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Analysis of multilayer thin-film structures containing magneto-optic and anisotropic media at oblique incidence using 2×2 matrices

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A complete analysis of multilayer structures containing an arbitrary number of dielectric, metal, magnetic, and birefringent/dichroic layers is presented. An algorithm, based on simple 2×2 matrices, is derived which allows reflection, transmission, absorption, magneto-optic conversion, birefringence, and dichroism of the structure to be computed on a personal computer. The incident beam is assumed to be plane monochromatic with arbitrary angle of incidence. There are no approximations involved, and the results are direct consequences of Maxwell's equations.

I. INTRODUCTION

Optical properties of multilayer structures are of great interest in a variety of technological applications. Methods for analysis and design of these structures have been developed in the past, and computer programs exist that can calculate their optical properties. The textbooks by Yeh¹ and Macleod² contain thorough descriptions of the analytic and numerical techniques available for the study of multilayers.

As long as the various layers of the structure are isotropic (i.e., simple dielectrics and metals), the computation of reflection and transmission involves only simple 2×2 matrices. When optical activity and/or anisotropy are introduced, however, the required matrices become 4×4 , and the analysis becomes substantially more complicated. Early investigators of magneto-optical phenomena in multilayers,^{3,4} for instance, used simplifying approximations and thus avoided the treatment of the problem in its most general form. More recently, several authors have attempted exact numerical computations for multilayers containing magnetic and birefringent media, predominantly in connection with optical data storage applications.⁵⁻⁸ These methods utilize the 4×4 matrix technique described by Yeh.^{1,5}

In this paper a general method of computing reflection, transmission, and absorption for structures containing anisotropic and optically active layers, using 2×2 matrices is presented. While the final results are the same as those obtained with the 4×4 matrix technique, the new approach has the advantage of simplicity, yielding significant insights into the peculiarities of multilayers.

In the next section the notation and formalism used throughout the paper are described. Then, in Secs. III and IV, plane-wave solutions of Maxwell's equations for media with optical activity and/or anisotropy are derived. Section V describes the algorithm for calculating reflection matrices at the various interfaces of a multilayer, while Sec. VI is concerned with transmission matrices. Section VII is a brief description of power computation using Poynting's theorem. Numerical results are the subject of Sec. VIII, and some conclusions and closing remarks are included in Sec. IX. Appendix A shows how to relate the dielectric tensors before and after a rotation of the coordinate system. Appendix B gives formulas for computing the roots of a fourth-

order polynomial equation encountered in calculating the propagation vector.

II. NOTATION AND FORMALISM

Let $\mathbf{u} = u_x \hat{\mathbf{x}} + u_y \hat{\mathbf{y}} + u_z \hat{\mathbf{z}}$ be a unit vector with real components in three-dimensional Cartesian space. We define the following matrices based on the components of \mathbf{u} :

$$\tilde{\mathbf{u}} = (u_x, u_y, u_z), \quad (1a)$$

$$\tilde{\tilde{\mathbf{u}}} = \begin{bmatrix} 0 & -u_z & u_y \\ u_z & 0 & -u_x \\ -u_y & u_x & 0 \end{bmatrix}. \quad (1b)$$

The dot product of two vectors $\mathbf{u} \cdot \mathbf{v}$ can be written either as $\tilde{\mathbf{u}}\tilde{\mathbf{v}}^T$ or as $\tilde{\tilde{\mathbf{u}}}\tilde{\mathbf{v}}$. Similarly, the cross product of these vectors $\mathbf{u} \times \mathbf{v}$ is written either as $\tilde{\tilde{\mathbf{u}}}\tilde{\mathbf{v}}^T$ or as $\tilde{\mathbf{u}}\tilde{\tilde{\mathbf{v}}}$. The concept is not restricted to unit vectors or to vectors with real components, and can be extended to arbitrary vectors with complex components. For instance, consider the propagation vector \mathbf{k} which, in general, is written

$$\mathbf{k} = (k_x + ik'_x)\hat{\mathbf{x}} + (k_y + ik'_y)\hat{\mathbf{y}} + (k_z + ik'_z)\hat{\mathbf{z}}. \quad (2a)$$

In Eq. (2a) the real and imaginary parts of the components of \mathbf{k} are explicitly identified. Defining \mathcal{K} as $(k_x^2 + k_y^2 + k_z^2)^{1/2}$ and \mathcal{K}' as $(k_x'^2 + k_y'^2 + k_z'^2)^{1/2}$, one can equivalently write \mathbf{k} as

$$\mathbf{k} = \mathcal{K}\mathbf{u} + i\mathcal{K}'\mathbf{u}'. \quad (2b)$$

In this equation \mathbf{u} and \mathbf{u}' are two unit vectors having, in general, different orientations. With this notation we will have

$$\tilde{\mathbf{k}} = \mathcal{K}\tilde{\mathbf{u}} + i\mathcal{K}'\tilde{\mathbf{u}}', \quad (3a)$$

$$\tilde{\tilde{\mathbf{k}}} = \mathcal{K}\tilde{\tilde{\mathbf{u}}} + i\mathcal{K}'\tilde{\tilde{\mathbf{u}}}'. \quad (3b)$$

When defining the dot and cross products of two complex vectors, one must be careful in generalizing to the complex domain the concepts from the domain of real vectors. For instance, the complex electric field vector \mathbf{E}_0 and the complex propagation vector \mathbf{k} specify the generalized plane wave

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0 \exp[i(\mathbf{k} \cdot \mathbf{r} - \omega t)]. \quad (4)$$

The magnetic field vector \mathbf{H}_0 , being proportional to the cross product of \mathbf{k} and \mathbf{E}_0 , can be written

$$\tilde{\mathbf{H}}_0^T \propto \tilde{\mathbf{k}} \tilde{\mathbf{E}}_0^T. \quad (5a)$$

The concept of orthogonality, however, cannot be applied to these complex vectors. This becomes evident as one expresses Eq. (5a) in terms of the real and imaginary components of the vectors:

$$(\mathcal{H}_0 \tilde{\mathbf{w}} + i\mathcal{H}'_0 \tilde{\mathbf{w}}')^T \propto (\mathcal{H} \tilde{\mathbf{u}} + i\mathcal{H}' \tilde{\mathbf{u}}')(\mathcal{E}_0 \tilde{\mathbf{v}} + i\mathcal{E}'_0 \tilde{\mathbf{v}}')^T. \quad (5b)$$

Clearly, \mathbf{w} and \mathbf{w}' are linear combinations of $\mathbf{u} \times \mathbf{v}$, $\mathbf{u} \times \mathbf{v}'$, $\mathbf{u}' \times \mathbf{v}$, and $\mathbf{u}' \times \mathbf{v}'$, and as such, no simple relationship (i.e., orthogonality) can be identified among pairs of these vectors.

Both \mathbf{k} and \mathbf{E}_0 are complex vectors in three-dimensional space, but we will find it useful to interpret them differently. \mathbf{k} is the propagation vector and, when written as $\mathcal{H}\mathbf{u} + i\mathcal{H}'\mathbf{u}'$, specifies two directions in space: \mathbf{u} is the direction of phase propagation, whereas \mathbf{u}' is the direction along which the wave amplitude undergoes an exponential decay. In other words, the planes perpendicular to \mathbf{u} have constant phase, while those perpendicular to \mathbf{u}' have constant amplitude. The interpretation of $\mathbf{E}_0 = \mathcal{E}_0\mathbf{v} + i\mathcal{E}'_0\mathbf{v}'$ is as follows: At any given point in space, the electric field vector is $\mathbf{E}_0 \exp(-i\omega t)$. One may consider either the real part or the imaginary part of this vector and show that, as time progresses, the tip of the vector travels around an ellipse confined to the plane of \mathbf{v} and \mathbf{v}' . The unit vectors \mathbf{v} and \mathbf{v}' therefore define the plane of polarization of the wave described by Eq. (4).

