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Revisit of optical properties of an absoptive thin film

Don Groom

SNAP CCD Group
Lawrence Berkeley National Laboratory
Berkeley, CA 94720

ABSTRACT

In the course of discussions with Steve Holland nearly 10 years ago, I wrote IDL code to calculate the internal quantum efficiency of our CCD with thin films of indium tin oxide (ITO) and SiO_2 on the back (light entrance side). Unavoidably, there was also an *in-situ* doped polysilicon (ISDP) layer 100–200 Å thick between the Si wafer and the ITO film. The optical properties of the ISDP are similar to those of pure Si, but it is conductive and hence absorptive. This is important at the blue end of spectrum, where the absorption length for light in Si is comparable to the ITO thickness. The unique feature of our analysis was treating the entire substrate as just one more thin film. The difference between incident intensity and transmitted intensity was understood to be the internal quantum efficiency, and in fact provided a good description over a central wavelength range, where the transmitted and reflected intensities were virtually identical.

Maximilian Fabricius made important contributions to the problem, not only rewriting the code in Java but in generalizing the number of layers possible and treating the ISDP as just one more layer. But our treatment of absorption was *ad hoc* at best, and the small absorption by the ITO was neglected. Our reference books assumed transparent media, so we explicitly inserted absorption—almost, but not quite right. This note is a discussion of the theory and coding considerations as necessary steps in updating/rewriting the code along more rigorous and more useful lines.

1. Introduction

Our previous analysis [1] was based on the multilayer film formalism presented in Pedrotti & Pedrotti's *Introduction to Optics* [2] (hereafter P^2), developed for nonabsorptive materials (real index of refraction). Simply replacing the indices with complex ones was probably too glib and in any case was not done consistently. Oblique incidence was not considered, but it is included here. The "by-hand" inclusion of aborption in silicon amounted to a first-order approximation to the correct treatment; this made little difference if the complex part of the index of refraction was small compared with the real part, as is usually true. In addition, the signs are questionable in Eq. (6) of Ref. 1.

The problem is illustrated in Fig. 1.1. Light is incident on a multilayered antireflective (AR) coating, which is slightly absorptive, goes through a thin *in-situ* doped polyslicon (ISDP) layer which is extremely absorptive at the blue end of the specrum, and. except in the near infrared (IR), is absorbed in the (depleted) silicon substrate. In the IR light is multiply reflected in the Si wafer, producing fringing, and is partly transmitted to get lost in the final substrate. Since the *e*-*h* pairs produced in the ISDP can diffuse into the depleted region, treating only the absorption, as we continue to do here, underestimates the quantum efficiency (QE) at the blue end of the spectrum.

In the last section, questions about the role of the front surface structure and its substrate in the far IR are considered with the conclusion that spot-o-matic profile measurements in this region should have high priority.

This revisit was inspired by the work of Maximilian Fabricius [3], who rewrote the IDL code used for Ref. 1 in JAVA, made it cleaner and more general, and, of special importance, treated the ISDP layer between the indium-tin oxide (ITO) and the silicon as a part of the antireflective (AR) coating. He also calculated the transmission of the AR coating and extended the treatment to any number of layers. The plan is to improve the IDL code along these lines, incorporating the formalism of this note.

Of course this is an old subject, and there is nothing in this note which is not in the literature already. But there are some difficulties with the standard sources: Most optics books do not consider absorption; after all, one tries to make optical coatings out of transparent materials! But once it is introduced, there is a confusion of sign conventions which result in different definitions of the complex index ($n_c = n + ik$ and $n_c = n - ik$). In this writeup we try to follow the treatment by, by Macleod, in his book *Thin-Film Optical Filters* [4] (who uses a different sign convention than P^2) does.

It is also no surprise that there are a variety of engineering-level (and very expensive) programs Such big guns should eventually be brought in, eventually, for the SNAP CCD's. But (a) we are physicists, and want to start with basic premises, and (b) our treatment is already unusual, in that we treat the silicon substrate itself as one or more "thin films," since the absorption in silicon is essentially the internal quantum efficiency (QE) of the device.

Given its purposes as a discussion of the physics and a reference for those interested in the code, this writeup is intentionally verbose—and for the most part elementary.

2. The boundary condition problem in one film

One need only calculate the reflectivity, absorption, and transmission of one layer. The electric and magnetic fields at the two surfaces can be related by a 2 × 2 matrix involving only the properties of the material in that layer. Multiple layers can be handled by sucessive matrix multiplications.

At a dielectric discontinuity with no surface charge $E_\parallel$ and $H_\parallel (= B_\parallel/\mu)$ are continuous, and since no cases of interest here involve magnetic materials, $\mu_0 = \mu_0$. The fields for a (thin) film are defined in Fig. 1.2 for the polarization case with $\boldsymbol{E}$ parallel to the surface. The figure is adapted from P^2's Fig. 19-1. These boundary conditions are also given by P^2's Eqs. (19-6)–(19.9).

The index of the film enters in two places:

1. In calculating the transmitted intensity. In a nonabsorptive medium with index of refraction n, $B = (n/c)E$. I did not find it obvious that n rather than $|n_c|$ appears in the Pointing vector.
2. In the phase shift and absorption of the reflected/refracted light after one "bounce," e.g. E_{r1} by the two successive paths shown in Fig. 1.2. The real and imaginary parts of the complex index of refraction appear in a slightly complicated way.

