Constraint on the optical constants of a film-substrate system for operation as an external-reflection retarder at a given angle of incidence

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Constraint on the optical constants of a film-substrate system for operation as an external-reflection retarder at a given angle of incidence

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Given a transparent film of refractive index $n_1$ on an absorbing substrate of complex refractive index $n_2 - jk_2$, we examine the constraint on $n_1$, $n_2$, and $k_2$ such that the film-substrate system acts as an external-reflection retarder of specified retardance $\Delta$ at a specified angle of incidence $\phi$. The constraint, which takes the form $f(n_1, n_2, k_2; \phi, \Delta) = 0$, is portrayed graphically by equi-$n_1$ contours in the $n_2, k_2$ plane at $\phi = 45^\circ$ and for $\Delta = \pm 90^\circ$ and $\pm 180^\circ$, corresponding to quarterwave and halfwave retarders (QWR and HWR), respectively. The required film thickness as a fraction of the film thickness period and the polarization-independent device reflectance $R$ are also studied graphically as functions of the optical constants. It is found that as $n_2 \to 0$, $R \to 1$, so that a metal substrate such as Ag is best suited for high-reflectance QWR ($\phi > 45^\circ$) and HWR ($\phi \leq 45^\circ$). However, films that achieve QWR at $k < 45^\circ$ are excellent antireflection coatings of the underlying dielectric, semiconductor, or metallic substrate.

I. Introduction

It has been shown$^{1-3}$ that, for a given optically isotropic system of a transparent thin film on an absorbing (or transparent) substrate, the $p$- and $s$-polarized components of incident monochromatic light can be reflected with equal attenuations and with a specified differential phase shift $\Delta$; hence the system functions as an external-reflection retarder. This is achieved simply by selecting the proper angle of incidence $\phi$ and film thickness $d$.

This paper deals with such a film-substrate reflection retarder from a different and global point of view. Specifically, we consider the constraint on the optical constants of the film and substrate such that a specified retardance $\Delta$ is achieved at a given $\phi$. The required film thickness as a fraction of the film thickness period, $\zeta$, and the polarization-independent device reflectance (insertion loss), $R$, are also computed. The results are presented graphically over a wide range of optical constants, without reference to a specific wavelength, for generality.

To keep the paper within reasonable bounds, we consider only two angles of incidence, $\phi = 45$, $70^\circ$ and two retardances $\Delta = \pm 90$, $\pm 180^\circ$, corresponding to quarterwave and halfwave retarders (QWR and HWR), respectively. Results at other $\phi, \Delta$ were obtained but are not given here. This paper also contains tables that give the characteristics of high-reflectance QWRs and HWRs using a thin-film-coated Ag substrate for several visible and near-IR wavelengths.

II. Basic Relations

The complex $p$- and $s$-reflection coefficients of a film-substrate system are$^4$

$$R_p = \frac{(r_{01} + r_{13}X)/(1 + r_{01}r_{13}X)}{(1 + r_{01}r_{13}X)}, \quad p = p, s,$$  (1)

and their ratio

$$\rho = R_p/R_s$$  (2)

is given by

$$\rho = \frac{(A + BX + CX^2)}{(D + EX + FX^2)},$$  (3)

where

$$X = \exp(-j2\pi\zeta),$$  (4)

$$A = r_{01}r_{13}, \quad B = r_{12} + r_{01}r_{13}r_{12}, \quad C = r_{01}r_{12}r_{13},$$

$$D = r_{01}, \quad E = r_{12} + r_{01}r_{13}r_{12}, \quad F = r_{01}r_{12}r_{13},$$  (5)

In Eq. (4), $\zeta$ is the normalized film thickness,

$$\zeta = d/D_\phi,$$  (6)

where

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Equation (10) follows from Eqs. (4), (6), and (7), where we assume $n_0$, $N_1$ (real), and $N_2$ (complex) are the refractive indices of the medium of incidence (0), film (1), and substrate (2), respectively. In Eqs. (1) and (5) $r_{ij}$ denotes the (complex-amplitude) Fresnel reflection coefficient of the $ij$ interface for the $v$ polarization. Such coefficients are given in standard optics texts.