We shall find it convenient to define the divergence ($\nabla \cdot$) and curl ($\nabla \times$) operators in our matrix notation as follows:

$$\text{Divergence: } \tilde{\nabla} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right). \quad (6)$$

$$\text{Curl: } \tilde{\nabla} = \begin{pmatrix} 0 & -\frac{\partial}{\partial z} & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & 0 & -\frac{\partial}{\partial x} \\ -\frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \end{pmatrix}. \quad (7)$$

In the next section Maxwell's equations will be expressed in matrix form, and general formulas for plane-wave propagation in homogeneous media will be derived. Readers familiar with the electromagnetic wave theory may find this exercise somewhat redundant, but the author believes that it will help preserve the continuity of the argument and clarify subsequent derivations.

III. MAXWELL'S EQUATIONS AND PLANE-WAVE PROPAGATION

In a medium with neither free charges nor currents, the Maxwell equations are

$$\nabla \cdot \mathbf{D} = 0, \quad (8a)$$

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t}, \quad (8b)$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \quad (8c)$$

$$\nabla \cdot \mathbf{B} = 0. \quad (8d)$$

Let the time dependence be $\exp(-i\omega t)$, with ω in the optical frequency range. It is generally believed that in this regime $\mathbf{B} = \mu_0 \mathbf{H}$, where μ_0 is the permeability of free space. Under these circumstances the constitutive relation that describes the interaction of light with the medium of propagation will be

$$\mathbf{D} = \epsilon_0 \tilde{\epsilon} \mathbf{E}. \quad (8e)$$

Here ϵ_0 is the permittivity of free space, and $\tilde{\epsilon}$, a 3×3 matrix, is the dielectric tensor of the propagation medium. In the matrix notation of the previous section, Maxwell's equations are written

$$\tilde{\nabla} \tilde{\epsilon} \tilde{\mathbf{E}}^T = 0, \quad (9a)$$

$$\tilde{\nabla} \tilde{\mathbf{H}}^T = -i\omega \epsilon_0 \tilde{\epsilon} \tilde{\mathbf{E}}^T, \quad (9b)$$

$$\tilde{\nabla} \tilde{\mathbf{E}}^T = i\omega \mu_0 \tilde{\mathbf{H}}^T, \quad (9c)$$

$$\tilde{\nabla} \tilde{\mathbf{H}}^T = 0. \quad (9d)$$

In the MKSA system of units, the electric field has units of V/m, the magnetic field is in A/m, $\mu_0 = 4\pi \times 10^{-7}$ H/m, and $\epsilon_0 = 8.82 \times 10^{-12}$ F/m. We shall normalize the electric field by the so-called impedance of free space, $Z_0 = (\mu_0/\epsilon_0)^{1/2} = 377 \Omega$, and use $\hat{\mathbf{E}}$ instead of \mathbf{E} to indicate the normalized electric field. Also introducing the propagation constant in free space, k_0 , defined as

$$k_0 = \frac{2\pi}{\lambda_0} = \sqrt{\mu_0 \epsilon_0} \omega, \quad (10)$$

one can rewrite Eqs. (9) as follows:

$$\tilde{\nabla} \hat{\mathbf{E}}^T = 0, \quad (11a)$$

$$\tilde{\nabla} \tilde{\mathbf{H}}^T = -ik_0 \tilde{\epsilon} \hat{\mathbf{E}}^T, \quad (11b)$$

$$\tilde{\nabla} \hat{\mathbf{E}}^T = ik_0 \tilde{\mathbf{H}}^T, \quad (11c)$$

$$\tilde{\nabla} \tilde{\mathbf{H}}^T = 0. \quad (11d)$$

In this streamlined version of Maxwell's equations both $\hat{\mathbf{E}}$ and \mathbf{H} are in units of A/m, k_0 is in $(\text{m})^{-1}$, and $\tilde{\epsilon}$ is dimensionless. The generalized plane wave described by Eq. (4) [with a similar expression for the magnetic field distribution $\mathbf{H}(\mathbf{r}, t)$] will be a solution of Maxwell's equations, provided that the following equations are satisfied:

$$\tilde{\mathbf{k}} \hat{\mathbf{E}}_0^T = 0, \quad (12a)$$

$$\tilde{\mathbf{k}} \tilde{\mathbf{H}}_0^T = -k_0 \tilde{\epsilon} \hat{\mathbf{E}}_0^T, \quad (12b)$$

$$\tilde{\mathbf{k}} \hat{\mathbf{E}}_0^T = k_0 \tilde{\mathbf{H}}_0^T, \quad (12c)$$

$$\tilde{\mathbf{k}} \tilde{\mathbf{H}}_0^T = 0. \quad (12d)$$

Only two of the above four equations are independent. To see this, note that for any complex vector \mathbf{k}

$$\tilde{\mathbf{k}} \tilde{\mathbf{k}} = 0. \quad (13)$$

Therefore, if Eq. (12b) is multiplied on both sides with $\tilde{\mathbf{k}}$, Eq. (12a) is obtained. Similarly, multiplication of Eq. (12c) by $\tilde{\mathbf{k}}$ leads to Eq. (12d). Thus the first and the last of Eqs. (12) need not be considered any longer. Now if Eq. (12c) is multiplied by $\tilde{\mathbf{k}}$ and if the right side of the resulting equation is replaced from Eq. (12b), we obtain

$$[(\tilde{k}/k_0)^2 + \tilde{\epsilon}] \hat{E}_0^T = 0, \quad (14a)$$

$$H_0^T = (\tilde{k}/k_0) \hat{E}_0^T. \quad (14b)$$

Equations (14) are the fundamental equations of plane-wave propagation in a homogeneous medium characterized by the dielectric tensor $\tilde{\epsilon}$. The first equation will have a non-trivial solution when the determinant of the coefficient matrix vanishes, yielding the characteristic equation

$$|(\tilde{k}/k_0)^2 + \tilde{\epsilon}| = 0. \quad (15)$$

Equation (15) imposes certain restrictions on the propagation vector \mathbf{k} , depending on the dielectric tensor of the medium. To give a simple example, consider the case of propagation in an isotropic medium where $\tilde{\epsilon} = \epsilon I$. Here ϵ is a complex constant and I is the identity matrix. Equation (15) in this case reduces to

$$k_x^2 + k_y^2 + k_z^2 = k_0^2 \epsilon. \quad (16)$$

In other words, any wave vector \mathbf{k} satisfying Eq. (16) is an acceptable solution to Maxwell's equations for propagation in the corresponding isotropic medium. In practice, the imposed restrictions by the characteristic equation are augmented by other restrictions (such as those imposed by the Snell's law), limiting the acceptable values of \mathbf{k} to a handful of wave vectors. For each acceptable wave vector Eq. (14a) must be solved for the components of \hat{E}_0 . Since the three linear equations implied by Eq. (14a) are not independent, they do not yield a unique solution for \hat{E}_0 ; rather they place certain constraints on the electric field vector. Complete identification of \hat{E}_0 is made possible only after additional constraints (such as continuity of fields at the interfaces) are taken into account.

Finally, Eq. (14b) is used to determine the magnetic field vector \mathbf{H}_0 for acceptable wave vectors \mathbf{k} once the corresponding electric field vector \mathbf{E}_0 has been identified.