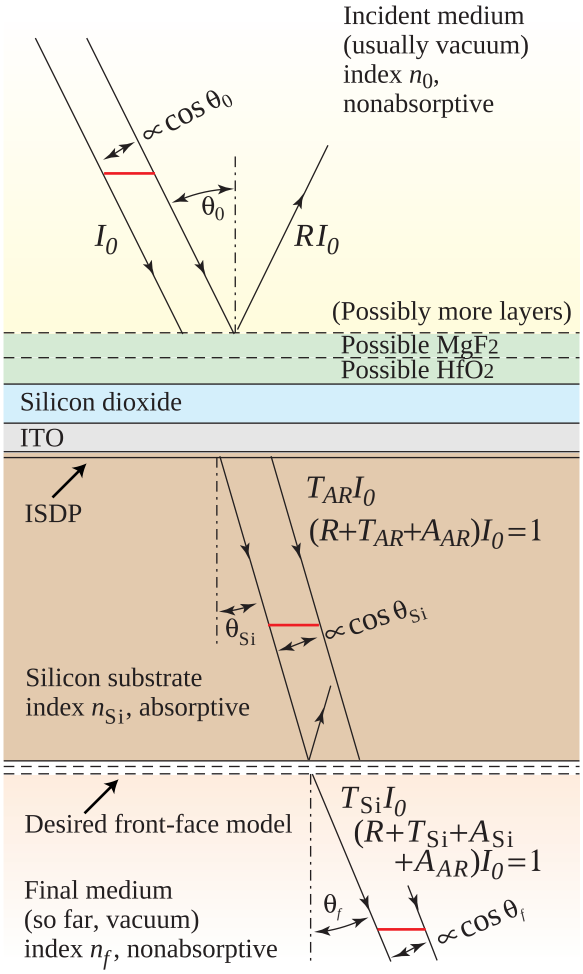

Figure 1.1: The problem: Light is incident on a CCD at zenith angle θ_0. It is reflected/transmitted/absorbed through a number of AR coatings (presently two), a thin layer of ISDP, the silicon wafer, and the front-surface gate structure, finally exiting into a substrate which at present is considered monolithic.

3. Ratio of $\boldsymbol{E}$ to $\boldsymbol{B}$

The most direct approach is to start with Maxwell's equations in the form

$$\nabla\times\boldsymbol{E} = -\partial_t\boldsymbol{B} \qquad \nabla\cdot\boldsymbol{B}=0 \tag{3.1a}$$

$$\nabla\times\boldsymbol{B} = \sigma\mu_0\boldsymbol{E}+\epsilon\mu_0\partial_t\boldsymbol{E} \qquad \nabla\cdot\boldsymbol{E}=0\ . \tag{3.1b}$$

There is no charge density, but we allow absorption through conductivity σ. This is a fair description for indium-tin oxide, but in the case of silicon e-h pair production accounts for most of the absorption in the wavelength range of interest. It doesn't really matter much; in the end only absorption length and the imaginary part of the index (proportional to its reciprocal) are of importance.

Combining Eqs. 3.1 yields a wave equation whose solution for a plane wave traveling in the $+z$ direction is

$$\boldsymbol{E} = \boldsymbol{E}_0\, e^{i\omega(z/v-t)} \qquad \boldsymbol{B}=\boldsymbol{B}_0\, e^{i\omega(z/v-t)} \tag{3.2a}$$

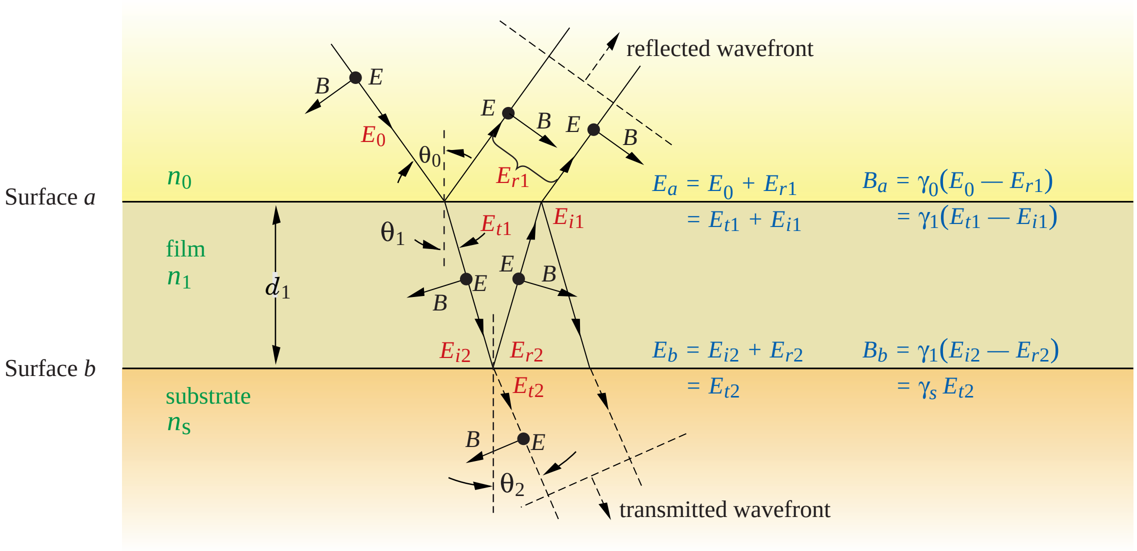

Figure 1.2: Reflected and transmitted electric field intensities from a film with index of refraction n_{c1} and thickness d_1, for $\boldsymbol{E}$ parallel to the surface. n_0 is required to be real, but n_{c1} and n_s are in general complex. Adapted from P^2 Eq. 19-1.

or, "equivalently,"

$$\boldsymbol{E} = \boldsymbol{E}_0\, e^{i\omega(t-z/v)} \qquad \boldsymbol{B} = \boldsymbol{B}_0\, e^{i\omega(t-z/v)} \; . \tag{3.2b}$$

The innocent-looking sign difference actually causes a lot of trouble, notably the differences between references in the sign of the imaginary part of the index of refraction.*

