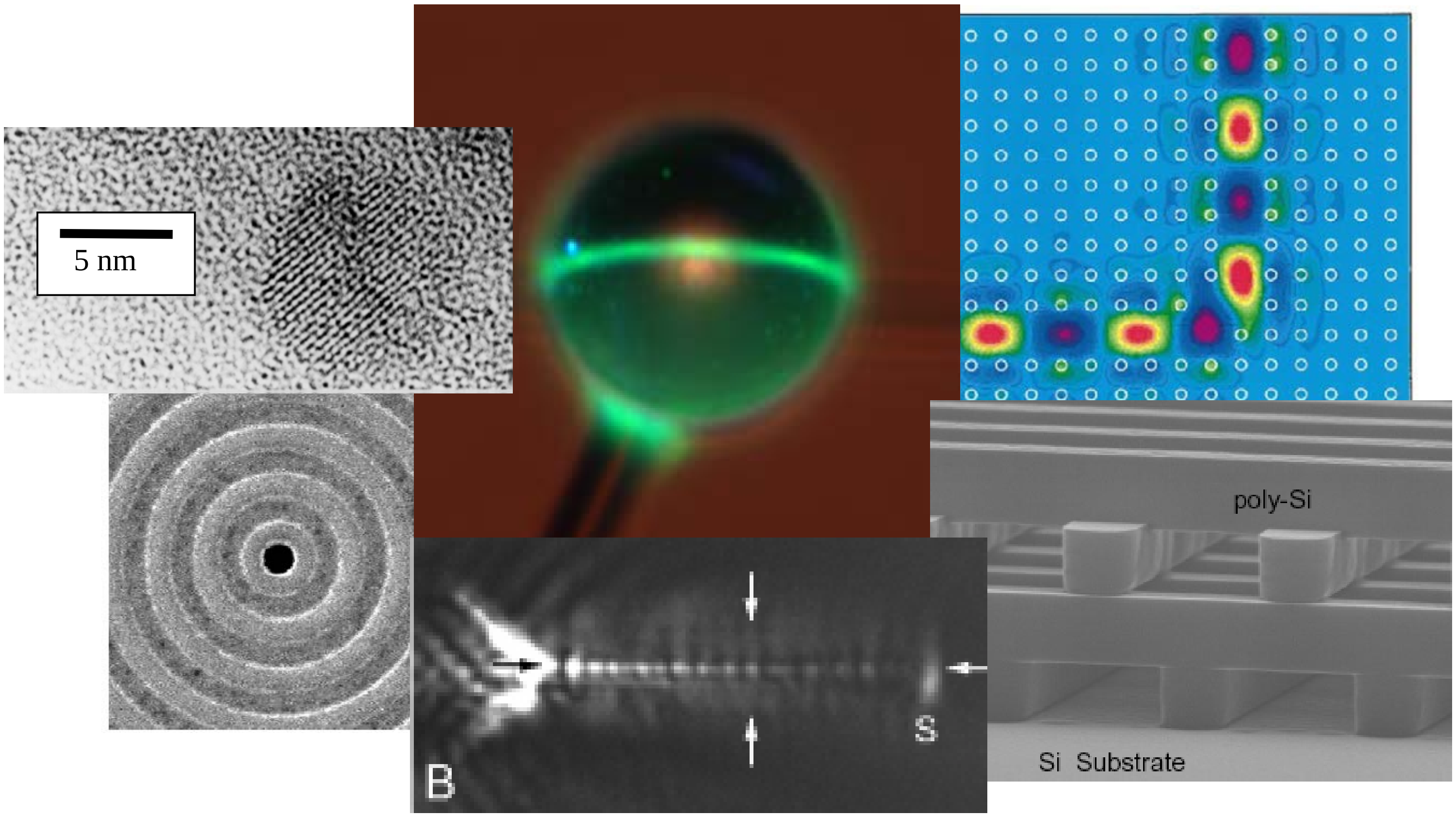
# Lecture 2: Dispersion in Materials



# Course Info

## Course webpage

- Is now up and running
www.ecepurdue.edu/~shalaev

## Let me know what you think!

- Direct questions
- Topics ?
- Format ?
- **Big** comments on the nanocourse are most welcome!
- Ask questions any time……….

# Previous Lecture: Maxwell + Wave Equation

## Speed of the EM wave:

Compare $\nabla^2 \boldsymbol{E} = \mu_0 \varepsilon_0 \varepsilon_r \frac{\partial^2 \boldsymbol{E}}{\partial t^2}$ and general wave Equation: $\nabla^2 \boldsymbol{U}(r,t) = \frac{1}{v^2} \frac{\partial^2 \boldsymbol{U}(r,t)}{\partial \boldsymbol{t}^2}$

$$\Rightarrow \quad v^2 = \frac{1}{\mu_0 \varepsilon_0} \frac{1}{\varepsilon_r} = \frac{c_0^2}{\varepsilon_r}$$

