

Drude Model

for dielectric constant of metals.

- Conduction Current in Metals
- EM Wave Propagation in Metals
- Skin Depth
- Plasma Frequency

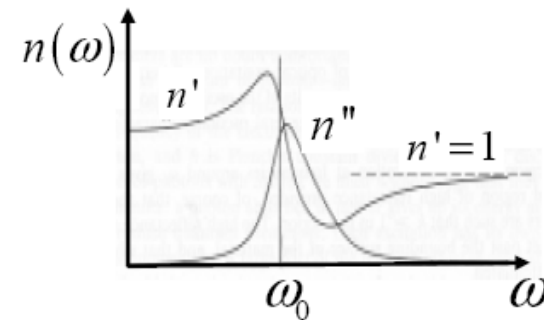
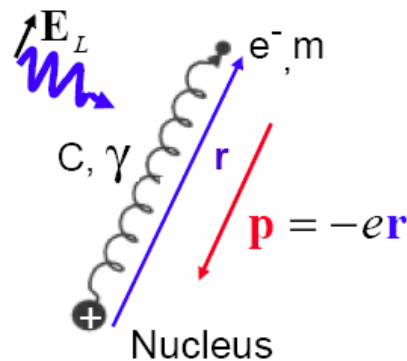
Ref : Prof. Robert P. Lucht, Purdue University

Drude model

- Drude model : Lorentz model (Harmonic oscillator model) without restoration force (that is, free electrons which are not bound to a particular nucleus)

Linear Dielectric Response of Matter

Lorentz model (harmonic oscillator model)



Charges in a material are treated as harmonic oscillators

$$m \mathbf{a}_{el} = \mathbf{F}_{E, Local} + \mathbf{F}_{Damping} + \mathbf{F}_{Spring} \quad (\text{one oscillator})$$

$$m \frac{d^2 \mathbf{r}}{dt^2} + m\gamma \frac{d\mathbf{r}}{dt} + C\mathbf{r} = -e\mathbf{E}_L \exp(-i\omega t)$$

Conduction Current in Metals

The equation of motion of a free electron (not bound to a particular nucleus; $C = 0$),

$$m_e \frac{d^2 \vec{r}}{dt^2} = -C \vec{r} - \frac{m_e}{\tau} \frac{d\vec{r}}{dt} - e \vec{E} \Rightarrow m_e \frac{d\vec{v}}{dt} + m_e \gamma \vec{v} = -e \vec{E}$$

($\tau = \frac{1}{\gamma}$: relaxation time $\approx 10^{-14}$ s)

*Lorentz model
(Harmonic oscillator model)*

If $C = 0$, it is called Drude model

The current density is defined :

$$\vec{J} = -N e \vec{v} \quad \text{with units of } \left[\frac{C}{s \cdot m^2} \right]$$

Substituting in the equation of motion we obtain :

$$\frac{d\vec{J}}{dt} + \gamma \vec{J} = \left(\frac{N e^2}{m_e} \right) \vec{E}$$

Conduction Current in Metals

Assume that the applied electric field and the conduction current density are given by:

$$\vec{E} = \vec{E}_0 \exp(-i\omega t) \quad \vec{J} = \vec{J}_0 \exp(-i\omega t) \quad \leftarrow \text{Local approximation to the current-field relation}$$

Substituting into the equation of motion we obtain:

$$\begin{aligned} \frac{d[\vec{J}_0 \exp(-i\omega t)]}{dt} + \gamma \vec{J}_0 \exp(-i\omega t) &= -i\omega \vec{J}_0 \exp(-i\omega t) + \gamma \vec{J}_0 \exp(-i\omega t) \\ &= \left(\frac{N e^2}{m_e} \right) \vec{E}_0 \exp(-i\omega t) \end{aligned}$$

Multiplying through by $\exp(+i\omega t)$:

$$(-i\omega + \gamma) \vec{J}_0 = \left(\frac{N e^2}{m_e} \right) \vec{E}_0$$

$$\text{or equivalently} \quad (-i\omega + \gamma) \vec{J} = \left(\frac{N e^2}{m_e} \right) \vec{E}$$

Conduction Current in Metals

For static fields ($\omega = 0$) we obtain :

$$\vec{J} = \left(\frac{N e^2}{m_e \gamma} \right) \vec{E} = \sigma \vec{E} \quad \Rightarrow \quad \sigma = \frac{N e^2}{m_e \gamma} = \text{static conductivity}$$

For the general case of an oscillating applied field :

$$\vec{J} = \left[\frac{\sigma}{1 - (i\omega / \gamma)} \right] \vec{E} = \sigma_\omega \vec{E} \quad \sigma_\omega = \text{dynamic conductivity}$$

For very low frequencies, $(\omega / \gamma) \ll 1$, the dynamic conductivity is purely real and the electrons follow the electric field.

