chem 249

A. Classical Description of Electromagnetic Radiation

1. Maxwells Equations & Plane Electromagnetic Waves

a. Vector Fields & Notation

$$\vec{A} = A_x \hat{i} + A_y \hat{j} + A_z \hat{k}$$

$$\vec{A} \cdot \vec{B} = A_x B_x + A_y B_y + A_z B_z$$ dot product

$$\vec{A} \times \vec{B} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ A_x & A_y & A_z \\ B_x & B_y & B_z \end{vmatrix} = (A_y B_z - B_y A_z)\hat{i} + (A_z B_x - B_z A_x)\hat{j} + (A_x B_y - B_x A_y)\hat{k}$$

$$\vec{\nabla} f = \frac{\partial f}{\partial x}\hat{i} + \frac{\partial f}{\partial y}\hat{j} + \frac{\partial f}{\partial z}\hat{k}$$ grad f

$$\vec{\nabla} \cdot \vec{A} = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}$$ div A

$$\vec{\nabla} \times \vec{A} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \end{vmatrix}$$ curl A

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} \quad ; \quad \nabla^2 \vec{A} = \vec{\nabla}(\vec{\nabla} \cdot \vec{A}) - \vec{\nabla} \times \vec{\nabla} \times \vec{A}$$

b. EM fields & superposition

test charge q: $\vec{F} = q(\vec{E} + \vec{v} \times \vec{B})$

$\vec{E}(\vec{r}, t)$ & $\vec{B}(\vec{r}, t)$

$\vec{E}_{TOT} = \vec{E}_1 + \vec{E}_2$ Principle of Superposition

Other EM Fields:

$\vec{P} = \epsilon_0 \underbrace{\chi}_{\text{susceptibility}} \vec{E}$ polarization of a dielectric

$\vec{D} = \epsilon_0 \vec{E} + \vec{P} = \epsilon_0 (1 + \chi) \vec{E} = \epsilon_0 \epsilon_r \vec{E} = \underbrace{\epsilon}_{\text{dielectric constant}} \vec{E}$

$\vec{M} = \chi_m \vec{H}$ Magnetization & Magnetic susceptibility

$\vec{B} = \mu_0 (\vec{H} + \vec{M}) = \mu_0 (1 + \chi_M) \vec{H} = \mu_0 \mu_r \vec{H} = \mu \vec{H}$

magnetic permeability

c. Maxwells Equations (in free space):

$$\vec{\nabla} \cdot \vec{E} = 0$$

$$\vec{\nabla} \cdot \vec{H} = 0$$

$$\vec{\nabla} \times \vec{H} = \epsilon_0 \frac{\partial \vec{E}}{\partial t}$$

$$\vec{\nabla} \times \vec{E} = -\mu_0 \frac{\partial \vec{H}}{\partial t}$$

$$\vec{\nabla} \times \vec{E} = -\mu_0 \, \partial \vec{H}/dt$$

$$\vec{\nabla} \times \vec{\nabla} \times \vec{E} = -\mu_0 \frac{\partial}{\partial t} \vec{\nabla} \times \vec{H}$$

$$\vec{\nabla}(\underbrace{\vec{\nabla} \cdot \vec{E}}_{0}) - \nabla^2 \vec{E} = -\mu_0 \epsilon_0 \frac{\partial^2 \vec{E}}{\partial t^2}$$

$$\nabla^2 \vec{E} = \epsilon_0 \mu_0 \frac{\partial^2 \vec{E}}{\partial t^2} \qquad c = 3.00 \cdot 10^{10} \text{ cm s}^{-1}$$

Likewise:

$$\nabla^2 \vec{H} = \epsilon_0 \mu_0 \frac{\partial^2 \vec{H}}{\partial t^2} \qquad \epsilon_0 \mu_0 \equiv \frac{1}{c^2}$$

These are the EM Wave Equations. The solutions are

$$\vec{E}(\vec{r}, t) = \vec{E}_0 \exp(i \vec{k} \cdot \vec{r} - i \omega t) \qquad |\vec{k}| = \frac{\omega}{c}$$

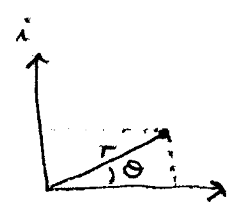
$$\vec{H}(\vec{r}, t) = \vec{H}_0 \exp(i \vec{k} \cdot \vec{r} - i \omega t) \qquad \omega = 2\pi\nu$$

$\vec{E}$ & $\vec{H}$ are in complex notation: $\qquad e^{i\theta} + e^{-i\theta} = 2\cos\theta$

$$e^{i\theta} = \cos\theta + i \sin\theta \qquad \text{Euler's Formula}$$

$$z = x + iy = r(\cos\theta + i\sin\theta) = re^{i\theta}$$

$$Re(z) = r\cos\theta$$



complex plane.

$$Im(z) = r\sin\theta$$

d. EM Plane Waves

1-d harmonic travelling wave equation:

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 \psi}{\partial t^2}$$

$$\psi(x,t) = A \sin k(x - vt) \qquad \text{general solution}$$

Spatial Periodicity: $\psi(x,t) = \psi(x+\lambda, t)$

$$A \sin k(x+\lambda - vt) \;;\quad k\lambda = 2\pi \;;\quad k = \frac{2\pi}{\lambda}$$

Temporal Periodicity: $\psi(x,t) = \psi(x, t+\tau)$

$$A \sin k(x - v(t+\tau)) \;;\quad |kv\tau| = 2\pi$$

$$\frac{2\pi}{\lambda} v \tau = 2\pi$$

$$v\tau = \lambda \qquad \nu = \text{frequency} \equiv \frac{1}{\tau}$$

$$v = \lambda \nu$$

$\omega \equiv 2\pi\nu \rightarrow$ angular frequency ; $kv = \frac{2\pi v}{\lambda} = 2\pi\nu = \omega$

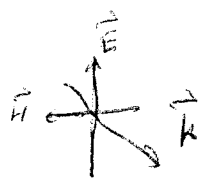
$$\psi(x,t) = A \sin(kx - kvt) = A \sin(kx - \omega t)$$