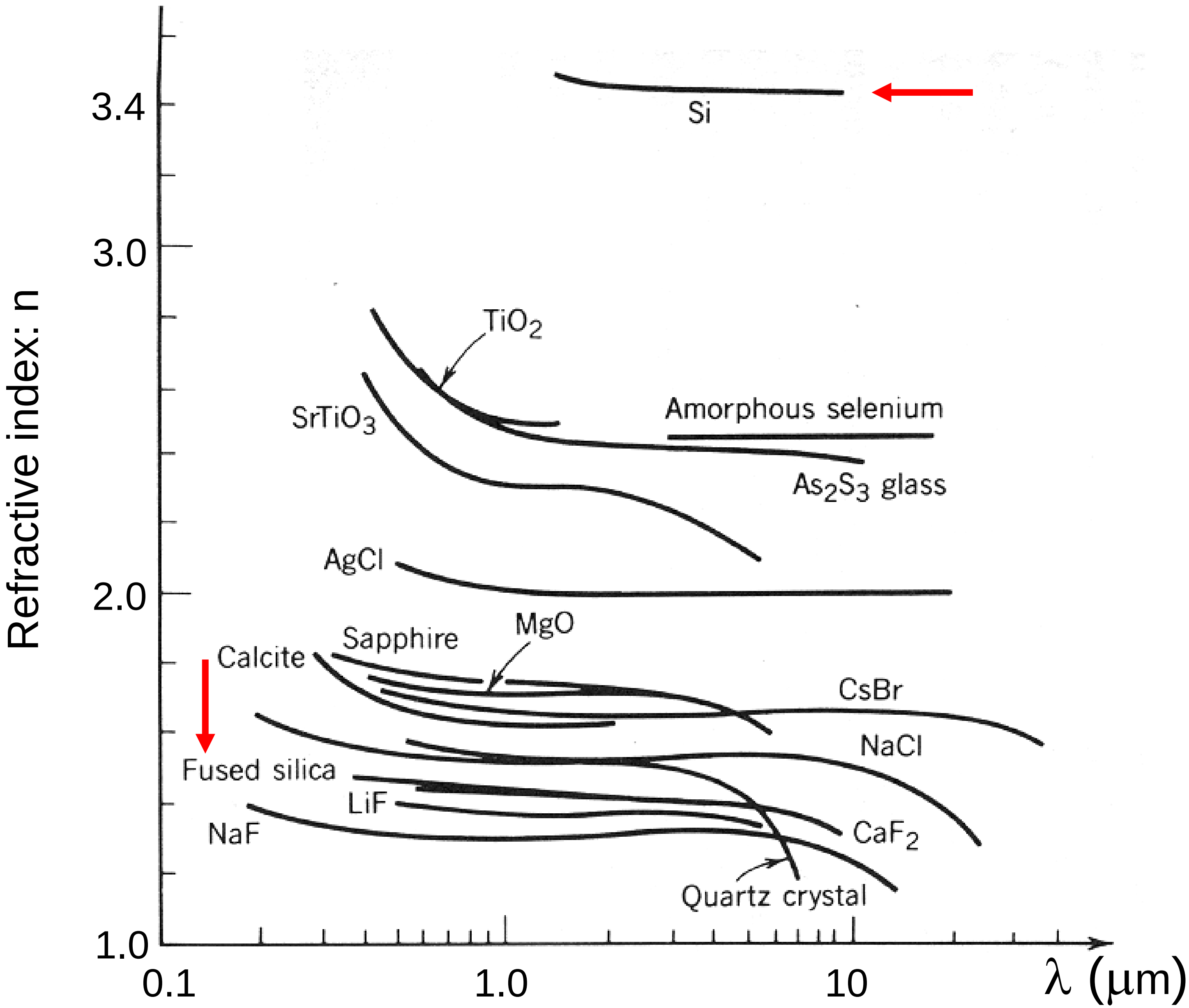
Where $c_0^2 = 1/(\varepsilon_0\ \mu_0) = 1/((8.85 \times 10^{-12}\ C^2/m^3 kg)\ (4\pi \times 10^{-7}\ m\ kg/C^2)) = (3.0 \times 10^8\ m/s)^2$

## Optical refractive index

Refractive index is defined by: $n = \frac{c_0}{v} = \sqrt{\varepsilon_r} = \sqrt{1 + \chi}$

Note: Including polarization results in same wave equation with a different $\varepsilon_r$ $\Rightarrow$ $c_0$ becomes $v$

# Refractive Index Various Materials



# Dispersion Relations

## Dispersion relation: ω = ω(k)

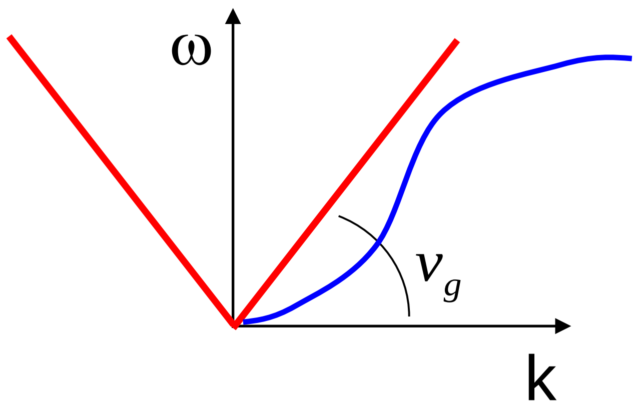
Derived from wave equation $$\nabla^2 \boldsymbol{E}(\boldsymbol{r},t) = \frac{n^2}{c^2}\frac{\partial^2 \boldsymbol{E}(\boldsymbol{r},t)}{\partial \boldsymbol{t}^2}$$