As the frequency of the applied field increases, the inertia of electrons introduces a phase lag in the electron response to the field, and the dynamic conductivity is complex.

For very high frequencies, $(\omega / \gamma) \gg 1$, the dynamic conductivity is purely imaginary and the electron oscillations are 90° out of phase with the applied field.

Propagation of EM Waves in

Metals

Maxwell's relations give us the following wave equation for metals:

$$\nabla^2 \vec{E} = \frac{1}{c^2} \frac{\partial^2 \vec{E}}{\partial t^2} + \frac{1}{\epsilon_0 c^2} \frac{\partial \vec{J}}{\partial t} \quad \leftarrow \vec{P} = 0, \vec{J} \neq 0$$

But
$$\vec{J} = \left[\frac{\sigma}{1 - (i\omega/\gamma)} \right] \vec{E}$$

Substituting in the wave equation we obtain:

$$\nabla^2 \vec{E} = \frac{1}{c^2} \frac{\partial^2 \vec{E}}{\partial t^2} + \frac{1}{\epsilon_0 c^2} \left[\frac{\sigma}{1 - (i\omega/\gamma)} \right] \frac{\partial \vec{E}}{\partial t}$$

The wave equation is satisfied by electric fields of the form:

$$\vec{E} = \vec{E}_0 \exp \left[i(\vec{k} \cdot \vec{r} - \omega t) \right]$$

where

$$k^2 = \frac{\omega^2}{c^2} + i \left[\frac{\sigma \omega \mu_0}{1 - (i\omega/\gamma)} \right] \quad c^2 = \frac{1}{\epsilon_0 \mu_0}$$

Skin Depth

Consider the case where ω is small enough that k^2 is given by:

$$k^2 = \frac{\omega^2}{c^2} + i \left[\frac{\sigma \omega \mu_0}{1 - (i\omega/\gamma)} \right] \cong i \sigma \omega \mu_0 = \exp\left(i \frac{\pi}{2}\right) \sigma \omega \mu_0$$

$$\text{Then, } \tilde{k} \cong \sqrt{\exp\left(i \frac{\pi}{2}\right) \sigma \omega \mu_0} = \exp\left(i \frac{\pi}{4}\right) \sqrt{\sigma \omega \mu_0} = \left[\cos\left(\frac{\pi}{4}\right) + i \sin\left(\frac{\pi}{4}\right) \right] \sqrt{\sigma \omega \mu_0} = (1+i) \sqrt{\frac{\sigma \omega \mu_0}{2}}$$

$$k_R = k_I = \sqrt{\frac{\sigma \omega \mu_0}{2}} \quad n_R = \left(\frac{c}{\omega}\right) k_R = \sqrt{\frac{\sigma c^2 \mu_0}{2\omega}} = \sqrt{\frac{\sigma}{2\omega \epsilon_0}} = n_I$$

In the metal, for a wave propagating in the z -direction:

$$\vec{E} = \vec{E}_0 \exp(-k_I z) \exp[i(k_R z - \omega t)] = \vec{E}_0 \exp\left(-\frac{z}{\delta}\right) \exp[i(k_R z - \omega t)]$$

The skin depth δ is given by:

$$\delta = \frac{1}{k_I} = \sqrt{\frac{2}{\sigma \omega \mu_0}} = \sqrt{\frac{2\epsilon_0 c^2}{\sigma \omega}}$$

For copper the static conductivity $\sigma = 5.76 \times 10^7 \text{ } \Omega^{-1} \text{m}^{-1} = 5.76 \times 10^7 \frac{\text{C}^2 - \text{s}}{\text{J} - \text{m}} \rightarrow \delta = 0.66 \mu\text{m}$

Plasma Frequency

Now consider again the general case:

$$k^2 = \frac{\omega^2}{c^2} + i \left[\frac{\sigma \omega \mu_0}{1 - (i\omega/\gamma)} \right]$$

$$n^2 = \frac{c^2}{\omega^2} k^2 = 1 + i \left\{ \frac{\sigma c^2 \mu_0}{\omega [1 - (i\omega/\gamma)]} \right\} = 1 + i \frac{i\gamma}{i\gamma} \left\{ \frac{\sigma c^2 \mu_0}{\omega [1 - (i\omega/\gamma)]} \right\}$$

$$n^2 = 1 - \frac{\gamma \sigma c^2 \mu_0}{\omega^2 + i\omega\gamma}$$

The plasma frequency is defined:

$$\omega_p^2 = \gamma \sigma c^2 \mu_0 = \gamma \left(\frac{N e^2}{m_e \gamma} \right) c^2 \mu_0 = \frac{N e^2}{m_e \epsilon_0}$$

The refractive index of the medium is given by

$$n^2 = 1 - \frac{\omega_p^2}{\omega^2 + i\omega\gamma}$$

Plasma Frequency

If the electrons in a plasma are displaced from a uniform background of ions, electric fields will be built up in such a direction as to restore the neutrality of the plasma by pulling the electrons back to their original positions.