For simplicity, and without loss of generality, we define relative film and substrate refractive indices as follows:

$$\frac{N_1}{N_0} = n_1, \quad \frac{N_2}{N_0} = n_2 - jk_2.$$  \hspace{1cm} (8)

Often the medium of incidence is air ($N_0 = 1$) and the distinction between the relative and actual refractive indices disappears.

The constraint on $n_1,n_2,k_2$ such that a given $\rho$ is realized at a given $\phi$ is obtained by solving Eq. (3) for $X$,

$$X = -\frac{D_0}{2} (1 - N_0^2 \sin^2 \phi)^{-1/2}.$$  \hspace{1cm} (7)

Equation (10) follows from Eqs. (4), (6), and (7), where we assume $N_1 > N_0 \sin \phi$, i.e., the absence of total internal reflection at the incidence medium–film interface.

Equation (10), where $X$ is given by the right-hand side of Eq. (9), represents the desired constraint on the optical constants $n_1$, $n_2$, and $k_2$ for given $\phi$ and $\rho$. It can be put in the functional form

$$f(n_1, n_2, \phi, \rho) = 0.$$  \hspace{1cm} (11)

With $\phi$ and $\rho$ specified, Eq. (11) is represented graphically by contours of constant film refractive index ($n_1 = \text{constant}$) in the $n_2,k_2$ plane. To generate one such contour, $n_1$ is assigned a fixed value, $n_2$ is scanned over a certain range, and for each $n_2$ Eq. (11) is solved for $k_2$ as its only unknown by numerical iteration. Only positive $k_2$ values are sought and two roots may in general be obtained that correspond to the double roots of $X$ (the $\pm$ signs) in Eq. (9). That a proper root has been found is verified by substituting $n_1, n_2, k_2, \rho, \phi$ into the right-hand side of Eq. (9) and checking that

$$|X| - 1 < 10^{-6}.$$  \hspace{1cm} (12)

The required normalized film thickness $\xi$ is obtained from complex $X$ via Eq. (4),

$$\xi = -\arg(X)/2\pi.$$  \hspace{1cm} (13)

The proper multiple of $2\pi$ is added to $\arg X$, so that $\xi$ is in the reduced range

$$0 < \xi < 1.$$  \hspace{1cm} (14)

The device reflectance is computed from Eq. (1),

$$R_v = |R_v|^2,$$  \hspace{1cm} (15)

and is ascertained to be the same for the $v = \rho$ and $v = s$ polarizations.

As indicated in Sec. I, we limit ourselves to film–substrate external-reflection quarterwave and halfwave retarders, $\rho = \pm j$ (QWR) and $\rho = -1$ (HWR) at two angles of incidence $\phi = 70^\circ$ and $\phi = 45^\circ$. Only $n_1$ values $>1$ are taken (i.e., the film is assumed to be more optically dense than the medium of incidence), and, with one exception, we restrict ourselves to a square of side 10 in the $n_2,k_2$ plane (i.e., $0 < n_2 \leq 10, 0 < k_2 < 10$). This corresponds to most substrate materials in the NUV–VIS–NIR spectral range. The $n_1$ values are selected to generate reasonably well-spaced equi-$n_1$ contours in the $n_2,k_2$ plane.

III. Quarterwave and Halfwave Retarders at $70^\circ$

Angle of Incidence

A. $\rho = +j$ QWR

Let us first consider $\rho = j$, which corresponds to a QWR with $\rho$ fast axis (i.e., parallel to the plane of incidence) at $\phi = 70^\circ$. Figure 1 shows a family of ten equi-$n_1$ contours in the $n_2,k_2$ plane, for $n_1$ values (marked by each curve) from 1.25 to 1.70 in equal steps (marked by each curve) from 1.25 to 1.70 in equal steps of 0.05. This is the only case where we allowed $n_2$ and $k_2$ to assume values $>10$. (The extended rectangular range $0 < n_2 \leq 10, 0 < k_2 \leq 50$ covers the optical constants of metals beyond the near and into the middle IR spectrum.) Refractive indices in the range 1.25 to 1.70 are realized with many film–substrate combinations at different wavelengths, with light incident from air or vacuum.

