

Theory of Multilayer Films

INTRODUCTION

The physics of interference in single-layer dielectric films has been treated, in its essentials, in Chapter 10. Many useful and interesting applications of thin films, however, make use of multilayer stacks of films. It is possible to evaporate multiple layers while maintaining control over both refractive index (choice of material) and individual layer thickness. Such techniques provide a great deal of flexibility in designing interference coatings with almost any specified frequency-dependent reflectance or transmittance characteristics. Useful applications of such coatings include antireflecting multilayers for use on the lenses of optical instruments and display windows; multipurpose broad and narrow band-pass filters, available from near ultraviolet to near infrared wavelengths; thermal reflectors and cold mirrors, which reflect and transmit infrared, respectively, and are used in projectors; dichroic mirrors consisting of band-pass filters deposited on the faces of prismatic beam splitters to divide light into red, green, and blue channels in color television cameras; and highly reflecting dielectric mirrors for use in gas lasers and in Fabry-Perot interferometers.

Computer techniques have made routine the rather detailed calculations involved in the analysis of multilayer film performance. The design of a multilayer stack that will meet arbitrary prespecified characteristics, however, remains a formidable task. In this chapter we develop a *transfer matrix* to represent the film and characterize its performance. The approach differs from that used in treating

multiple reflections from a thin film in Chapter 11. There we added the amplitudes of all the individual reflected or transmitted beams to find the resultant reflectance or transmittance. It will be more efficient, in the general treatment that follows, to consider all transmitted or reflected beams as already summed in corresponding electric fields that satisfy the general boundary conditions required by Maxwell's equations.

The relationships we require from electromagnetic theory, already presented in Chapter 8, are summarized here. The energy of a plane, electromagnetic wave propagates in the direction of the Poynting vector, given by

$$\mathbf{S} = \epsilon_0 c^2 \mathbf{E} \times \mathbf{B} \quad (19-1)$$

The magnitudes of electric and magnetic fields in the wave are related by

$$E = vB \quad (19-2)$$

where the wave speed can also be expressed by the refractive index,

$$n = \frac{c}{v} \quad (19-3)$$

The wave speed in vacuum is a constant, equal to

$$c = \frac{1}{\sqrt{\epsilon_0 \mu_0}} \quad (19-4)$$

where ϵ_0 and μ_0 are the permittivity and permeability, respectively, of free space. Combining Eqs. (19-2), (19-3), and (19-4), the magnitudes of the magnetic and electric fields can also be related by

$$B = \frac{E}{v} = \left(\frac{n}{c}\right)E = n\sqrt{\epsilon_0 \mu_0}E \quad (19-5)$$

19-1 TRANSFER MATRIX

Our analysis is carried out in terms of the quantities defined in Figure 19-1. An incident beam is shown, with \mathbf{E} chosen for the moment in a direction perpendicular to the plane of incidence. (Keep in mind, however, that for normal incidence E_\perp and E_\parallel are equivalent since a unique plane of incidence cannot be specified.) The beam undergoes external reflection at the plane interface (a) separating the external medium of index n_0 from the nonmagnetic ($\mu = \mu_0$) film of index n_1 . The transmitted portion of the beam undergoes an internal reflection and transmission at the plane interface (b) separating the film from the substrate of index n_s . Along each beam the \mathbf{E} -field is shown—by the usual dot notation—to be pointing out of the page ($-z$ -direction), and the \mathbf{B} -field is shown in a direction consistent with Eq. (19-1). Notice that the y -component of \mathbf{B} must reverse on reflection. The insets define a terminology for the magnitudes of the electric fields *at the boundaries* (a) and (b). For example, E_{r1} represents the sum of all the multiply reflected beams at interface (a) in the process of emerging from the film, E_{t2} represents the sum of all the multiple beams at interface (b) and directed toward the substrate, and so on. In this way, we account for multiple beams in the interference.