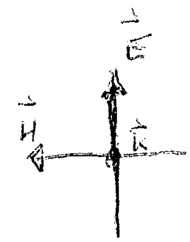
In 3 dimensions,
$$\nabla^2 \psi = \frac{1}{v^2}\frac{\partial^2 \psi}{\partial t^2}$$

$$\psi(\vec{r},t) = A \exp(i\vec{k}\cdot\vec{r} - i\omega t) \qquad |\vec{k}| = \frac{\omega}{c}$$

$\Rightarrow \quad \vec{E}(\vec{r},t)$ & $\vec{H}(\vec{r},t)$ have this format.

d. ~~Polarization~~
$$\vec{k}\cdot\vec{E} = \vec{k}\cdot\vec{H} = 0$$
$$\vec{k}\times\vec{E} = \omega\mu_0 \vec{H}$$
$$\vec{k}\times\vec{H} = -\omega\epsilon_0 \vec{E}$$





$$H_0 = (\epsilon_0/\mu_0)^{1/2} E_0$$

= If $\vec{k} = k\hat{k}$, $\quad \vec{E}(\vec{r},t) = E_0 \sin(~~\omega t~~\ kz - \omega t)\,\hat{x}$

e. EM Waves in Dielectrics $\quad \epsilon_0 \to \epsilon$
$$\nabla^2\vec{E} - \epsilon\mu_0\frac{\partial^2\vec{E}}{\partial t^2} = 0 \ ; \ \nabla^2\vec{H} - \epsilon\mu_0\frac{\partial^2\vec{H}}{\partial t^2} = 0$$

$$\epsilon\mu_0 = \frac{1}{u^2} \Rightarrow \quad u = (\epsilon\mu_0)^{-1/2} = \frac{c}{\epsilon_r^{1/2}} \equiv \frac{c}{n}$$

index of refraction
$n = \epsilon_r^{1/2}$

$$H_0 = \left(\frac{\epsilon}{\mu_0}\right)^{1/2} E_0$$

Electric Energy $= \frac{1}{2}\epsilon E^2$

$$k = \frac{\omega}{u} = n\frac{\omega}{c}$$

$$\frac{k\cdot c}{\omega} = n \quad ; \quad \left(\frac{kc}{\omega}\right)^2 = n^2 = \epsilon = 1 + \chi$$

f. Poynting Vector

$$\vec{S} = \vec{E} \times \vec{H}$$

the energy crossing unit area in unit time (watts cm^{-2})

$$|S| = \left(\frac{\epsilon_0}{\mu_0}\right)^{1/2} |E^2|$$

$$= \epsilon_0 c \cdot |E^2|$$

$$\langle S_{av} \rangle = c\,\epsilon_0 \langle E^2 \rangle_{av} \qquad \langle E^2 \rangle_{av} = \tfrac{1}{2} E_0^2$$

$$= c \cdot \tfrac{1}{2} \epsilon_0 E_0^2 \qquad = \text{velocity} \times \text{energy}$$

In a dielectric

$$|S| = \left(\frac{\epsilon}{\mu_0}\right)^{1/2} |E^2| = u\,\underbrace{\epsilon}_{n^2\epsilon_0}\,|E^2| = \text{phase velocity} \times \text{energy}$$

$$u = \frac{c}{n}$$

$$= n c \cdot \tfrac{1}{2} \epsilon_0 E_0^2$$

Numerical Example: p 5 (465), C & L.

20 gigawatt laser beam

2 mm diameter

$$S_{av} = c\,\epsilon_0 \underbrace{E_{av}^2}_{= \frac{1}{2} E_0^2} = 2.66 \cdot 10^{-3} E_{rms}^2 \text{ watts } m^{-2}$$

$$E_0 = \sqrt{2}\, E_{rms} = \sqrt{2} \left(\frac{1}{2.66 \cdot 10^{-3}} \cdot \frac{20 \times 10^9}{\pi \times 10^{-6}} \right)^{1/2} = \underline{\underline{2.2 \cdot 10^9 \text{ V/meter}}}$$

$$B_0 = \frac{E_0}{c} = \frac{2.2 \times 10^9}{3 \times 10^8} = 7.3 \text{ Tesla}$$

g. ~~Radiat~~ Polarization

~~E~~ Consider two waves.

$$\vec{E}_x(z,t) = \hat{\imath}\, E_{0x} \cos(kz - \omega t)$$

$$\vec{E}_y(z,t) = \hat{\jmath}\, E_{0y} \cos(kz - \omega t + \varepsilon)$$

$$\vec{E}(z,t) = \vec{E}_x + \vec{E}_y$$

linear again

if $\varepsilon = 0$, $\quad \vec{E} = (\hat{\imath} E_{0x} + \hat{\jmath} E_{0y}) \cos(kz - \omega t)$

linear again

if $\varepsilon = \pi$ $\quad \vec{E} = (\hat{\imath} E_{0x} - \hat{\jmath} E_{0y}) \cos(kz - \omega t)$

if $\varepsilon = \pi/2$ $\quad \vec{E} = E_0 [\hat{\imath} \cos(kz - \omega t) + \hat{\jmath} \sin(kz - \omega t)]$

& $E_{0x} = E_{0y} = E_0$

at $t = 0$ $\quad \vec{E}_x = \hat{\imath} E_0 \cos kz_0$

$z = z_0$ $\quad \vec{E}_y = \hat{\jmath} E_0 \sin kz_0$

at $t = \frac{kz_0}{\omega}$ $\quad \vec{E}_x = \hat{\imath} E_0$

$\vec{E}_y = 0$.

clockwise rotation - right circular polarization

left circular polarization $\quad \vec{E} = E_0[\hat{\imath} \cos(kz - \omega t) - \hat{\jmath} \sin(kz - \omega t)]$

if E_0 is not equal $\Rightarrow$ elliptical polarization

2. Fresnel Calculations & Total Internal Reflection

a. Fresnel Calculations

Consider an EM wave at an interface. Two new waves are created, a reflected and a transmitted wave. Following the notation of L & C.

$$\vec{E}_i = \vec{E}_{0i} \exp(i\omega_i t - i\vec{k}_i \cdot \vec{r}) \qquad \text{where } \vec{k}_i = \frac{n_1 \omega}{c} \hat{n}_i$$

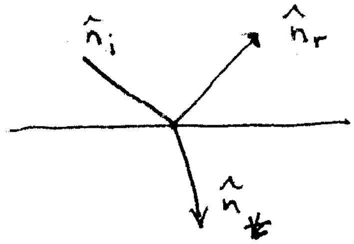
$$= \vec{E}_{0i} \exp i\omega_i \left(t - \frac{\hat{n}_i \cdot \vec{r}}{u_1}\right) \qquad u_1 = \frac{c}{n_1}$$

Also

$$\vec{E}_r = \vec{E}_{0r} \exp i\omega_r \left(t - \frac{\hat{n}_r \cdot \vec{r}}{u_1}\right)$$

&

$$\vec{E}_t = \vec{E}_{0t} \exp i\omega_t \left(t - \frac{\hat{n}_t \cdot \vec{r}}{u_2}\right)$$



Fresnel Calculations use the fact that ~~E~~ the tangential components of $\vec{E}$ + $\vec{H}$ must be continuous across the interface.

