Part III Optical Properties of Materials

Chap. 10 The optical constants

Chap. 11 Atomistic Theory of the Optical Properties

Chap. 12 Quantum Mechanical Treatment of the Optical Properties

Chap. 13 Applications

Introduction

✓ The interactions of light with the valence electrons of a material is postulated to be responsible for the optical properties.

✓ Light comprises only extremely small segment of the entire electromagnetic spectrum (Fig 10.1)

✓ Optical methods are among the most important tools for elucidating the electron structure of matter

✓ Optical devices : lasers, photodetectors, waveguides, light-emitting diodes, flat-panel displays

✓ Applications for communication : fiber optics, medical diagnostics, night viewing, solar applications, optical computing and etc..

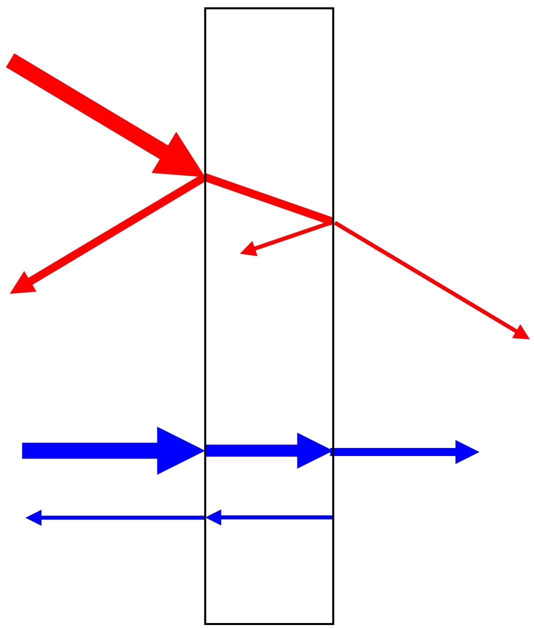
✓ Traditional utilizations: widows, antireflection coating; lenses, mirrors, etc..

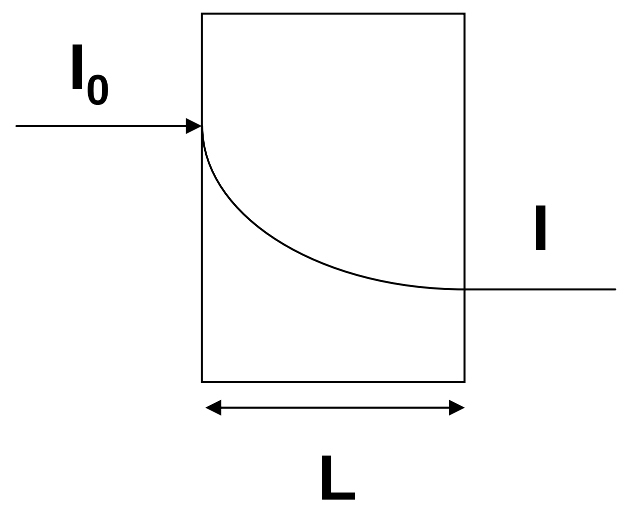
cf) BBR (black body radiation)

Introduction

Interactions between light and matter

- Refraction
- Reflection
- Transmission
- Absorption
- Luminescence





$I/I_0 = ?$

What is light?

Light

- Speed: c~3x10^{10} cm/s in vacuum
- Ray: geometric optics such as lens, mirror
- Electromagnetic wave: refraction, reflection, interference, diffraction, hollogram, etc.
- A stream of photons: absorption and emission

Spectrum (wavelength) of light

γ-ray (10^{-2} Å) ~ X-ray (1 Å) ~ UV(100 nm)
~ visible (400nm (blue) ~ 700nm (red))
~ IR (~10 μm) ~ microwave (GHz) ~ radio (MHz-KHz)