As physicists, we are used to separating Schrödinger's equation in cases where an energy eigenfunction can be found: $\Psi(\boldsymbol{r},t) = \psi(\boldsymbol{r})f(t)$, with solution $f(t) = \exp(-i\omega t)$. It is thus more natural to use the first form, Eq. (3.2a). Engineering books, in particular optics books, tend to use Eq. (3.2b). At risk of belaboring the point too much, for the moment we write

$$\boldsymbol{E} = \boldsymbol{E}_0\, e^{\pm i(\omega/v)z \mp i\omega t} \qquad \boldsymbol{B} = \boldsymbol{B}_0\, e^{\pm i(\omega/v)z \mp i\omega t} \; . \tag{3.3}$$

For a wave of this form it follows trivially from the two divergence equations that E_z and B_z vanish: there is no field in the direction of propagation. By direct substitution the remaining (space-space) curl equations give us

$$\partial_y E_z - \partial_z E_y = -\partial_t B_x \quad \Longrightarrow \quad \mp i\,(\omega/v)\,E_y = \pm i\omega B_x \tag{3.4a}$$

$$\partial_z E_x - \partial_x E_z = -\partial_t B_y \quad \Longrightarrow \quad \pm i\,(\omega/v)\,E_x = \pm i\omega B_y \tag{3.4b}$$

$$\partial_y B_z - \partial_z B_y = \sigma\mu_0 E_x + \epsilon\mu_0 \partial_t E_x \quad \Longrightarrow \quad \mp i\,(\omega/v)\,B_y = (\sigma\mu_0 \mp i\omega\epsilon\mu_0)\,E_x \tag{3.4c}$$

$$\partial_z B_x - \partial_x B_z = \sigma\mu_0 E_y + \epsilon\mu_0 \partial_t E_y \quad \Longrightarrow \quad \pm i\,(\omega/v)\,B_x = (\sigma\mu_0 \mp i\omega\epsilon\mu_0)\,E_y \; . \tag{3.4d}$$

from which we find

$$\frac{E_x}{B_y} = v = \frac{\mp i\,(\omega/v)}{\sigma\mu_0 \mp i\omega\epsilon\mu_0} = \frac{\omega/v}{\epsilon\mu_0\omega \pm i\sigma\mu_0} \; . \tag{3.5}$$

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* In H. J. Lipkin's *Lie Groups for Pedestrians,* the statement, "…confusion and errors are avoided by using the same convention throughout a particular calculation" is footnoted with, "Do not believe this sentence. There are always confusion and errors. You have to live with them."

(The ratio E_y/B_x yields no new information.) Then

$$\begin{aligned}
(\omega/v)^2 &= \omega^2\,(\epsilon\mu_0 \pm i\sigma\mu_0/\omega) && (3.6a)\\
v &= \frac{1}{\sqrt{\epsilon\mu_0 \pm i\sigma\mu_0/\omega}} && (3.6b)\\
&= \frac{c}{\sqrt{n^2 \pm i\sigma\mu_0 c^2/\omega}} \equiv \frac{c}{n_c} && (3.6c)\\
E_y/B_x &= E_y/\mu_0 H_x = c/n_c\ , && (3.6d)
\end{aligned}$$

where n is the index in a nonconductive (nonabsorptive) medium ($\sigma = 0$). The complex index n_c is

$$\begin{aligned}
n_c &\equiv \sqrt{n^2 \pm i\sigma\mu_0 c^2/\omega} && (3.7a)\\
&\equiv n \pm ik && (3.7b)\\
&\approx n \pm i\sigma\mu_0 c^2/2n\omega\ . && (3.7c)
\end{aligned}$$

The approximate form is valid if $k \equiv \sigma\mu_0 c^2/2n\omega \ll n$. This is true for silicon for $\lambda \gtrsim 400$ nm. When $1/v$ is replaced by $n_c/c = (n \pm ik)/c$ in Eq. (3.3) becomes

$$\boldsymbol{E} = \boldsymbol{E}_0\, e^{\mp i\omega(t-nz/c)-k\omega z/c} \qquad \boldsymbol{B} = \boldsymbol{B}_0\, e^{\mp i\omega(t-nz/c)-k\omega z/c}\ . \tag{3.8}$$

So both sign options lead to attenuation, as desired (and required). In the following, we arbitrarily follow Macleod in choosing the bottom sign.

4. Poynting vector

The flow of energy across a unit area is given by

$$\boldsymbol{S} = \boldsymbol{E} \times \boldsymbol{H}\,(= \boldsymbol{E} \times \boldsymbol{B}/\mu_0)\ . \tag{4.1}$$

At this point, we must remember that our complex notation for the field variables means that the real physical fields were the real (or imaginary) parts. Since $\boldsymbol{S}$ is a nonlinear combination of them, we must retreat from the complex notation, and use either the real or imaginary parts. Denoting the real part of $\boldsymbol{S}$ by $\boldsymbol{I}$, we use an obscure identity* to write

$$\boldsymbol{I} = \tfrac{1}{2}\Re\,(\boldsymbol{E}^* \times \boldsymbol{H})\ , \tag{4.2}$$

Remembering that $\boldsymbol{E}$ and $\boldsymbol{H}$ are perpendicular (with scaler complex magnitudes E and H), and that $H = (n_c/\mu_0 c)\,E$, the scaler intensity is

$$I = \tfrac{1}{2}\Re\,((n_c/\mu_0 c)\ EE^*) = \tfrac{1}{2}\,(n/\mu_0 c)\,EE^*\ . \tag{4.3}$$