*Because of their inertia, the electrons will overshoot and oscillate around their equilibrium positions with a characteristic frequency known as the **plasma frequency**.*

$E_s = \sigma_o / \epsilon_o = Ne(\delta x) / \epsilon_o$: electrostatic field by small charge separation δx

$\delta x = \delta x_o \exp(-i\omega_p t)$: small-amplitude oscillation

$$m \frac{d^2(\delta x)}{dt^2} = (-e)E_s \quad \Rightarrow \quad -m\omega_p^2 = -\frac{Ne^2}{\epsilon_o} \quad \Rightarrow \quad \therefore \omega_p^2 = \frac{Ne^2}{m\epsilon_o}$$

Plasma Frequency

$$n^2 = \left(\frac{c}{\omega} k \right)^2 = 1 + \frac{i\sigma c^2 \mu_0}{\omega(1 - i\omega/\gamma)} = 1 - \frac{\sigma c^2 \mu_0 \gamma}{\omega^2 + i\omega\gamma}$$

$$n^2 = (n_R + in_I)^2 = 1 - \frac{\omega_p^2}{\omega^2 + i\omega\gamma}$$

$$n^2 = 1 - \frac{\omega_p^2}{\omega^2} \quad \text{by neglecting } \gamma, \text{ valid for high frequency } (\omega \gg \gamma).$$

For $\omega < \omega_p$, n is complex and radiation is attenuated.

For $\omega > \omega_p$, n is real and radiation is not attenuated (transparent).

Plasma Frequency

$$\lambda_c = \lambda_p = \frac{2\pi c}{\omega_p}$$

TABLE XXVIII

The critical wavelengths λ_c below which the alkali metals become transparent, and above which they are opaque and highly reflecting

Metal	Lithium	Sodium	Potassium	Rubidium	Caesium
$(\lambda_c)_{\text{obs}}$	2050 Å	2100 Å	3150 Å	3600 Å	4400 Å
$(\lambda_c)_{\text{calc}}$	1500 Å	2100 Å	2900 Å	3200 Å	3600 Å
$\frac{N_{\text{eff}}}{N}$	0.54	1.00	0.85	0.79	0.67

Born and Wolf, Optics, page 627.

Plasma Frequency

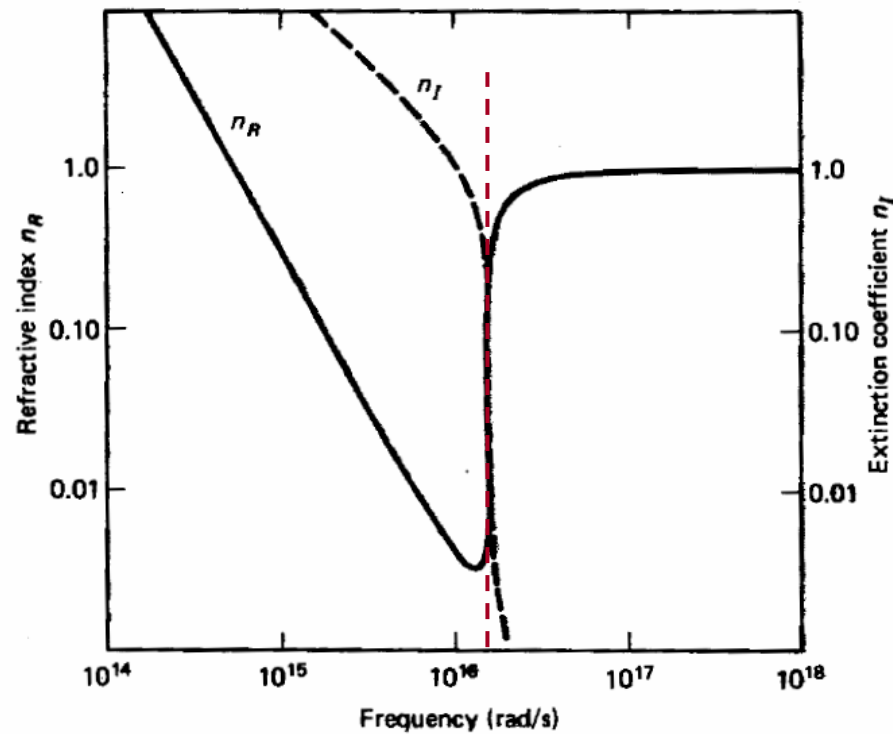


Figure 27-3 Angular frequency dependence of the refractive index n_R and the extinction coefficient n_I for copper. Values assumed are $\omega_p = 1.63 \times 10^{16} \text{ s}^{-1}$ and $\gamma = 4.1 \times 10^{13} \text{ s}^{-1}$. The crossover point of the curves coincides with the plasma frequency.

