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FINAL REPORT

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ELLIPSOMETRIC MEASUREMENTS OF EPITAXIAL GaAs LAYERS ON A GaAs SUBSTRATE

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When this project was initially undertaken, we felt that we were well prepared and that it would not be too difficult to construct an ellipsometer for measurement of the thickness and uniformity of epitaxial layers of GaAs on a GaAs substrate of different refractive index. The state of the art at that time was that the mathematics for the analysis of ellipsometric data for conventional isotropic surfaces and films was well understood. While there is always room for interpretation of data, we felt that we were adequately prepared for this problem.

Upon subsequent reading of the most current literature (1) (some of which was not in print at the time this proposal was first submitted) and in discussions with some groups involved with epitaxial layers we were forced to the unfortunate conclusion that epitaxial thin films would probably be anisotropic in nature. The equations available for ellipsometry of isotropic surfaces and thin films are completely inadequate for the analysis of anisotropic surfaces and films and if the isotropic equations are used when the surface or film under study is not isotropic then the thickness of the film deduced from the use of these equations would have little, if any, relation to the true thickness of the film. We, therefore, undertook an extensive examination of the ellipsometric equations for anisotropic surfaces and thin films. Some of these results are summarized herein.

We let P, A, and Q represent the angular settings of the polarizer, analyzer, and compensator of an ellipsometer configured such that the compensator elliptically polarizes the beam prior to striking the sample surface.

These angles are measured counter-clockwise for an observer looking into the beam and are considered to be zero when the transmission axes of the polarizer and analyzer and the fast axis of the compensator are in the plane of incidence. If we assume for a moment that we are dealing with a compensator with quarter-wave retardation, then the polarization of light immediately before it strikes the surface of the sample is given by (2)

$$\begin{pmatrix} E_{p,i} \\ E_{s,i} \end{pmatrix} = \begin{pmatrix} \cos Q \cos(P - Q) + i \sin Q \sin(P - Q) \\ \sin Q \cos(P - Q) - i \cos Q \sin(P - Q) \end{pmatrix} \qquad (1)$$

where $E_{p,i}$ and $E_{s,i}$ is the Jones vector (3) which represents the polarization of the light immediately before it strikes the sample surface. Immediately after reflection from the surface, the polarization of light is given by the Jones vector.

$$\begin{pmatrix} E_{p,r} \\ E_{s,r} \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} \begin{pmatrix} E_{p,i} \\ E_{s,i} \end{pmatrix} \qquad (2)$$

Now, if we use the ellipsometer as a nulling instrument and we can find a setting of the analyzer which will extinguish all of the light reflected from the surface, then it is evident from Eq. (2) that the phases of the two components of the Jones vector for the reflected radiation must be equal, or equivalently, the imaginary part of the ratio of $E_{p,r}/E_{s,r}$ must be zero. Using this fact, a bit of tedious algebra demonstrates that there are two settings of polarizer which will yield a null. These are

$$P_1 = \tfrac{1}{2}\{\sin^{-1}(H/(F^2 + G^2)^{\frac{1}{2}}) - \tan^{-1}(G/F)\} + Q \tag{3a}$$

and

$$P_2 = \tfrac{1}{2}\{\pi - \sin^{-1}(H/(F^2 + G^2)^{\frac{1}{2}}) - \tan^{-1}(G/F)\} + Q \tag{3b}$$

Here F, G, and H are related to the elements of the matrix R by

$$\begin{aligned} F &= \mathrm{Re}(R_{11} R_{22}^*) - \mathrm{Re}(R_{12}R_{21}^*), \\ G &= \mathrm{Im}(R_{12}R_{21}^* + R_{11}R_{22}^*) \sin 2Q \\ &\quad + \mathrm{IM}(R_{11}R_{21}^* - R_{12}R_{22}^*) \cos 2Q, \end{aligned} \tag{4}$$

and

$$H = -\mathrm{Im}(R_{11}R_{21}^*) - \mathrm{Im}\,(R_{12}R_{22}^*);$$

where '*' denotes complex congigate.

Each of these values can be used in turn to calculate an associated setting of the analyzer which will extinguish this polarized light.

The equation which applies here is

$$\tan A = -\frac{R_{11}\, E_{p,i} + R_{12}\, E_{s,i}}{R_{21}\, E_{p,i} + R_{22}\, E_{s,i}} \tag{5}$$

which gives two values for A, one for each of the values of P in Eqs. (3).

It is convenient here to mention the fact that the equations of ellipsometry applied to isotropic systems have the off-diagonal elements of the matrix R in Eq. (2) equal to zero. In fact, for an isotropic surface or any combination of isotropic surfaces and films one need not write out Eq. (2) in the form given, since in isotropic cases one can calculate reflection coefficients, and a matrix formulation is not necessary.

The problem is now reduced to the calculation or determination of the matrix R for an anisotropic surface or a combination of anisotropic surfaces and films. This is a problem of considerable difficulty. We initially approached the problem by considering a situation similar to that depicted in Figure 1. This figure represents polarized light incident on, and reflected from, a biaxial substrate with principal values of the refractive index n_x, n_y, and n_z. Our approach was to note that there will be two independent polarizations which propagate through the anisotropic medium. From Snell's law, plus Fresnel's equation for light propagating through a biaxial medium, we were able to find numerical solutions for the two angles of refraction and subsequently for the two refractive indices which correspond to these two angles. Given these quantities, it is a relatively simple matter (4) to find the direction numbers associated with the electric and magnetic fields in the anisotropic medium. Finally, boundary conditions require that the tangential components of the electric and magnetic fields be continuous across the interface. The fact that these boundary conditions must hold gives four linear equations in six unknowns, and this set of equations, written in matrix form, can be reduced to a set of two equations and magnetic fields for the transmitted beams. Thus, the matrix R can be calculated for this particular single surface, provided the optical constants of the surface are known.