Substitute: $$\boldsymbol{E}(z,t) = \mathrm{Re}\left\{\boldsymbol{E}(z,\omega)\exp(-ikz + i\omega t)\right\}$$

Result: $$k^2 = \frac{n^2}{c^2}\omega^2$$

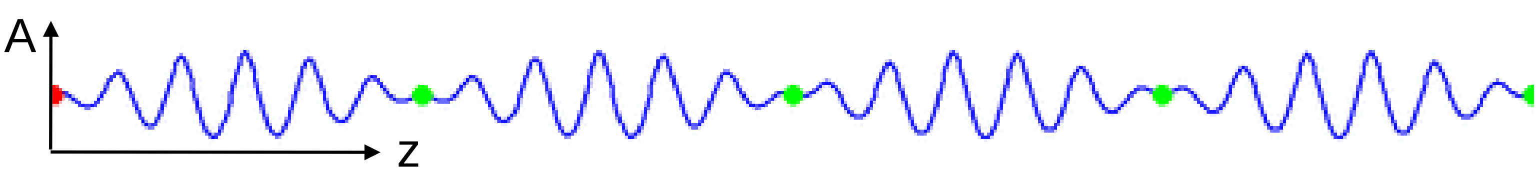
Check this!

$$\omega^2 = \frac{c^2}{n^2}k^2$$




Group velocity: $$v_g \equiv \frac{d\omega}{dk} = \frac{\omega}{k} = \frac{c}{n} = \frac{c}{\sqrt{\varepsilon_r}} = \frac{c}{\sqrt{1+\chi}}$$

Phase velocity: $$v_{ph} \equiv \frac{\omega}{k}$$



# Absorption and Dispersion of EM Waves

Transparent materials can be described by a purely real refractive index n

EM wave: $\boldsymbol{E}(z,t) = \mathrm{Re}\left\{\boldsymbol{E}(z,\omega)\exp(-ikz + i\omega t)\right\}$

Dispersion relation $\omega^2 = \frac{c^2}{n^2}k^2 \Rightarrow k = \pm\frac{\omega}{c}n$

Absorbing materials can be described by a complex n: $n = n' + in''$

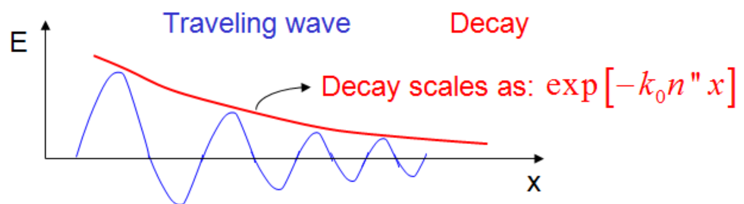
It follows that: $k = \pm\frac{\omega}{c}(n' + in'') = \pm\left(\frac{\omega}{c}n' + i\frac{\omega}{c}n''\right) \equiv \pm\left(\beta - i\frac{\alpha}{2}\right)$

Investigate + sign: $\boldsymbol{E}(z,t) = \mathrm{Re}\left\{\boldsymbol{E}(z,\omega)\exp\left(-i\beta z - \frac{\alpha}{2}z + i\omega t\right)\right\}$

Traveling wave ($-i\beta z$) Decay ($-\frac{\alpha}{2}z$)

Note: $\beta = \frac{\omega}{c}n' = kn' \Rightarrow$ n' acts as a regular refractive index

$\alpha = -2\frac{\omega}{c}n'' = -2kn'' \Rightarrow$ $\alpha$ is the absorption coefficient



# Summary and Future Directions

Maxwell's Equations

$$\nabla \cdot \boldsymbol{D} = \rho_f \qquad \nabla \cdot \boldsymbol{B} = 0 \qquad \nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial \boldsymbol{t}} \qquad \nabla \times \boldsymbol{H} = \frac{\partial \boldsymbol{D}}{\partial \boldsymbol{t}} + \boldsymbol{J}$$

Curl Equations lead to

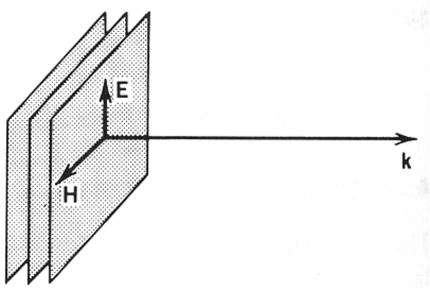
$$\nabla^2 \boldsymbol{E} = \mu_0 \varepsilon_0 \frac{\partial^2 \boldsymbol{E}}{\partial t^2} + \mu_0 \frac{\partial^2 \boldsymbol{P}}{\partial t^2}$$ (under certain conditions)

