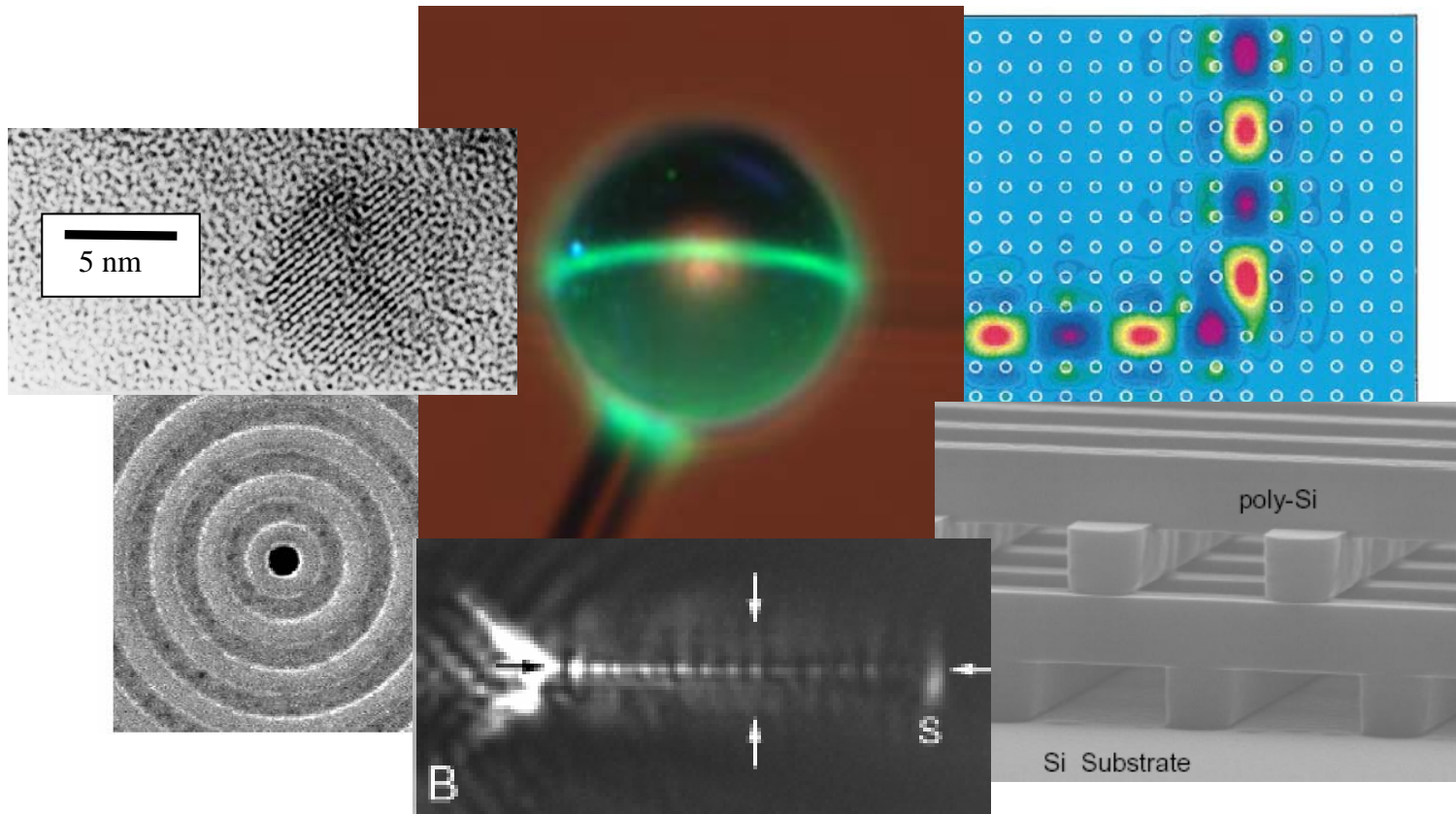


# Lecture 2: Dispersion in Materials



# Course Info

---

## Course webpage

- Is now up and running  
<http://shay.ecn.purdue.edu/~ece695s>

## Let me know what you think!

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

# What Happened in the Previous Lecture ?

## Maxwell's Equations

Bold face letters are vectors!