1) Since $\vec{E}_i$, $\vec{E}_r$ & $\vec{E}_t$ ~~are~~ must be identical functions of time,

$$\omega_i = \omega_r = \omega_t$$

2) All 3 vectors are identical functions of position r_I on the interface:

$$\frac{\hat{n}_i \cdot r_I}{u_1} = \frac{\hat{n}_r \cdot r_I}{u_1} = \frac{\hat{n}_t \cdot r_I}{u_2}$$

From these equations:

$$(n_i - n_r) \cdot r_I = 0 \quad \text{so}$$

$$n_r = -n_i \quad \& \quad \theta_i = \theta_r \qquad \text{law of reflection}$$

3) also from these eqution

$$\left(\frac{n_i}{u_1} - \frac{n_t}{u_2}\right) \cdot \vec{r}_I = 0$$

So that the tangential components of n_i/u_1 & n_t/u_2

$$\frac{\sin\theta_i}{u_1} = \frac{\sin\theta_t}{u_2}$$

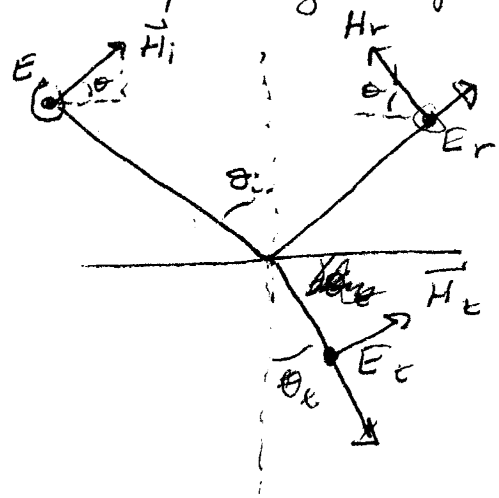
$$k_1 \sin\theta_i = k_2 \sin\theta_t$$

$$n_1 \sin\theta_i = n_2 \sin\theta_2 \qquad \text{Snell's law}$$

$$\sin\theta_2 = \frac{n_1}{n_2} \sin\theta_1, \qquad \text{critical } \angle \; \text{:} \; \sin\theta_c = \frac{n_2}{n_1}$$

~~$\sin\theta_t = 90°$~~

Fresnel calculation for s-polarized light ($E_x = E_z = 0$):



$$E_{0i} + E_{0r} = E_{0t}$$

$$H_{0i}\cos\theta_i - H_{0r}\cos\theta_i = H_{0t}\cos\theta_t$$

since $\frac{|E|}{|H|} = \frac{\omega\mu}{k}$

$$\frac{k_1}{\omega\mu_1}\left(E_{0i} - E_{0r}\right)\cos\theta_i = \frac{k_2}{\omega\mu_2} E_{0t}\cos\theta_t$$

Let $\mu_1 = \mu_2 = \mu$

$$\left(\frac{k}{\omega\mu} = \frac{n\frac{\omega}{c}\mu}{\omega} = \frac{n\mu}{c}\right)$$

Then if $\quad \xi_1 = n_1\cos\theta_i$

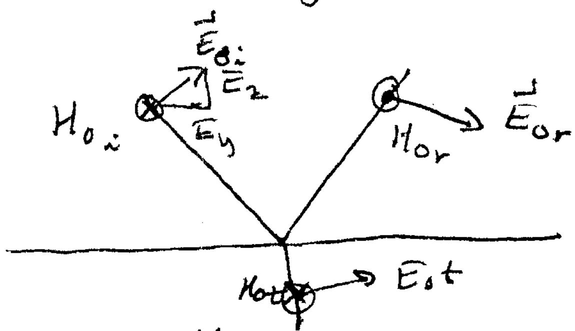
$\qquad\qquad \xi_2 = n_2\cos\theta_t$

$$\left(\frac{E_{0r}}{E_{0i}}\right) = \frac{\xi_1 - \xi_2}{\xi_1 + \xi_2}$$

for s-polarized light

$$\left(\frac{E_{0t}}{E_{0i}}\right) = \frac{2\xi_1}{\xi_1 + \xi_2}$$

Fresnel Equations for p-polarized light:



$\vec{E}_{0r}$ & $\vec{E}_{0t}$ chosen so that they are the same as the s-polarized case when $\theta_i = 0$.

Then, from continuity $\quad H_{0i} - H_{0r} = H_{0t}$

$$\frac{k_1}{\omega\mu_1}\left(E_{0i} - E_{0r}\right) = \frac{k_2}{\omega\mu_2} E_{0t}$$

$$\left(E_{0i} + E_{0r}\right)\cos\theta_i = E_{0t}\cos\theta$$

$$\frac{E_{0r}}{E_{0i}} = -\frac{\epsilon_2\xi_1 - \epsilon_1\xi_2}{\epsilon_2\xi_1 + \epsilon_1\xi_2} \qquad \begin{aligned}\epsilon_1 &= n_1^2\\ \epsilon_2 &= n_2^2\end{aligned}$$

Hecht doesn't have this because of E_{0r} definition difference

$$\frac{E_{0t}}{E_{0i}} = \frac{2\epsilon_2\xi_1}{\epsilon_2\xi_1 + \epsilon_1\xi_2}$$

