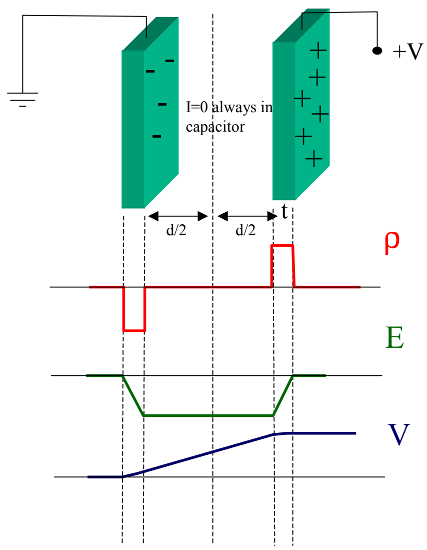
The Capacitor



$$\nabla \cdot E = \frac{\rho}{\varepsilon_o}$$

$$E = \int_{\frac{-d}{2}-t}^{\frac{-d}{2}} \frac{\rho}{\varepsilon_o} dx = \frac{\rho t}{\varepsilon_o} = \frac{Q}{A\varepsilon_o}$$

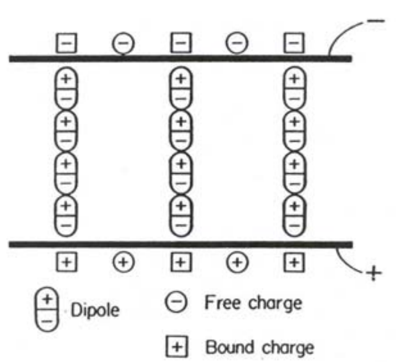
$$V = \int_{\frac{-d}{2}}^{\frac{d}{2}} E dx = \frac{Qd}{A\varepsilon_o}$$

$$\frac{Q}{C} = V = \frac{Qd}{A\varepsilon_o}$$

$$C = \frac{\varepsilon_o A}{d}$$

The Capacitor

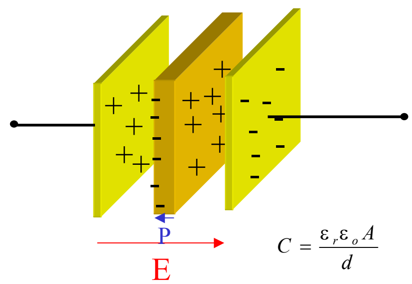
- The air-gap can store energy!
- If we can move charge temporarily without current flow, can store even more
- Bound charge around ion cores in a material can lead to dielectric properties



•Two kinds of charge can create plate charge:
- •surface charge
- •dipole polarization in the volume

•Gauss' law can not tell the difference (only depends on charge per unit area)

Material Polarization



$$C = \frac{\varepsilon_r \varepsilon_o A}{d}$$

$$D = \varepsilon_o E + P = \varepsilon E$$

$$\varepsilon = \varepsilon_r \varepsilon_o$$

$$\varepsilon_r = 1 + \frac{P}{\varepsilon_o E} = 1 + \chi$$

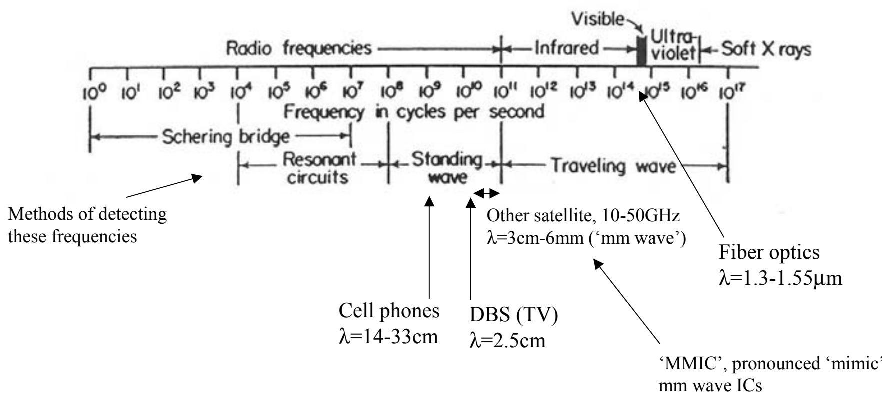
P is the Polarization
D is the Electric flux density or the Dielectric displacement
χ is the dielectric or electric susceptibility

All detail of material response is in ε_r and therefore P

Origin of Polarization

- We are interested in the true dipoles creating polarization in materials (not surface effect)
- As with the free electrons, what is the response of these various dipole mechanisms to various E-field frequencies?
- When do we have to worry about controlling
  - molecular polarization (molecule may have non-uniform electron density)
  - ionic polarization (E-field may distort ion positions and temporarily create dipoles)
  - electronic polarization (bound electrons around ion cores could distort and lead to polarization)
- Except for the electronic polarization, we might expect the other mechanisms to operate at lower frequencies, since the units are much more massive
- What are the applications that use waves in materials for frequencies below the visible?

