Drude Model

for dielectric constant of metals.

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

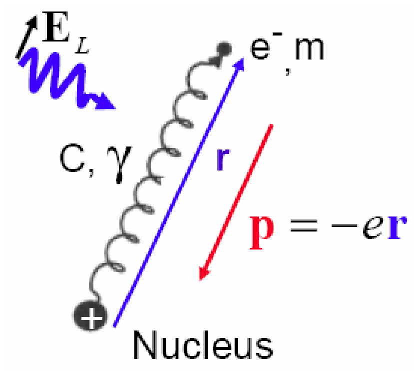
Ref : Prof. Robert P. Lucht, Purdue University

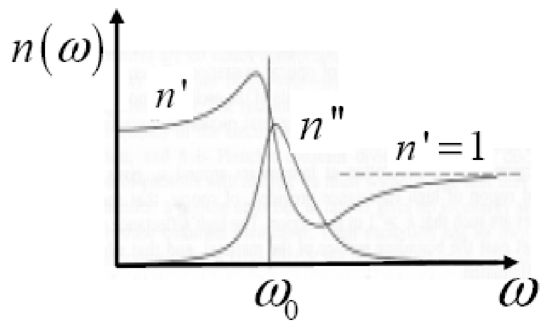
Drude model

- Drude model : Lorenz 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

$$m\mathbf{a}_{el} = \mathbf{F}_{E,Local} + \mathbf{F}_{Damping} + \mathbf{F}_{Spring}$$ (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

Conduction Current in Metals

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

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

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

Lorentz model
(Harmonic oscillator model)

If C = 0, it is called Drude model

The current density is defined :

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

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:

$$\vec{E} = \vec{E}_0 \exp(-i\omega t) \qquad \vec{J} = \vec{J}_0 \exp(-i\omega t)$$

Local approximation to the current-field relation

Substituting into the equation of motion we obtain:

$$\frac{d\left[\vec{J}_0 \exp(-i\omega t)\right]}{dt} + \gamma \vec{J}_0 \exp(-i\omega t) = -i\omega \vec{J}_0 \exp(-i\omega t) + \gamma \vec{J}_0 \exp(-i\omega t)$$

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

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

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

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

Conduction Current in Metals

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:

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

For very low frequencies, $(\omega/\gamma) << 1$, *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, $(\omega/\gamma) >> 1$, *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:

$$\nabla^2 \vec{E} = \frac{1}{c^2}\frac{\partial^2 \vec{E}}{\partial t^2} + \frac{1}{\varepsilon_0 c^2}\frac{\partial \vec{J}}{\partial t}$$

$$\vec{P} = 0, \quad \vec{J} \neq 0$$

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

Substituting in the wave equation we obtain:

$$\nabla^2 \vec{E} = \frac{1}{c^2}\frac{\partial^2 \vec{E}}{\partial t^2} + \frac{1}{\varepsilon_0 c^2}\left[\frac{\sigma}{1-\left(i\omega/\gamma\right)}\right]\frac{\partial \vec{E}}{\partial t}$$

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

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

where

$$k^2 = \frac{\omega^2}{c^2} + i\left[\frac{\sigma\,\omega\,\mu_0}{1-\left(i\omega/\gamma\right)}\right] \qquad c^2 = \frac{1}{\varepsilon_0\mu_0}$$

Skin Depth

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

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

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

$$k_R = k_I = \sqrt{\frac{\sigma\,\omega\,\mu_0}{2}} \qquad\qquad n_R = \left(\frac{c}{\omega}\right)k_R = \sqrt{\frac{\sigma\,c^2\,\mu_0}{2\omega}} = \sqrt{\frac{\sigma}{2\omega\varepsilon_0}} = n_I$$

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

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

The skin depth δ *is given by:* $\boxed{\delta = \frac{1}{k_I} = \sqrt{\frac{2}{\sigma\,\omega\,\mu_0}} = \sqrt{\frac{2\varepsilon_0 c^2}{\sigma\,\omega}}}$