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

## Curl Equations lead to

$$\nabla^2 \mathbf{E} = \mu_0 \epsilon_0 \frac{\partial^2 \mathbf{E}}{\partial t^2} + \mu_0 \frac{\partial^2 \mathbf{P}}{\partial t^2} \quad (\text{under certain conditions})$$

## Linear, Homogeneous, and Isotropic Media

$$\mathbf{P} = \epsilon_0 \chi \mathbf{E}$$

## Wave Equation

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

## Solutions: EM waves

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

Phase propagation      absorption

## In real life: Response of matter ( $\mathbf{P}$ ) is not instantaneous

$$\mathbf{P}(\mathbf{r}, t) = \epsilon_0 \int_{-\infty}^{+\infty} dt' \chi(t-t') \mathbf{E}(\mathbf{r}, t') \quad \Rightarrow \quad \left. \begin{array}{l} \chi' = \chi'(\omega) \\ \chi'' = \chi''(\omega) \end{array} \right\} \Leftrightarrow \left\{ \begin{array}{l} n' = n'(\omega) \\ n'' = n''(\omega) \end{array} \right. \quad \curvearrowright$$

# Today: Microscopic Origin $\omega$ -Response of Matter

---

## Origin frequency dependence of $\chi$ in real materials

- Lorentz model (harmonic oscillator model)
- Insulators (Lattice absorption, color centers...)
- Semiconductors (Energy bands, Urbach tail, excitons ...)
- Metals (AC conductivity, Plasma oscillations, interband transitions...)

## Real and imaginary part of $\chi$ are linked

- Kramers-Kronig

## But first.....

- When should I work with  $\chi$ ,  $\varepsilon$ , or  $n$  ?

They all seem to describe the optical properties of materials!

# n' and n'' vs χ' and χ'' vs ε' and ε''

All pairs (n' and n'', χ' and χ'', ε' and ε'') describe the same physics

For some problems one set is preferable for others another

n' and n'' used when discussing wave propagation

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

Phase propagation    absorption

χ' and χ''  
ε' and ε'' } used when discussing microscopic origin of optical effects

As we will see today...

## Inter relationships

Example: n and ε

From  $n = \sqrt{\epsilon_r}$

↓

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



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

$$\epsilon_r'' = 2n'n''$$

and

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

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

# Linear Dielectric Response of Matter

## Behavior of bound electrons in an electromagnetic field

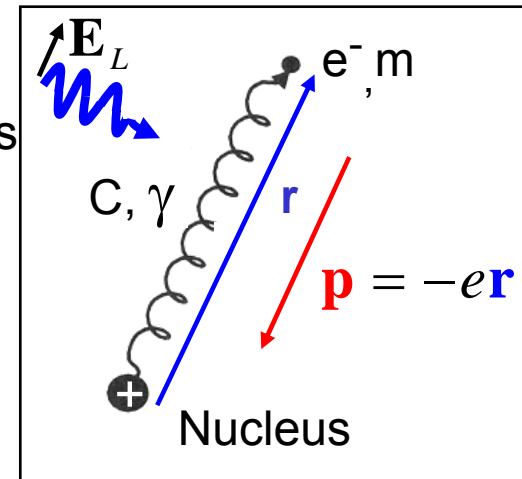
- Optical properties of insulators are determined by bound electrons

### Lorentz model

- Charges in a material are treated as harmonic oscillators

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

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



- 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:

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

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

# Atomic Polarizability

## Determination of atomic polarizability

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

⇒ 
$$-\omega^2 \mathbf{p}_0 - i\gamma\omega \mathbf{p}_0 + \frac{C}{m} \mathbf{p}_0 = \frac{e^2}{m} \mathbf{E}_L \quad (\text{Divide by } m)$$

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

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

Atomic polarizability (in SI units)

- Define atomic polarizability:  $\alpha(\omega) \equiv \frac{p_0}{\varepsilon_0 \mathbf{E}_L} = \frac{e^2}{\varepsilon_0 m} \frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega}$
- Resonance frequency      Damping term

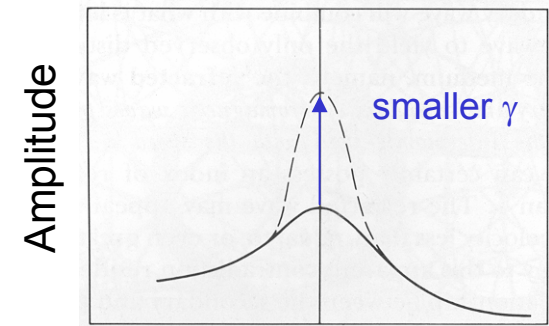
# Characteristics of the Atomic Polarizability