Application for Different E-M Frequencies



In communications, many E-M waves travel in insulating materials: What is the response of the material (ε_r) to these waves?

Wave Eqn. with Insulating Material and Polarization

$$\nabla x\vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\nabla x\vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t} \xrightarrow{nonmag} \nabla x\vec{B} = \vec{J} + \frac{\partial\left(\varepsilon_o\vec{E} + \vec{P}\right)}{\partial t} \xrightarrow{insulating} \nabla x\vec{B} = \varepsilon\frac{\partial \vec{E}}{\partial t}$$

$$(\vec{D} = \varepsilon_0\vec{E} + \vec{P} = \varepsilon\vec{E})$$

$$\nabla^2 E = \mu_0\varepsilon_0\varepsilon_r\frac{\partial^2 E}{\partial t^2} = \frac{\varepsilon_r}{c^2}\frac{\partial^2 E}{\partial t^2}$$

$$E = E_0 e^{i(k\bullet r - \varpi t)} = E_0 e^{ik\bullet r}e^{-i\varpi t} = E(r)e^{-i\varpi t}$$

$$\nabla^2 E(r) = -\frac{\omega^2\varepsilon_r E(r)}{c^2}$$

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

$$\omega = \frac{c}{\sqrt{\varepsilon_r}}k \xrightarrow{optical} \frac{c}{n}k$$

So polarization slows down the velocity of the wave in the material

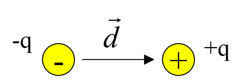
Compare Optical (index of refraction) and Electrical Measurements of ε

Material	Optical, n^2	Electrical, ε	
diamond	5.66	5.68	Only electronic polarization
NaCl	2.25	5.9	Electronic and ionic polarisation
H_2O	1.77	80.4	Electronic, ionic, and molecular polarisation

Polarization that is active depends on material and frequency

Microscopic Frequency Response of Materials

- Bound charge can create dipole through charge displacement.
- Hydrodynamic equation (Newtonian representation) will now have a restoring force.
- Review of dipole physics:



Dipole moment: $\vec{p} = q\vec{d}$

$\vec{p}$

Applied E-field rotates dipole to align with field:

Torque $\vec{\tau} = \vec{p} x \vec{E}$

Potential Energy $U = -\vec{p} \cdot \vec{E} = |\vec{p}||\vec{E}| \cos\theta$

Microscopic Frequency Response of Materials

- For a material with many dipoles:

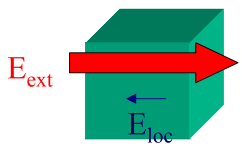
$$\vec{P} = N\vec{p} = N\alpha\vec{E} \ (\vec{p} = \alpha\vec{E})$$

(polarization=(#/vol)*dipole polarization)
α=polarizability

$$\chi = \frac{|\vec{P}|}{\varepsilon_o|\vec{E}|}, \text{ so } \chi = \frac{N\alpha}{\varepsilon_0}$$

$\vec{p} = \alpha\vec{E}$ Actually works well only for low density of dipoles, i.e. gases: little screening

For solids where there can be a high density: local field



For a spherical volume inside (theory of local field),

$$\vec{E}_{loc} = \vec{E}_{ext} + \frac{\vec{P}}{3\varepsilon_o}$$

Microscopic Frequency Response of Materials

- We now need to derive a new relationship between the dielectric constant and the polarizability

$$D = \varepsilon_r\varepsilon_o E_{ext} = \varepsilon_o E_{ext} + P$$

$$P = \varepsilon_r\varepsilon_o E_{ext} - \varepsilon_o E_{ext}$$

$$E_{loc} = E_{ext}\left(\frac{2+\varepsilon_r}{3}\right)$$

Plugging into $P=N\alpha E_{loc}$:

$$\varepsilon_r\varepsilon_o E_{ext} - \varepsilon_o E_{ext} = N\alpha\frac{(\varepsilon_r+2)}{3}E_{ext}$$

$$(\varepsilon_r - 1)\varepsilon_o = \frac{N\alpha}{3}(\varepsilon_r + 2)$$

Clausius-Mosotti Relation: $$\frac{\varepsilon_r - 1}{\varepsilon_r + 2} = \frac{N\alpha}{3\varepsilon_o} = \frac{\alpha}{3v\varepsilon_o}$$ Where v is the volume per dipole (1/N)

Macro Micro

Different Types of Polarizability

Highest natural frequency ↕ Lowest natural frequency

- Atomic or electronic, α_e
- Displacement or ionic, α_i
- Orientational or dipolar, α_o

Lightest mass ↕ Heaviest mass

$$\alpha = \alpha_e + \alpha_i + \alpha_o$$

As with free e-, we want to look at the time dependence of the E-field: $E = E_o e^{-i\omega t}$

$$m\frac{\partial^2 x}{\partial t^2} = \frac{m}{\tau}\frac{\partial x}{\partial t} - eE - Kx$$