For copper the static conductivity $\sigma = 5.76\times10^7\ \Omega^{-1}m^{-1} = 5.76\times10^7\ \frac{C^2-s}{J-m} \rightarrow \delta = 0.66\mu m$

Plasma Frequency

Now consider again the general case:

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

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

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

The plasma frequency is defined:

$$\omega_p^2 = \gamma\,\sigma\,c^2\mu_0 = \gamma\left(\frac{N\,e^2}{m_e\gamma}\right)c^2\mu_0 \quad = \frac{N\,e^2}{m_e\varepsilon_0}$$

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.

$$E_s = \sigma_o / \varepsilon_o = Ne(\delta x) / \varepsilon_o \text{ : electrostatic field by small charge separation } \delta x$$

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

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

Plasma Frequency

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

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

$n^2 = 1 - \dfrac{\omega_p^2}{\omega^2}$ by neglecting γ, valid for high frequency ($\omega >> \gamma$).

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
$(\lambda_c)_{obs}$	2050 Å	2100 Å	3150 Å	3600 Å	4400 Å
$(\lambda_c)_{calc}$ . . .	1500 Å	2100 Å	2900 Å	3200 Å	3600 Å
$\frac{N_{eff}}{N}$	0·54	1·00	0·85	0·79	0·67

Born and Wolf, Optics, page 627.

Plasma Frequency

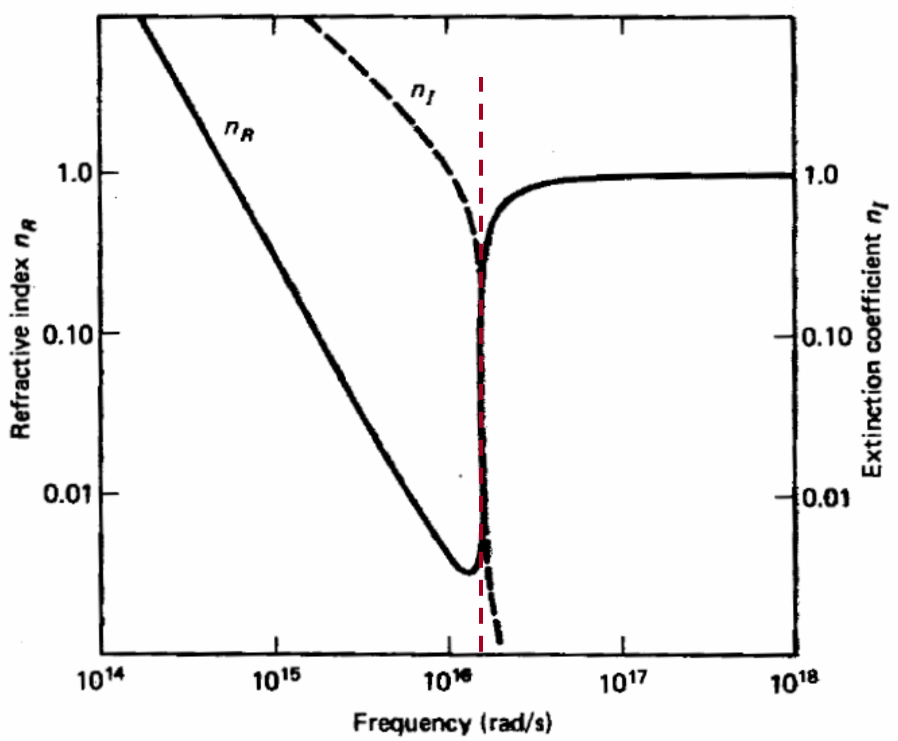


Figure 27-3 Angular frequency dependence of the refractive index n_R and the extinction coefficient n_I for copper. Values assumed are $\omega_p = 1.63 \times 10^{16}\ s^{-1}$ and $\gamma = 4.1 \times 10^{13}\ s^{-1}$. The crossover point of the curves coincides with the plasma frequency.