Introduction

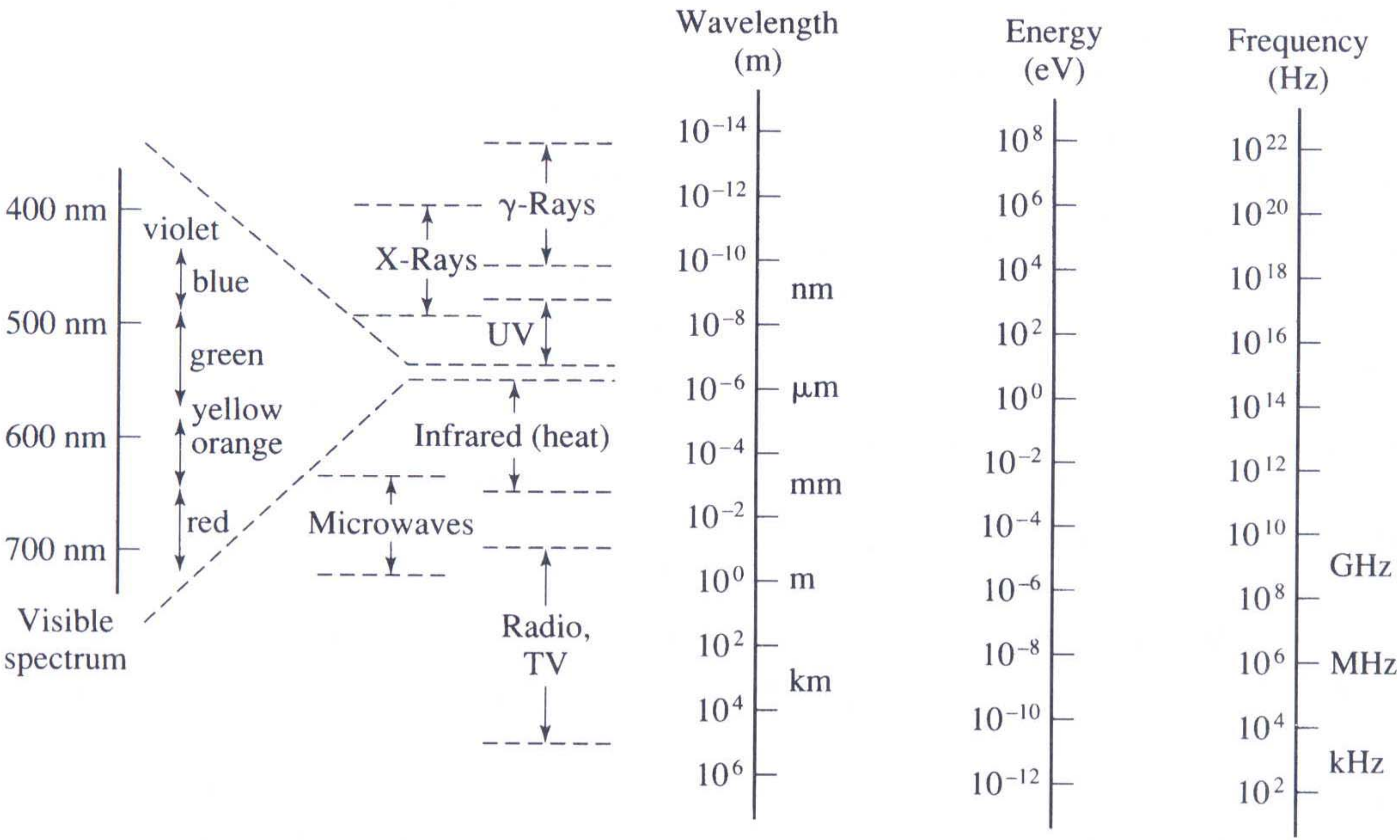
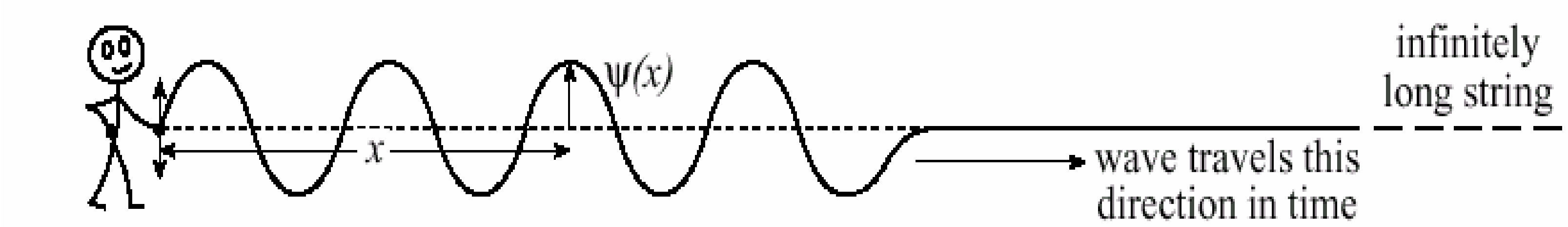