Using $\boldsymbol{E}$ from Eq. (3.8), we find

$$I = \tfrac{1}{2}\,(n/\mu_0 c)\,|\boldsymbol{E}_0|^2 e^{-2k\omega z/c}\ . \tag{4.4}$$

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* If $\boldsymbol{F}$ and $\boldsymbol{G}$ both vary as $e^{i\omega t}$, then $\overline{\Re(\boldsymbol{F})\cdot\Re(\boldsymbol{G})} = \frac{1}{2}\,\Re(\boldsymbol{F}\cdot\boldsymbol{G}^*) = \frac{1}{2}\,\Re(\boldsymbol{F}^*\cdot\boldsymbol{G})$, where an overline means a time average over 1 (or n) cycles [5]. This remarkable result can easily be shown longhand, for example starting with $\boldsymbol{F} = \boldsymbol{F}_0 \exp(i\phi)\exp(i\omega t)$ and $\boldsymbol{G} = \boldsymbol{G}_0 \exp(i\psi)\exp(i\omega t)$. $\boldsymbol{F}_0$ and $\boldsymbol{G}_0$ are real vectors or scalers.

It is convenient to make the following definitions involving the absorption coefficient:

$$2k\omega/c = 2k/\lambdabar = \alpha = 1/\ell \tag{4.5}$$

Here $\lambdabar = \lambda/2\pi$ is the wavenumber in vacuum, α is the usual (intensity) absorption coefficient, and ℓ is the (intensity) absorption length.

In the thin-film formalism discussed below, r is the fractional reflected electric field strength and t the fractional transmitted electric field strength. To convert these to reflection and transmission coefficients, one must include n, the real part of the index of refraction via Eq. (4.4):

$$R \ = |r|^2 \qquad T = n|t|^2 \ . \tag{4.6}$$

Since only ratios enter, the common factors $\frac{1}{2}\mu_0 c$ cancel.

But there are other worries. The field of the incident radiation, $\boldsymbol{E}_0$, is in a medium with index n_0 which might not be unity. (We find it convenient to change notation to that shown in Fig. 1.2, where the subscript "0" labels the medium in which the wave is considered incident, and "s" the "substrate." There may or may not be additional layers; we are simply interested in the transmitted intensity entering the substrate.) The incident Pointing vector is thus proportional to $n_0|\boldsymbol{E}|^2$. The factor n_0 is also present in the reflected wave, so its relative intensity is still $|r|^2$. But in the case of the transmitted wave, our factor $n_s|t|^2$ should become $(n_s/n_0)|t|^2$.

Finally, if the light is incident at an angle θ_0 and exits at an angle θ_s, then the perpendicular area of a cylinder of incident light goes into an area different by $\cos\theta_0/\cos\theta_s$; the intensity is changed by this factor. This situation is indicated in Fig. 1.1, where the red bar indicates the beam width for normal incidence. In summary,

$$T = \frac{\cos\theta_s}{\cos\theta_0}\frac{n_s}{n_0}|t|^2 \ . \tag{4.7}$$

5. Including absorption in the reflected and transmitted $\boldsymbol{E}$ fields at a thin film

In the first place, we make the enormous simplification that the incident medium and (usually) the substrate are nonabsorptive: θ_0 is real, and n_0 is real.

As a matter of simplicity, Eqs. 3.2, 3.3, and 3.8 described plane waves moving in the $+z$ direction. If instead the angle of incidence is θ_0 and the direction lies in the xy plane, then we can write

$$\text{Incident:}\ \exp\left[i\{\omega t - (n_0/\lambdabar)\,(x\sin\theta_0 + z\cos\theta_0)\}\right] \tag{5.1a}$$

$$\text{Transmitted:}\ \exp\left[i\{\omega t - (n_{c1}/\lambdabar)\,(x\sin\theta_1 + z\cos\theta_1)\}\right]\ , \tag{5.1b}$$

where $n_{c1} = n_1 - ik_1$. At $z = 0$ the two expressions must agree, yielding the complex version of Snell's law,

$$(n_1 - ik_1)\sin\theta_1 \ = n_0\sin\theta_0 \tag{5.2a}$$

which propagates from one film to another:

$$(n_j - ik_j)\sin\theta_j \ = n_0\sin\theta_0 \ . \tag{5.2b}$$

Since $n_0\sin\theta_0$ is real by definition, $\sin\theta_k$ and hence θ_k are complex if $k_j \neq 0$.

In discussing the phase shift in a film, we will usually need the product $n_{cj}\cos\theta_j$:

$$\begin{aligned}(n_j - ik_j)\cos\theta_j &= \sqrt{(n_j^2 - k_j^2 - n_0^2\sin^2\theta_0) - 2in_jk_j} \\ &\equiv a_j - ib_j \end{aligned} \tag{5.3}$$

Writing the first three terms under the radical in this way makes it manifest that only the last term introduces a complex quantity, even though $n_{c1}\sin\theta_1$ is real via Eq. 5.2. Equation 5.1*b* becomes

$$\exp\left[-b_i z/\bar{\lambda}\right]\exp\left[i\{\omega t - (x/\bar{\lambda})\,n_0\sin\theta_0 - a_i z/\bar{\lambda}\}\right] \ , \tag{5.4}$$

so that we have a damped wave, as expected and required.

5.1. Phase shift

The reflected wavefront E_{r1} is the superposition of an infinite number of refracted/reflected/refracted waves. The first such ray is delayed by a phase proportional to the path length in the film, $2d/\cos\theta_1$, but as can be seen from Fig. 1.2 the directly reflected wave is delayed as well (greater distance to the wavefront). Using Snell's Law and a clever geometrical argument,* P^2 shows that the optical path length difference is

$$\Delta_1 = 2d_1n_1\cos\theta_1 \ . \tag{5.5}$$

Using half this length, the phase lag in one traversal of the film is

$$\delta_1 = (d_1/\bar{\lambda})\,n_1\cos\theta_1 \ . \tag{5.6}$$

Thus in the absence of absorption

$$\begin{aligned} E_{i2} &= E_{t1}e^{-i\delta_1} \\ E_{i1} &= E_{r2}e^{-i\delta_1} \ . \end{aligned} \tag{5.7}$$

(P^2's Eqs. 19-15 and 19-16).