IV. SNELL'S LAW AND POSSIBLE SOLUTIONS OF THE WAVE EQUATION

With reference to Fig. 1, a plane wave incident at oblique angle (θ, ϕ) on the surface of a multilayer has the following wave vector:

$$\mathbf{k}^{(i)} = k_0 \mathbf{u}^{(i)} = -k_0 (\sin \theta \cos \phi \hat{x} + \sin \theta \sin \phi \hat{y} + \cos \theta \hat{z}) \quad (17)$$

(superscript i is for incident). The continuity of \mathbf{E} and \mathbf{H} at the interface between adjacent layers requires that the components of the propagation vector along \hat{x} and \hat{y} (i.e., k_x and k_y) be the same on both sides of the interface. Therefore, for all plane waves in all layers,

$$k_x = -k_0 \sin \theta \cos \phi, \quad (18a)$$

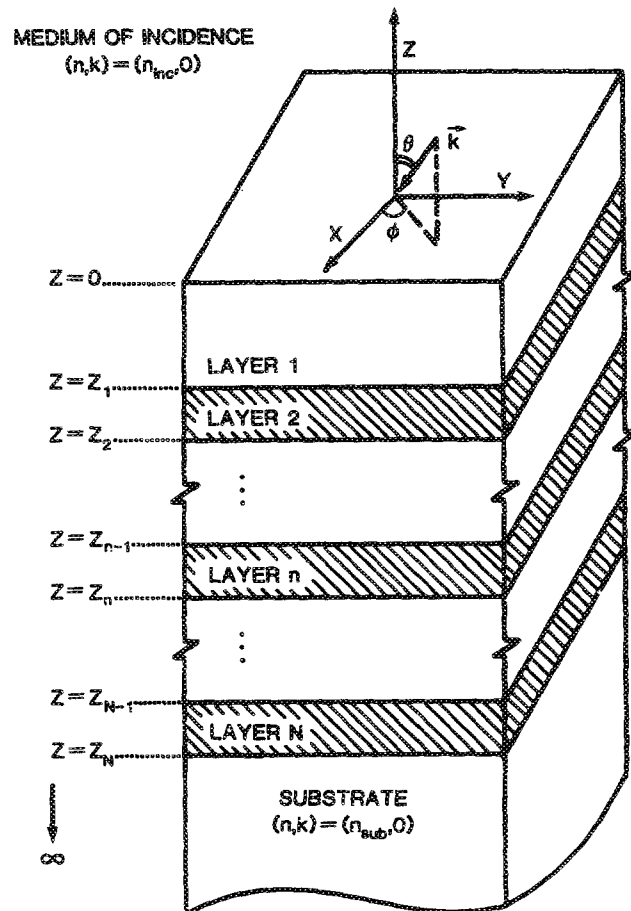


FIG. 1. Schematic diagram of a multilayer structure. The incident beam is in the upper semi-infinite medium with refractive index n_{inc} and has propagation vector \mathbf{k} .

$$k_y = -k_0 \sin \theta \sin \phi. \quad (18b)$$

Let us now examine the characteristic equation (15) for a medium with the general dielectric tensor:

$$\tilde{\epsilon} = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{pmatrix}. \quad (19)$$

Replacing $\tilde{\epsilon}$ of Eq. (19) in Eq. (15) and performing the algebraic manipulations, one obtains the following fourth-order equation for k_z :

$$\left(\frac{k_z}{k_0}\right)^4 + A \left(\frac{k_z}{k_0}\right)^3 + B \left(\frac{k_z}{k_0}\right)^2 + C \left(\frac{k_z}{k_0}\right) + D = 0. \quad (20)$$

The coefficients A , B , C , and D in Eq. (20) are given below:

$$A = \left(\frac{k_x}{k_0}\right) \frac{\epsilon_{xz} + \epsilon_{zx}}{\epsilon_{zz}} + \left(\frac{k_y}{k_0}\right) \frac{\epsilon_{yz} + \epsilon_{zy}}{\epsilon_{zz}},$$

$$B = \left(\frac{k_x}{k_0}\right)^2 \left(1 + \frac{\epsilon_{xx}}{\epsilon_{zz}}\right) + \left(\frac{k_y}{k_0}\right)^2 \left(1 + \frac{\epsilon_{yy}}{\epsilon_{zz}}\right) + \left(\frac{k_x k_y}{k_0^2}\right) \frac{\epsilon_{xy} + \epsilon_{yx}}{\epsilon_{zz}} + \left(\frac{\epsilon_{xz} \epsilon_{zx} + \epsilon_{yz} \epsilon_{zy}}{\epsilon_{zz}} - \epsilon_{xx} - \epsilon_{yy}\right),$$

$$\begin{aligned}
C &= \left(\frac{k_x^2 + k_y^2}{k_0^2} \right) \left[\left(\frac{k_x}{k_0} \right) \frac{\epsilon_{xz} + \epsilon_{zx}}{\epsilon_{zz}} + \left(\frac{k_y}{k_0} \right) \frac{\epsilon_{yz} + \epsilon_{zy}}{\epsilon_{zz}} \right] \\
&+ \left(\frac{k_x}{k_0} \right) \left(\frac{\epsilon_{xy}\epsilon_{yz} + \epsilon_{yx}\epsilon_{zy}}{\epsilon_{zz}} - \frac{\epsilon_{yy}}{\epsilon_{zz}} (\epsilon_{xz} + \epsilon_{zx}) \right) \\
&+ \left(\frac{k_y}{k_0} \right) \left(\frac{\epsilon_{xy}\epsilon_{zx} + \epsilon_{yx}\epsilon_{xz}}{\epsilon_{zz}} - \frac{\epsilon_{xx}}{\epsilon_{zz}} (\epsilon_{yz} + \epsilon_{zy}) \right), \\
D &= \left(\frac{k_x^2 + k_y^2}{k_0^2} \right) \left[\left(\frac{k_x}{k_0} \right)^2 \frac{\epsilon_{xx}}{\epsilon_{zz}} + \left(\frac{k_y}{k_0} \right)^2 \frac{\epsilon_{yy}}{\epsilon_{zz}} + \left(\frac{k_x k_y}{k_0^2} \right) \frac{\epsilon_{xy} + \epsilon_{yx}}{\epsilon_{zz}} - \frac{\epsilon_{xx}\epsilon_{yy}}{\epsilon_{zz}} \right] + \left(\frac{k_x}{k_0} \right)^2 \left(\frac{\epsilon_{xy}\epsilon_{yx} + \epsilon_{xz}\epsilon_{zx}}{\epsilon_{zz}} - \epsilon_{xx} \right) \\
&+ \left(\frac{k_y}{k_0} \right)^2 \left(\frac{\epsilon_{xy}\epsilon_{yx} + \epsilon_{yz}\epsilon_{zy}}{\epsilon_{zz}} - \epsilon_{yy} \right) + \left(\frac{k_x k_y}{k_0^2} \right) \left(\frac{\epsilon_{xz}\epsilon_{zy} + \epsilon_{zx}\epsilon_{yz}}{\epsilon_{zz}} - \epsilon_{xy} - \epsilon_{yx} \right) \\
&+ \left[\epsilon_{xx}\epsilon_{yy} + \frac{\epsilon_{xy}\epsilon_{yz}\epsilon_{zx} + \epsilon_{yx}\epsilon_{zy}\epsilon_{xz}}{\epsilon_{zz}} - \epsilon_{xy}\epsilon_{yx} - \left(\frac{\epsilon_{xx}}{\epsilon_{zz}} \right) \epsilon_{yz}\epsilon_{zy} - \left(\frac{\epsilon_{yy}}{\epsilon_{zz}} \right) \epsilon_{xz}\epsilon_{zx} \right].
\end{aligned}$$

In general, Eq. (20) has four complex solutions for k_z . Of these, two solutions are in the upper half and two in the lower half of the complex plane. The solutions with positive imaginary part propagate in the positive Z direction, while those with negative imaginary part propagate in the negative Z direction.