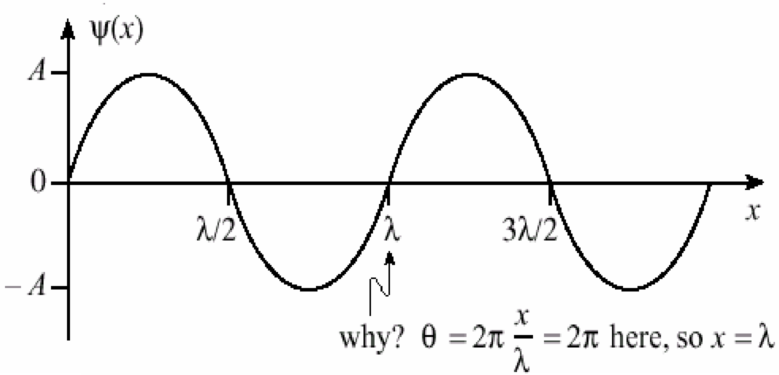
Figure 10.1. The spectrum of electromagnetic radiation. Note the small segment of this spectrum that is visible to human eyes.

Introduction

Electromagnetic Wave

Periodic displacement in time and position



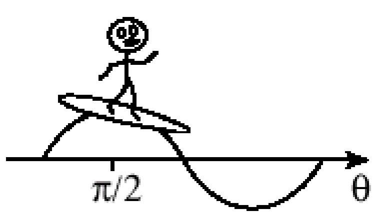


$$\psi(x,t) = A\sin\left(2\pi\frac{x}{\lambda} \pm 2\pi\nu t\right) = A\sin\left(2\pi\left[\frac{x}{\lambda} \pm \nu t\right]\right).$$

$$\boxed{k \equiv \frac{2\pi}{\lambda}} \text{ and } \boxed{\omega \equiv 2\pi\nu}.$$

$$\boxed{\psi(x,t) = A\sin(kx \pm \omega t)}.$$

$$\boxed{\psi(x,t) = A\cos(kx \pm \omega t)},$$



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

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

Introduction

Electromagnetic Wave

- $\mathbf{E} = \mathbf{A} \cos(kx - \omega t + \phi)$,
- $\mathbf{E} = \mathbf{A}/2\ [\exp\{i(kx - \omega t + \phi)\} + cc]$,
- $\mathbf{E} = \mathrm{Re}\ [\mathbf{A} \exp\{i(kx - \omega t + \phi)\}]$,
- $\mathbf{E} = \mathbf{A}\exp\{i(kx - \omega t + \phi)\}$ for convienence:
  - This, of course, is not strictly correct; when it happens, it is always understood that what is meant by this equation is the real part of Aexp$\{i(kx\text{-}wt)\}$. This representation is OK for linear mathematical operations, such as differentiation, integration, and summation, are concerned. The exception is the product or power.

- **E**: electric field
- **A**: amplitude, $I = \mathbf{E} \bullet \mathbf{E}^*$
- k: wavenumber, wavevector ($=2\pi/\lambda$)
- ω: angular frequency ($=2\pi\nu$)
- ϕ: phase

Intensity of a Light Wave, I: the quantity which determines the amount of energy per unit time per unit cross-sectional area that is carried by a wave:

$$I = \psi^2 = \frac{Energy}{Time \cdot Area} = \frac{Power}{Area}\left(\frac{\text{Watts}}{\text{meters}^2}\right).$$

Electromagnetic Wave

- Polarization state specified by the electric field vector, **E**(**r**,t)
- Assuming propagation in the z-direction
  - Transverse wave lies in xy-plane
  - Two mutually independent components are

$$E_x = A_x \cos(\omega t - kz + \delta_x)$$

$$E_y = A_y \cos(\omega t - kz + \delta_y)$$

  - A_x, A_y are independent positive amplitudes
  - δ_x, δ_y are independent phases
- These correspond to elliptic polarization with relative phase $\delta=\delta_y-\delta_x$.