Response of matter (**P**) is not instantaneous  $\Rightarrow$   $\omega$ -dependent response

- Atomic polarizability:  $\alpha(\omega) = \frac{p_0}{\epsilon_0 E_L} = \frac{e^2}{\epsilon_0 m} \frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega} = A \exp[i\theta(\omega)]$

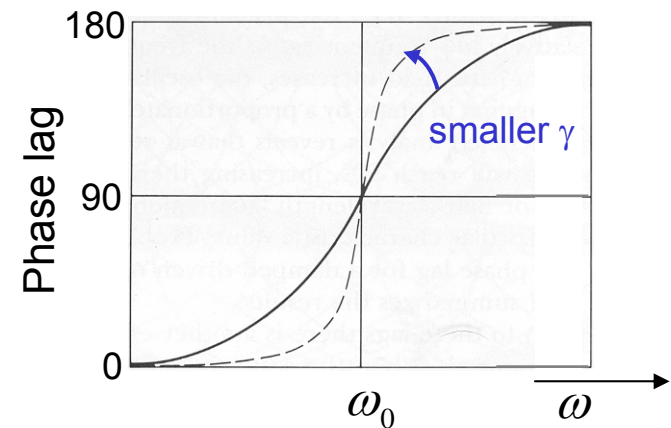
- Amplitude

$$A = \frac{e^2}{\epsilon_0 m} \frac{1}{\left[ (\omega_0^2 - \omega^2)^2 + \gamma^2 \omega^2 \right]^{1/2}}$$



- Phase lag of  $\alpha$  with **E**:

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





# Relation Atomic Polarizability ( $\alpha$ ) and $\chi$ : 2 cases

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

• Dipole moment of one atom, j :  $\mathbf{p}_j = \varepsilon_0 \alpha_j(\omega) \mathbf{E}_L$  ↖ E-field photon

• Polarization vector:  $\mathbf{P} = \frac{1}{V} \sum_j \mathbf{p}_j = \frac{\varepsilon_0}{V} \sum_j \alpha_j \mathbf{E}_L = \varepsilon_0 N \alpha_j \mathbf{E}_L$  ↖ Density

↑ Occurs in Maxwell's equation..

sum over all atoms

$$\alpha_j(\omega) = \frac{e^2}{\varepsilon_0 m} \frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

➡  $\mathbf{P} = \frac{Ne^2}{m} \frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega} \mathbf{E}_L \quad (= \varepsilon_0 \chi \mathbf{E}_L)$

➡ 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: $\epsilon$ and $n$ follow directly from $\chi$