In our earlier treatment, absorption was added in a way that seemed obvious: an additional factor $\exp(-d_1/(2\ell_1\cos\theta_1)) = \exp(-(k_1d_1/\bar{\lambda})/\cos\theta_1))$ is contributed by each transit:

$$\begin{aligned} E_{i2} &= E_{t1}e^{-(k_1/\bar{\lambda}_1)d_1/\cos\theta_1 - i(n_1/\bar{\lambda}_1)d_1\cos\theta_1} \\ &\equiv E_{t1}e^{-i\delta_{c1}} \ , \\ E_{i1} &= E_{r2}e^{-\delta_{c1}} \end{aligned} \tag{5.8}$$

where

$$\begin{aligned} \delta_{c1} &= \delta_1 - \frac{id_1}{2\ell_1\cos\theta_1} \\ &= \frac{d_1}{\bar{\lambda}}\left(n_1\cos\theta_1 - \frac{i\,k_1}{\cos\theta_1}\right) \ , \end{aligned} \tag{5.9}$$

and $\lambda = 2\pi\bar{\lambda}$ is the wavelength of the light in vacuum. In this argument θ_1 was assumed to be a real angle.

This form for the phase shift was physically reasonable and at the end gave a reasonable description of our AR coatings. However, it has a number of problems: $\cos\theta_1$ appears in a disturbingly

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* Variants of the argument can be found in virtually any optics book, e.g. Refs. 4, 6, and 7.

asymmetric way in the real and imaginary parts. In the case of normal incidence, $n_{c1} = n - ik$—even though P^2's sign conventions led to $n_{c1} = n + ik$. It was not noticed that a real θ_1 was inconsistent with any reasonable generalization of Snell's law.

Sense can be made of this if we expand Eq. 5.3 for the case $n_1 \gg k_1$, making use of Eq. 5.2 along the way:

$$(n_1 - ik_1)\cos\theta_1 = a_1 - ib_1 \;= \sqrt{n_1^2 - k_1^2 - n_0^2\sin^2\theta_0}\sqrt{1 - \frac{2in_1k_1}{n_1^2 - k_1^2 - n_0^2\sin^2\theta_0}} \tag{5.10a}$$

$$\approx \sqrt{n_1^2 - n_0^2\sin^2\theta_0}\left(1 - \frac{in_1k_1}{n_1^2 - n_0^2\sin^2\theta_0}\right) \tag{5.10b}$$

But in this limit the normal Snell's law is almost true: $n_1\sin\theta_1 \approx n_0\sin\theta_0$, so $n_1^2 - n_0^2\sin^2\theta_0 \approx n_1^2\cos^2\theta_1$, and

$$(n_1 - ik_1)\cos\theta_1 \approx n_1\cos\theta_1 - \frac{ik_1}{\cos\theta_1}\ . \tag{5.11}$$

As a sanity check, consider the case $n_0 = 1,\ \theta_1 = 30°$. With $n_1 = 1.6,\ k_1 = 0.1n_1$,

$$\begin{aligned} \text{Left side of Eq. 5.11:}\quad n_c &= 1.52077 - i\ 0.168336 \\ \text{Right side of Eq. 5.11:}\quad n_c &= 1.51987 - i\ 0.168436\ , \end{aligned} \tag{5.12}$$

Similarly, $\cos\theta_1$ as calculated from Eq. 5.10 is $(0.930653 - i\ 0.198275)$, while in the absence of absorption, $\cos\theta_1 = 0.949918 - i\ 0.00000$.

Even in the extreme case $n_1 = 1.6,\ k_1 = n_1$,

$$\begin{aligned} \text{Left side of Eq. 5.11:}\quad n_c &= 1.56143 - i\ 1.63953 \\ \text{Right side of Eq. 5.11:}\quad n_c &= 1.51987 - i\ 1.68436\ . \end{aligned} \tag{5.13}$$

Although there is no present reason to use the old form given by Eq. 5.9, we see that the approximation wasn't all that bad.

6. Case with *E* parallel to the surface

The variables in this section are defined in Fig. 1.2, which in turn is basically P^2 Fig. 19-1. $\boldsymbol{E}_\parallel$ and $\boldsymbol{H}_\parallel = (n/\mu_0 c)\ \boldsymbol{B}_\parallel\cos\theta$ are continuous, so for this case

$$\begin{aligned} E_a &= E_0 + E_{r1} &&= E_{t1} + E_{i1} \\ B_a &= \gamma_0\,(E_0 - E_{r1}) &&= \gamma_1\,(E_{t1} - E_{i1}) \\ E_b &= E_{r2} + E_{t1} &&= E_{t2} \\ B_b &= \gamma_1\,(E_{i2} - E_{r2}) &&= \gamma_s E_{t2}\ , \end{aligned} \tag{6.1}$$

where we use P^2's definitions*

$$\begin{aligned} \gamma_0 &= (n_0/c)\cos\theta_0 \\ \gamma_1 &= (n_{c1}/c)\cos\theta_1 \\ \gamma_s &= (n_{cs}/c)\cos\theta_s\ . \end{aligned} \tag{6.2}$$

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* An inspection of the final expressions for r (Eq . 6.6)and t (Eq. 6.7) below, together with the form of the transfer matrix (Eq. 6.3 below) shows that the factor of c cancels. We can thus use $\gamma_j = n_j\cos\theta_j$ (or $n_j/\cos\theta_j$ if $\boldsymbol{B}$ is parallel to the surface; see below).