Generalized Fresnel Formula: $\hat{n}_2 = n_2 + i k_2$

$$\hat{\epsilon}_2 = \hat{n}_2^2$$

And $\hat{\xi}_2 = \hat{n}_2 \cos\theta_2$

$\cos\theta_2$ can be >1 (θ_2 complex)

$$\hat{\xi}_2 = \left(\hat{n}_2^2 - n_1^2 \sin^2\theta_1\right)^{1/2}$$

from

$\hat{\xi}_2$ can be complex

$$\hat{n}_2 \cancel{\sin}\theta_2 = n_1 \sin\theta_1$$

$$\hat{n}_2^2 \sin^2\theta_2 = n_1^2 \sin^2\theta_1$$

$$\hat{n}_2^2 (1 - \cos^2\theta_2) = n_1^2 \sin^2\theta_1$$

$$\hat{n}_2^2 \cos^2\theta_2 = \hat{n}_2^2 - n_1^2 \sin^2\theta_1$$

The Reflection & Transmission coefficients R & T are defined as

$$R = \frac{E_{or}^2}{E_{o\cancel{t}}^2} = \left(\frac{S_{rav}}{S_{\cancel{t}av}}\right) \cancel{R = ZE}$$

$$T = \frac{S_{tav}}{S_{iav}} = \frac{n_2}{n_1} \frac{E_{ot}^2}{E_{oi}^2}$$

$$\boxed{R + T = 1}$$

Normally we use R_p, T_p or R_s, T_s.

b. Normal Incidence Reflectance

At normal incidence $R_s = R_p$ & $T_p = T_s$

$$\theta_i = \theta_t = \theta_r = 0$$

$$R = \frac{\left(\frac{n_1}{n_2} - 1\right)^2}{\left(\frac{n_1}{n_2} + 1\right)^2} = \frac{(n_1 - n_2)^2}{(n_1 + n_2)^2}$$

$$T = \frac{4 n_1 n_2}{(n_1 + n_2)^2}$$

If $n_1 = n_2$, no reflection, otherwise, there is a loss of energy at the interface.

For example, if $n_1 = 1$ air & $n_2 = 3$ (ZnSe?)

$$R = \frac{(1-3)^2}{(1+3)^2} = \frac{4}{16} = 0.25$$

$$T = \frac{4 \cdot 3 \cdot 1}{(1+3)^2} = \frac{3}{4} = 0.75$$

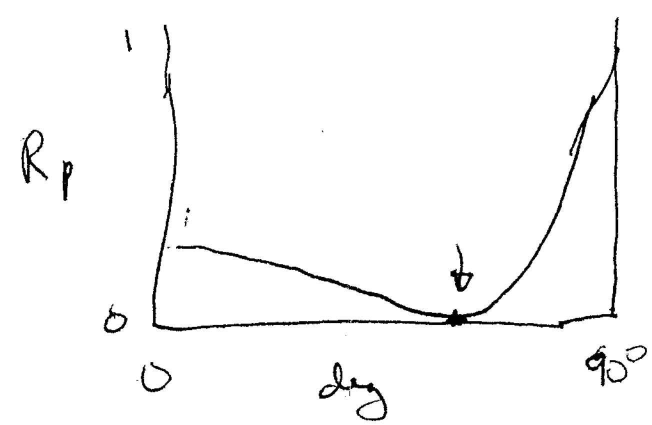
25% reflection loss. Same for $n_1 = 3$, $n_2 = 1$

so a say ZnSe uncoated ~~window~~. $T_{TOT} = 9/16$

c. Brewster's Angle

In §12.3 L & C discuss the phase of the reflected & transmitted light at an interface w/ n_1, n_2 real. For s-polarized light, the transmitted wave is always in phase with the incident light. For reflected light, the Electric fields are <u>in phase</u> if $n_1 > n_2$, or 180° (π) out of phase in $n_1 < n_2$.

For p-polarized light where $n_1 < n_2$, the transmitted wave is <u>in phase</u>, but the reflected wave is either in or out of phase. A minimum is observed in the reflectivity



At this minimum, $R_p = 0$ (of course) and $\theta_i + \theta_t = \frac{\pi}{2}$:

$$R_p = \frac{\epsilon_2 \xi_1 - \epsilon_1 \xi_2}{\epsilon_2 \xi_1 + \epsilon_1 \xi_2} = 0$$

$$\epsilon_2 \xi_1 - \epsilon_1 \xi_2 = 0$$

$$n_2^2 (n_1 \cos\theta_1) - n_1^2 n_2 \cos\theta_2 = 0$$

$$n_2 \cos\theta_1 - n_1 \cos\theta_2 = 0$$

But from Snell's Law: $n_1 \sin\theta_1 = n_2 \sin\theta_2$

$$n_1 = \frac{n_2 \sin\theta_2}{\sin\theta_1}$$

So $$n_2 \cos\theta_1 - \frac{n_2 \sin\theta_2}{\sin\theta_1} \cos\theta_2 = 0$$

$$\cos\theta_1 \sin\theta_1 - \sin\theta_2 \cos\theta_2 = 0$$

or $$\cos\theta_1 \sin\theta_1 = \cos\theta_2 \sin\theta_2$$

which is true if $\theta_2 = \frac{\pi}{2} - \theta_1$.

This angle is called Brewster's Angle, and is used to create polarize light, either on purpose or by accident.

d. Total Internal Reflection

If $n_1 > n_2$ then from Snell's Law.

$$n_1 \sin\theta_i = n_2 \sin\theta_t$$

$$\sin\theta_t = \frac{n_1}{n_2}\sin\theta_i \qquad \text{L.H.S. can be } > 1$$

If $\sin\theta_t = 1 = \frac{n_1}{n_2}\sin\theta_{ic}$

$$\sin\theta_{ic} = \frac{n_2}{n_1}$$

θ_{ic} is called the critical angle. For all angles θ_i greater than θ_{ic}, $R_{\ddagger} = 1$. This occurs for both R_s & R_p. This phenomenon is called Total (Internal) Reflection. The phase of the reflected wave ~~of~~ relative to the input phase is $0°$ at θ_{ic} & moves smoothly to $180°$ at $90°$ (grazing incidence).