For each value of k_z the corresponding electric field must satisfy Eq. (14a). Since the determinant of the coefficient matrix has been set to zero, the three equations in the three unknowns E_x , E_y , and E_z can be solved for two of the E field components in terms of the third one. The best strategy is to arrange the four values of k_z such that k_{z1} and k_{z2} are in the lower half of the complex plane (i.e., propagating downward), while k_{z3} and k_{z4} are in the upper half (i.e., propagating upward). Then, for beams with k_{z1} and k_{z3} , express E_y and E_z in terms of the corresponding E_x . Similarly, for beams with k_{z2} and k_{z4} , E_x and E_z must be related to E_y . Table I summarizes this strategy. The coefficients a_m and b_m in Table I are obtained from Eq. (14a) using $k_z = k_{zm}$. For each beam, the magnetic field components can be obtained from Eq. (14b). The results for the H field are also given in Table I.

The number of parameters that remain to be identified has now been reduced to four: E_{x1} , E_{y2} , E_{x3} , and E_{y4} . As will be shown in the next section, by matching the tangential field components at the various interfaces, it is possible to deter-

mine the values of these parameters for each layer in an arbitrary multilayer stack.

V. BOUNDARY CONDITIONS AT THE INTERFACE BETWEEN TWO LAYERS

Figure 1 shows a multilayer structure with interface planes at $Z = Z_1, Z_2, \dots$. The surface is at $Z = 0$, and the bottom layer (substrate) extends to infinity along the negative Z axis. We develop the boundary conditions for layer n whose upper and lower surfaces are at Z_{n-1} and Z_n , respectively. We shall use the plane $Z = Z_n$ as the reference plane for the four beams in layer n , so that each beam is described by the equation

$$\mathbf{E} = \mathbf{E}_0 \exp[i(k_x x + k_y y + k_z(z - z_n))]. \quad (21)$$

The reflectivity matrix R_n at the lower interface is defined as follows:

$$\begin{pmatrix} E_{x3} \\ E_{y4} \end{pmatrix} = R_n \begin{pmatrix} E_{x1} \\ E_{y2} \end{pmatrix} = \begin{pmatrix} r_{11} & r_{12} \\ r_{21} & r_{22} \end{pmatrix} \begin{pmatrix} E_{x1} \\ E_{y2} \end{pmatrix}. \quad (22)$$

The components of \mathbf{E} parallel to the plane at Z_n are thus given by

TABLE I. Relationship among the various components of \mathbf{E} and \mathbf{H} for plane waves in homogeneous media. The four beams described here have the same k_x and k_y .

	Beam 1	Beam 2	Beam 3	Beam 4
k_z	k_{z1} , lower half	k_{z2} , lower half	k_{z3} , upper half	k_{z4} , upper half
E_x	adjustable	$a_2 E_{y2}$	adjustable	$a_4 E_{y4}$
E_y	$a_1 E_{x1}$	adjustable	$a_3 E_{x3}$	adjustable
E_z	$b_1 E_{x1}$	$b_2 E_{y2}$	$b_3 E_{x3}$	$b_4 E_{y4}$
$k_0 H_x$	$(-k_{z1} a_1 + k_y b_1) E_{x1}$	$(-k_{z2} + k_y b_2) E_{y2}$	$(-k_{z3} a_3 + k_y b_3) E_{x3}$	$(-k_{z4} + k_y b_4) E_{y4}$
$k_0 H_y$	$(k_{z1} - k_x b_1) E_{x1}$	$(k_{z2} a_2 - k_x b_2) E_{y2}$	$(k_{z3} - k_x b_3) E_{x3}$	$(k_{z4} a_4 - k_x b_4) E_{y4}$
$k_0 H_z$	$(-k_y + k_x a_1) E_{x1}$	$(-k_y a_2 + k_x) E_{y2}$	$(-k_y + k_x a_3) E_{x3}$	$(-k_y a_4 + k_x) E_{y4}$

$$\begin{pmatrix} E_x \\ E_y \end{pmatrix}_{Z_n^+} = \sum_{m=1}^4 \begin{pmatrix} E_{xm} \\ E_{ym} \end{pmatrix} = \begin{pmatrix} 1 & a_2 \\ a_1 & 1 \end{pmatrix} \begin{pmatrix} E_{x1} \\ E_{y2} \end{pmatrix} + \begin{pmatrix} 1 & a_4 \\ a_3 & 1 \end{pmatrix} \begin{pmatrix} E_{x3} \\ E_{y4} \end{pmatrix},$$

where Z_n^+ stands for points just above Z_n . Defining the 2×2 matrices in the preceding equation as A_{12} and A_{34} , and with the aid of Eq. (22), the preceding equation is written

$$\begin{pmatrix} E_x \\ E_y \end{pmatrix}_{Z_n^+} = (A_{12} + A_{34}R)_n \begin{pmatrix} E_{x1} \\ E_{y2} \end{pmatrix}_n. \quad (23)$$

The tangential components of the magnetic field at Z_n^+ are

$$k_0 \begin{pmatrix} H_x \\ H_y \end{pmatrix}_{Z_n^+} = (B_{12} + B_{34}R)_n \begin{pmatrix} E_{x1} \\ E_{y2} \end{pmatrix}_n, \quad (24)$$

where

$$B_{12} = \begin{pmatrix} -k_{z1}a_1 + k_yb_1 & -k_{z2} + k_yb_2 \\ k_{z1} - k_xb_1 & k_{z2}a_2 - k_xb_2 \end{pmatrix}, \quad (25)$$

with a similar expression for B_{34} . The tangential components of \mathbf{E} and \mathbf{H} at the upper boundary of the layer n , namely, at Z_{n-1} , are

$$\begin{pmatrix} E_x \\ E_y \end{pmatrix}_{Z_{n-1}^-} = (A_{12}C_{12} + A_{34}C_{34}R)_n \begin{pmatrix} E_{x1} \\ E_{y2} \end{pmatrix}_n, \quad (26)$$

$$\begin{pmatrix} H_x \\ H_y \end{pmatrix}_{Z_{n-1}^-} = (B_{12}C_{12} + B_{34}C_{34}R)_n \begin{pmatrix} E_{x1} \\ E_{y2} \end{pmatrix}_n. \quad (27)$$

The matrix C_{12} in Eqs. (26)–(27) is

$$C_{12} = \begin{pmatrix} \exp(ik_{z1}d_n) & 0 \\ 0 & \exp(ik_{z2}d_n) \end{pmatrix}, \quad (28)$$

where d_n is the thickness of layer n . A similar expression describes C_{34} .