As can be verified from Fig. 1.2, the right set of equalities in Eq. 6.1 refer only to

The (real) angle of incidence is θ_0 and the (possibly complex) refracted angles in the film and in the substrate are θ_1 and θ_s. As mentioned above, the incident medium has real index n_0. The other indices can be complex.

That said, we can follow P^2 exactly: δ_1 is given by Eq. 5.6, except that $n_1 \cos\theta_1$ is now the complex form given by Eq. 5.3. We can then use Eq. 5.8 (or, now equivalently, Eq. 5.7) to eliminate E_{i2} and E_{r2} in the left set of equalities in Eqs. (6.1), to find

$$\begin{aligned} \begin{pmatrix} E_a \\ \\ B_a \end{pmatrix} &= \begin{pmatrix} \cos\delta_1 & \dfrac{i\,\sin\delta_1}{\gamma_1} \\ i\,\gamma_1 \sin\delta_1 & \cos\delta_1 \end{pmatrix} \begin{pmatrix} E_b \\ \\ B_b \end{pmatrix} \\ &\equiv \mathcal{M}_1 \begin{pmatrix} E_b \\ \\ B_b \end{pmatrix} \ . \end{aligned} \tag{6.3}$$

Magically, $\mathcal{M}_1$ refers only to the parameters of film 1: It is a transfer matrix relating the fields at the incident surface to the fields at the rear surface. It is thus possible to describe the fields of an N-layer configuration by simply multiplying them together:

$$\begin{pmatrix} E_a \\ B_a \end{pmatrix} = \mathcal{M}_1 \mathcal{M}_2 \dots \mathcal{M}_N \begin{pmatrix} E_N \\ B_N \end{pmatrix} \tag{6.4a}$$

$$= \mathcal{M} \begin{pmatrix} E_N \\ B_N \end{pmatrix} \ . \tag{6.4b}$$

We can now use the rightmost equalities in Eqs. (6.1) to find

$$\begin{aligned} 1 + r &= m_{11} t + m_{12} \gamma_s t \\ \gamma_0 (1 - r) &= m_{21} t + m_{22} \gamma_s t \ , \end{aligned} \tag{6.5}$$

where the matrix elements are the components of $\mathcal{M}$. The reflected E field relative to the incident field is the reflection coefficient $r = E_{r1}/E_0$, and $t = E_{t2}/E_0$ is the relative transmission coefficient. It is easy to solve for r and t:

$$r = \frac{(\gamma_0 m_{11} + \gamma_0 \gamma_s m_{12}) - (m_{21} + \gamma_s m_{22})}{(\gamma_0 m_{11} + \gamma_0 \gamma_s m_{12}) + (m_{21} + \gamma_s m_{22})} \tag{6.6}$$

$$t = \frac{2\gamma_0}{(\gamma_0 m_{11} + \gamma_0 \gamma_s m_{12}) + (m_{21} + \gamma_s m_{22})} \tag{6.7}$$

The reflected intensity fraction R is just $|r|^2$. As per Eq. 4.7, the fractional transmitted intensity T is $|t|^2 (n_s \cos\theta_s)/(n_0 \cos\theta_0)$, where n_s is the real part of the index of the substrate (which might be air). (These are the same as P^2 Eqs. 19-36 and 19-35.)

However, this time there is a problem: If we are calculating the fraction transmitted to the silicon substrate in order to obtain the absorption in the AR coating, then $\cos\theta_1$ is complex, and there is no clear way to deal with it in Eq. 4.7. We return to this problem in Sec. 7.

6.1. Absorption in the AR coating and in the CCD

In the nonabsorptive case, $R + T = 1$. Using the notation from Fig. 1.1,

$$\begin{aligned} A_{AR} &= 1 - (R + T_{AR}) && (6.8a) \\ A_{\text{total}} = A_{\text{Si}} + A_{AR} &= 1 - (R + T_{\text{total}}) \ , && (6.8b) \end{aligned}$$

where A_{AR} and A_{Si} are the intensity fractions absorbed in the AR coating and in the silicon, respectively. A_{Si} is to be identified with the QE at wavelengths were the internal QE of the silicon is 100%. To calculate these absorption fractions, it is convenient to write

$$\begin{aligned} \begin{pmatrix} E_a \\ B_a \end{pmatrix} &= \mathcal{M}_{\text{AR}} \begin{pmatrix} E_{a\text{Si}} \\ B_{a\text{Si}} \end{pmatrix} && (6.9a) \\ &= \mathcal{M}_{\text{AR}} \mathcal{M}_{\text{Si}} \begin{pmatrix} E_{b\text{Si}} \\ B_{b\text{Si}} \end{pmatrix} \ . && (6.9b) \end{aligned}$$

In this somewhat confusing notation, $\mathcal{M}_{\text{AR}}$ represents the transfer matrix of the AR coating alone. $E_{a\text{Si}}$ and $B_{a\text{Si}}$ are the fields at the entry surface of the Si substrate. Thus R and T_{AR} can be found, and Eq. 6.8a then yields A_{AR}. Similarly, Eq. 6.9b, where $E_{b\text{Si}}$ and $B_{b\text{Si}}$ are the fields at the exit of the Si (surface of the substrate), can then be used to find A_{Si}.

These equations are written somewhat more elegantly in Macleod [4] (his Eqs. 2.106, 2.108, and 2.109), but Eqs. 6.8 seem sufficient.