We are compelled to point out here that this method of calculating R, even for a single surface, requires that the surface be biaxial. The equations used for finding direction numbers of the electric and magnetic fields become singular if the material under consideration is not biaxial. Any generalization of this method to thin films would require that the thin films be biaxial. Therefore, another method for calculating the reflection matrix was sought.

A recent development in the calculation of the optical properties of liquid crystals under certain conditions ultimately provides what is probably the most general and economical method of calculating the reflection matrix for an arbitrary, but known, surface or combination of arbitrary surfaces and films. This method has been best described by Berreman (5). This formalism involves writing Maxwell's equations in 6 x 6 matrix form and, by applying appropriate boundary conditions at proper points in the development of the formalism, reducing the equation for the propagation of light through an anisotropic medium to an eigenvalue problem using a 4 x 4 matrix.

It would not be in order here to extensively discuss this formalism since it has been presented succinctly and accurately by Berreman. However, we should point out that it does eliminate the problem of singularities mentioned above and it generalizes quite easily to the ellipsometry of anisotropic thin films.

A computer program employing this formalism has been written for the analysis of ellipsometric data for anisotropic films. This program was debugged and ran successfully approximately four weeks ago. Examination of the output of the program using artificial optical constants shows that ellipsometry is capable of measuring the thickness of an anisotropic film accurately provided that data are taken at several angles of incidence and also at several orientations of the sample relative to the plane of incidence. We now believe that we have the problem of ellipsometry of anisotropic surfaces and films solved, at least in principle.

The construction of the infrared ellipsometer has not proceeded quite as we had hoped, partly because we were preoccupied with the problems associated with the interpretation of ellipsometric data for anisotropic systems. The polarizer and analyzer of the infrared ellipsometer were mounted and tested and these components proved adequate. We did experience some unexpected difficulties in aligning the ellipsometer as well as with the various infrared detectors purchased. However, we shall continue our efforts to develop an infrared ellipsometer. When we succeed this instrument will be made available to NASA.

We intend to incorporate the information we have assembled and discussed in this report as part of a paper which we will submit to the Journal of the Optical Society of America within the next month. The publication of this paper represents a significant step forward in the development of ellipsometry as a tool for the study of surfaces and thin films.

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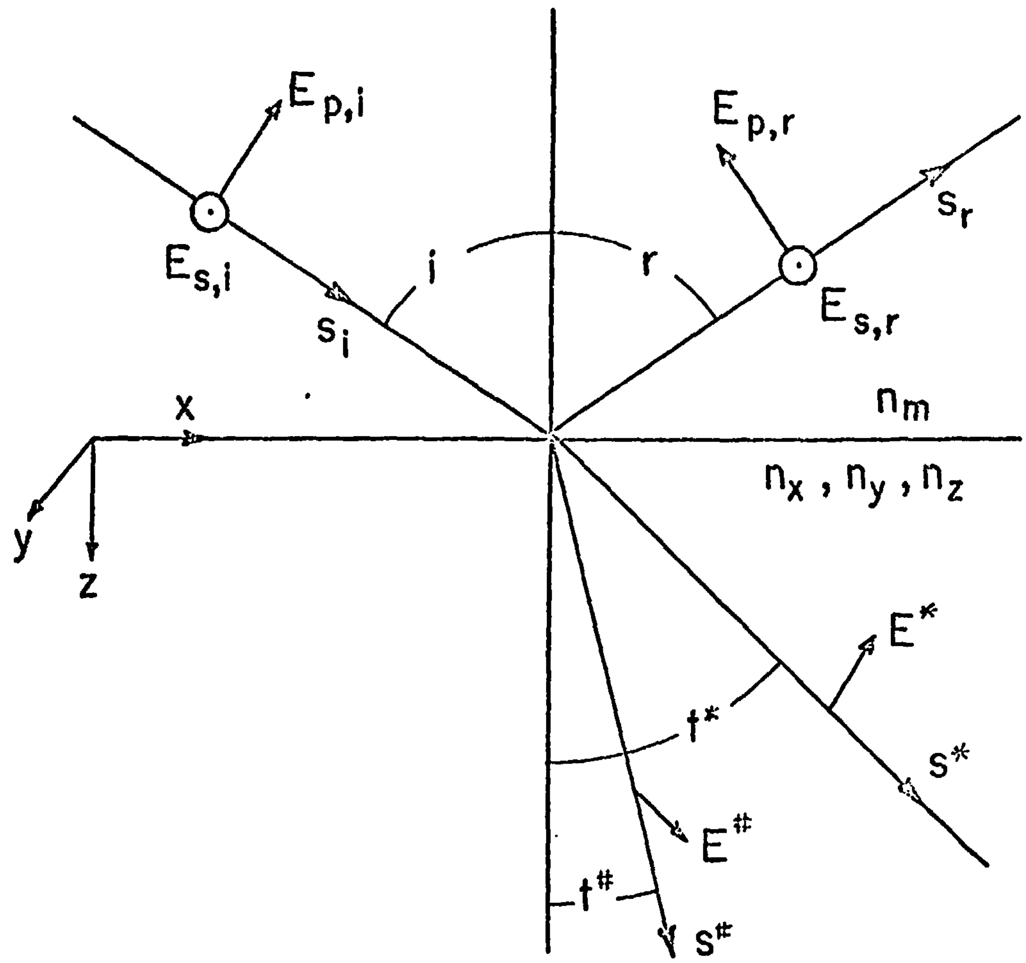

Figure 1