Continuity of tangential \mathbf{E} and \mathbf{H} at the interface $Z = Z_n$ implies that

$$\begin{aligned} (A_{12} + A_{34}R)_n \begin{pmatrix} E_{x1} \\ E_{y2} \end{pmatrix}_n \\ = (A_{12}C_{12} + A_{34}C_{34}R)_{n+1} \begin{pmatrix} E_{x1} \\ E_{y2} \end{pmatrix}_{n+1}, \end{aligned} \quad (29)$$

$$\begin{aligned} (B_{12} + B_{34}R)_n \begin{pmatrix} E_{x1} \\ E_{y2} \end{pmatrix}_n \\ = (B_{12}C_{12} + B_{34}C_{34}R)_{n+1} \begin{pmatrix} E_{x1} \\ E_{y2} \end{pmatrix}_{n+1}. \end{aligned} \quad (30)$$

Eliminating $\begin{pmatrix} E_{x1} \\ E_{y2} \end{pmatrix}_{n+1}$ from these equations and then equating the coefficients of $\begin{pmatrix} E_{x1} \\ E_{y2} \end{pmatrix}_n$, we obtain

$$\begin{aligned} (A_{12}C_{12} + A_{34}C_{34}R)_{n+1}^{-1} (A_{12} + A_{34}R)_n \\ = (B_{12}C_{12} + B_{34}C_{34}R)_{n+1}^{-1} (B_{12} + B_{34}R)_n. \end{aligned} \quad (31)$$

Let us define the matrix F_{n+1} as follows:

$$\begin{aligned} F_{n+1} &= (B_{12}C_{12} + B_{34}C_{34}R)_{n+1} \\ &\times (A_{12}C_{12} + A_{34}C_{34}R)_{n+1}^{-1}. \end{aligned} \quad (32)$$

Then, Eq. (31) is written

$$F_{n+1}(A_{12} + A_{34}R)_n = (B_{12} + B_{34}R)_n, \quad (33)$$

or, equivalently,

$$R_n = (F_{n+1}A_{34}^{(n)} - B_{34}^{(n)})^{-1}(B_{12}^{(n)} - F_{n+1}A_{12}^{(n)}). \quad (34)$$

Equation (34) gives R_n in terms of R_{n+1} . Realizing that R for the substrate is zero, one can calculate R_n iteratively, starting at the substrate and moving up the multilayer until surface reflectivity R_0 is obtained.

In practice, it is useful to express the state of polarization of the incident and reflected beams at the surface in terms of the P and S components of polarization. We now express the relationship between the P and S components of reflected and incident beams in terms of the matrix R_0 . Assuming that the incident \mathbf{k} vector has spherical coordinates (θ, ϕ) , one can write

$$\begin{pmatrix} E_x \\ E_y \end{pmatrix} = \begin{pmatrix} \cos \theta \cos \phi & -\sin \phi \\ \cos \theta \sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} E_p \\ E_s \end{pmatrix}. \quad (35)$$

Denote the coefficient matrix in Eq. (35) by P_{inc} , and define the reflectivity matrix R for the multilayer by the relation

$$\begin{pmatrix} E_p \\ E_s \end{pmatrix}_{\text{ref}} = R \begin{pmatrix} E_p \\ E_s \end{pmatrix}_{\text{inc}}. \quad (36)$$

Then,

$$R = P_{\text{inc}}^{-1}R_0P_{\text{inc}}. \quad (37)$$

Given R and the state of incident polarization, one can calculate the polarization state of the reflected beam from Eq. (36).

VI. TRANSMISSION OF PLANE WAVES THROUGH MULTILAYERS

Having found the matrices R_n from the recursive relation (34), we go back to Eq. (29) and rewrite it as follows:

$$\begin{pmatrix} E_{x1} \\ E_{y2} \end{pmatrix}_{n+1} = T_n \begin{pmatrix} E_{x1} \\ E_{y2} \end{pmatrix}_n, \quad (38)$$

where

$$T_n = (A_{12}C_{12} + A_{34}C_{34}R)_{n+1}^{-1} (A_{12} + A_{34}R)_n. \quad (39)$$

All the matrices on the right side of Eq. (39) are known; thus it is possible to calculate T_n for all layers. The total transmission matrix is then given by

$$\hat{T} = T_0T_1T_2 \cdots T_N. \quad (40)$$

\hat{T} relates the incident E_x and E_y to the transmitted E_x and E_y . To find the relation between the P and S components of polarization in the incident wave and those of the transmitted wave, we must first find the direction of transmission, namely, the angles (θ_s, ϕ_s) that describe the propagation direction in the substrate. Assuming that the substrate is transparent with refractive index n_{sub} , and that the medium of incidence (also transparent) has refractive index n_{inc} , one obtains the following relations from the Snell's law:

$$\sin \theta_s = \left(\frac{n_{\text{inc}}}{n_{\text{sub}}} \right) \sin \theta, \quad (41a)$$

$$\phi_s = \phi. \quad (41b)$$

If the right side of Eq. (41a) happens to be greater than unity, the wave in the substrate will be evanescent, and no power transmission to the substrate will occur. On the other hand, when Eq. (41a) has a real solution for θ_s , we define the matrix P_{sub} as

$$P_{\text{sub}} = \begin{pmatrix} \cos \theta_s \cos \phi & -\sin \phi \\ \cos \theta_s \sin \phi & \cos \phi \end{pmatrix}. \quad (42)$$

The total transmission matrix T (for the P and S components of polarization) is defined as

$$\begin{pmatrix} E_p \\ E_s \end{pmatrix}_{\text{trans}} = T \begin{pmatrix} E_p \\ E_s \end{pmatrix}_{\text{inc}}. \quad (43)$$

This matrix is related to \hat{T} of Eq. (40) by the relation

$$T = P_{\text{sub}}^{-1} \hat{T} P_{\text{inc}}. \quad (44)$$

Given T and the state of incident polarization, one can calculate the polarization state of the transmitted beam from Eq. (44).

VII. POWER COMPUTATION USING POYNTING'S THEOREM

The total electric field at a point (x, y, z) within the layer n is the sum of the four plane-wave amplitudes at that point, namely,

$$\tilde{E}(z) = \sum_{m=1}^4 \tilde{E}_0^{(m)} \exp[i(k_x x + k_y y + k_{zm}(z - z_n))]. \quad (45)$$

The magnetic field is also the sum of four magnetic amplitudes as follows:

$$\tilde{H}^T(z) = \frac{1}{k_0} \sum_{m=1}^4 \tilde{k}^{(m)} (\tilde{E}_0^{(m)})^T \times \exp[i(k_x x + k_y y + k_{zm}(z - z_n))]. \quad (46)$$

The values of \tilde{k} and \tilde{E}_0 for each layer can be calculated with the methods described in the previous sections. Therefore, the total electromagnetic field can be computed from Eqs. (45) and (46). The Poynting's theorem now yields

$$\begin{aligned} S &= \frac{1}{2} \text{Re}(\mathbf{E} \times \mathbf{H}^*) \\ &= \frac{1}{2k_0} \text{Re} \left(\sum_{m=1}^4 \sum_{m'=1}^4 \tilde{E}_0^{(m)} \tilde{k}^{*(m')} (\tilde{E}_0^{*(m')})^T \right. \\ &\quad \left. \times \exp[i(k_{zm} - k_{zm'}^*)(z - z_n)] \right). \end{aligned} \quad (47)$$

As expected, the Poynting vector is independent of x and y . The component of the Poynting vector \mathbf{S} along the Z axis, S_z , is the time-averaged rate of flow of energy per unit area in the Z direction. S_z is the quantity of interest in most calculations.

VIII. NUMERICAL RESULTS AND DISCUSSION

We now present numerical results based on the algorithm developed in the preceding sections. We study a quadrilayer magneto-optic device which has also been investigated by Balasubramanian, Marathay, and Macleod using

the 4×4 matrix technique.⁷ Our findings are in full agreement with the reported instances in Ref. 7; in addition, we have studied other situations that were not reported in that article, but are of sufficient potential value to warrant their presentation in this paper.