Linear, Homogeneous, and Isotropic Media

$$\boldsymbol{P} = \varepsilon_0 \chi \boldsymbol{E}$$

Wave Equation with v = c/n

$$\nabla^2 \boldsymbol{E}(\boldsymbol{r},t) = \frac{n^2}{c^2} \frac{\partial^2 \boldsymbol{E}(\boldsymbol{r},t)}{\partial \boldsymbol{t}^2}$$ ⇒ Solutions:




Today: In real life the relation between $\boldsymbol{P}$ and $\boldsymbol{E}$ is dynamic

⇒ $$\boldsymbol{P}(\boldsymbol{k},\omega) = \varepsilon_0 \chi(\omega) \boldsymbol{E}(\boldsymbol{k},\omega)$$

Materials have a response time

Lorentz model: Helps to understand the optical response of real materials

$\chi(\omega)$, $\varepsilon(\omega)$, $n(\omega)$

# n' and n'' vs χ' and χ'' vs $\varepsilon_r$' and $\varepsilon_r$''

All pairs (n' and n'', χ' and χ'', $\varepsilon_r$' and $\varepsilon_r$'') describe the same physics

For some problems one set is preferable for others another

n' and n'' used when discussing wave propagation

$$\boldsymbol{E}(z,t) = \mathrm{Re}\left\{\boldsymbol{E}(z,\omega)\exp\left(-i\beta z - \frac{\alpha}{2}z + i\omega t\right)\right\}$$ where $\beta = k_0 n'$ and $\alpha = -2k_0 n''$

Phase propagation absorption

χ' and χ''
$\varepsilon_r$' and $\varepsilon_r$''
} used when discussing microscopic origin of optical effects

As we will see today…

Inter relationships

Example: n and $\varepsilon_r$

From $n = \sqrt{\varepsilon_r}$

$$n' + in'' = \sqrt{\varepsilon_r' + i\varepsilon_r''}$$

$$\varepsilon_r' = (n')^2 - (n'')^2$$
$$\varepsilon_r'' = 2n'n''$$

and

$$n' = \sqrt{\frac{\sqrt{(\varepsilon_r')^2 + (\varepsilon_r'')^2} + \varepsilon_r'}{2}}$$

$$n'' = \sqrt{\frac{\sqrt{(\varepsilon_r')^2 + (\varepsilon_r'')^2} - \varepsilon_r'}{2}}$$

# Light Propagation Dispersive Media

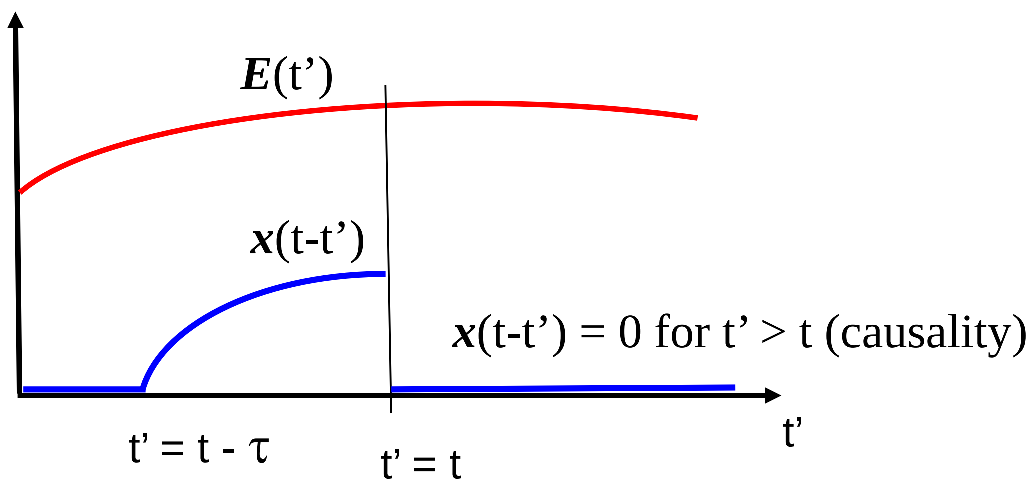
## Relation between *P* and *E* is dynamic

The relation : $\boldsymbol{P}(\boldsymbol{r},t)=\varepsilon_0\chi\boldsymbol{E}(\boldsymbol{r},t)$ assumes an instantaneous response

In real life: $$\boldsymbol{P}(\boldsymbol{r},t)=\varepsilon_0\int_{-\infty}^{+\infty}dt'\,x(\underline{t-t'})\,\boldsymbol{E}(\boldsymbol{r},t')$$

***P*** results from response to ***E*** over some characteristic time $\tau$ :

Function *x*(t) is a scalar function lasting a characteristic time $\tau$ :



# EM waves in Dispersive Media

Relation between ***P*** and ***E*** is dynamic

$$\boldsymbol{P}(\boldsymbol{r},t)=\varepsilon_0\int_{-\infty}^{+\infty}dt'\,x(t-t')\,\boldsymbol{E}(\boldsymbol{r},t')$$

EM wave:

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

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

Relation between complex amplitudes

$$\boxed{\boldsymbol{P}(\boldsymbol{k},\omega)=\varepsilon_0\chi(\omega)\boldsymbol{E}(\boldsymbol{k},\omega)}$$

(Slow response of matter ⇨ ω-dependent behavior)

This follows by equation of the coefficients of exp(iωt) ..check this!