6.2. Case with $\boldsymbol{B}$ parallel to the surface

In this case, it is the component of $\boldsymbol{E}$ parallel to the surface which is continuous. This slightly changed situation is shown in Fig. 6.1. Eqs. (6.1) become

$$\begin{aligned} E_a &= (E_0 + E_{r1}) \cos\theta_0 &&= (E_{t1} + E_{i1}) \cos\theta_1 \\ B_a &= (n_0/c)\,(E_0 - E_{r1}) &&= (n_{c1}/c)\,(E_{t1} - E_{i1}) \\ E_b &= (E_{r2} + E_{t1}) \cos\theta_1 &&= E_{t2} \cos\theta_s \\ B_b &= (n_{c1}/c)\,(E_{i2} - E_{r2}) &&= (n_s/c)\,E_{t2} \ , \qquad (6.10) \end{aligned}$$

The phase shift δ_c depends on optical and geometrical path lengths, and so is the same as for the other polarization. Proceeding to find E_a and B_a as functions of E_b and B_b, we find that $\mathcal{M}_1$ has become

$$\mathcal{M}_1\,(\boldsymbol{B}\text{ parallel}) = \begin{pmatrix} \cos\delta_{c1} & \dfrac{i\cos\theta_1\ \sin\delta_{c1}}{n_{c1}/c} \\ \dfrac{i(n_{c1}/c)\ \sin\delta_{c1}}{\cos\theta_1} & \cos\delta_{c1} \end{pmatrix} \ . \qquad (6.11)$$

This is exactly the same as Eq. (6.3) except that $\cos\theta$ has been replaced by $1/\cos\theta$ (but not in δ_1). The solution of the rightmost versions of Eqs. (6.10) using the new $\mathcal{M}_1$ proceeds as before, except that all occurences of $\gamma = (n/c)\cos\theta$ are replaced by $\gamma = (n/c)/\cos\theta$.

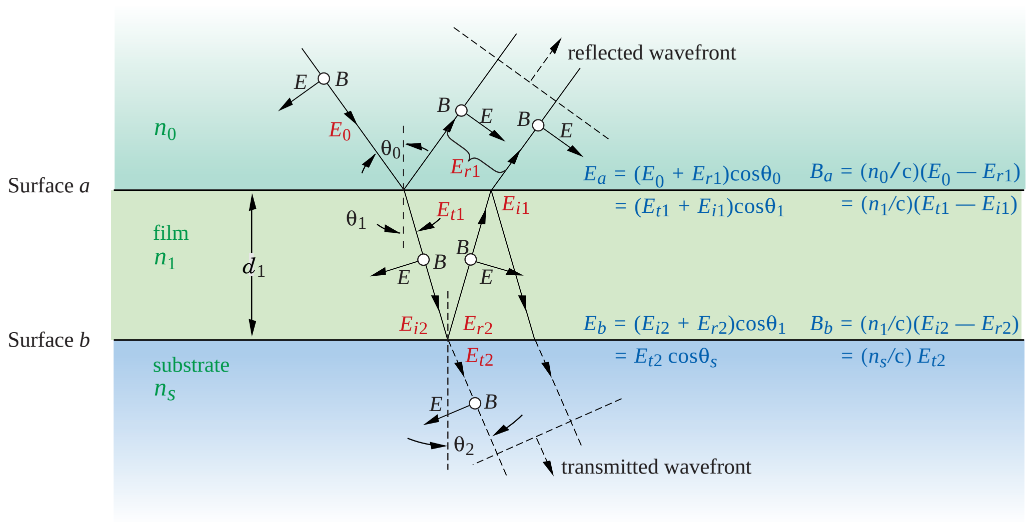

Figure 6.1: Reflected and transmitted electric field intensities from a film with index of refraction. n_{c1} and thickness d, for $\boldsymbol{B}$ parallel to the surface.

7. Remaining problems

7.1. Oblique incidence

Macleod [4] introduces the tangential components of $\boldsymbol{E}$ and $\boldsymbol{H}$, so that Eqs. 6.1 and 6.10 take on a much simpler form. He then obtains somewhat different looking solutions for r and t. The expression for r then reduces to Eq. 6.6. One motivation is to maintain the $R+T=1$ rule in the case of oblique incidence.* However, t is different that that obtained from Eq. 6.7. He merely says "…the reflection coefficients in Eq. …and Eq. …are identical, and since much more use is made of reflection coeficients confusion is rare."

But transmission is the object of the present calculation. It would be simple enough to use Eq. 4.7 if the two $\cos\theta$ terms were real. However, part of the present problem is to calculate A_{AR}, and in this case the "substrate" is the silicon itself, which is absorptive.

The problem appears to be profound [8]. In the absorptive material, the wavefront is normal to the refracted direction, while the intensity falls exponentially with distance from the surface. This makes calculation of A_{AR} problematical in the oblique incidence case. There is no problem with transmission through the whole assembly, so calculation of $A_{AR}+A_T$ has no formal obstacles.

The AR coating absorption is at most a few percent, and its angular variation is of secondary importance. We plan to proceed with the coding using normal incidence, and analyze this problem numerically if it becomes relevant. Thus Eqns. 5.3, 5.6, and 6.2 become

$$n_j - ik_j = a_j - ib_j \tag{7.1a}$$

$$\delta_j = d_j n_j/\lambda \tag{7.1b}$$

$$\gamma_j = n_j/c \tag{7.1c}$$

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* The cosine factors in Eq. 4.7 probably take care of this if they are real.