We assume that the film is both homogeneous and isotropic. We assume further that the film thickness is of the order of the wavelength of light, so that the path difference between multiply reflected and transmitted beams remains small compared with the coherence length of the monochromatic light. This ensures that the

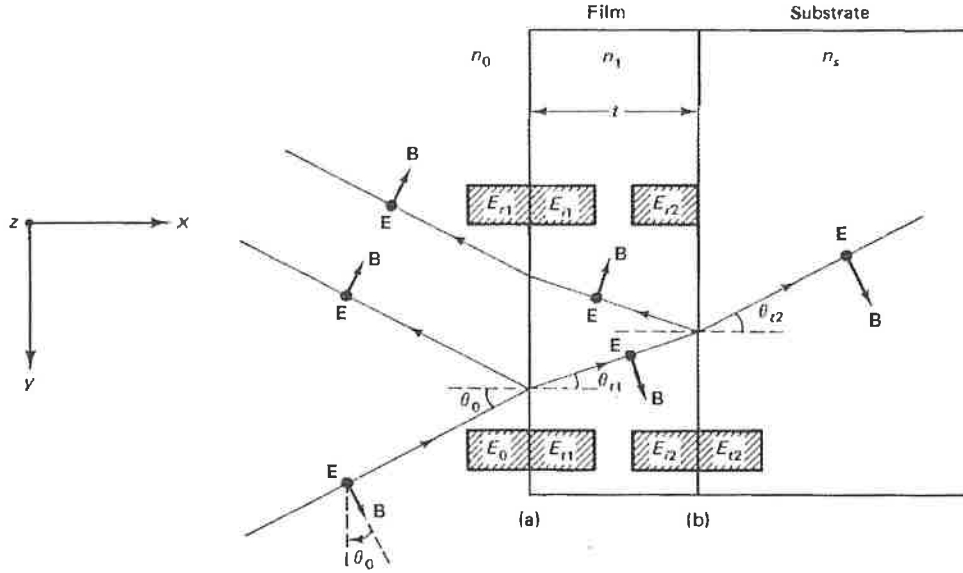


Figure 19-1 Reflection of a beam from a single layer. The diagram defines quantities used in applying boundary conditions to write Eqs. (19-6)–(19-9). Note that a bold dot is used to denote directions perpendicular to the plane of incidence.

beams are essentially coherent. The width of the incident beam, finally, is assumed to be large compared with its lateral displacement due to the many reflections that contribute significantly to the resultant reflected and transmitted beams.

Boundary conditions for the electric and magnetic fields of plane waves incident on the interfaces (a) and (b) are simply stated: The tangential components of the resultant **E**- and **B**-fields are continuous across the interface, that is, their magnitudes on either side are equal. For the case considered in Figure 19-1, **E** is everywhere tangent to the planes at (a) and (b), whereas **B** consists of both a tangential component (*y*-direction) and a perpendicular component (*x*-direction). Thus the boundary conditions for the electric field at the two interfaces become

$$E_a = E_0 + E_{r1} = E_{i1} + E_{i1} \quad (19-6)$$

$$E_b = E_{i2} + E_{r2} = E_{i2} \quad (19-7)$$

Corresponding equations for the magnetic field are

$$B_a = B_0 \cos \theta_0 - B_{r1} \cos \theta_0 = B_{i1} \cos \theta_{11} - B_{i1} \cos \theta_{11} \quad (19-8)$$

$$B_b = B_{i2} \cos \theta_{11} - B_{r2} \cos \theta_{11} = B_{i2} \cos \theta_{12} \quad (19-9)$$

Rewriting Eqs. (19-8) and (19-9) in terms of electric fields with the help of Eq. (19-5),

$$B_a = \gamma_0(E_0 - E_{r1}) = \gamma_1(E_{i1} - E_{i1}) \quad (19-10)$$

$$B_b = \gamma_1(E_{i2} - E_{r2}) = \gamma_s E_{i2} \quad (19-11)$$

where we have written

$$\gamma_0 \equiv n_0 \sqrt{\epsilon_0 \mu_0} \cos \theta_0 \quad (19-12)$$

$$\gamma_1 \equiv n_1 \sqrt{\epsilon_0 \mu_0} \cos \theta_{11} \quad (19-13)$$

$$\gamma_s \equiv n_s \sqrt{\epsilon_0 \mu_0} \cos \theta_{12} \quad (19-14)$$

Now E_{i2} differs from E_{i1} only because of a phase difference δ that develops due to one traversal of the film. Using half the phase difference calculated in Eq. (10-33) for two traversals of the film, we have

$$\delta = k_0 \Delta = \left(\frac{2\pi}{\lambda_0} \right) n_1 t \cos \theta_{i1} \quad (19-15)$$