Electromagnetic Wave

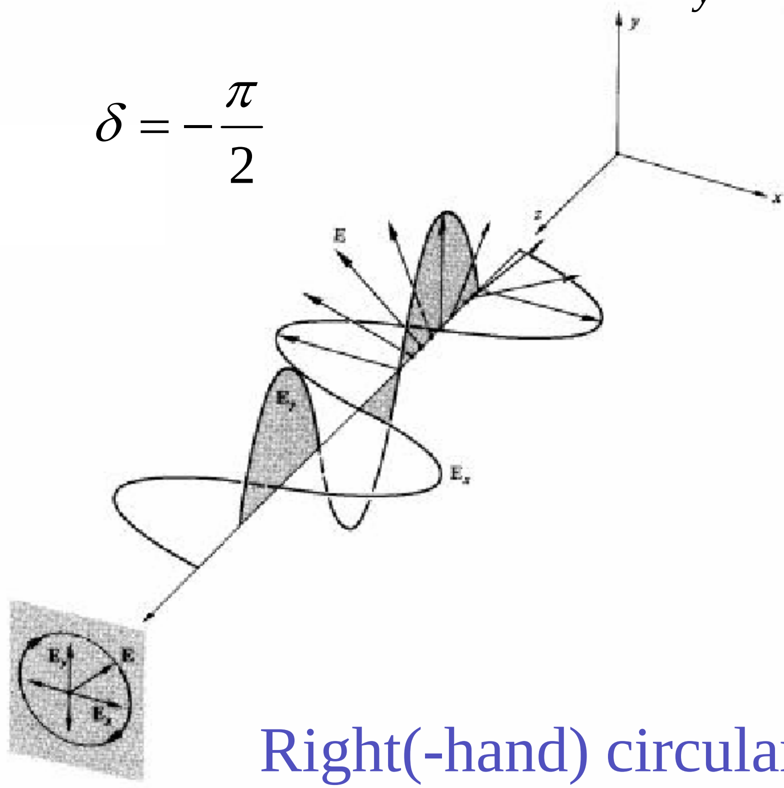
Polarization of light-circular polarization

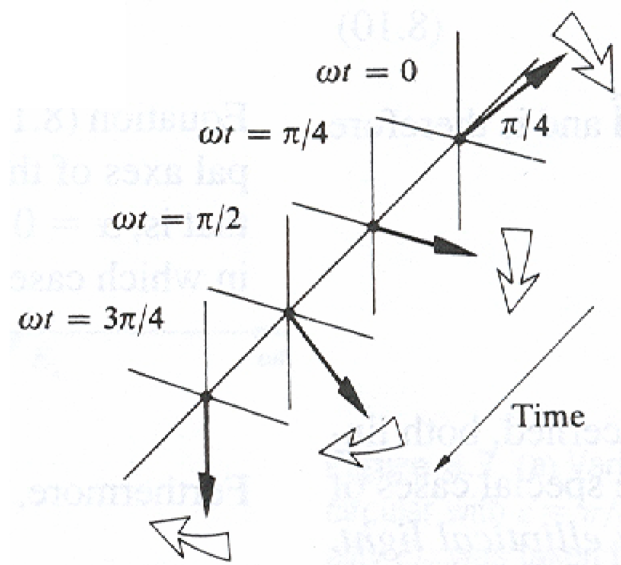
$\delta=\delta_y-\delta_x=\pm\pi/2$, $A_y = A_x$

$$E_x = A_x \cos(\omega t - kz + \delta_x)$$

$$E_y = A_y \cos(\omega t - kz + \delta_y)$$

$$\delta = -\frac{\pi}{2}$$





Right(-hand) circularly polarized

(look back at the source)

Electromagnetic Wave

Polarization of light-circular polarization

Beam of light is circularly polarized if the electric field vector undergoes uniform rotation in the xy-plane

$$\delta = \delta_y - \delta_x = \pm\pi/2$$

$$A_y = A_x$$

Beam of light is right-hand circularly polarized when $\delta = -\pi/2$ which corresponds to counter-clockwise rotation of the E field vector in xy-plane

Beam of light is left-hand circularly polarized when $\delta = +\pi/2$ which corresponds to clockwise rotation of the E field vector in xy-plane.