7.2. What if there is too much absorption?

If the index is complex, $\delta = \delta_R + i\delta_I = n_c d/\lambdabar = d(n - ik)/\lambdabar$. Then

$$\begin{aligned}
\cos\delta &= \cos\delta_R \cos i\delta_I - \sin\delta_R \sin i\delta_I \\
&= \cos\delta_R \cosh\delta_I - i \sin\delta_R \sinh\delta_I && (7.2) \\
\sin\delta &= \sin\delta_R \cos i\delta_I + \cos\delta_R \sin i\delta_I \\
&= \sin\delta_R \cosh\delta_I + i \cos\delta_R \sinh\delta_I \ . && (7.3)
\end{aligned}$$

(Note that δ_I is always negative.) For $-\delta_I > 88$ (single precision) or $-\delta_I > 710.$ (double precision), IDL yields "Infinity" for $\cosh\delta_I$ or $\sinh\delta_I$. For a 250 μm silicon substrate, $2\pi kd/\lambda = 29.6, 229, 1520,$ and 21792 for $\lambda = 600, 500, 400,$ and 300 nm, respectively. Clearly, special care must be taken for large (negative) δ_I. A useful (arbitrary) threshold might be at $\delta_I = -10$, where $\cosh\delta_I \approx -\sinh\delta_I = 11013.2$: If $\delta_I < -10.$, then $\delta_I = -10$.

It is convenient to factor out the $\exp(-\delta_I)$ part of $\cos\delta$ and $\sin\delta$. Rewriting Eq. (7.2),

$$\begin{aligned}
\cos\delta &= \tfrac{1}{2}\left[\cos\delta_R \left(e^{\delta_I} + e^{-\delta_I}\right) - i \sin\delta_R \left(e^{\delta_I} - e^{-\delta_I}\right)\right] \\
&= e^{-\delta_I}\tfrac{1}{2}\left[\cos\delta_R \left(1 + e^{2\delta_I}\right) + i \sin\delta_R \left(1 - e^{2\delta_I}\right)\right] \\
&\equiv e^{-\delta_I}\,\mathrm{Fcos}\left(\delta_R, \delta_I\right) && (7.4)
\end{aligned}$$

Similarly,

$$\begin{aligned}
\sin\delta &= e^{-\delta_I}\tfrac{1}{2}\left[\sin\delta_R \left(1 + e^{2\delta_I}\right) - i \cos\delta_R \left(1 - e^{2\delta_I}\right)\right] \\
&\equiv e^{-\delta_I}\,\mathrm{Fsin}\left(\delta_R, \delta_I\right) && (7.5)
\end{aligned}$$

With these definitions, $\mathcal{M}$ as defined in Eq. (6.3) becomes

$$\begin{aligned}
\mathcal{M}_j &= e^{-\delta_{Ij}} \begin{pmatrix} \mathrm{Fcos}\left(\delta_{Rj}, \delta_{Ij}\right) & \dfrac{i\,\mathrm{Fsin}(\delta_{Rj}, \delta_{Ij})}{\gamma_j} \\ i\,\gamma_j \mathrm{Fsin}\left(\delta_{Rj}, \delta_{Ij}\right) & \mathrm{Fcos}\left(\delta_{Rj}, \delta_{Ij}\right) \end{pmatrix} \\
\mathcal{M}_j &\equiv e^{-\delta_{Ij}} \mathcal{M}_j^F && (7.6)
\end{aligned}$$

Eq. (6.4) then becomes

$$\begin{aligned}
\begin{pmatrix} E_a \\ B_a \end{pmatrix} &= e^{-\delta_{I1}} \mathcal{M}_1^F \; e^{-\delta_{I2}} \mathcal{M}_2^F \;\ldots\; e^{-\delta_{IN}} \mathcal{M^F}_N \begin{pmatrix} E_N \\ B_N \end{pmatrix} && (7.7) \\
&= \exp\left(-\textstyle\sum \delta_{Ij}\right)\, \mathcal{M}^F \begin{pmatrix} E_N \\ B_N \end{pmatrix} \ . && (7.8)
\end{aligned}$$

Following the discussion of Sec. 6, Eqs. 6.6 and 6.7 become

$$\begin{aligned}
r &= \frac{(\gamma_0 m_{11}^F + \gamma_0\gamma_s m_{12}^F) - (m_{21}^F + \gamma_s m_{22}^F)}{(\gamma_0 m_{11}^F + \gamma_0\gamma_s m_{12}^F) + (m_{21}^F + \gamma_s m_{22}^F)} && (7.9) \\
t &= \frac{2\gamma_0 \exp\left(\sum \delta_{Ij}\right)}{(\gamma_0 m_{11}^F + \gamma_0\gamma_s m_{12}^F) + (m_{21}^F + \gamma_s m_{22}^F)} && (7.10)
\end{aligned}$$

Thus the reflected amplitude r is calculable for any amount of absorption, since the exponential factors cancel, while the transmitted amplitude t is (essentially) zero for high absorption, as expected. We can calculate the reflectivity from thick absorptive layers without numerical analysis problems.

How shall we treat $\mathcal{M}$ in thin-film cases? It really doesn't matter if the positive exponential part is factored out or not. It is easiest to *always* use Eq. (7.6), *i.e.*, use the same IDL procedure for all cases.

8. Reflections on the front surface and substrate

In previous calculations, it was assumed that the index of the material after the Si, n_s, is just 1.00—air. In reality there is no sharp boundary; it is all of the irregular ISDP and oxide layers making up the gate structure, the thicker passivation layer, epoxy, and the AlN substrate. It is not clear how to represent this material, although it makes a difference only in the near IR, where light is actually penetrating the Si active region. Not only is the amplitude of the fringes affected, but light probably scatters irregularly from this surface, producing halation.

If the AlN were like "dark glass" rather than amorphous and diffusive, it would not matter if it were white or black—only its interface with the the epoxy is operative, since all the light would be absorbed in the AlN anyway. But it is diffusive, and the gate structures are irregular optically.

Only studies of the beam spot profile in the near IR will shed light on this problem.

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