The transmitted wave is a damped exponential normal to the interface w/ a damping factor of

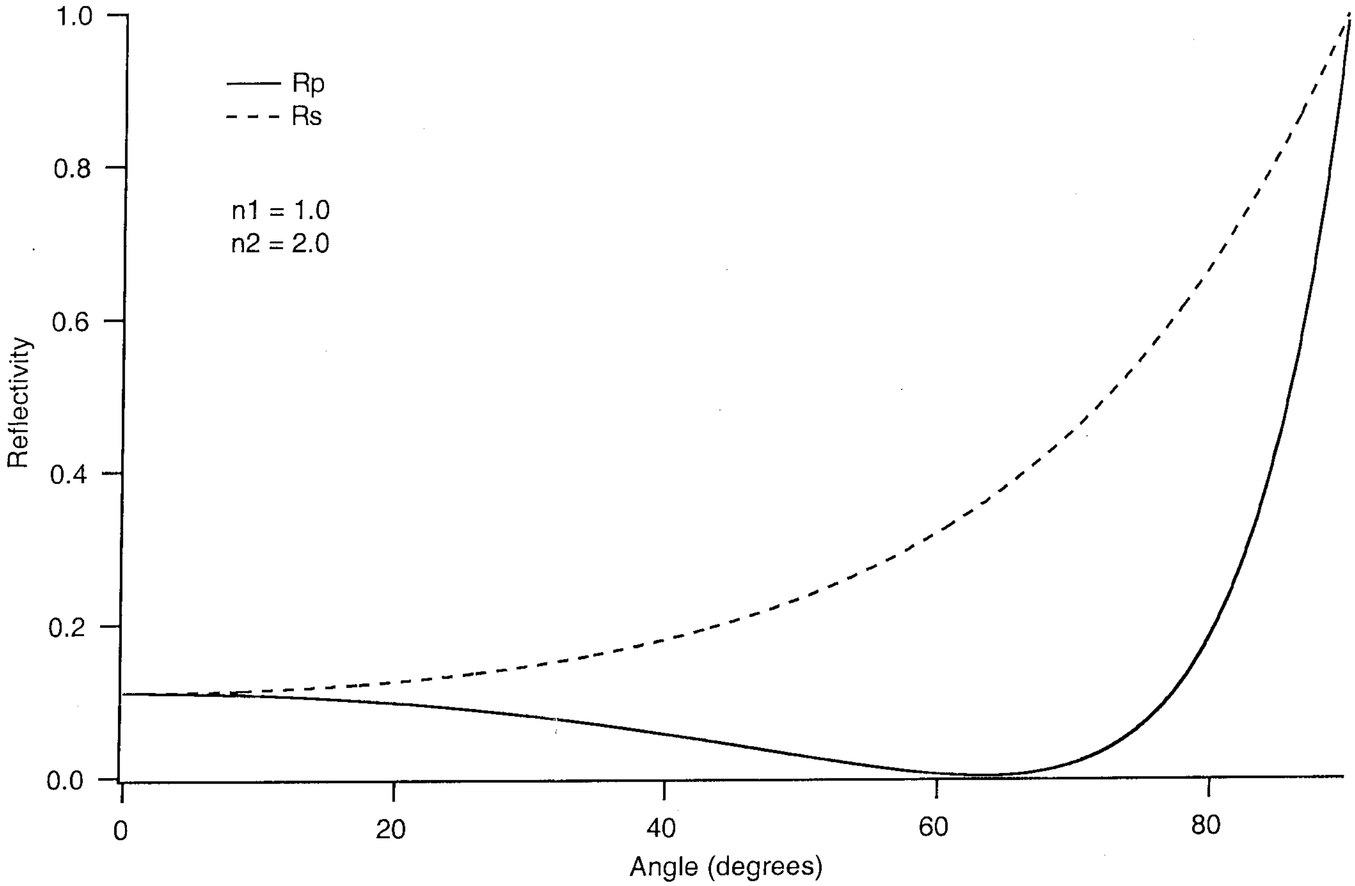
$$\delta_z = \frac{\lambda}{2\pi\left(\left(\frac{n_1}{n_2}\right)^2 \sin^2\theta_i - 1\right)^{1/2}}$$

Using the Eqns in Hansen, we can calculate the Electric Field intensity ratio, $\left\langle \frac{E_{xyz}}{E_{0i}} \right\rangle^2$ at the surface for the TIR (or any other geometry. The enhancement factors are always largest at θ_{ic}, and is always 4 for s-polarized light, and for p-polarized light $\langle E_x \rangle^2 = 0$ & $\left\langle \frac{E_z}{E_i} \right\rangle^2 = 4\left(\frac{n_1}{n_1+n_2}\right)^2$