Thus

$$E_{i2} = E_{i1} e^{-i\delta} \quad (19-16)$$

In the same way,

$$E_{i1} = E_{r2} e^{-i\delta} \quad (19-17)$$

Using Eqs. (19-16) and (19-17) we may eliminate the fields E_{i2} and E_{r2} in the boundary conditions at (b), expressed by Eqs. (19-7) and (19-11), as follows:

$$E_b = E_{i1} e^{-i\delta} + E_{i1} e^{i\delta} = E_{i2} \quad (19-18)$$

$$B_b = \gamma_1 (E_{i1} e^{-i\delta} - E_{i1} e^{i\delta}) = \gamma_s E_{i2} \quad (19-19)$$

Disregarding for the moment the rightmost members, these equations may be solved simultaneously for E_{i1} and E_{i1} in terms of E_b and B_b , yielding

$$E_{i1} = \left(\frac{\gamma_1 E_b + B_b}{2\gamma_1} \right) e^{i\delta} \quad (19-20)$$

$$E_{i1} = \left(\frac{\gamma_1 E_b - B_b}{2\gamma_1} \right) e^{-i\delta} \quad (19-21)$$

Finally, substituting the expressions from Eqs. (19-20) and (19-21) into the equations (19-6) and (19-10) for boundary (a), the result is

$$E_a = E_b \cos \delta + B_b \left(\frac{i \sin \delta}{\gamma_1} \right) \quad (19-22)$$

$$B_a = E_b (i\gamma_1 \sin \delta) + B_b \cos \delta \quad (19-23)$$

where we have used the identities

$$2 \cos \delta \equiv e^{i\delta} + e^{-i\delta} \quad \text{and} \quad 2i \sin \delta \equiv e^{i\delta} - e^{-i\delta}$$

Equations (19-22) and (19-23) relate the net fields at one boundary with those at the other. They may be written in matrix form as

$$\begin{bmatrix} E_a \\ B_a \end{bmatrix} = \begin{bmatrix} \cos \delta & \frac{i \sin \delta}{\gamma_1} \\ i\gamma_1 \sin \delta & \cos \delta \end{bmatrix} \begin{bmatrix} E_b \\ B_b \end{bmatrix} \quad (19-24)$$

The 2×2 matrix is called the *transfer matrix* of the film, represented in general by

$$\mathcal{M} = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} \quad (19-25)$$

If boundary (b) is the interface of another film layer, rather than the substrate, Eq. (19-24) is still valid. The fields E_b and B_b are then related to the fields E_c and B_c at the back boundary of the second film layer by a second transfer matrix. Generalizing, then for a multilayer of arbitrary number N of layers,

$$\begin{bmatrix} E_a \\ B_a \end{bmatrix} = \mathcal{M}_1 \mathcal{M}_2 \mathcal{M}_3 \cdots \mathcal{M}_N \begin{bmatrix} E_N \\ B_N \end{bmatrix}$$

An overall transfer matrix, \mathcal{M}_T , representing the entire multilayer stack is the product of the individual transfer matrices, in the order in which the light encounters them,

$$\mathcal{M}_T = \mathcal{M}_1 \mathcal{M}_2 \mathcal{M}_3 \cdots \mathcal{M}_N \quad (19-26)$$

We return now to Eqs. (19-6), (19-7), (19-10), and (19-11) to make use of those members previously ignored in first finding the transfer matrix. Those remaining equations are

$$E_a = E_0 + E_{r1} \quad (19-27)$$

$$E_b = E_{t2} \quad (19-28)$$

$$B_a = \gamma_0(E_0 - E_{r1}) \quad (19-29)$$

$$B_b = \gamma_s E_{t2} \quad (19-30)$$

For the fields as represented by Eqs. (19-27) to (19-30), the transfer matrix, Eqs. (19-24) and (19-25), may be written as

$$\begin{bmatrix} E_0 + E_{r1} \\ \gamma_0(E_0 - E_{r1}) \end{bmatrix} = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} \begin{bmatrix} E_{t2} \\ \gamma_s E_{t2} \end{bmatrix} \quad (19-31)$$

Equation (19-31) is equivalent to the two equations,

$$1 + r = m_{11}t + m_{12}\gamma_s t \quad (19-32)$$

$$\gamma_0(1 - r) = m_{21}t + m_{22}\gamma_s t \quad (19-33)$$

where we have used the reflection and transmission coefficients defined by

$$r \equiv \frac{E_{r1}}{E_0} \quad \text{and} \quad t \equiv \frac{E_{t2}}{E_0} \quad (19-34)$$