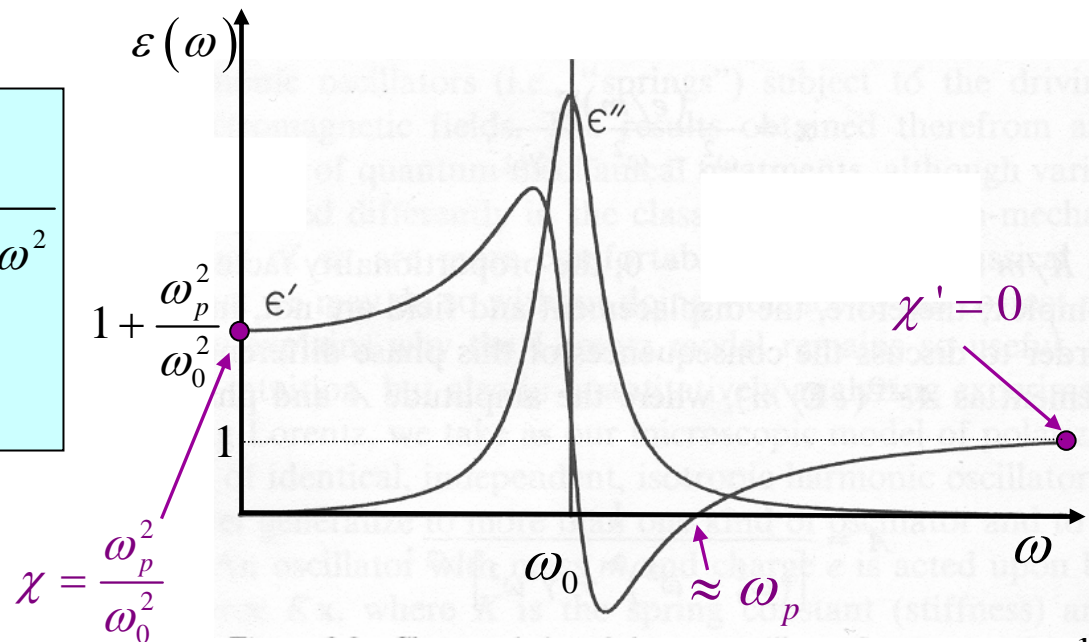
### Frequency dependence $\epsilon$

- Relation of  $\epsilon$  to  $\chi$ :  $\epsilon = 1 + \chi = 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\gamma\omega}$

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

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

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



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

## Relation between $n$ and $\epsilon$

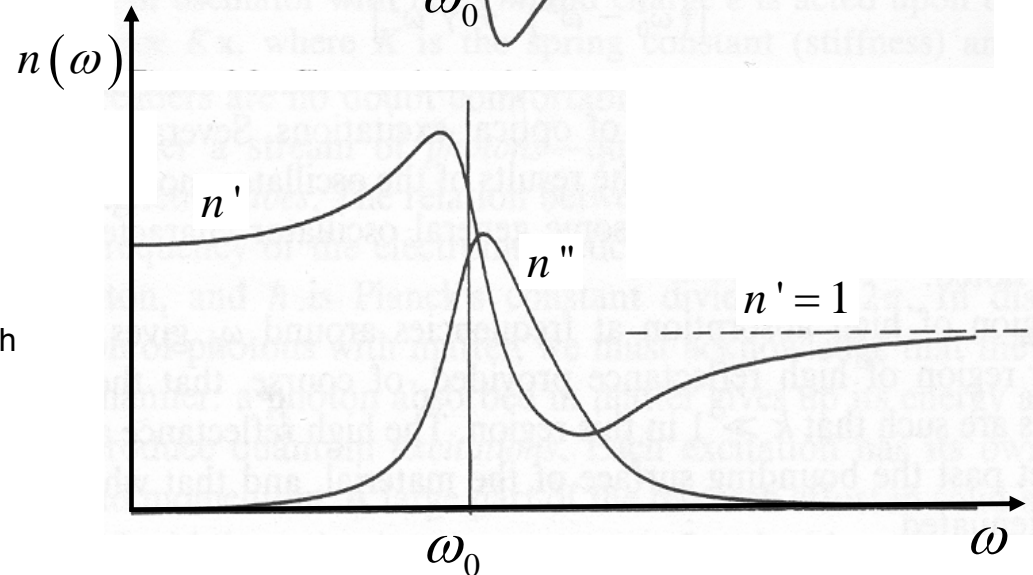
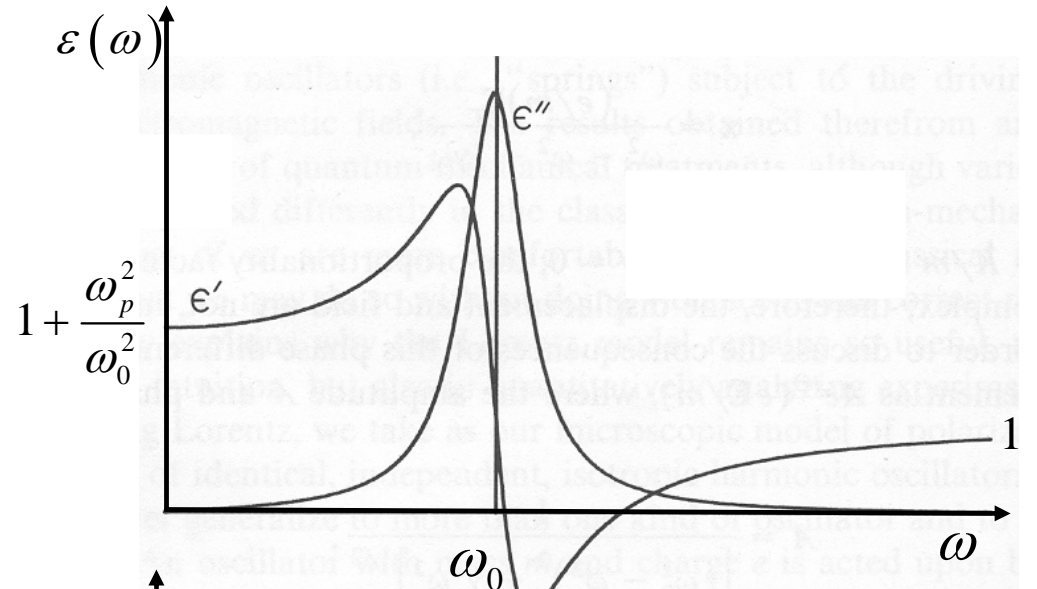
$$n = \sqrt{\epsilon}$$