Dielectric constant of metal : Drude model

$$\varepsilon(\omega) = \varepsilon_R + i\varepsilon_I = n^2$$

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

$$= (n_R^2 - n_I^2) + i2n_R n_I$$

$$= \left(1 - \frac{\omega_p^2}{\omega^2 + \gamma^2}\right) + i\left(\frac{\omega_p^2 \gamma}{\omega^3 + \omega\gamma^2}\right)$$

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

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

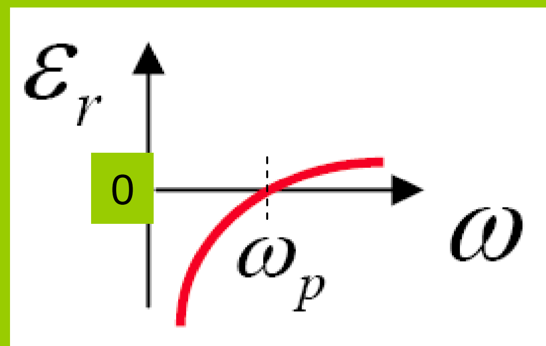
Ideal case : metal as a free-electron gas

Dielectric constant of a free electron gas

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

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

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



Plasma waves (plasmons)

What is a plasmon ?

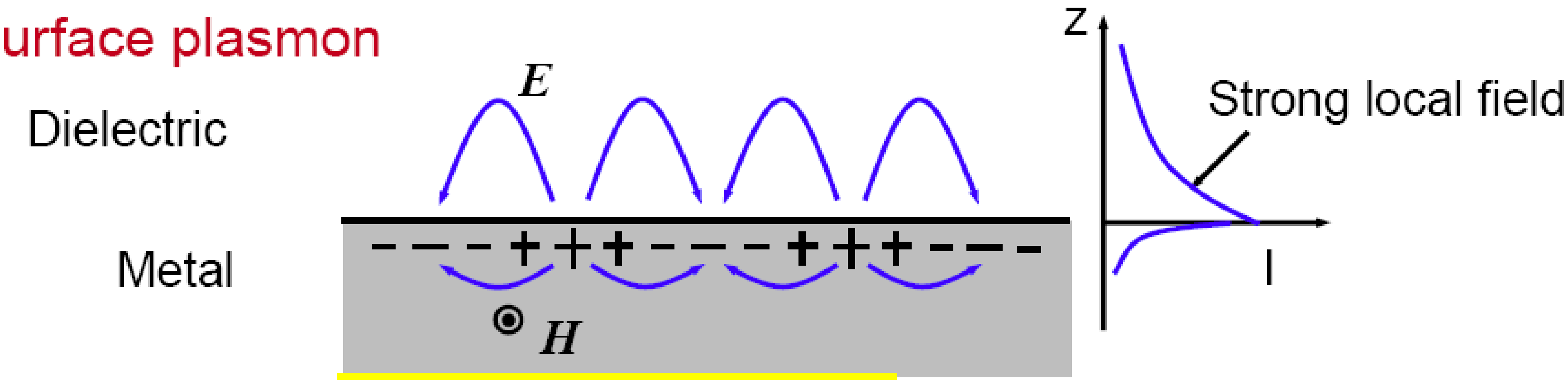
- Compare electron gas in a metal and real gas of molecules
- Metals are expected to allow for electron density waves: plasmons

Bulk plasmon

- Metals allow for EM wave propagation above the plasma frequency

They become transparent!

Surface plasmon

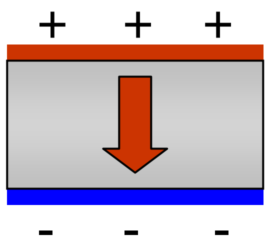


Note: SP is a TM wave!