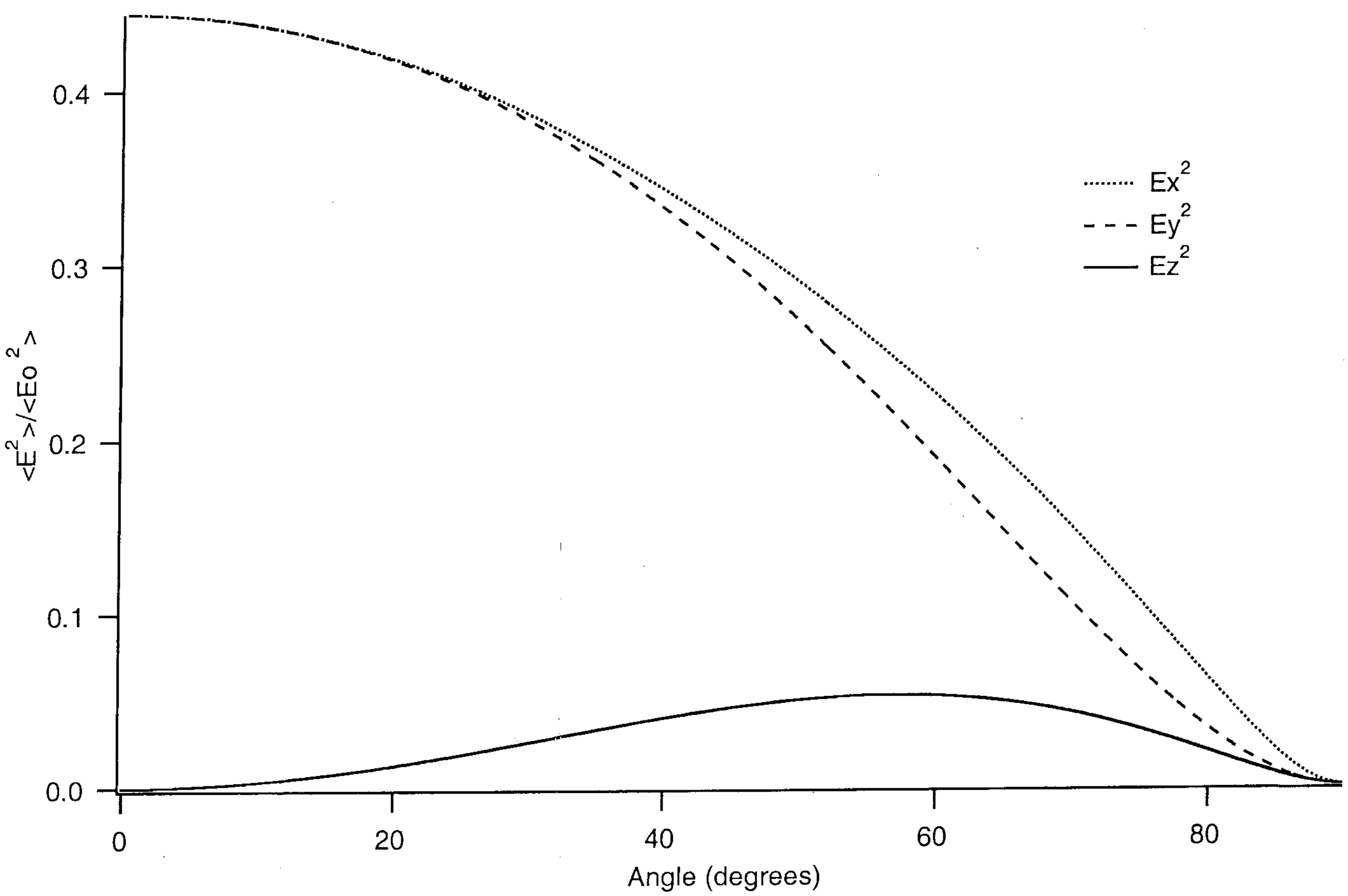
e. Metal Surfaces.

Similar Fresnel Calculations can be made for metal surfaces, where now $\hat{n}_2 = \underbrace{0.1}_{\text{small real}} + \overbrace{5i}^{\text{large imaginary part.}}$

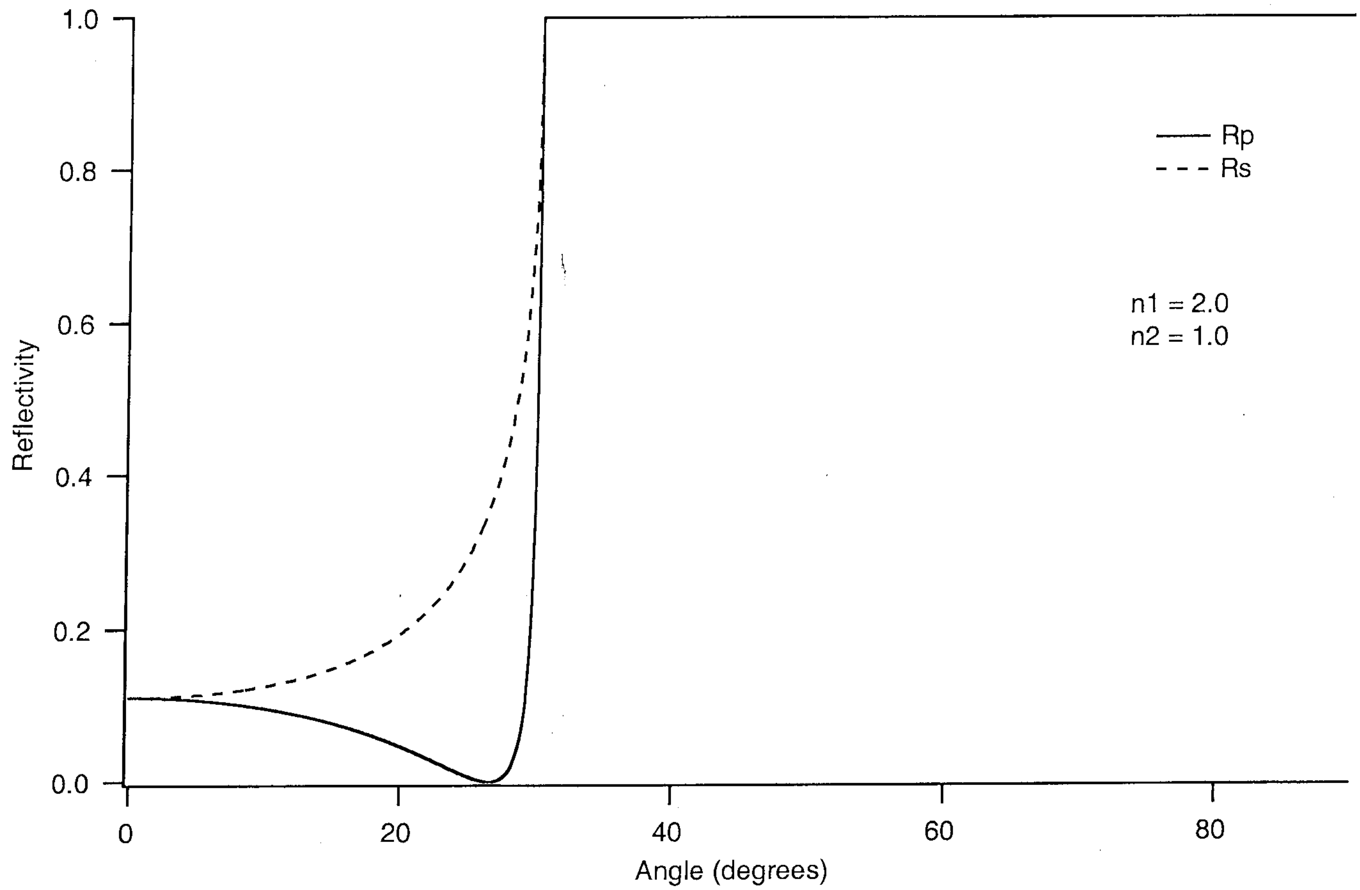
See graphs & homework.