Figure 2 shows the variation of the normalized film thickness $\xi$ (required to achieve QWR at $\phi = 70^\circ$) along...
Fig. 2. Film thickness as a fraction of the film thickness period \( \xi \), required to achieve \( \rho = j \) QWR at \( \phi = 70^\circ \), plotted as a function of \( n_2 \) at constant \( n_1 \) (marked by each curve). \( n_1, n_2 \) specify a particular film–substrate QWR completely, because \( k_2 \) can be deduced from Fig. 1. The contour \( AB \) describes the variation of \( \xi \) with \( n_2 \) along the similarly marked \( n_1 = 1.6 \) contour in Fig. 1.

Fig. 3. Polarization-independent reflectance \( R \) of film–substrate \( \rho = j \) QWRs at \( \phi = 70^\circ \) plotted as a function of \( n_2 \) at constant \( n_1 \) (marked by each curve) along the equi-\( n_1 \) contours of Fig. 1.

Fig. 4. Same as Fig. 1 except that \( \rho = -j \) (QWR with \( s \) fast axis).

each and every one of the \( n_1 = \) constant contours of Fig. 1. The \( n_1 = 1.6 \) contour has been marked by its end points \( A \) and \( B \) in Figs. 1 and 2 [and 3] and by an arrow pointing from \( A \) to \( B \). In Fig. 1 points \( A \) and \( B \) represent the limiting states of the substrate being perfectly metallic (\( n_2 = 0 \)) and perfectly dielectric (\( k_2 = 0 \)), respectively. As a point moves along the \( n_1 = 1.6 \) contour from \( A \) to \( B \) in Fig. 1, \( \xi \) varies (increases monotonically) from \( \xi_A \) to \( \xi_B \) along the corresponding \( (n_1 = 1.6) \) contour of Fig. 2. It is significant to note that \( \xi \) occupies only a narrow range, \( 0.275 < \xi < 0.375 \), for all \( \rho = j \) QWRs at \( \phi = 70^\circ \), represented in Fig. 1.

Figure 3 describes the variation with \( n_2 \) of the reflectance \( R \) (which is the same for the \( p \) and \( s \) polarizations) along each and every \( n_1 = \) constant contour of Fig. 1. In Figs. 2 and 3 an \( (n_1, n_2) \) pair defines one device completely, because \( k_2 \) can be obtained from Fig. 1. It is evident from Fig. 3 that \( R = 1 \) when \( n_2 = 0 \), hence an ideal, lossless (total-reflection) QWR is obtained. This most desirable characteristic can be very nearly achieved by using a metallic substrate such as Ag\(^0\) in the visible and near IR, as will be demonstrated in Sec. V. Movement along any equi-\( n_1 \) contour in Fig. 1 from the \( n_2 = 0 \) point (such as \( A \)) to the \( k_2 = 0 \) point (such as \( B \)) is accompanied by a monotonic decrease of the reflectance \( R \) from a maximum of 1 to a certain minimum \( R_m \) that depends on \( n_1 \), \( R_m \), hence the device reflectance in general, increases as \( n_1 \) is increased. It is also evident from Fig. 1 that higher values of the film refractive index \( n_1 \) are associated with higher substrate optical constants \( n_2, k_2 \), or higher \( (n_2^2 + k_2^2)^{1/2} \) in particular.

B. \( \rho = -j \) QWR

The case of \( \rho = -j \) represents a QWR with the fast axis in the \( s \) direction (perpendicular to the plane of incidence). Again we take \( \phi = 70^\circ \).

Figure 4 shows a family of equi-\( n_1 \) contours, corresponding to \( n_1 \) from 1.3 to 2.3 in equal steps of 0.1, in the \( n_2, k_2 \) plane. (From now on, \( n_2 \) and \( k_2 \) are limited to a maximum of 10.) All curves appear to emanate from the point \( n_2 = 1, k_2 = 0 \). Contours that correspond to \( n_1 \leq 1.7 \) terminate on the \( n_2 \) axis \( (k_2 = 0) \), whereas those for \( n_1 \geq 1.8 \) terminate on the \( k_2 \) axis \( (n_2 = 0) \). Again with an air or vacuum ambient this range of \( n_1 \) corresponds to a variety of suitable thin-film coating materials,\(^7\)\(^8\) so that \( \rho = -j \) QWRs are readily realizable.
Comparing Figs. 3 and 6 we find that, for films of $n_1 < 1.7$, reflectance is generally lower for the $\rho = -j$ QWR than it is for the $\rho = j$ QWR at the same ($\phi = 70^\circ$) angle of incidence. (Of course, the constraint on $n_1, n_2, k_2$ to achieve $\rho = -1$ at $\phi = 70^\circ$ is very sensitive to small changes of $n_1$ ($\Delta n_1 = 0.001$) around $n_1 = 1$. All curves emanate from the point $n_2 = 1$, $k_2 = 0$ and terminate either on the $n_2$ or the $k_2$ axis. Data for $n_1 < 1.3$ are meaningful only if a dense medium of incidence ($N_0 > 1$) is assumed (which may serve as the substrate if it is a solid phase). For light incident from vacuum or air, HWRs at $\phi = 70^\circ$ require films with $n_1 > 1.3$ on substrates with $n_2 < 1$ and $k_2 < 2$. The latter optical constants are typical of some metals in the UV.