It also follows that: $\varepsilon_r(\omega)=\varepsilon_0\left[1+\chi(\omega)\right]$

Next: We will model the frequency dependence of χ, ε, and n

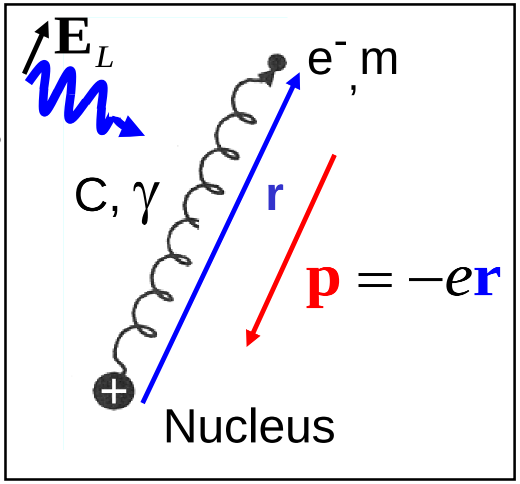
# Linear Dielectric Response of Matter

## Behavior of bound electrons in an electromagnetic field

- Optical properties of insulators are determined by bound electrons

## Lorentz 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)

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

- The electric dipole moment of this system is: $\mathbf{p} = -e\mathbf{r}$

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

- Guess a solution of the form:

$$\mathbf{p} = \mathbf{p}_0 \exp(-i\omega t)\ ;\ \frac{d\mathbf{p}}{dt} = -i\omega\mathbf{p}_0 \exp(-i\omega t)\ ;\ \frac{d^2\mathbf{p}}{dt^2} = -\omega^2\mathbf{p}_0 \exp(-i\omega t)$$

$\Rightarrow$ $-m\omega^2\mathbf{p}_0 - im\gamma\omega\mathbf{p}_0 + C\mathbf{p}_0 = e^2\mathbf{E}_L$ $\Rightarrow$ Solve for $\mathbf{p}_0(\mathbf{E}_L)$

# Atomic Polarizability

## Determination of atomic polarizability

- Last slide: $-m\omega^2\mathbf{p}_0 - im\gamma\omega\mathbf{p}_0 + C\mathbf{p}_0 = e^2\mathbf{E}_L$

$$\Rightarrow \quad -\omega^2\mathbf{p}_0 - i\gamma\omega\mathbf{p}_0 + \frac{C}{m}\mathbf{p}_0 = \frac{e^2}{m}\mathbf{E}_L$$

(Divide by m)

Define as $\omega_0^2$ (turns out to be the resonance $\omega$)

$$\Rightarrow \quad \mathbf{p}_0 = \frac{e^2}{m}\frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega}\mathbf{E}_L$$

Atomic polarizability (in SI units)

- Define atomic polarizability: $\alpha(\omega) \equiv \frac{p_0}{\mathrm{E}_L} = \frac{e^2}{m}\frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega}$

Resonance frequency

Damping term

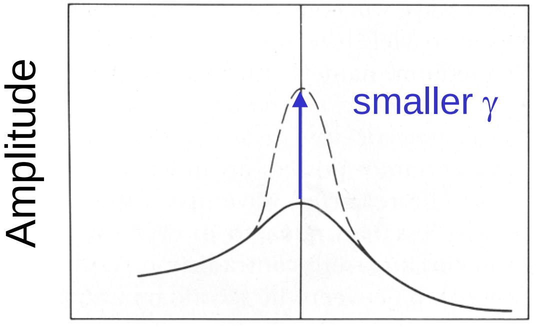
# Characteristics of the Atomic Polarizability

Response of matter (***P***) is not instantaneous ⇨ ω-dependent response

- Atomic polarizability: $\alpha(\omega) = \frac{p_0}{E_L} = \frac{e^2}{m}\frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega} = A\exp\left[i\theta(\omega)\right]$

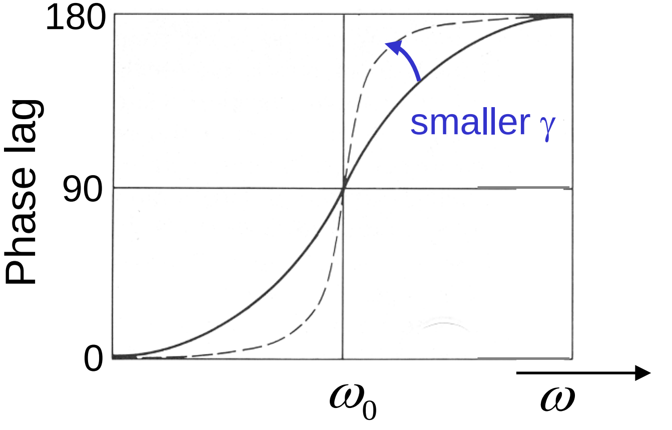
- Amplitude

$$A = \frac{e^2}{m}\frac{1}{\left[\left(\omega_0^2 - \omega^2\right)^2 + \gamma^2\omega^2\right]^{1/2}}$$