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

$$\epsilon_r'' = 2n'n''$$

- $\omega \ll \omega_0$  : High  $n'$   $\Rightarrow$  low  $v_{ph} = c/n'$
- $\omega \approx \omega_0$  : Strong  $\omega$  dependence  $v_{ph}$   
Large absorption ( $\sim n''$ )
- $\omega \gg \omega_0$  :  $n' = 1$   $\Rightarrow$   $v_{ph} = c$



# Realistic Rarefied Media

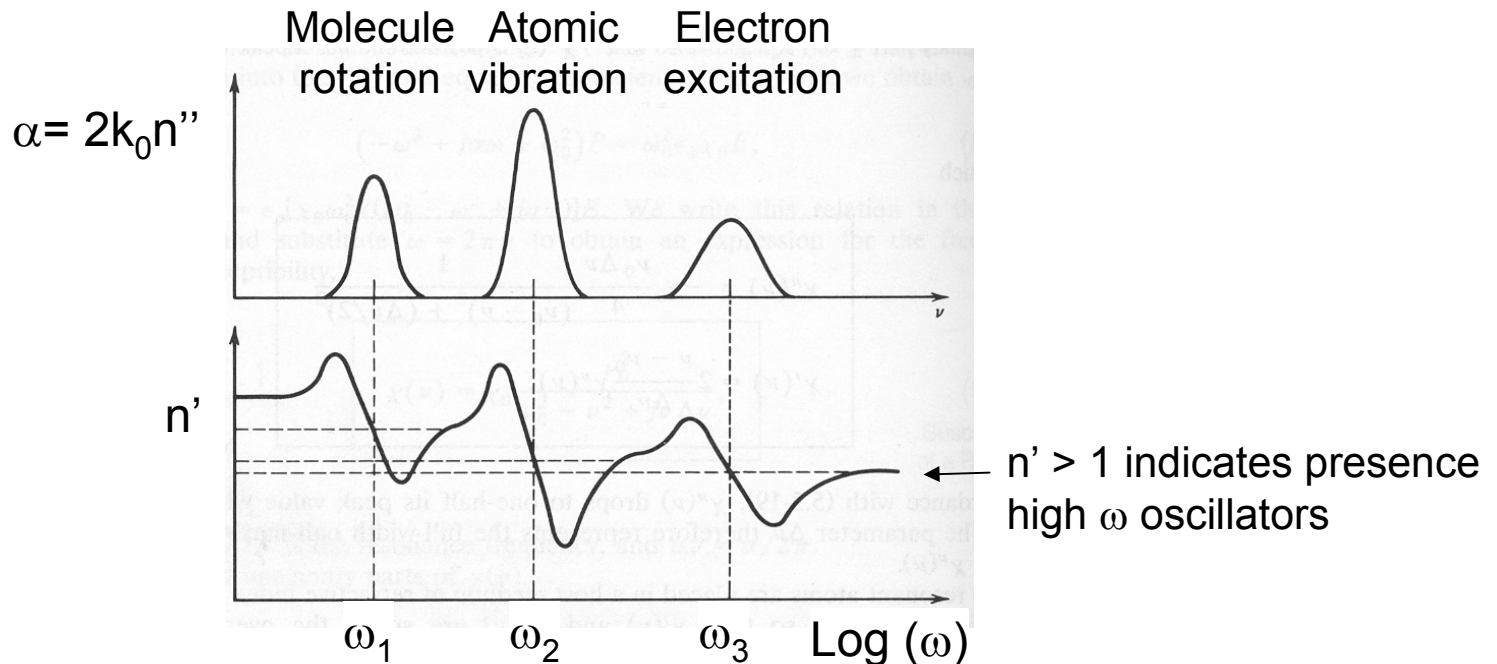
## Realistic atoms have many resonances

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

$$\Rightarrow \chi = \sum_k \frac{N_k e^2}{\epsilon_0 m} \frac{1}{\omega_k^2 - \omega^2 - i\gamma\omega}$$