Figures 8 and 9 show the variation of $\xi$ and $R$, respectively, with $n_2$ along each and every $n_1$ constant contour in Fig. 7. In Fig. 8 it appears that $\xi \to 0$ as $n_2 \to 1$. In Fig. 9 we see that, for $n_1 > 1.16$, $R = 1$ at $n_2 = 0$; this represents totally reflecting HWRs at $\phi = 70^\circ$. Note also that, for $n_1 \geq 1.3$, $R$ decreases steeply from 1 to 0 as $n_2$ increases from 0 to 1.

IV. Quarterwave and Halfwave Retarders at 45° Angle of Incidence

We now present and briefly discuss the results obtained when the procedure of Sec. II is applied with $\rho = j$ (QWR, $p$ fast axis), $\rho = -j$ (QWR, $s$ fast axis), and $\rho = -1$ (HWR) at $\phi = 45^\circ$ as another (perhaps more attractive) angle of incidence. The $\rho = j$ QWR is illustrated by Figs. 10, 11, and 12 which show the equi-$n_1$ contours in the $n_2, k_2$ plane, $\xi$ vs $n_2$ at constant $n_1$, and $R$ vs $n_2$ at constant $n_1$, respectively. The $\rho = -j$ QWR is represented by Figs. 13–15 in the same fashion.
These graphical results should now be self-explanatory in view of the 70° cases already discussed in Sec. III.

The most remarkable observation is that the reflectance \( R \), which is the same for the \( p \) and \( s \) (hence for all incident) polarizations, becomes very low (<7% in all cases). Consequently, the film that produces QWR is also an efficient antireflection coating at 45°, especially with \( n_1 < 2 \). This is portrayed by Figs. 12 and 15, which also indicate that lower reflectances accompany the \(-90°\) rather than the \(+90°\) retardance. What adds to the importance of these (and other) results is the global way in which a vast range of substrates and films is considered.

Finally, Figs. 16–18 illustrate HWRs (\( \rho = -1 \)) at \( \phi = 45° \). Compared with HWRs that we obtained earlier at \( \phi = 70° \) (Figs. 7–9), HWRs at \( \phi = 45° \) can be constructed from many combinations of films and substrates with refractive indices covering wide and realistic ranges and with the medium of incidence conveniently being air or vacuum.

Figure 17 shows that the normalized film thickness \( \xi \) required to achieve \( \rho = -1 \) at \( \phi = 45° \) is between 0 and 0.5.

In Fig. 18 we observe that high reflectance \( \mathcal{R} \) (approaching 100%) is again achieved when \( n_2 \ll 1 \). This is further demonstrated in Sec. V which provides data on HWRs at \( \phi = 45° \) using a Ag substrate at several wavelengths in the visible and near IR.
V. Quarterwave and Halfwave Retarders Using a Ag Substrate Coated by a Dielectric Thin Film

So far we have kept general our discussion of the constraint on \( n_1, n_2, k_2 \) such that a film–substrate system functions as an external-reflection retarder with specified retardance at a specified angle of incidence. Figures 1–18 are applicable to a wide range of ambient, film, and substrate materials and over a wide range of wavelengths. However, we have already remarked in Secs. III and IV that a high-reflectance metal substrate, such as Ag, would be ideally suited for high-reflectance devices. In this section we present specific examples of Ag-based QWRs and HWRs in the visible and near IR, and we examine their sensitivity to small errors of incidence angle and of film refractive index and thickness. The assumed optical constants \( n_2, k_2 \) of Ag are those cited in Ref. 9.