A linear polarized wave can be synthesized from two oppositely polarized circular or elliptic waves of equal amplitude.

Contents

10 The optical Constants

The Optical Constants

10.2 Index of Refraction, *n*

Snell's law : refractive power of a material

$$\frac{\sin\alpha}{\sin\beta} = \frac{n_{\text{med}}}{n_{\text{vac}}} = n$$

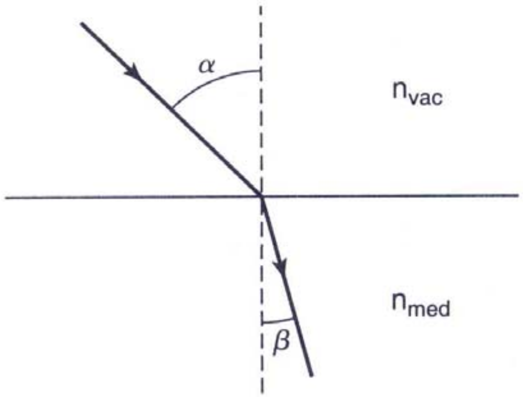


Figure 10.2. Refraction of a light beam when traversing the boundary from an optically thin medium into an optically denser medium.

The index of refraction of vacuum, n_{vac} is arbitrarily set to be unity

$$\frac{\sin\alpha}{\sin\beta} = \frac{c_{\text{vac}}}{c_{\text{med}}} \quad \text{thus} \quad n = \frac{c_{\text{vac}}}{c_{\text{med}}} = \frac{c}{\upsilon}$$

light passes from vacuum into a medium

Dispersion: the property that the magnitude of the refractive index, *n* depends on the wavelength of the incident light. In metals, *n* also varies with ω

When light passes from vacuum into a medium, its velocity as well as its wavelength decreases in order to keep the frequency constant.

10.3 Damping Constant, *k*

Consider a plane-polarized wave propagating along the positive *z*-axis and which vibrates in the *x*-direction. (Fig.10.3) We neglect possible magnetic effects. The electromagnetic wave equation may be written as

$$c^2 \frac{\partial^2 E_x}{\partial z^2} = \varepsilon \frac{\partial^2 E_x}{\partial t^2} + \frac{\sigma}{\varepsilon_0} \frac{\partial E_x}{\partial t}$$

See (A. 26) in Appendix 1

Where E_x is the *x*-component of the electric field strength, ε is the dielectric constant, σ is the (a.c.) conductivity and ε_0 is a constant, called permittivity of empty space

The solution to the above wave equation

$$E_x = E_0 \exp\left[i\omega \left(t - \frac{zn}{c} \right) \right]$$

E_0 is the maximal value of the electric field strength and $\omega = 2\pi\nu$ is the angular frequency

10.3 Damping Constant, *k*

Differentiating the above equation once with respect to time and twice with respect to time and *z*, and inserting these values into the wave equation yields

$$\hat{n}^2 = \varepsilon - \frac{\sigma}{\varepsilon_0 \omega} i = \varepsilon - \frac{\sigma}{2\pi\varepsilon_0 \nu} i \qquad \text{and} \qquad \hat{n} = n_1 - in_2$$

***n_2* is often denoted by *k* and then (10.7) written as** $\hat{n} = n - ik$

***n_2* or *k* is the damping constant (sometimes called, *absorption constant*, attenuation index, or *extinction coefficient*).**

$$\hat{n}^2 = n^2 - k^2 - 2nki = \varepsilon - \frac{\sigma}{2\pi\varepsilon_0 \nu} i$$

Then $\varepsilon = n^2 - k^2 \qquad \sigma = 4\pi\varepsilon_0 nk\nu$

And $\hat{n}^2 = n^2 - k^2 - 2nik \equiv \hat{\varepsilon} = \varepsilon_1 - i\varepsilon_2$

$$\varepsilon_1 = n^2 - k^2 \qquad \varepsilon_2 = 2nk = \frac{\sigma}{2\pi\varepsilon_0 \nu}$$