Equations (19-32) and (19-33) can be solved for the transmission and reflection coefficients in terms of the transfer-matrix elements to give

$$t = \frac{2\gamma_0}{\gamma_0 m_{11} + \gamma_0 \gamma_s m_{12} + m_{21} + \gamma_s m_{22}} \quad (19-35)$$

$$r = \frac{\gamma_0 m_{11} + \gamma_0 \gamma_s m_{12} - m_{21} - \gamma_s m_{22}}{\gamma_0 m_{11} + \gamma_0 \gamma_s m_{12} + m_{21} + \gamma_s m_{22}} \quad (19-36)$$

Equations (19-35) and (19-36), together with the transfer-matrix elements as defined by Eq. (19-24), now enable one to evaluate the reflective and transmissive properties of the single or multilayer film represented by the transfer matrix.

Before continuing with applications of these equations, we must take into account the necessary modification of the theory that results when the incident electric field of Figure 19-1 has the other polarization, that is, in the plane of incidence. Suppose that \mathbf{E} is chosen in the original direction of \mathbf{B} and \mathbf{B} is rotated accordingly to maintain the same wave direction. If the equations are developed along the same lines, one finds that only a minor alteration of the transfer matrix becomes necessary: In the expression for γ_1 , Eq. (19-13), the cosine factor now appears in the denominator rather than in the numerator. Summarizing,

$$\begin{aligned} \mathbf{E} \perp \text{plane of incidence:} \quad \gamma_1 &= n_i \sqrt{\epsilon_0 \mu_0} \cos \theta_{i1} \\ \mathbf{E} \parallel \text{plane of incidence:} \quad \gamma_1 &= n_i \frac{\sqrt{\epsilon_0 \mu_0}}{\cos \theta_{i1}} \end{aligned} \quad (19-37)$$

Notice that for normal incidence, where E_{\perp} and E_{\parallel} are indistinguishable, we have $\cos \theta_{t1} = 1$, and the expressions are equivalent. For oblique incidence, however, results must be calculated for each polarization. An average can be taken for unpolarized light. For example, the reflectance becomes

$$R = \frac{1}{2}(R_{\parallel} + R_{\perp}) \quad (19-38)$$

19-2 REFLECTANCE AT NORMAL INCIDENCE

We apply the theory now for the case of normally incident light, the case most commonly found in practice. Results apply quite well also to cases of near-normal incidence. The beam remains normal at all interfaces, so that all angles are zero. In Eqs. (19-12) to (19-14), the cosine factors in the γ -terms are all unity. The matrix elements from Eq. (19-24), appropriately modified to become

$$\begin{aligned} m_{11} &= \cos \delta & m_{12} &= \frac{i \sin \delta}{n_1 \sqrt{\epsilon_0 \mu_0}} \\ m_{21} &= i n_1 \sqrt{\epsilon_0 \mu_0} \sin \delta & m_{22} &= \cos \delta \end{aligned} \quad (19-39)$$

are substituted into Eq. (19-36). After cancellation of the constant $\sqrt{\epsilon_0 \mu_0}$ and some simplification, we find

$$r = \frac{n_1(n_0 - n_s) \cos \delta + i(n_0 n_s - n_1^2) \sin \delta}{n_1(n_0 + n_s) \cos \delta + i(n_0 n_s + n_1^2) \sin \delta} \quad (19-40)$$

The reflectance R , which measures the reflected exitance, is defined by

$$R = |r|^2 \quad (19-41)$$

To calculate R , first notice that the reflection coefficient r is complex and that it has the general form

$$r = \frac{A + iB}{C + iD}$$

so that

$$|r|^2 = rr^* = \frac{A + iB}{C + iD} \frac{A - iB}{C - iD} = \frac{A^2 + B^2}{C^2 + D^2}$$

By inspection then, we may write

normal incidence

$$R = \frac{n_1^2(n_0 - n_s)^2 \cos^2 \delta + (n_0 n_s - n_1^2)^2 \sin^2 \delta}{n_1^2(n_0 + n_s)^2 \cos^2 \delta + (n_0 n_s + n_1^2)^2 \sin^2 \delta} \quad (19-42)$$

Example

A 400-Å thick film of ZrO_2 ($n = 2.10$) is deposited on glass ($n = 1.50$). Determine the normal reflectance for sodium light.

Solution The phase difference is given by

$$\delta = \frac{2\pi}{\lambda}(n_1 t) = \frac{2\pi}{589.3}(2.1)(40) = 0.8956 \text{ rad}$$