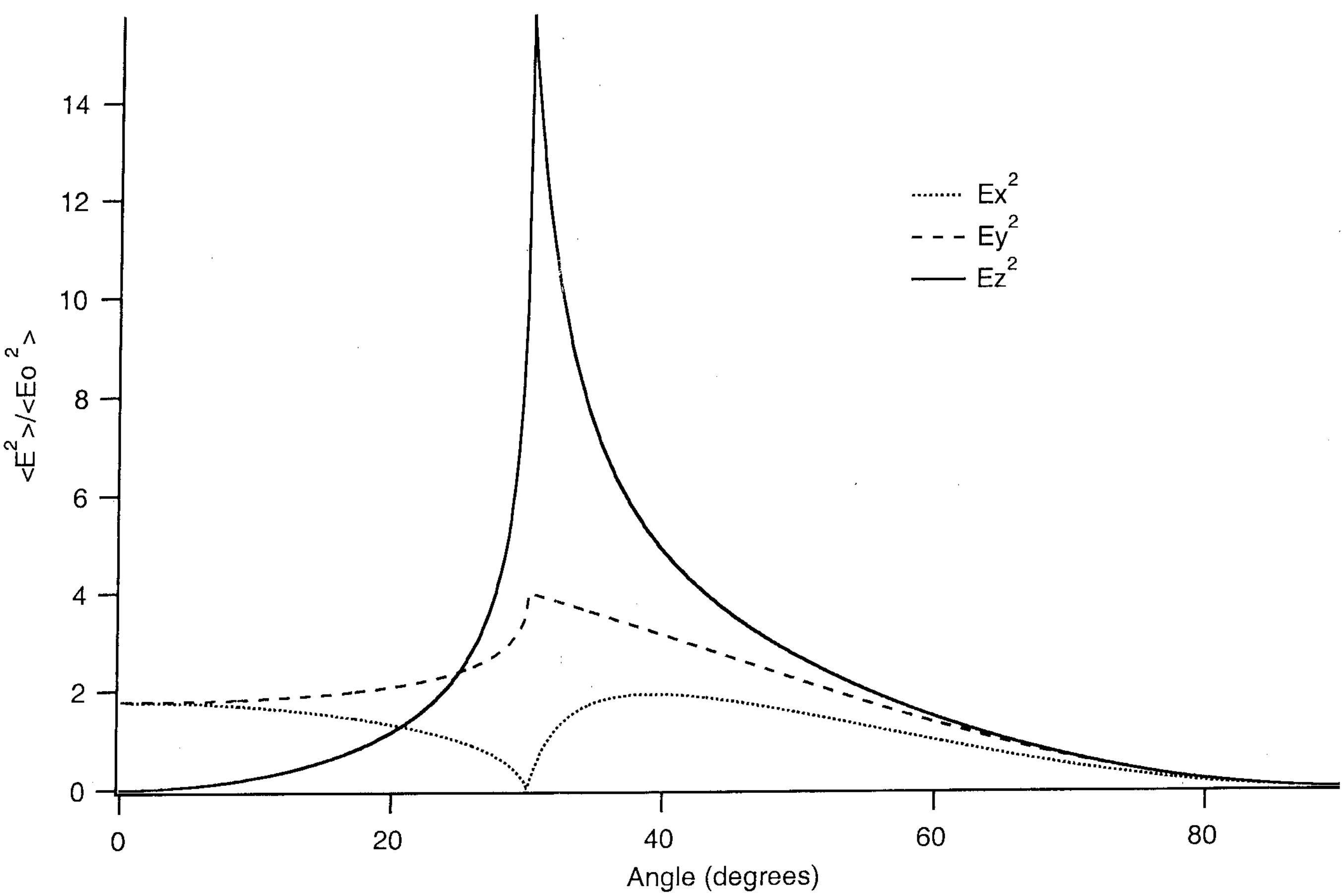


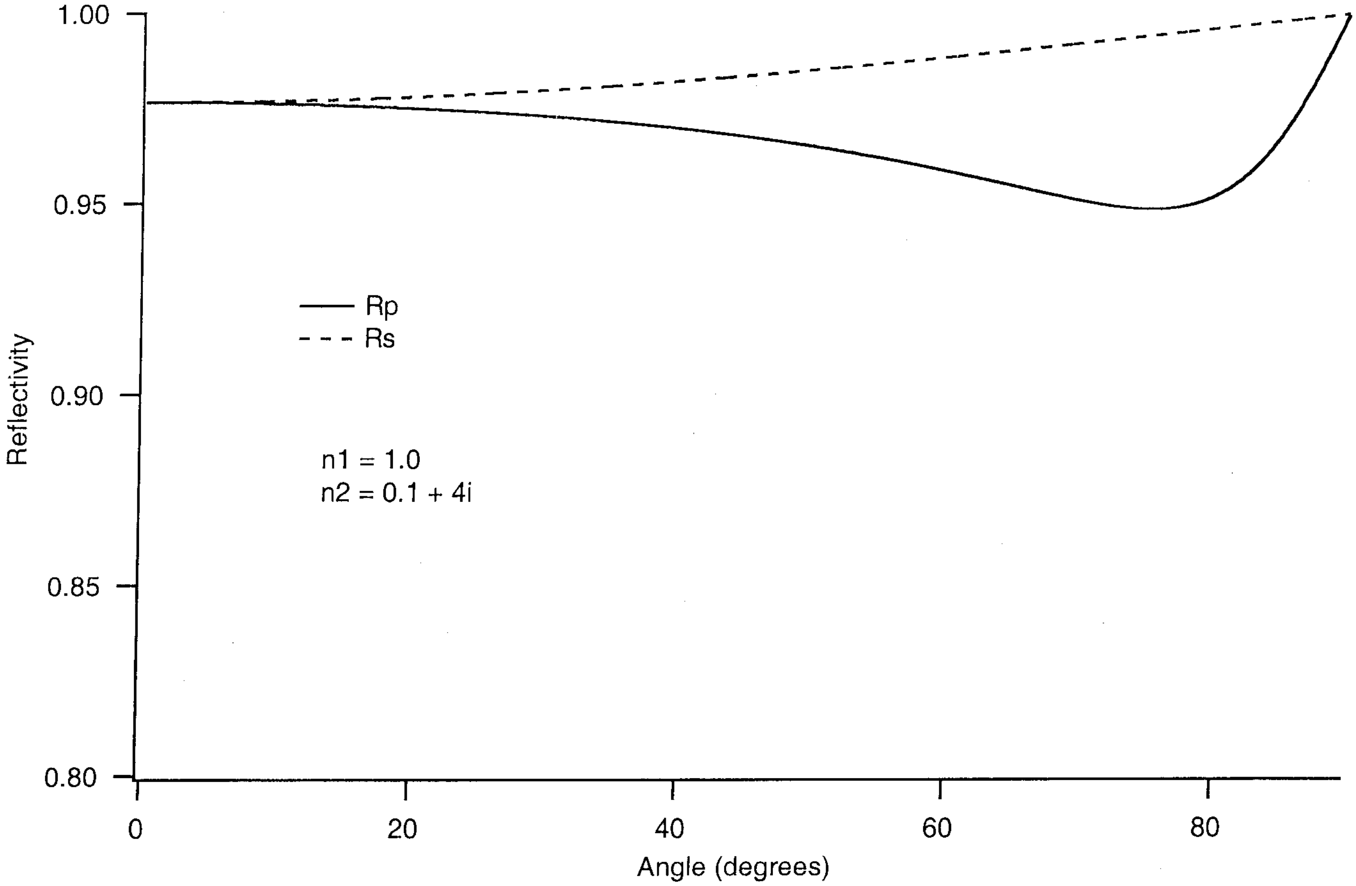
Rp
Rs
n1 = 1.0
n2 = 2.0
Reflectivity
1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
Angle (degrees)