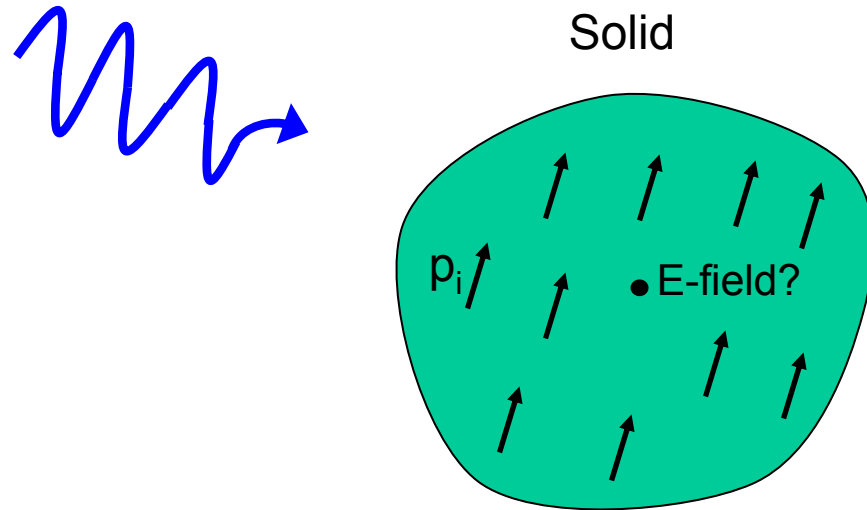
Where  $N_k$  is the density of the electrons/atoms with a resonance at  $\omega_k$

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



# Back to Relation Atomic Polarizability ( $\alpha$ ) and $\chi$ :

## 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                      Field without matter                      Induced dipolar field from all the other atoms

# Electric Susceptibility of a Solid

## Local field

- Local field:

$$\mathbf{E}_L = \mathbf{E}_0 + \mathbf{E}_I$$

Local field
Field without matter
All the other atoms

## Induced dipolar field

- Example: For cubic symmetry:  $\mathbf{E}_I = \frac{\mathbf{P}}{3\epsilon_0}$  (Solid state Phys. Books, e.g. Kittel, Ashcroft..)

$$\Rightarrow \mathbf{E}_L = \mathbf{E}_0 + \frac{\mathbf{P}}{3\epsilon_0} \quad (\text{Similar relations can be derived for any solid})$$

## Polarization of a solid

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

$$\mathbf{P} = \epsilon_0 \sum_j N_j \alpha_j \mathbf{E}_L = \epsilon_0 \sum_j N_j \alpha_j \left( \mathbf{E}_0 + \frac{\mathbf{P}}{3\epsilon_0} \right) = \epsilon_0 \sum_j N_j \alpha_j \mathbf{E}_0 + \sum_j N_j \alpha_j \frac{\mathbf{P}}{3}$$

$\underbrace{\hspace{2em}}_{p_j}$

$$\Rightarrow \mathbf{P} \left( 1 - \frac{1}{3} \sum_j N_j \alpha_j \right) = \epsilon_0 \sum_j N_j \alpha_j \mathbf{E}_0 \Rightarrow$$

$$\chi = \frac{P}{\epsilon_0 E} = \frac{\sum_j N_j \alpha_j}{1 - \frac{1}{3} \sum_j N_j \alpha_j}$$

# Clausius-Mossotti Relation

## Polarization of a solid

- Susceptibility:

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

- Limit of low atomic concentration:  
....or weak polarizability:  
pretty good for gasses and glasses

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

## Clausius-Mossotti

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

$$\frac{\varepsilon - 1}{\varepsilon + 2} = \frac{1}{3\varepsilon_0} \sum_j N_j \alpha_j \quad \text{III}$$

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