10.3 Damping Constant, *k*

ε_1, ε_2: The real and the imaginary parts of the complex dielectric constant

ε_2: absorption (product)

For insulator ($\sigma \approx 0$) it follows from (10.11) that $k \approx 0$. then (10.10) reduces to $\varepsilon = n^2$ (Maxwell relation).

$$n^2 = \frac{1}{2}\left(\sqrt{\varepsilon^2 + \left(\frac{\sigma}{2\pi\varepsilon_0\nu}\right)^2} + \varepsilon\right) = \frac{1}{2}\left(\sqrt{\varepsilon_1^2 + \varepsilon_2^2} + \varepsilon_1\right)$$

$$k^2 = \frac{1}{2}\left(\sqrt{\varepsilon^2 + \left(\frac{\sigma}{2\pi\varepsilon_0\nu}\right)^2} - \varepsilon\right) = \frac{1}{2}\left(\sqrt{\varepsilon_1^2 + \varepsilon_2^2} - \varepsilon_1\right)$$

Table 10.1. Characteristic Penetration Depth, W, and Damping Constant, k, for Some Materials ($\lambda = 589.3$ nm).

Material	Water	Flint glass	Graphite	Gold
W(cm)	32	29	6×10^{-6}	1.5×10^{-6}
k	1.4×10^{-7}	1.5×10^{-7}	0.8	3.2

The Optical Constants

10.3 Damping Constant, *k*

Return to (10.5)

$$E_x = E_0 \exp\left[i\omega\left(t - \frac{zn}{c} \right) \right]$$

Replace the index of refraction by complex index of refraction (10.8)

$$E_x = E_0 \exp\left[i\omega\left(t - \frac{z(n-ik)}{c} \right) \right]$$

$$E_x = E_0 \exp\underbrace{\left[-\frac{\omega k}{c} z \right]}_{\text{damped}} \cdot \exp\underbrace{\left[i\omega\left(t - \frac{zn}{c} \right) \right]}_{\text{undamped}}$$

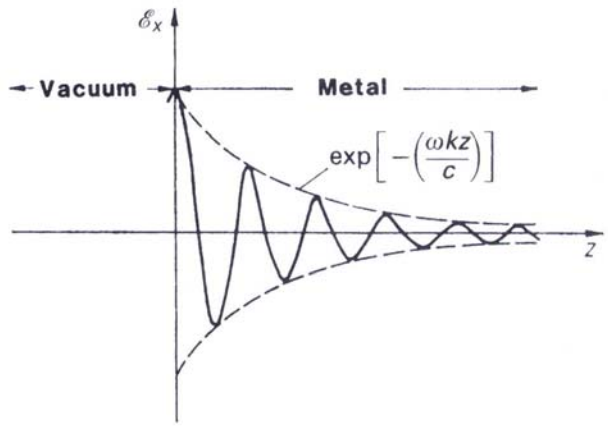


Figure 10.4. Modulated light wave. The amplitude decreases exponentially in an optically dense material. The decrease is particularly strong in metals, but less intense in dielectric materials, such as glass.

Damping constant, *k* determines how much the amplitude decreases : the degree of damping of the light wave

At high frequencies the electromagnetic wave are conducted only on the outer surface of wire : *skin effect*

The Optical Constants

10.4 Characteristic Penetration Depth, W, and Absorbance, α

The damping term in (10.18)

$$I = E^2 = I_0 \exp\left(-\frac{2\omega k}{c} z\right)$$

$$\frac{I}{I_0} = \frac{1}{e} = e^{-1}$$

We define a characteristic penetration depth, *W*, as that distance at which the intensity of the light wave, which travels through a material, has decreased to 1/e of its original value

in conjunction with (10.19)

$$z = W = \frac{c}{2\omega k} = \frac{c}{4\pi \nu k} = \frac{\lambda}{4\pi k}$$

The inverse of W is called attenuation or the absorbance

By making use of (10.21), (10.14), and (10,11)

$$\alpha = \frac{4\pi k}{\lambda} = \frac{2\pi \varepsilon_2}{\lambda n} = \frac{\sigma}{n c \varepsilon_0} = \frac{2\omega k}{c}$$