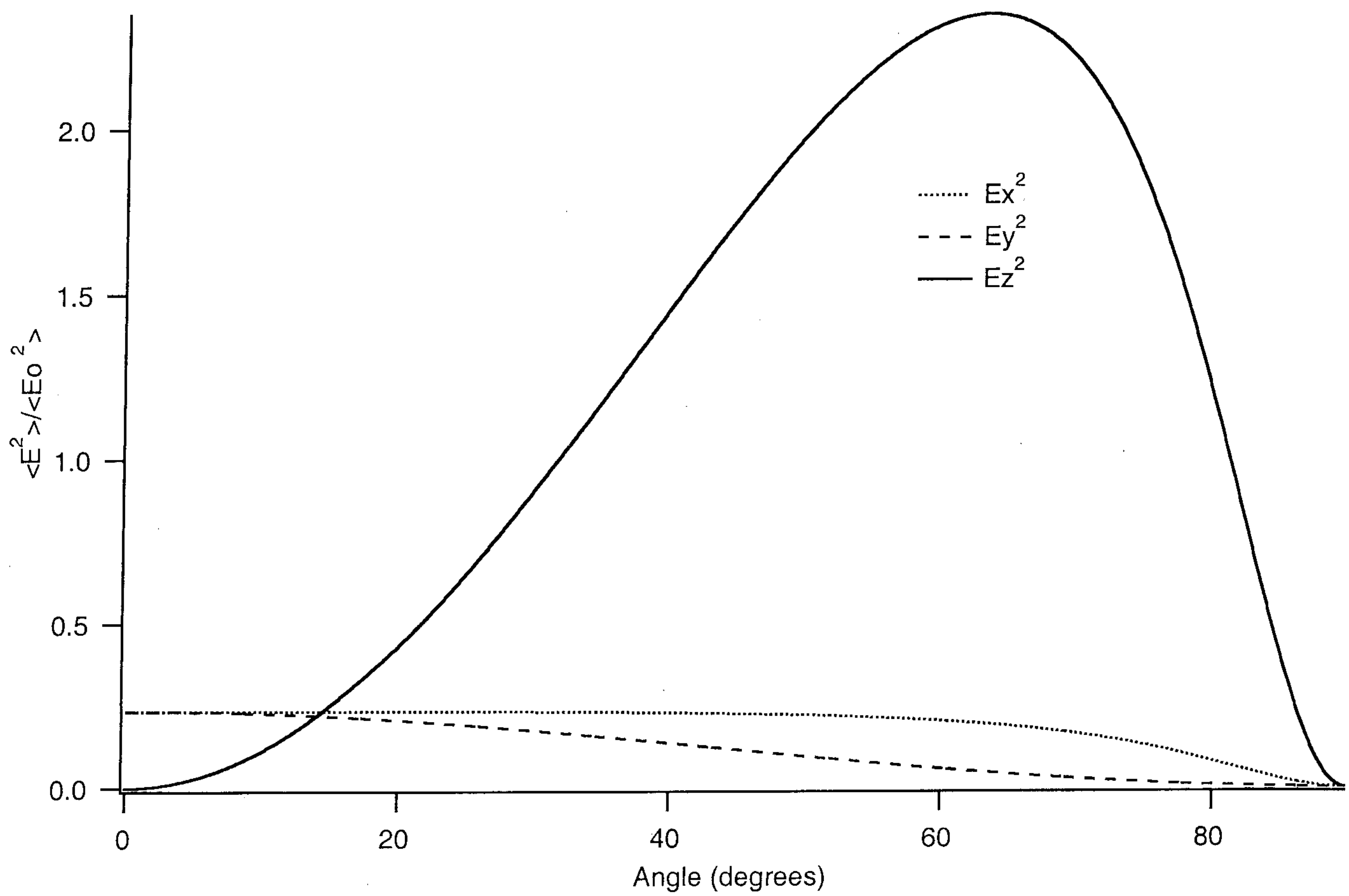


Ex^2
Ey^2
Ez^2
$<E^2>/<Eo^2>$
0.4
0.3
0.2
0.1
0.0
0
20
40
60
80
Angle (degrees)


1.0
0.8
0.6
0.4
0.2
0.0
Reflectivity
0
20
40
60
80
Angle (degrees)
Rp
Rs
n1 = 2.0
n2 = 1.0


14
12
10
8
6
4
2
0
$<E^2>/<Eo^2>$
0
20
40
60
80
Angle (degrees)
Ex^2
Ey^2
Ez^2


1.00
0.95
0.90
0.85
0.80
Reflectivity
Rp
Rs
n1 = 1.0
n2 = 0.1 + 4i
0
20
40
60
80
Angle (degrees)


2.0
1.5
1.0
0.5
0.0
$<E^2>/<Eo^2>$
Ex^2
Ey^2
Ez^2
0
20
40
60
80
Angle (degrees)