Dielectric constant of metal : Drude model

$$\begin{aligned}\varepsilon(\omega) &= \varepsilon_R + i\varepsilon_I = n^2 \\ &= (n_R + in_I)^2 = 1 - \frac{\omega_p^2}{\omega^2 + i\omega\gamma} \\ &= (n_R^2 - n_I^2) + i2n_Rn_I \\ &= \left(1 - \frac{\omega_p^2}{\omega^2 + \gamma^2}\right) + i\left(\frac{\omega_p^2\gamma}{\omega^3 + \omega\gamma^2}\right)\end{aligned}$$

Dielectric constant at $\omega \approx \omega_{\text{visible}}$

$$\omega \gg \gamma = \frac{1}{\tau} \quad \Rightarrow \quad \varepsilon(\omega) = \left(1 - \frac{\omega_p^2}{\omega^2}\right) + i\left(\frac{\omega_p^2}{\omega^3 / \gamma}\right)$$

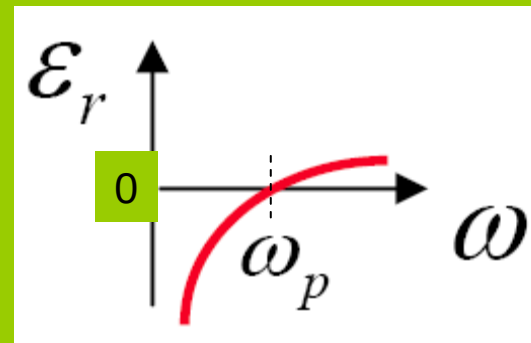
Ideal case : metal as a free-electron gas

Dielectric constant of a free electron gas

- no decay (infinite relaxation time)
- no interband transitions

$$\varepsilon(\omega) \xrightarrow[\gamma \rightarrow 0]{\tau \rightarrow \infty} \varepsilon(\omega) = \left(1 - \frac{\omega_p^2}{\omega^2} \right)$$

$$\varepsilon_r = 1 - \frac{\omega_p^2}{\omega^2}$$



Plasma waves (plasmons)

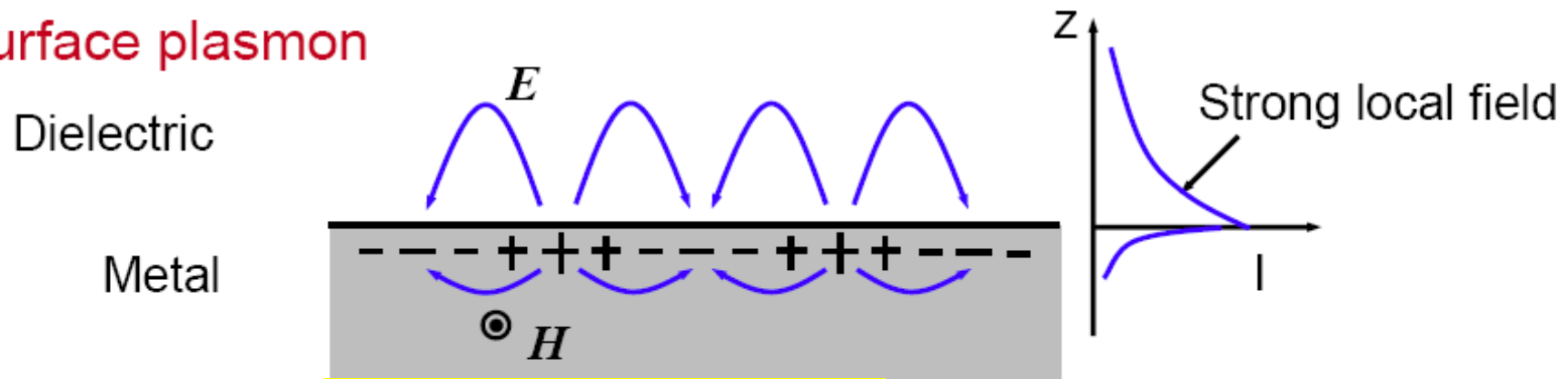
What is a plasmon ?

- Compare electron gas in a metal and real gas of molecules
- Metals are expected to allow for electron density waves: plasmons

Bulk plasmon

- Metals allow for EM wave propagation above the plasma frequency
 ↖ They become transparent!