To obtain the required film characteristics, the sequence of calculations is altered slightly from what we indicated in the discussion following Eq. (11). Here the substrate optical constants \( n_2, k_2 \) (and \( \rho, \phi \)) are specified...
and Eq. (11) is solved for $n_1$ as its only unknown by iteration. Subsequently, the normalized and actual film thicknesses ($\zeta$, $d$) and the device reflectance ($R$) are computed as before.

Table I gives the characteristics of $p = +j$ QWRs for $\phi = 70^\circ$ at several wavelengths. The required refractive index $n_1$, normalized thickness $\zeta$, and actual thickness $d$ (nm) of the thin dielectric film on Ag are all listed. The polarization-independent device reflectance, which appears in the last column of Table I, exceeds 97% at all wavelengths $\geq$ 500 nm.

We have also examined the effect of small errors of (a) angle of incidence ($\Delta \phi = 0.1^\circ$), (b) film refractive index ($\Delta n_1 = 0.01$), and (c) film thickness ($\Delta d = 1$ nm) on the device performance as represented by the ratio $\rho$ of the complex $p$- and $s$-reflection coefficients. Specifically, we have calculated the magnitude error $|\rho| - 1$, and phase error $\text{arg}(\rho) - \Delta_{\text{nom}}$, where $\Delta_{\text{nom}}$ is the nominal retardance in degrees ($\Delta_{\text{nom}} = 90^\circ$ for the $p = +j$ QWR, and $\Delta_{\text{nom}} = \pm 180^\circ$ for the HWR). The results are listed in Table II. All errors fall within rea-

Table I. Characteristics of Quarterwave Retarders ($QWR$, $p = +j$) at $70^\circ$ Angle of Incidence Using a Dielectric Thin Film on a Ag Substrate at Several Wavelengths

<table>
<thead>
<tr>
<th>$\lambda$ (nm)</th>
<th>$n_2$</th>
<th>$k_2$</th>
<th>$n_1$</th>
<th>$\zeta$</th>
<th>$d$ (nm)</th>
<th>$R$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>400</td>
<td>0.075</td>
<td>1.93</td>
<td>1.219154</td>
<td>0.277011</td>
<td>71.33</td>
<td>94.09</td>
</tr>
<tr>
<td>500</td>
<td>0.050</td>
<td>2.87</td>
<td>1.291322</td>
<td>0.278983</td>
<td>78.72</td>
<td>97.72</td>
</tr>
<tr>
<td>600</td>
<td>0.060</td>
<td>3.75</td>
<td>1.349785</td>
<td>0.285499</td>
<td>88.39</td>
<td>98.20</td>
</tr>
<tr>
<td>700</td>
<td>0.075</td>
<td>4.62</td>
<td>1.396728</td>
<td>0.292587</td>
<td>99.10</td>
<td>98.72</td>
</tr>
<tr>
<td>800</td>
<td>0.090</td>
<td>5.45</td>
<td>1.433078</td>
<td>0.308224</td>
<td>110.48</td>
<td>98.55</td>
</tr>
<tr>
<td>950</td>
<td>0.110</td>
<td>6.56</td>
<td>1.471883</td>
<td>0.306027</td>
<td>128.32</td>
<td>98.72</td>
</tr>
<tr>
<td>2000</td>
<td>0.480</td>
<td>14.40</td>
<td>1.601287</td>
<td>0.322617</td>
<td>256.69</td>
<td>98.69</td>
</tr>
</tbody>
</table>

$^a$ $\lambda$ is the wavelength of light. $n_2, k_2$ are the real and imaginary parts of the Ag substrate complex refractive index (from Ref. 9). $n_1$ is the film refractive index obtained by solving Eq. (11) with $p = +j$ and $\phi = 70^\circ$. $\zeta$ and $d$ are the normalized and actual (least) film thicknesses, respectively, and $R$ is the polarization-independent reflectance of the QWR.
The characteristics of QWRs operating at the (desirable) incidence angle of 45° and at the same wavelengths selected in Table I. Note that $R > 96\%$ for all $\lambda \geq 500$ nm, indicating an efficient device. The magnitude and phase errors that result from $\Delta \phi = 0.1^\circ$ angle-of-incidence error, $\Delta n_1 = 0.01$ film-refractive-index error, and $\Delta d = 1$ nm film-thickness error are all listed in Table IV. Again, the errors fall within reasonable limits so that good, but not very stringent, control on film deposition is required. Particularly noticeable in Table IV is the negligible sensitivity as a fraction of the film thickness period and the polarization-independent device reflectance for the HWR.