10.5 Reflectivity, R, and Transmittance T

Determination for the reflectivity $R = \frac{I_R}{I_0}$

I_R the reflected intensity

I_0 incoming intensity

transmissivity, or transmittance $T = \frac{I_T}{I_0}$

Experiments have shown that for insulators, *R* depends solely on the index of refraction. For perpendicular incidence one finds.

$$R = \frac{(n-1)^2}{(n+1)^2}$$

Also, can be derived from Maxwell equations

n is generally a complex quantity. *R* should be real. Thus, *R* becomes

$$R = \left|\frac{\hat{n}-1}{\hat{n}+1}\right|^2$$

$$R = \frac{(n-ik-1)}{(n-ik+1)} \cdot \frac{(n+ik-1)}{(n+ik+1)} = \frac{(n-1)^2+k^2}{(n+1)^2+k^2}$$

10.5 Reflectivity, *R*, and Transmittance *T*

The reflectivity is also a function of ε_1, ε_2

$$R = \frac{n^2 + k^2 + 1 - 2n}{n^2 + k^2 + 1 + 2n}$$

(1) $$n^2 + k^2 = \sqrt{(n^2 + k^2)^2} = \sqrt{n^4 + 2n^2k^2 + k^2}$$

$$= \sqrt{n^4 - 2n^2k^2 + k^4 + 4n^2k^2} = \sqrt{(n^2 - k^2)^2 + 4n^2k^2}$$

$$= \sqrt{\varepsilon_1^2 + \varepsilon_2^2}$$

(2) $$2n = \sqrt{4n^2} = \sqrt{2(n^2 + k^2 + n^2 - k^2)} = \sqrt{2(\sqrt{\varepsilon_1^2 + \varepsilon_2^2} + \varepsilon_1)}$$

Inserting (1) and (2) into (10.26)

$$R = \frac{\sqrt{\varepsilon_1^2 + \varepsilon_2^2} + 1 - \sqrt{2(\sqrt{\varepsilon_1^2 + \varepsilon_2^2} + \varepsilon_1)}}{\sqrt{\varepsilon_1^2 + \varepsilon_2^2} + 1 + \sqrt{2(\sqrt{\varepsilon_1^2 + \varepsilon_2^2} + \varepsilon_1)}}$$

10.6 Hagen-Ruben Relation

To find relationship between reflectivity and conductivity

For small frequency (i.e $\nu < 10^{13} s^{-1}$) the ratio $\sigma/2\pi\varepsilon_0\nu$ for metals is very large $\sigma/2\pi\varepsilon_0\nu \approx 10^{17} s^{-1}$. with $\varepsilon \approx 10$ we obtain

$$\frac{\sigma}{2\pi\varepsilon_0\nu} \approx \frac{10^{17}}{10^{13}} \gg \varepsilon$$

Then (10.15) and (10.16) reduce to $n^2 \approx \frac{\sigma}{2\pi\varepsilon_0\nu} \approx k^2$

By combing the slightly modified equation (10.26) with (10.31)

$$R = \frac{n^2 + 2n + k^2 + 1 - 4n}{n^2 + 2n + 1 + k^2} = 1 - \frac{4n}{2n^2 + 2n + 1}$$

10.6 Hagen-Ruben Relation

If $2n+1$ is neglected as small compared to $2n^2$ (which can be done only for small frequencies for which n is much larger than 1), then (10.32) reduces by using (10.31) to

$$R = 1 - \frac{2}{n} = 1 - 2\sqrt{\frac{\nu}{\sigma}\pi\varepsilon_0}$$

Set $\sigma = \sigma_0$ which is again only permissible for small frequencies, i.e., in the infrared region of the spectrum . This yields the Hagen-Ruben equation

$$R = 1 - 2\sqrt{\frac{\nu}{\sigma_0}\pi\varepsilon_0}$$

The Hagen-Ruben relation is only valid at frequencies below 10^{13} s^{-1}, or equivalently, at wavelength larger than about 30μm