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

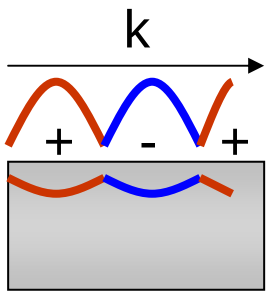
Plasmons

Plasma oscillation = density fluctuation of free electrons

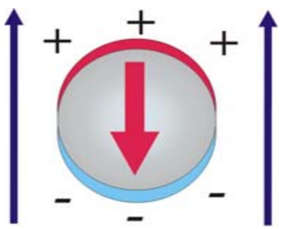


Plasmons in the bulk oscillate at ω_p determined by the free electron density and effective mass

$$\omega_p^{drude} = \sqrt{\frac{Ne^2}{m\varepsilon_0}}$$



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



$$\omega_{particle}^{drude} = \sqrt{\frac{1}{3}\frac{Ne^2}{m\varepsilon_0}}$$

Confinement effects result in resonant SPP modes in nanoparticles

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

Determination of dispersion relation for bulk plasmons

- The wave equation is given by:

$$\frac{\varepsilon_r}{c^2}\frac{\partial^2 \boldsymbol{E}(\boldsymbol{r},t)}{\partial \boldsymbol{t}^2} = \nabla^2 \boldsymbol{E}(\boldsymbol{r},t)$$

- Investigate solutions of the form:

$$\boldsymbol{E}(\boldsymbol{r},t) = \mathrm{Re}\left\{\boldsymbol{E}(\boldsymbol{r},\omega)\exp(i\boldsymbol{k}\cdot\boldsymbol{r} - i\omega t)\right\}$$

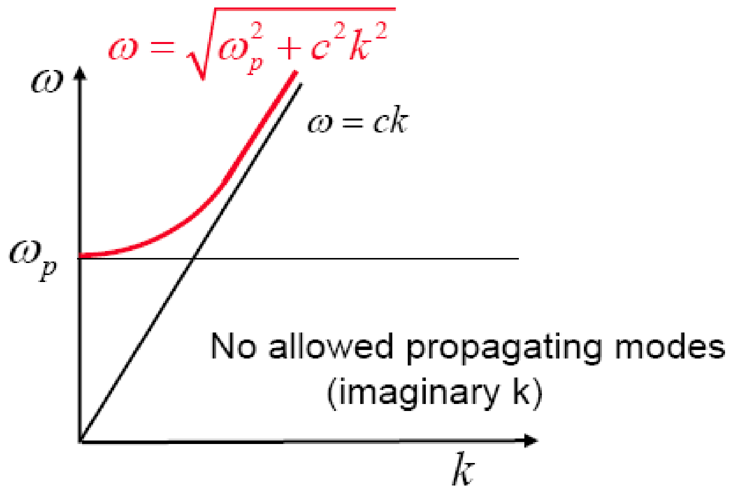
$$\Rightarrow \quad \omega^2 \varepsilon_r = c^2 k^2$$

- Dielectric constant: $\varepsilon_r = 1 - \dfrac{\omega_p^2}{\omega^2}$

$$\Rightarrow \quad \omega^2\left(1 - \frac{\omega_p^2}{\omega^2}\right) = \boxed{\omega^2 - \omega_p^2 = c^2 k^2}$$

- Dispersion relation:

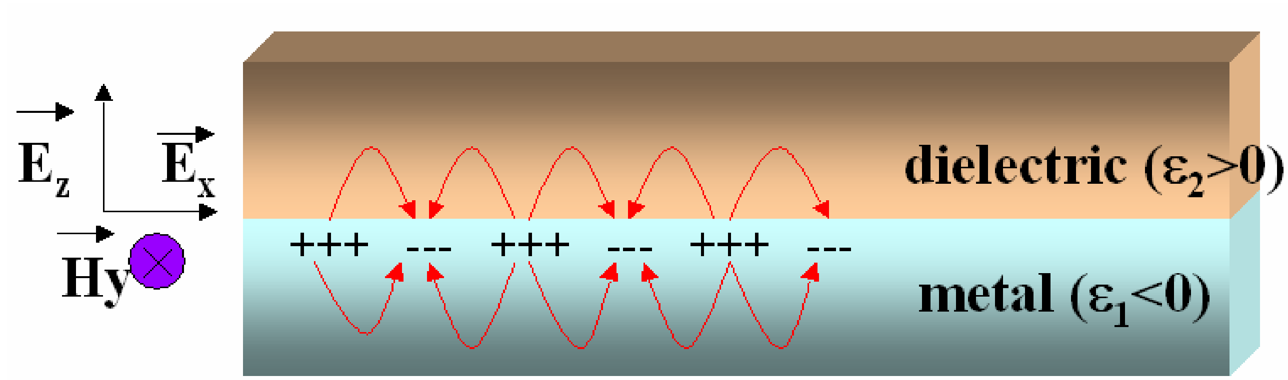
$$\boxed{\omega = \omega(k)}$$

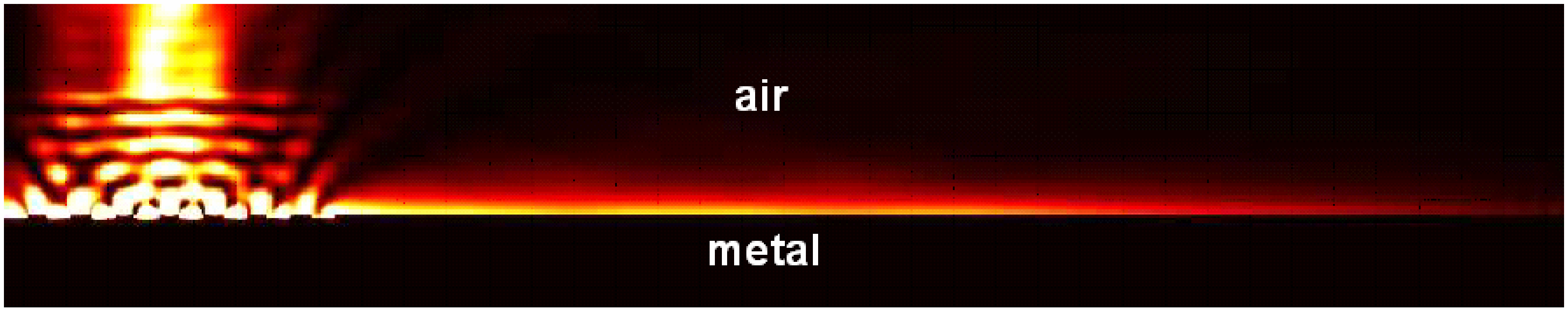


Note1: Solutions lie above light line

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

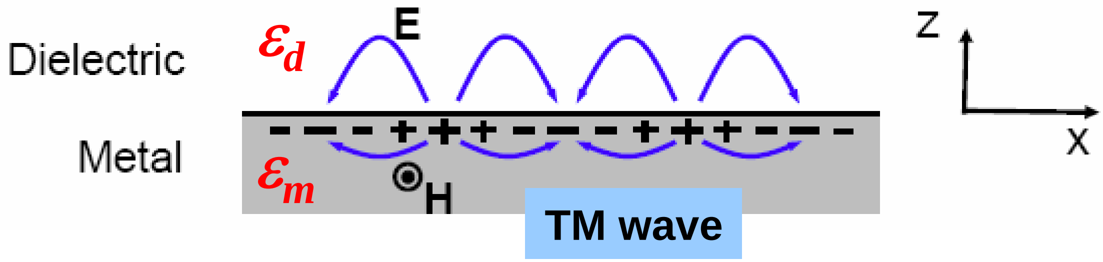




Dispersion relation for surface plasmon polaritons

Solve Maxwell's equations with boundary conditions

- We are looking for solutions that look like:



- Mathematically:

z > 0

$$\begin{cases} \boldsymbol{H}_d = (0, H_{yd}, 0)\exp i(k_{xd}x + k_{zd}z - \omega t) \\ \boldsymbol{E}_d = (E_{xd}, 0, E_{zd})\exp i(k_{xd}x + k_{zd}z - \omega t) \end{cases}$$

z < 0

$$\begin{cases} \boldsymbol{H}_m = (0, H_{ym}, 0)\exp i(k_{xm}x + k_{zm}z - \omega t) \\ \boldsymbol{E}_m = (E_{xm}, 0, E_{zm})\exp i(k_{xm}x + k_{zm}z - \omega t) \end{cases}$$

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

$$\nabla \cdot \varepsilon_i \boldsymbol{E} = 0 \qquad \nabla \cdot \boldsymbol{H} = 0 \qquad \nabla \times \boldsymbol{E} = -\mu_0 \frac{\partial \boldsymbol{H}}{\partial \boldsymbol{t}} \qquad \nabla \times \boldsymbol{H} = \varepsilon_i \frac{\partial \boldsymbol{E}}{\partial \boldsymbol{t}}$$

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

$$E_{xm} = E_{xd} \qquad H_{ym} = H_{yd} \qquad \varepsilon_m E_{zm} = \varepsilon_d E_{zd}$$

Dispersion relation for surface plasmon polaritons

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

$$\nabla \times \boldsymbol{H}_i = \varepsilon_i \frac{\partial \boldsymbol{E}_i}{\partial \boldsymbol{t}}$$

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

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

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

$$k_{zi}H_{yi} = \omega\varepsilon_i E_{xi} \Rightarrow \begin{cases} k_{zm}H_{ym} = \omega\varepsilon_m E_{xm} \\ k_{zd}H_{yd} = \omega\varepsilon_d E_{xd} \end{cases}$$

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

$$\Rightarrow \frac{k_{zm}}{\varepsilon_m} H_{ym} = \frac{k_{zd}}{\varepsilon_d} H_{yd}$$

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

Combine with: $\frac{k_{zm}}{\varepsilon_m} H_{ym} = \frac{k_{zd}}{\varepsilon_d} H_{yd}$

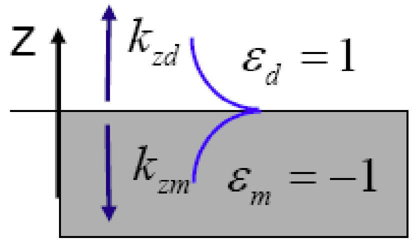
$$\Rightarrow \boxed{\frac{k_{zm}}{\varepsilon_m} = \frac{k_{zd}}{\varepsilon_d}}$$

Dispersion relation for surface plasmon polaritons

Relations between k vectors

- Condition for SP's to exist: $\dfrac{k_{zm}}{\varepsilon_m} = \dfrac{k_{zd}}{\varepsilon_d}$

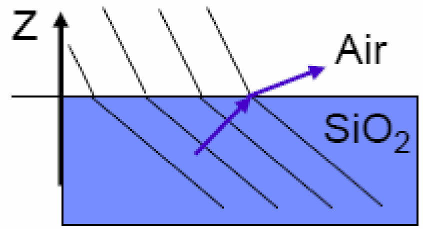
Example



- Relation for k_x (Continuity $E_{//}$, $H_{//}$) : $k_{xm} = k_{xd}$

true at any boundary

Example



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

- Both in the metal and dielectric: $k_{sp} = k_x = \sqrt{\varepsilon_i \left(\dfrac{\omega}{c}\right)^2 - k_{zi}^2}$

$$\frac{k_{zm}}{\varepsilon_m} = \frac{k_{zd}}{\varepsilon_d}$$

SP Dispersion Relation

$$\Rightarrow \boxed{k_x = \frac{\omega}{c}\sqrt{\frac{\varepsilon_m \varepsilon_d}{\varepsilon_m + \varepsilon_d}}}$$