The quadrilayer consists of a glass substrate with refractive index $n_{\text{sub}} = 1.5$, coated with a reflecting (aluminum) layer of thickness 500 nm and complex refractive index $(n, k) = (2.75, 8.31)$. A quarter-wave-thick layer of SiO_x (thickness = 143.2 nm) with $(n, k) = (1.449, 0)$ separates the aluminum layer from the magneto-optic film which is 20 nm thick and the nonzero elements of its dielectric tensor are $\epsilon_{xx} = \epsilon_{yy} = \epsilon_{zz} = (-4.8984 + i19.415)$ and $\epsilon_{xy} = -\epsilon_{yx} = (0.4322 + i0.0058)$. The magnetic film is coated with another quarter-wave-thick layer of SiO_x , and the medium of incidence is air ($n_{\text{inc}} = 1$). The incident beam is plane with wavelength $\lambda = 830$ nm.

Figure 2(a) shows the various reflectivities as a function of the angle of incidence θ . (Only the magnitudes of the complex reflectivities are shown.) r_{pp} and r_{ps} are, respectively, the P and S components of the reflected beam when the incident polarization is P . Similarly, r_{sp} and r_{ss} correspond to S -polarized incident light. It is observed that r_{ps} and r_{sp} are identical. Note also that, unlike reflection from a single interface where r_{pp} usually shows a dip around Brewster's angle, the dip for this multilayer appears in the r_{ss} curve. Figure 2(b) shows the Kerr rotation angle and ellipticity as functions of θ for P -polarized incident light. The corresponding curves for S polarization are shown in Fig. 2(c). Even though the effective magneto-optic signals are the same in the two cases (i.e., $r_{ps} = r_{sp}$), the Kerr angle and ellipticity are totally different for P and S polarizations.

Figure 3 shows the magnitude of the Poynting vector S_z when a linearly polarized beam with unit power density illuminates the quadrilayer at normal incidence. This is a plot of the average power density that crosses planes parallel to the XY plane at various positions along the Z axis. The power density is constant in the transparent layers, but drops rather sharply in the absorbing layers, as expected.

Let us now consider the magneto-optic signal at normal incidence while the magnetization vector \mathbf{M} is being pulled out into the plane of the film, a situation that arises in optical measurements of magnetic anisotropy.^{9,10} For a linearly polarized, normally incident beam Figure 4 shows the calculated values of the Kerr rotation angle versus Θ_M , the angle between \mathbf{M} and the Z axis. It is found that the polar Kerr effect is proportional to $\cos \Theta_M$ and that this result is independent of the relative orientation of the magnetization vector \mathbf{M} and the polarization vector.

Finally, in Fig. 5 we show some manifestations of the longitudinal Kerr effect when the magnetic film in our quadrilayer becomes in-plane magnetized. (By definition, the longitudinal Kerr effect occurs when the magnetization \mathbf{M} lies in the plane of the film as well as in the plane of incidence.) Figure 5(a) shows the magnitudes of r_{sp} and r_{ps} , which are again identical, as was the case with the polar Kerr effect in Fig. 2(a). The largest magneto-optic signal in the longitudinal case, however, occurs at $\theta = 65^\circ$. Figure 5(b) shows plots of the Kerr rotation angle and ellipticity versus θ

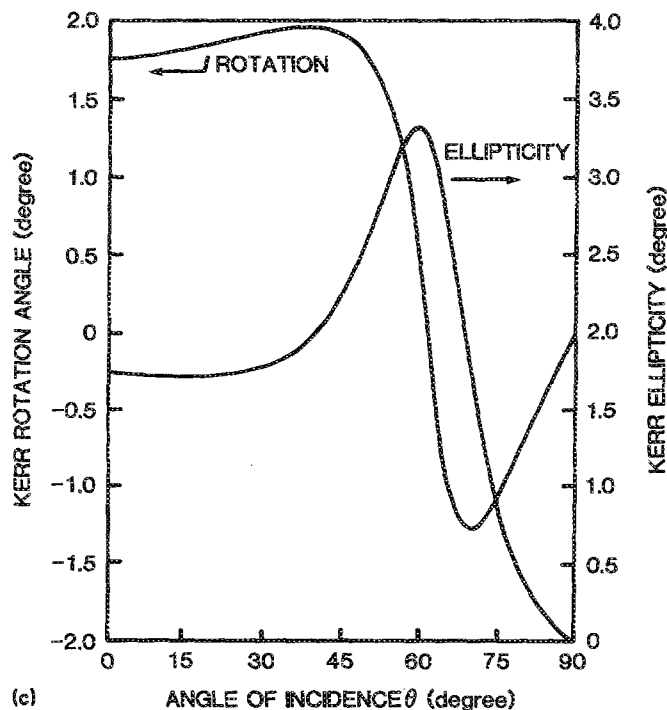
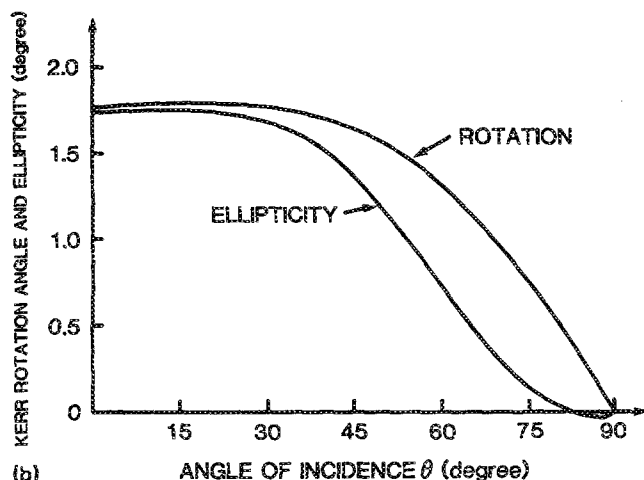
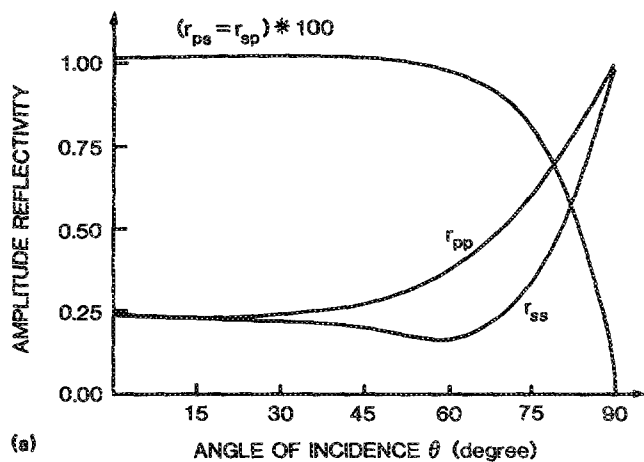


FIG. 2. Magneto-optic Kerr effect for a quadrilayer structure with perpendicular magnetization. (a) Magnitudes of r_{pp} , r_{ss} , r_{ps} , and r_{sp} vs angle of incidence θ . Note that $r_{ps} = r_{sp}$ and that the corresponding curve is magnified by a factor of 100. (b) Kerr rotation and ellipticity vs θ for P -polarized incident light. (c) Kerr rotation and ellipticity for S -polarized incident light. Note that the curves are plotted on different scales.