- Phase lag of $\boldsymbol{\alpha}$ with ***E*:**

$$\theta = \tan^{-1}\frac{\gamma\omega}{\omega_0^2 - \omega^2}$$



# Relation Atomic Polarizability (α) and χ: 2 cases

## Case 1: Rarified media (.. gasses)

- Dipole moment one atom, j : $\mathbf{p}_j = \alpha_j(\omega)\mathbf{E}_L$ ← E-field photon

- Polarization vector: $\mathbf{P} = \frac{1}{V}\sum_j \mathbf{p}_j = \frac{1}{V}\sum_j \alpha_j \mathbf{E}_L = N\alpha\langle\mathbf{E}_L\rangle$ ← Density

Occurs in Maxwell's equation..

sum over all atoms

$$\alpha(\omega) = \frac{e^2}{m}\frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

⇨ $$\mathbf{P} = \frac{Ne^2}{m}\frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega}\langle\mathbf{E}_L\rangle = \varepsilon_0\chi\langle\mathbf{E}_L\rangle = \varepsilon_0\chi\mathbf{E}$$

⇨ Microscopic origin susceptibility: $$\chi(\omega) = \frac{Ne^2}{\varepsilon_0 m}\frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

- Plasma frequency defined as: $\omega_p^2 = \frac{Ne^2}{\varepsilon_0 m}$ ⇨ $\chi(\omega) = \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\gamma\omega}$

# Remember: ε and n follow directly from χ

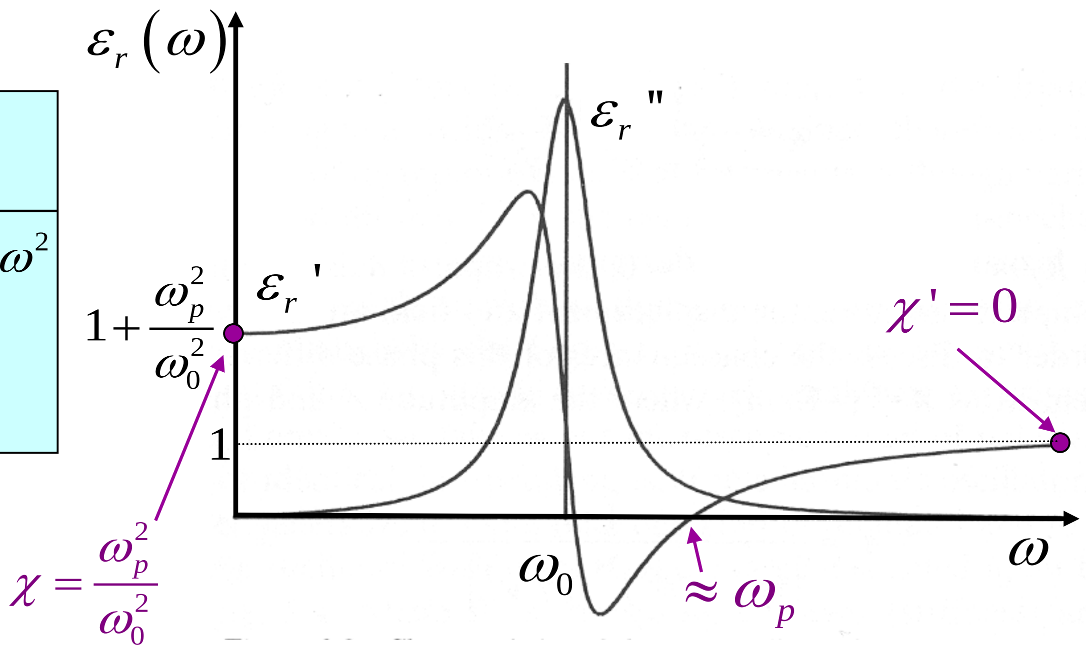
## Frequency dependence ε

- Relation of ε to χ : $\varepsilon_r = 1 + \chi = 1 + \dfrac{\omega_p^2}{\omega_0^2 - \omega^2 - i\gamma\omega}$

$$\Rightarrow \quad \varepsilon_r' + i\varepsilon_r'' = 1 + \chi' + i\chi'' = 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

$$\varepsilon_r' = 1 + \chi'(\omega) = 1 + \frac{\omega_p^2\left(\omega_0^2 - \omega^2\right)}{\left(\omega_0^2 - \omega^2\right)^2 + \gamma^2\omega^2}$$

$$\varepsilon_r'' = \chi''(\omega) = \frac{\omega_p^2\gamma\omega}{\left(\omega_0^2 - \omega^2\right)^2 + \gamma^2\omega^2}$$