Surface plasmon

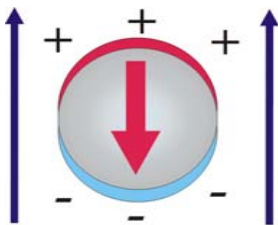
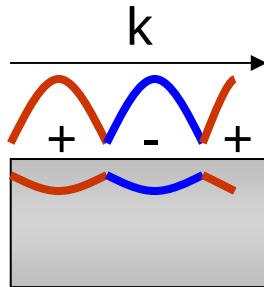
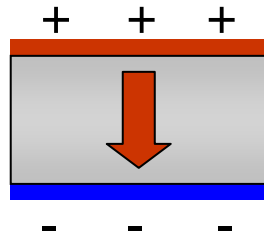


Note: SP is a TM wave!

- Sometimes called a surface plasmon-polariton (strong coupling to EM field)

Plasmons

Plasma oscillation = density fluctuation of free electrons



Plasmons **in the bulk** oscillate at ω_p determined by the free electron density and effective mass

$$\omega_p^{drude} = \sqrt{\frac{Ne^2}{m\epsilon_0}}$$

Plasmons **confined to surfaces** that can interact with light to form propagating “surface plasmon polaritons (SPP)”

Confinement effects result in resonant SPP modes **in nanoparticles**

$$\omega_{particle}^{drude} = \sqrt{\frac{1}{3} \frac{Ne^2}{m\epsilon_0}}$$

Dispersion relation for EM waves in electron gas (bulk plasmons)

Determination of dispersion relation for bulk plasmons

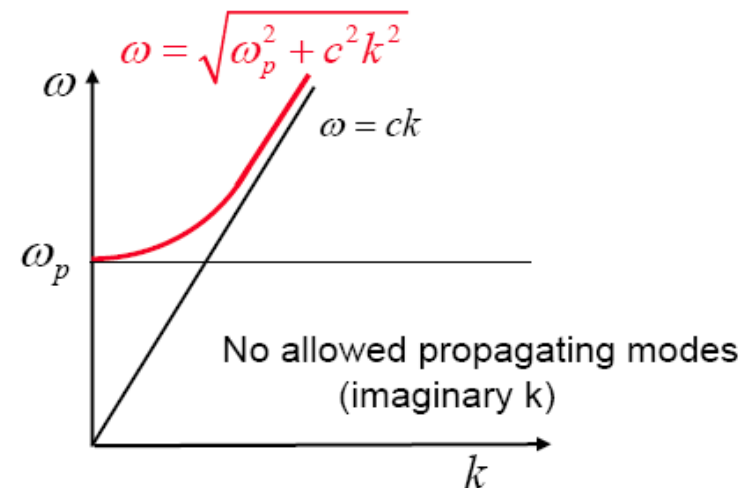
- The wave equation is given by:
$$\frac{\epsilon_r}{c^2} \frac{\partial^2 \mathbf{E}(\mathbf{r}, t)}{\partial t^2} = \nabla^2 \mathbf{E}(\mathbf{r}, t)$$

- Investigate solutions of the form:
$$\mathbf{E}(\mathbf{r}, t) = \text{Re} \{ \mathbf{E}(\mathbf{r}, \omega) \exp(i\mathbf{k} \cdot \mathbf{r} - i\omega t) \}$$

- Dielectric constant:
$$\left. \begin{array}{l} \Rightarrow \omega^2 \epsilon_r = c^2 k^2 \\ \epsilon_r = 1 - \frac{\omega_p^2}{\omega^2} \end{array} \right\} \Rightarrow \omega^2 \left(1 - \frac{\omega_p^2}{\omega^2} \right) = \boxed{\omega^2 - \omega_p^2 = c^2 k^2}$$

- Dispersion relation:

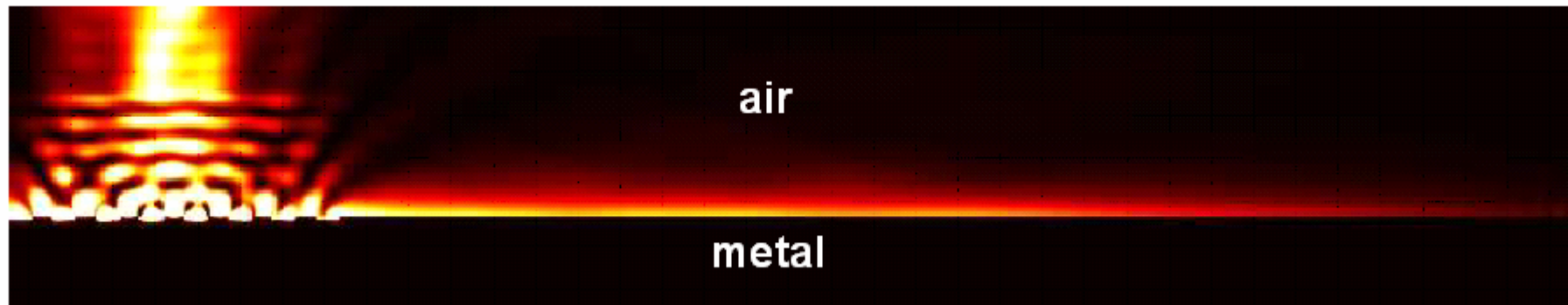
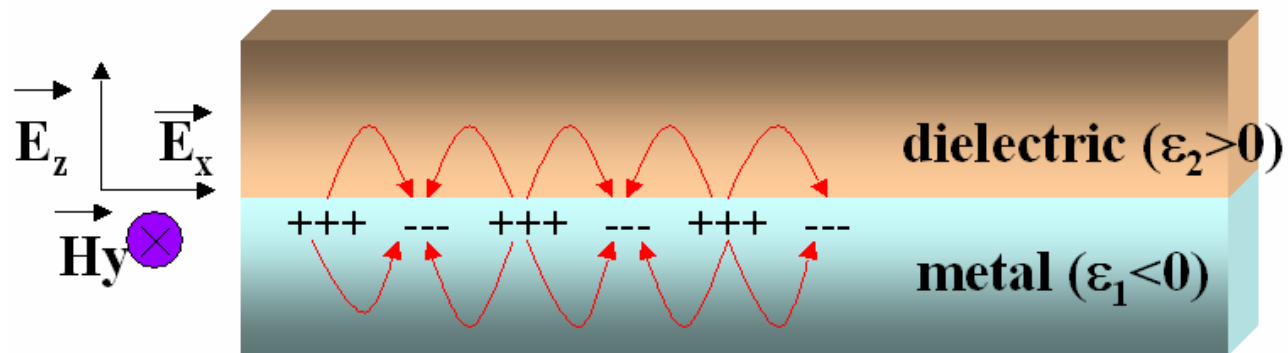
$$\boxed{\omega = \omega(k)}$$



Note1: Solutions lie above light line

Note2: Metals: $\hbar\omega_p \approx 10$ eV; Semiconductors $\hbar\omega_p < 0.5$ eV (depending on dopant conc.)

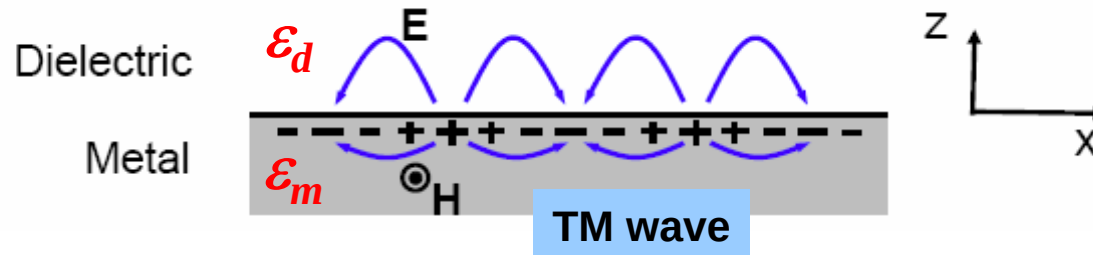
Dispersion relation of surface-plasmon for dielectric-metal boundaries



Dispersion relation for surface plasmon polaritons

Solve Maxwell's equations with boundary conditions

- We are looking for solutions that look like:



- Mathematically:

$$\begin{aligned}
 z > 0 \quad & \begin{cases} H_d = (0, H_{yd}, 0) \exp i(k_{xd}x + k_{zd}z - \omega t) \\ E_d = (E_{xd}, 0, E_{zd}) \exp i(k_{xd}x + k_{zd}z - \omega t) \end{cases} \\
 z < 0 \quad & \begin{cases} H_m = (0, H_{ym}, 0) \exp i(k_{xm}x + k_{zm}z - \omega t) \\ E_m = (E_{xm}, 0, E_{zm}) \exp i(k_{xm}x + k_{zm}z - \omega t) \end{cases}
 \end{aligned}$$

- Maxwell's Equations in medium i (i = metal or dielectric):

$$\nabla \cdot \epsilon_i \mathbf{E} = 0 \quad \nabla \cdot \mathbf{H} = 0 \quad \nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t} \quad \nabla \times \mathbf{H} = \epsilon_i \frac{\partial \mathbf{E}}{\partial t}$$