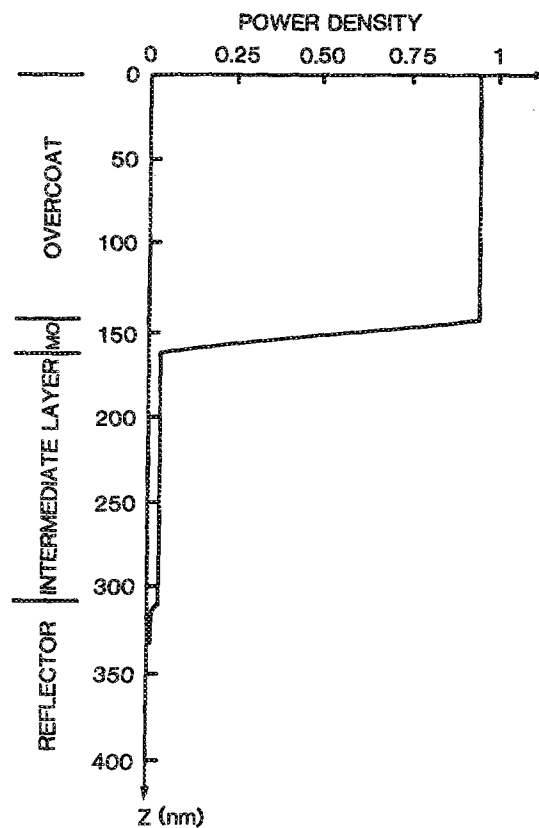


FIG. 3. Poynting vector throughout the quadrilayer with perpendicular magnetization. The normally incident beam is assumed to have unit power density and linear polarization. Note that the bulk of the absorption (about 91% of the total incident power) takes place in the magneto-optic (MO) layer, while the reflector absorbs only 3%. The remaining 6% of the incident power is reflected back towards the medium of incidence.

for P -polarized incident light. Similar results for S polarization are shown in Fig. 5(c). Notice that these values are smaller than the corresponding polar Kerr values in Fig. 2 by more than an order of magnitude.

IX. CONCLUDING REMARKS

In this paper we have presented a complete analysis of reflection, absorption, and transmission of plane waves at

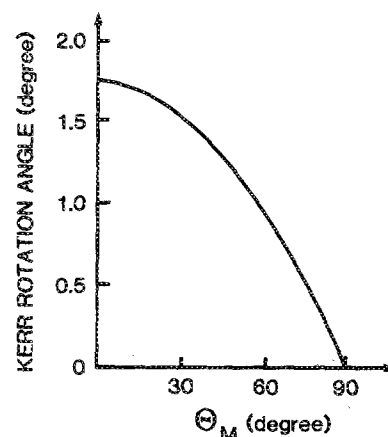


FIG. 4. The magneto-optic Kerr rotation angle vs Θ_M (the angle between the magnetization vector \mathbf{M} and the Z axis) for normally incident, linearly polarized light. The curve is proportional to a plot of $\cos \Theta_M$.

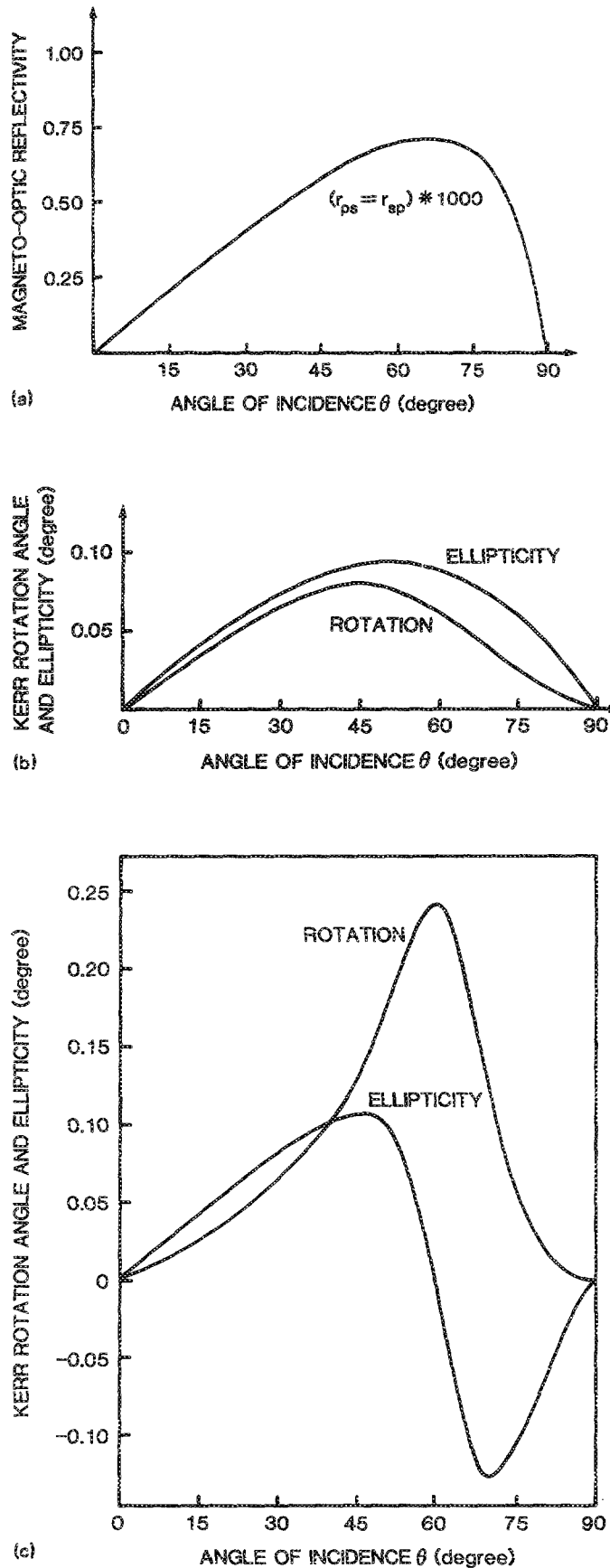


FIG. 5. Longitudinal magneto-optic Kerr effect for a quadrilayer structure with in-plane magnetization. (a) Magnitudes of r_{ps} and r_{sp} vs angle of incidence θ (note that $r_{ps} = r_{sp}$). The curve is magnified by a factor of 1000. (b) Polarization rotation and ellipticity vs θ for P-polarized incident light. (c) Polarization rotation and ellipticity vs θ for S-polarized incident light.

oblique incidence on multilayer structures. The considered multilayer is quite general in the sense that it can contain any number of layers, each with its own (arbitrary) dielectric tensor. Only 2×2 matrices are needed for the implementation of the proposed algorithm, which results in considerable simplification. A computer program was developed, and extensive comparisons of the numerical results with similar calculations based on the "standard" 4×4 matrix technique confirmed the validity of the new approach.

