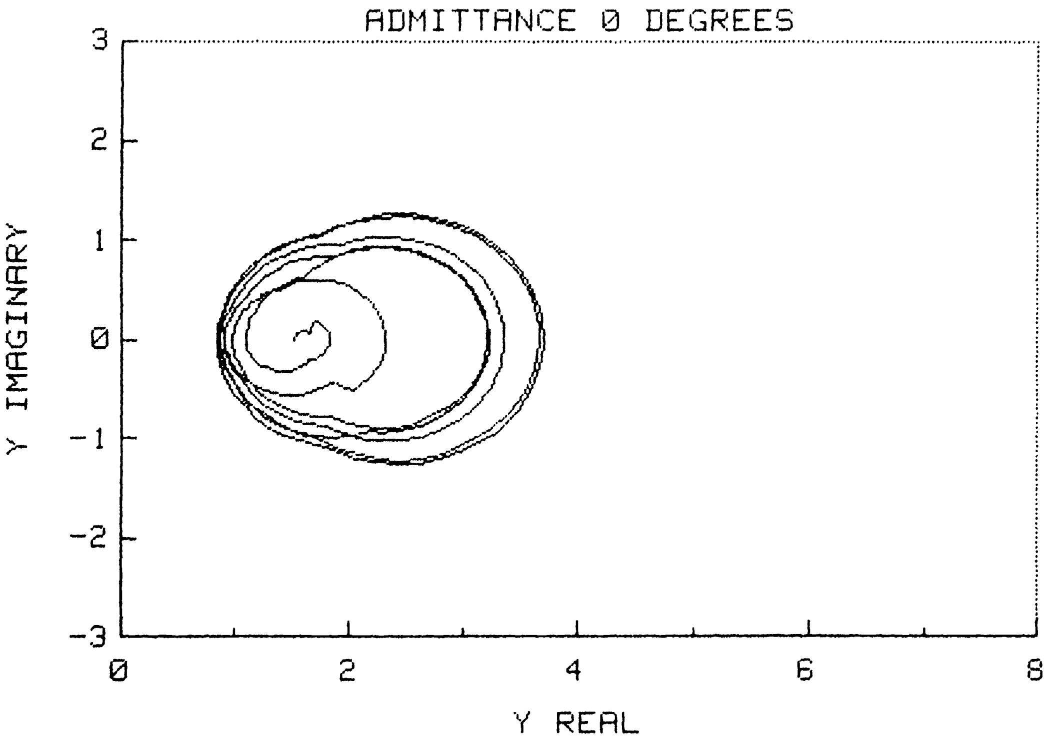


FIG. 11. ADMITTANCE DIAGRAM (AMPLITUDE AND PHASE) OF THE AR DESIGN AT 900NM FOR 0 DEGREES.

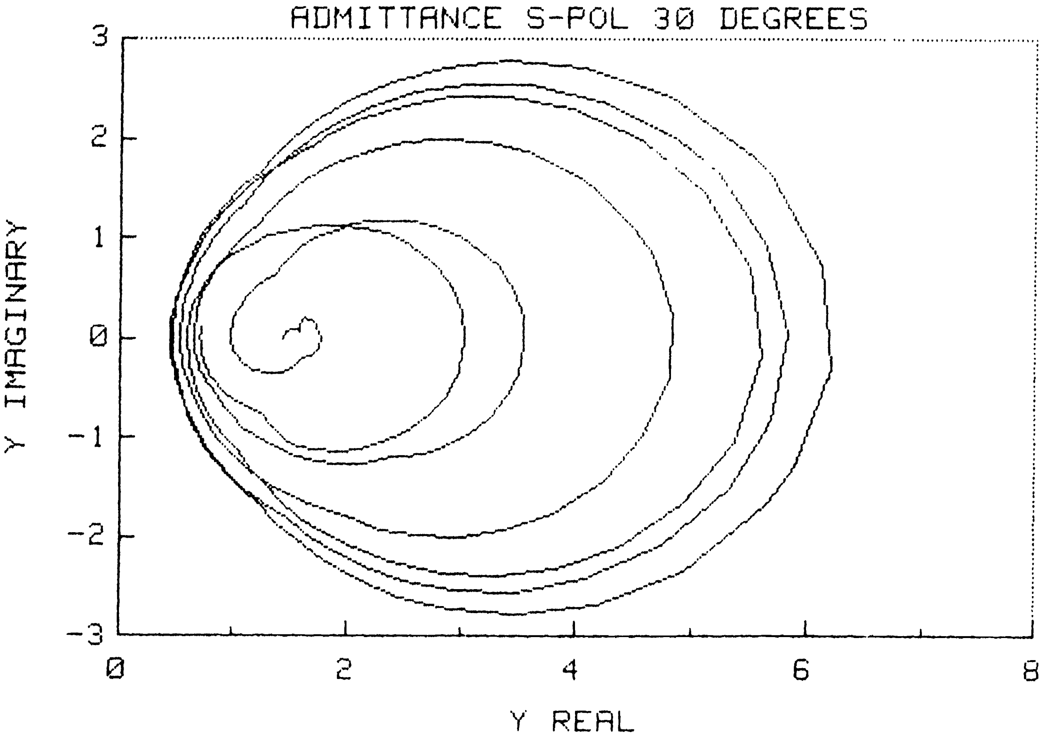


FIG. 12. ADMITTANCE DIAGRAM OF THE AR DESIGN AT 900NM FOR 30 DEGREES AND S-POLARIZATION.