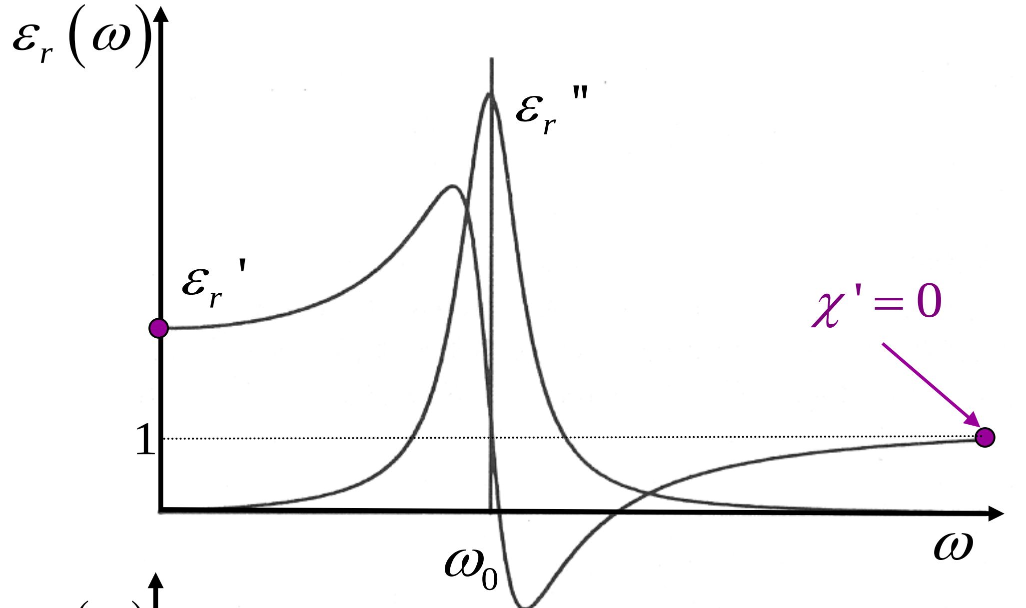
# Propagation of EM-waves: Need n' and n''

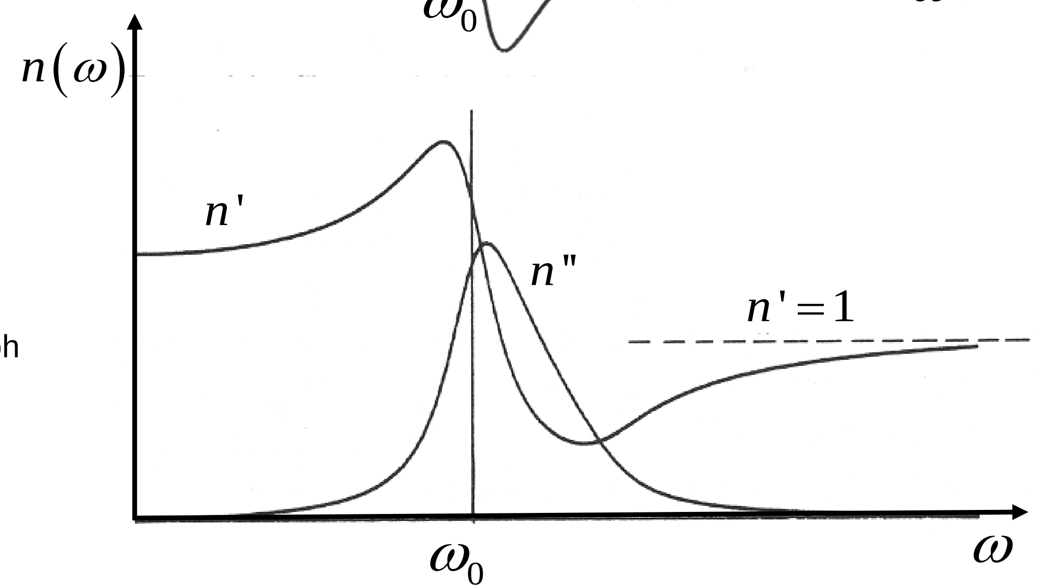
## Relation between n and $\varepsilon_r$

$$n = \sqrt{\varepsilon_r}$$

$$\varepsilon_r' = (n')^2 - (n'')^2$$

$$\varepsilon_r'' = 2n'n''$$




- $\omega \ll \omega_0$ : High n' ⇨ low $v_{ph}$ =c/n'
- $\omega \approx \omega_0$ : Strong $\omega$ dependence $v_{ph}$

  Large absorption (~ n'')
- $\omega \gg \omega_0$ : n' = 1 ⇨ $v_{ph}$ =c

# Realistic Rarefied Media

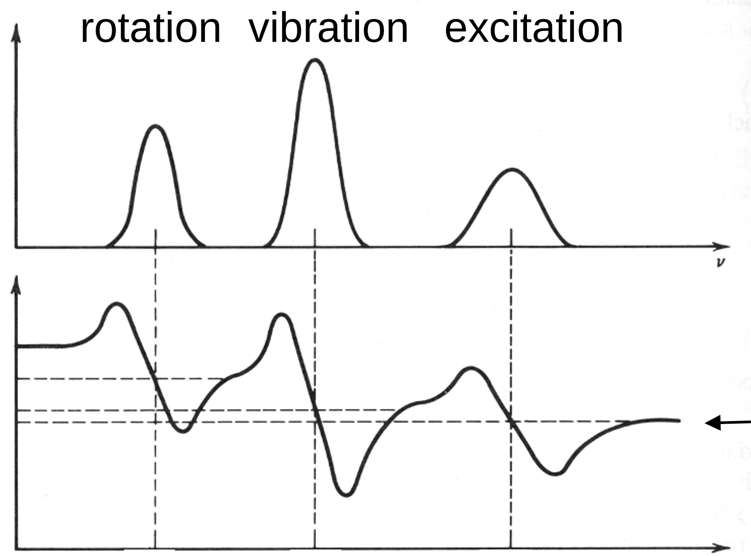
## Realistic atoms have many resonances

- Resonances occur due to motion of the atoms (low $\omega$) and electrons (high $\omega$)

$$\Rightarrow \quad \chi = \sum_k \frac{N_k e^2}{\varepsilon_0 m} \frac{1}{\omega_k^2 - \omega^2 - i\gamma\omega}$$