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APPENDIX A

In this Appendix we describe the transformation of dielectric tensors caused by a rotation of the coordinate system. Consider two Cartesian coordinate systems XYZ and $X'Y'Z'$, which share the origin O . In general three angles Θ , Φ , and Ψ specify the relative orientation of these systems. Θ and Φ are the spherical coordinates of Z' in the XYZ system. Imagine a rotation of $X'Y'Z'$ that takes place by keeping Φ constant while reducing Θ to zero. After this rotation, Z and Z' will be aligned, but the angle between X and X' will not necessarily be zero. This angle is denoted by Ψ and is measured counterclockwise from the positive X axis. Keeping Z and Z' aligned while rotating $X'Y'Z'$ through the angle Ψ will bring the two systems into complete alignment. (Ψ , Θ , and $\Phi - \Psi$ are the Euler angles.) It is thus possible to express the unit vectors $\hat{x}', \hat{y}', \hat{z}'$ in terms of the unit vectors $\hat{x}, \hat{y}, \hat{z}$ as follows:

$$\hat{x}' = a_{11}\hat{x} + a_{12}\hat{y} + a_{13}\hat{z}, \quad (A1)$$

$$\hat{y}' = a_{21}\hat{x} + a_{22}\hat{y} + a_{23}\hat{z}, \quad (A2)$$

$$\hat{z}' = a_{31}\hat{x} + a_{32}\hat{y} + a_{33}\hat{z}, \quad (A3)$$

where

$$a_{11} = \cos \Theta \cos \Phi \cos(\Phi - \Psi) + \sin \Phi \sin(\Phi - \Psi), \quad (A4)$$

$$a_{12} = \cos \Theta \sin \Phi \cos(\Phi - \Psi) - \cos \Phi \sin(\Phi - \Psi), \quad (A5)$$

$$a_{13} = -\sin \Theta \cos(\Phi - \Psi), \quad (A6)$$

$$a_{21} = \cos \Theta \cos \Phi \sin(\Phi - \Psi) - \sin \Phi \cos(\Phi - \Psi), \quad (A7)$$

$$a_{22} = \cos \Theta \sin \Phi \sin(\Phi - \Psi) + \cos \Phi \cos(\Phi - \Psi), \quad (A8)$$

$$a_{23} = -\sin \Theta \sin(\Phi - \Psi), \quad (A9)$$

$$a_{31} = \sin \Theta \cos \Phi, \quad (A10)$$

$$a_{32} = \sin \Theta \sin \Phi, \quad (A11)$$

$$a_{33} = \cos \Theta. \quad (A12)$$

Now, let \mathbf{E} and \mathbf{D} be the electric field vector and the

displacement vector in the XYZ coordinate system. The dielectric tensor $\tilde{\epsilon}$ in this system relates \mathbf{E} and \mathbf{D} as follows:

$$\mathbf{D} = \tilde{\epsilon}\mathbf{E}. \quad (\text{A13})$$

Similarly, in the $X'Y'Z'$ system, we have

$$\mathbf{D}' = \tilde{\epsilon}'\mathbf{E}', \quad (\text{A14})$$

but $\tilde{\mathbf{E}} = \tilde{\mathbf{E}}'P$ and $\tilde{\mathbf{D}} = \tilde{\mathbf{D}}'P$, where

$$P = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \quad (\text{A15})$$

is the rotation matrix between XYZ and $X'Y'Z'$. Therefore, Eqs. (A13) and (A14) yield

$$\tilde{\epsilon} = P^{-1}\tilde{\epsilon}'P. \quad (\text{A16})$$

Here, $P^T = P^{-1}$ because P is unitary. Equation (A16) shows the transformation of the dielectric tensor from the $X'Y'Z'$ system to the XYZ system.

As an example, consider a magneto-optic material with direction of magnetization along Z' . Then, in $X'Y'Z'$, the dielectric tensor is that of a polar Kerr material, i.e.,

$$\tilde{\epsilon}' = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & 0 \\ -\epsilon_{xy} & \epsilon_{xx} & 0 \\ 0 & 0 & \epsilon_{zz} \end{pmatrix}. \quad (\text{A17})$$

The rotation angles Θ and Φ specify the magnetization vector in the XYZ coordinate system, but Ψ is arbitrary. Using Eq. (A16), we find the dielectric tensor in the new XYZ coordinates as follows:

$$\tilde{\epsilon} = \begin{pmatrix} \epsilon_{xx} & \cos \Theta \epsilon_{xy} & -\sin \Theta \sin \Phi \epsilon_{xy} \\ -\cos \Theta \epsilon_{xy} & \epsilon_{xx} & \sin \Theta \cos \Phi \epsilon_{xy} \\ \sin \Theta \sin \Phi \epsilon_{xy} & -\sin \Theta \cos \Phi \epsilon_{xy} & \epsilon_{zz} \end{pmatrix}.$$

Note that the dielectric tensor in XYZ is independent of Ψ , and that it reduces to the familiar forms for longitudinal and transverse Kerr effects when $(\Theta = 90^\circ, \Phi = 0)$ and $(\Theta = 90^\circ, \Phi = 90^\circ)$, respectively.

APPENDIX B

In this Appendix we describe a method for computing the roots of the fourth-order equation

$$S^4 + AS^3 + BS^2 + CS + D = 0. \quad (\text{B1})$$

The first step is to calculate the roots of the following third-order polynomial equation:

$$8S^3 - 4BS^2 + 2(AC - 4D)S - [C^2 + D(A^2 - 4B)] = 0 \quad (\text{B2})$$

To this end, we define y_1, y_2, x_1 , and x_2 as follows:

$$y_i = \frac{AC}{12} - \frac{D}{3} - \frac{B^2}{36}, \quad (\text{B3})$$

$$y_2 = \left(\frac{B}{6}\right)^3 + \frac{A^2D + C^2}{16} - \frac{ABC}{48} - \frac{BD}{6}, \quad (\text{B4})$$

$$x_1 = (y_2 + \sqrt{y_1^3 + y_2^2})^{1/3}, \quad (\text{B5})$$

$$x_2 = (y_2 - \sqrt{y_1^3 + y_2^2})^{1/3}. \quad (\text{B6})$$

Since a complex number has three possible cube roots, x_1 and x_2 can each have three different values. Of these, the only acceptable ones are those that satisfy the equality

$$x_1x_2 + y_1 = 0. \quad (\text{B7})$$

It is not difficult to verify that only three pairs (x_1, x_2) satisfy Eq. (B7). The solutions of Eq. (B2) in terms of the acceptable pairs (x_1, x_2) are

$$S_0, S_1, S_2 = x_1 + x_2 + (B/6). \quad (\text{B8})$$

The next step is to choose one of the solutions of the third-order equation (say, S_0) and form two quadratic equations as follows:

$$S^2 + \left[\frac{A}{2} + \left(\frac{A^2}{4} - B + 2S_0\right)^{1/2}\right]S + [S_0 + (S_0^2 - D)^{1/2}] = 0. \quad (\text{B9})$$

$$S^2 + \left[\frac{A}{2} - \left(\frac{A^2}{4} - B + 2S_0\right)^{1/2}\right]S + [S_0 - (S_0^2 - D)^{1/2}] = 0. \quad (\text{B10})$$

The four roots of the original equation (B1) will be the roots of the quadratic equations (B9) and (B10). Because square roots of complex numbers appear in these equations, the question arises as to which root belongs in which equation. The answer is found by setting the product of Eqs. (B9) and (B10) equal to Eq. (B1). It turns out that the complex square roots must satisfy the relation

$$(S_0^2 - D)^{1/2} \left(\frac{A^2}{4} - B + 2S_0\right)^{1/2} = \frac{AS_0 - C}{2}. \quad (\text{B11})$$

Although the procedure described here is exact, in practice, numerical errors rapidly accumulate and give inaccurate results. To overcome this difficulty, we used an iterative technique that pushes the inexact solutions towards the correct roots. Since the analytic solutions obtained are fairly close to the desired roots, the algorithm does not have to be sophisticated. For instance, let \hat{S} be an estimated root of Eq. (B1). By moving along the slope of the polynomial function at \hat{S} , we find a better estimate $\hat{\hat{S}}$ as follows:

$$\hat{S} = \hat{S} - \frac{\hat{S}^4 + A\hat{S}^3 + B\hat{S}^2 + C\hat{S} + D}{4\hat{S}^3 + 3A\hat{S}^2 + 2B\hat{S} + C}. \quad (\text{B12})$$

By repeating the procedure described in Eq. (B12), we have been able to get arbitrarily close to the exact roots.

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