- At the boundary (continuity of the tangential E_x , H_y , and the normal D_z):

$$E_{xm} = E_{xd} \quad H_{ym} = H_{yd} \quad \epsilon_m E_{zm} = \epsilon_d E_{zd}$$

Dispersion relation for surface plasmon polaritons

- Start with curl equation for $\mathbf{H}$ in medium i

$$\left. \begin{aligned} \nabla \times \mathbf{H}_i &= \epsilon_i \frac{\partial \mathbf{E}_i}{\partial t} \\ \text{where } \mathbf{H}_i &= (0, H_{yi}, 0) \exp i(k_{xi}x + k_{zi}z - \omega t) \\ \mathbf{E}_i &= (E_{xi}, 0, E_{zi}) \exp i(k_{xi}x + k_{zi}z - \omega t) \end{aligned} \right\} \Rightarrow$$

$$\left(\frac{\partial H_{zi}}{\partial y} - \frac{\partial H_{yi}}{\partial z}, \frac{\partial H_{xi}}{\partial z} - \frac{\partial H_{zi}}{\partial x}, \frac{\partial H_{yi}}{\partial x} - \frac{\partial H_{xi}}{\partial y} \right) = (\underline{-ik_{zi}H_{yi}}, 0, \underline{ik_{xi}H_{yi}}) = (\underline{-i\omega\epsilon_i E_{xi}}, 0, \underline{-i\omega\epsilon_i E_{zi}})$$

$$k_{zi}H_{yi} = \omega\epsilon_i E_{xi} \Rightarrow \left\{ \begin{aligned} k_{zm}H_{ym} &= \omega\epsilon_m E_{xm} \\ k_{zd}H_{yd} &= \omega\epsilon_d E_{xd} \end{aligned} \right\} \Rightarrow \frac{k_{zm}}{\epsilon_m} H_{ym} = \frac{k_{zd}}{\epsilon_d} H_{yd}$$

- $E_{\parallel}$ across boundary is continuous: $E_{xm} = E_{xd}$

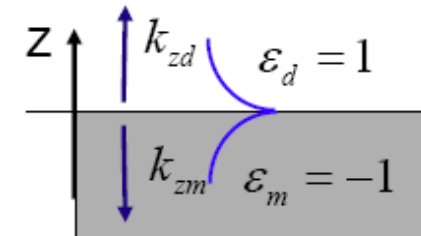
- $H_{\parallel}$ across boundary is continuous: $H_{ym} = H_{yd}$

$$\left. \begin{aligned} \text{Combine with: } \frac{k_{zm}}{\epsilon_m} H_{ym} &= \frac{k_{zd}}{\epsilon_d} H_{yd} \end{aligned} \right\} \Rightarrow \frac{k_{zm}}{\epsilon_m} = \frac{k_{zd}}{\epsilon_d}$$

Dispersion relation for surface plasmon polaritons

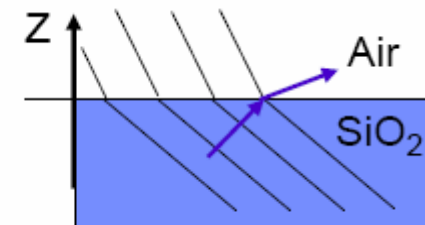
Relations between k vectors

- Condition for SP's to exist: $\frac{k_{zm}}{\epsilon_m} = \frac{k_{zd}}{\epsilon_d}$ Example



- Relation for k_x (Continuity $E_{||}$, $H_{||}$): $k_{xm} = k_{xd}$
true at any boundary

Example



- For any EM wave: $k^2 = \epsilon_i \left(\frac{\omega}{c} \right)^2 = k_x^2 + k_{zi}^2$, where $k_x \equiv k_{xm} = k_{xd}$

- Both in the metal and dielectric: $k_{sp} = k_x = \sqrt{\epsilon_i \left(\frac{\omega}{c} \right)^2 - k_{zi}^2}$
 $\frac{k_{zm}}{\epsilon_m} = \frac{k_{zd}}{\epsilon_d}$ } $\Rightarrow$ **SP Dispersion Relation**
 $k_x = \frac{\omega}{c} \sqrt{\frac{\epsilon_m \epsilon_d}{\epsilon_m + \epsilon_d}}$

Dispersion relation for surface plasmon polaritons

x-direction: $k_x = k'_x + ik''_x = \frac{\omega}{c} \left(\frac{\epsilon_m \epsilon_d}{\epsilon_m + \epsilon_d} \right)^{1/2} \quad \epsilon_m = \epsilon'_m + i\epsilon''_m$

z-direction: $k_{zi}^2 = \epsilon_i \left(\frac{\omega}{c} \right)^2 - k_x^2 \rightarrow k_{zi} = k'_{zi} + ik_{zi} = \pm \frac{\omega}{c} \left(\frac{\epsilon_i^2}{\epsilon_m + \epsilon_d} \right)^{1/2}$