Dispersion relation for surface plasmon polaritons

x-direction: $$k_x = k'_x + ik''_x = \frac{\omega}{c}\left(\frac{\varepsilon_m \varepsilon_d}{\varepsilon_m + \varepsilon_d}\right)^{1/2} \qquad \varepsilon_m = \varepsilon_m' + i\varepsilon_m''$$

z-direction: $$k_{zi}^2 = \varepsilon_i \left(\frac{\omega}{c}\right)^2 - k_x^2 \longrightarrow k_{zi} = k'_{zi} + ik_{zi} = \pm\frac{\omega}{c}\left(\frac{\varepsilon_i^2}{\varepsilon_m + \varepsilon_d}\right)^{1/2}$$

For a bound SP mode:

k_{zi} must be imaginary: $\varepsilon_m + \varepsilon_d < 0$

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

+ for z < 0
- for z > 0

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

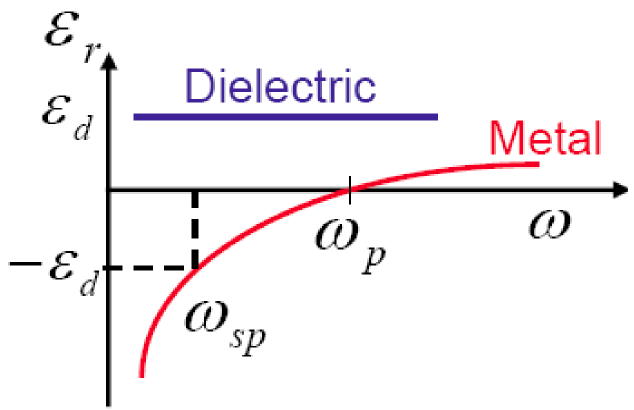
$$\boldsymbol{H}_i = (0, H_{yi}, 0)\exp i(k_{xi}x + k_{zi}z - \omega t)$$
$$\boldsymbol{E}_i = (E_{xi}, 0, E_{zi})\exp i(k_{xi}x + k_{zi}z - \omega t)$$

So, $$\boxed{\varepsilon_m' < -\varepsilon_d}$$

Plot of the dispersion relation

- Plot of the dielectric constants:

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



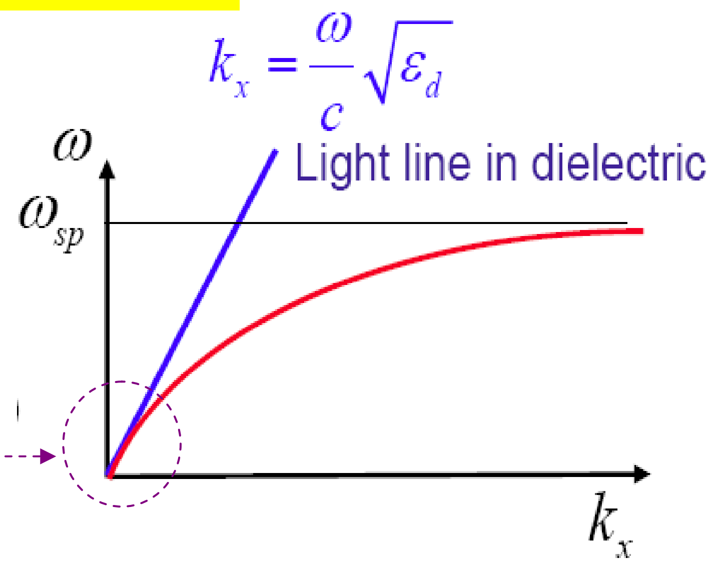
- Plot of the dispersion relation:

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

- When $\varepsilon_m \to -\varepsilon_d$,

$$\Rightarrow \quad \mathrm{k_x} \to \infty, \ \omega \equiv \omega_{sp} = \frac{\omega_p}{\sqrt{1+\varepsilon_d}}$$

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



Surface plasmon dispersion relation

$$k_x = \frac{\omega}{c}\left(\frac{\varepsilon_m \varepsilon_d}{\varepsilon_m + \varepsilon_d}\right)^{1/2} \qquad k_{zi} = \frac{\omega}{c}\left(\frac{\varepsilon_i^2}{\varepsilon_m + \varepsilon_d}\right)^{1/2}$$