A wide selection of thin-film coating materials is availableootnote{Ref. 3} with the requisite refractive indices listed in the fourth column of Tables I and III.

### VI. Summary

Comprehensive results have been presented of film–substrate QWR and HWR at 70° and 45° angles of incidence. The constraint on the optical constants of the film ($n_1$) and substrate ($n_2$, $k_2$), such that a given ratio $\rho$ of the complex $n$ and $s$ reflection is achieved at a given angle of incidence, is elucidated with graphs showing equi-$n_1$ contours in the $n_2$, $k_2$ plane for $\rho = -j$ (QWR) and $\rho = -1$ (HWR). The required film thickness, as a fraction of the film thickness period and the polarization-independent device reflectance, are also studied graphically as functions of the optical constants. Films that achieve QWR at 45° angle of incidence are excellent antireflection coatings for the underlying dielectric, semiconducting, or metallic substrate.

The characteristics of high-reflectance QWRs (at $\phi = 70^\circ$) and HWRs (at $\phi = 45^\circ$) using a Ag substrate coated by a dielectric thin film at several wavelengths in the visible and near IR are listed in Tables I and III. The sensitivity of these designs to errors of angle of incidence is elucidated with graphs showing equi-$n_1$ contours in the $n_2$, $k_2$ plane for $\rho = -j$ (QWR) and $\rho = -1$ (HWR). The required film thickness, as a fraction of the film thickness period and the polarization-independent device reflectance, are also studied graphically as functions of the optical constants. Films that achieve QWR at 45° angle of incidence are excellent antireflection coatings for the underlying dielectric, semiconducting, or metallic substrate.

A wide selection of thin-film coating materials is availableootnote{Ref. 3} with the requisite refractive indices listed in the fourth column of Tables I and III.
cidence, film refractive index, and film thickness has been determined and the results appear in Tables II and IV.

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References
4. See, for example, R. M. A. Azzam and N. M. Bashara, Ellipsometry and Polarized Light (North-Holland, Amsterdam, 1977), Sec. 4.3.
6. If the incident light is linearly polarized at 45° azimuth with respect to the plane of incidence, so that the p and s components of the incident electric vector are equal and inphase, the p component of the electric vector of the reflected light will lead the s component by 90°, when p = j, hence the identification of the p direction as the fast axis. The $\exp(j\omega t)$ harmonic time dependence is assumed.

Meetings Schedule

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21–24 May 1985 CLEO 85, OSA/IEEE CONFERENCE ON LASERS AND ELECTROOPTICS, Baltimore Information: Meetings Department at OSA

10–13 June 1985 INTERNATIONAL LENS DESIGN CONFERENCE, Cherry Hill Information: Meetings Department at OSA

10–14 June 1985 SPRING CONFERENCE ON APPLIED OPTICS, Cherry Hill Information: Meetings Department at OSA

12–14 June 1985 WORKSHOP ON OPTICAL FABRICATION AND TESTING, Cherry Hill Information: Meetings Department at OSA

18–21 June 1985 INSTABILITIES AND DYNAMICS OF LASERS AND NONLINEAR OPTICAL SYSTEMS TOPICAL MEETING, Rochester Information: Meetings Department at OSA

15–17 October 1985 OPTICAL STORAGE DATA TOPICAL MEETING, Washington D.C. Information: Meetings Department at OSA

15–18 October 1985 ANNUAL MEETING OPTICAL SOCIETY OF AMERICA, Washington D.C. Information: Meetings Department at OSA

10–13 June 1986 CLEO 86, OSA/IEEE CONFERENCE ON LASERS AND ELECTROOPTICS, San Francisco Information: Meetings Department at OSA

21–24 October 1986 ANNUAL MEETING OPTICAL SOCIETY OF AMERICA, Los Angeles Information: Meetings Department at OSA