For a bound SP mode:

k_{zi} must be imaginary: $\epsilon_m + \epsilon_d < 0$

$$k_{zi} = \pm \sqrt{\epsilon_i \left(\frac{\omega}{c} \right)^2 - k_x^2} = \pm i \sqrt{k_x^2 - \epsilon_i \left(\frac{\omega}{c} \right)^2} \Rightarrow |k_x| > \sqrt{\epsilon_i} \left(\frac{\omega}{c} \right)$$

+ for $z < 0$
- for $z > 0$

k'_x must be real: $\epsilon_m < 0$

So,

$$\epsilon'_m < -\epsilon_d$$

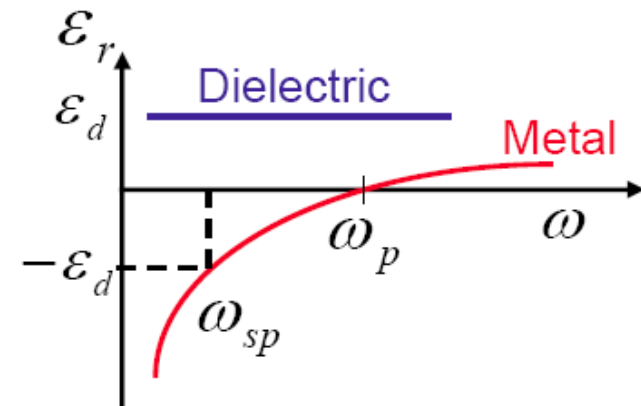
$$H_i = (0, H_{yi}, 0) \exp i(k_{xi}x + k_{zi}z - \omega t)$$

$$E_i = (E_{xi}, 0, E_{zi}) \exp i(k_{xi}x + k_{zi}z - \omega t)$$

Plot of the dispersion relation

- Plot of the dielectric constants:

$$\epsilon_m(\omega) = 1 - \frac{\omega_p^2}{\omega^2}$$



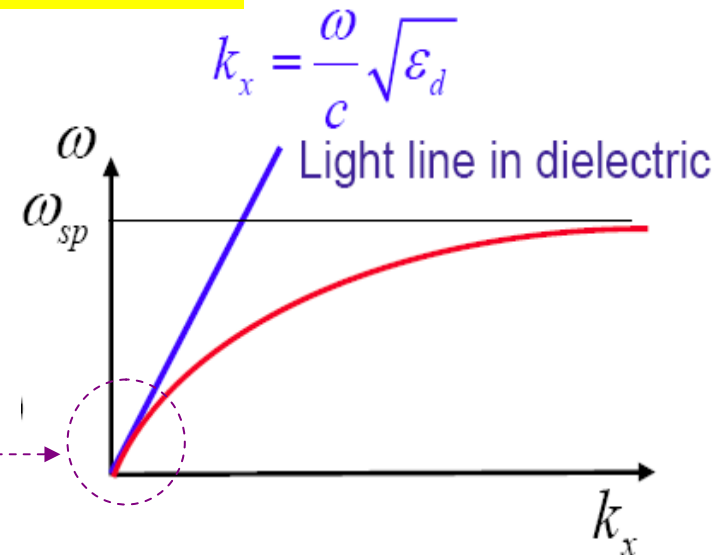
- Plot of the dispersion relation:

$$k_x = \frac{\omega}{c} \sqrt{\frac{\epsilon_m \epsilon_d}{\epsilon_m + \epsilon_d}} \quad \Rightarrow \quad k_x = k_{sp} = \frac{\omega}{c} \sqrt{\frac{(\omega^2 - \omega_p^2) \epsilon_d}{(1 + \epsilon_d) \omega^2 - \omega_p^2}}$$

- When $\epsilon_m \rightarrow -\epsilon_d$,

$$\Rightarrow k_x \rightarrow \infty, \quad \omega \equiv \omega_{sp} = \frac{\omega_p}{\sqrt{1 + \epsilon_d}}$$

- Low ω : $k_x = \frac{\omega}{c} \lim_{\epsilon_m \rightarrow -\infty} \left(\frac{\epsilon_m \epsilon_d}{\epsilon_m + \epsilon_d} \right)^{1/2} \approx \frac{\omega}{c} \sqrt{\epsilon_d}$



Surface plasmon dispersion relation

$$k_x = \frac{\omega}{c} \left(\frac{\epsilon_m \epsilon_d}{\epsilon_m + \epsilon_d} \right)^{1/2} \quad k_{zi} = \frac{\omega}{c} \left(\frac{\epsilon_i^2}{\epsilon_m + \epsilon_d} \right)^{1/2}$$