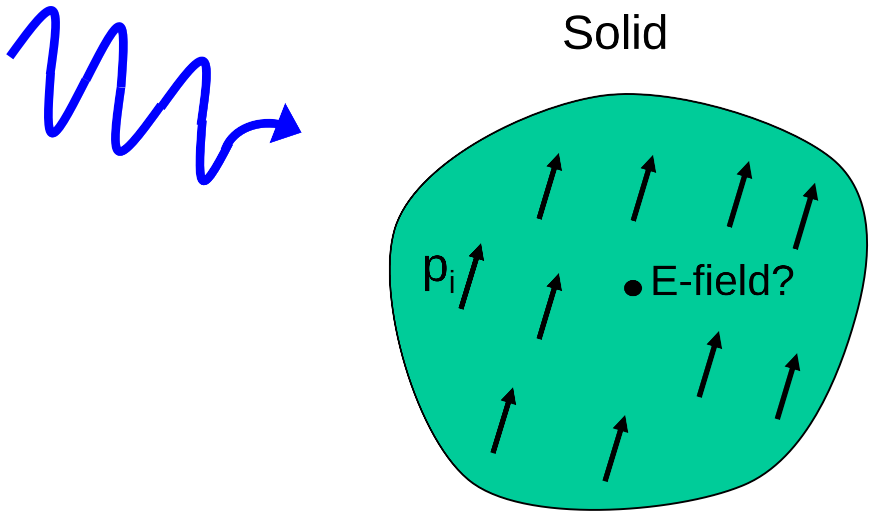
Where $N_k$ is the density of the electrons/atoms with a resonance at $\omega_k$

## Example of a realistic dependence of n' and n''



# Back to Relation Atomic Polarizability (α) and χ:

Case 2: Solids




- Atom “feels” field from: 1) Incident light beam

  2) Induced dipolar field from other atoms, $p_i$

- Local field: $$\mathbf{E}_L = \mathbf{E}_0 + \mathbf{E}_I$$

Local field ($\mathbf{E}_L$)

Field without matter ($\mathbf{E}_0$)

Induced dipolar field from all the other atoms ($\mathbf{E}_I$)

# Electric Susceptibility of a Solid

## Local field

- Local field: $\mathbf{E}_L = \mathbf{E}_0 + \mathbf{E}_I$

Local field — $\mathbf{E}_L$; Field without matter — $\mathbf{E}_0$; All the other atoms — $\mathbf{E}_I$

## Induced dipolar field

- Example: For cubic symmetry: (Solid state Phys. Books, e.g. Kittel p381-390)

$$\mathbf{E}_L = \mathbf{E} + \frac{\mathbf{P}}{3\varepsilon_0}$$

(Similar relations can be derived for any solid)

## Polarization of a solid

- Solid consists of atom type j at a concentration $N_j$

$$\mathbf{P} = \sum_j \varepsilon_0 N_j \underbrace{\alpha_j \mathbf{E}_L}_{p_j} = \sum_j \varepsilon_0 N_j \alpha_j \left( \mathbf{E} + \frac{\mathbf{P}}{3\varepsilon_0} \right) = \varepsilon_0 \sum_j N_j \alpha_j \mathbf{E} + \sum_j N_j \alpha_j \frac{\mathbf{P}}{3}$$

$$\Rightarrow \mathbf{P}\left(1 - \frac{1}{3}\sum_j N_j \alpha_j\right) = \varepsilon_0 \sum_j N_j \alpha_j \mathbf{E} \Rightarrow$$

$$\chi = \frac{P}{\varepsilon_0 E} = \frac{\sum_j N_j \alpha_j}{1 - \frac{1}{3}\sum_j N_j \alpha_j}$$

# Clausius-Mossotti Relation

## Polarization of a solid

- Susceptibility:

$$\chi = \frac{P}{\varepsilon_0 E} = \frac{\sum_j N_j \alpha_j}{1 - \frac{1}{3}\sum_j N_j \alpha_j} \qquad \text{I}$$

- Limit of low atomic concentration:

….or weak polarizability:

pretty good for gasses and glasses

$$\chi \approx \sum_j N_j \alpha_j \qquad \text{II}$$

## Clausius-Mossotti

- By definition: $\varepsilon = 1 + \chi$
- Rearranging I gives

$$\frac{\varepsilon - 1}{\varepsilon + 2} = \frac{1}{3}\sum_j N_j \alpha_j \qquad \text{III}$$

- Conclusion: Dielectric properties solids related to atomic polarizability
- This is very general!!