Response, Drag, Driving Force, Restoring Force

$$m\ddot{x} = -eE - Kx$$

$$x = x_o e^{-i\omega t}$$

$$m(-\omega^2)x_o = -eE_o - Kx_o$$

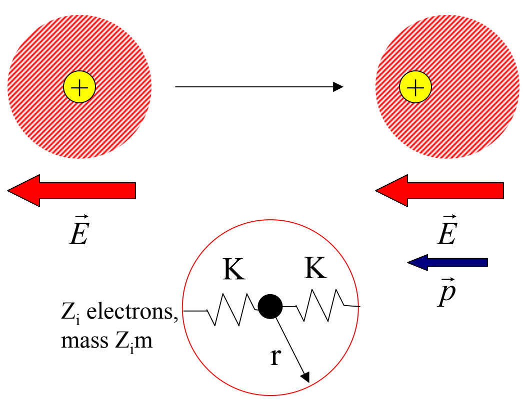
$$x_o = \frac{eE_o}{m\left(\omega^2 - \frac{K}{m}\right)} = \frac{eE_o}{m\left(\omega^2 - \omega_o^2\right)}$$

$$\omega_o = \sqrt{\frac{K}{m}}$$

So lighter mass will have a higher critical frequency

Classical Model for Electronic Polarizability

- Electron shell around atom is attached to nucleus via springs



$$Z_i m\ddot{r} = -Kr - Z_i eE_{loc}, \text{ assume } r = r_o e^{-i\omega t}$$

Electronic Polarizability

$$r_o = \frac{eE_o}{m(\omega^2-\omega_{oe}^2)};\ \omega_{oe} = \sqrt{\frac{K}{mZ_i}}$$

$$r_o = \frac{eE_o}{m\left(\omega^2 - \frac{K}{mZ_i}\right)}$$

$$p = qd = -Z_i er;\ p = p_o e^{-i\omega t}$$

$$p_o = \frac{Z_i e^2}{m(\omega^2-\omega_o^2)}E_o = \alpha_e E_o$$

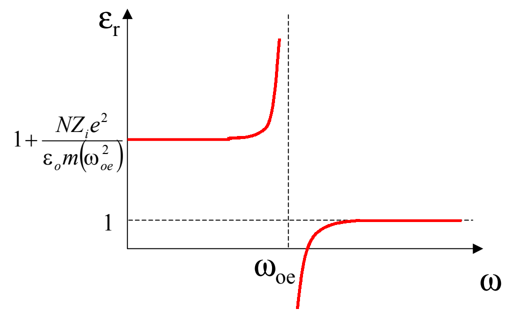
$$\alpha_e = \frac{Z_i e^2}{m(\omega^2-\omega_{oe}^2)}$$

$$\omega >> \omega_{oe},\ \alpha_e = 0$$

$$\omega << \omega_{oe},\ \alpha_e = \frac{Z_i e^2}{m\omega_{oe}^2}$$

If no Clausius-Mosotti,

$$\varepsilon_r = 1 + \frac{N\alpha_e}{\varepsilon_o} = 1 + \frac{NZ_i e^2}{\varepsilon_o m(\omega^2-\omega_{oe}^2)} = n^2$$



QM Electronic Polarizability

- At the atomic electron level, QM expected: electron waves
- QM gives same answer qualitatively
- QM exact answer very difficult: many-bodied problem

E_1 ————

E_0 ————

$$\alpha_e(\omega) = \frac{e^2}{m}\frac{f_{10}}{\omega_{10}^2-\omega^2};\ \omega_{10} = \frac{E_1-E_0}{\hbar}$$

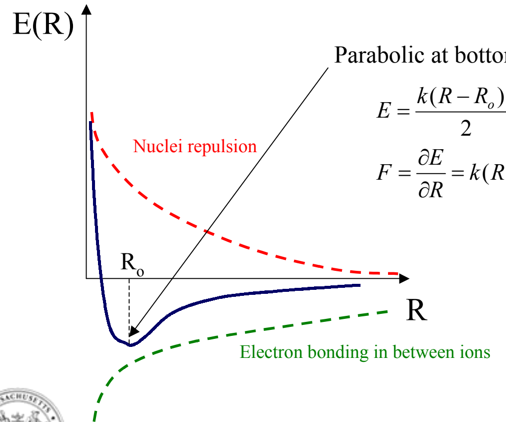
f_{10} is the oscillator strength of the transition (ψ_1 couples to ψ_o by E-field)

For an atom with multiple electrons in multiple levels:

$$\alpha_e(\omega) = \frac{e^2}{m}\sum_{j\neq 0}\frac{f_{j0}}{j_{10}^2-\omega^2};\ \omega_{j0} = \frac{E_j-E_0}{\hbar}$$

Ionic Polarizability

- Problem reduces to one similar to the electronic polarizability
- Critical frequency will be less than electronic since ions are more massive
- The restoring force between ion positions is the interatomic potential



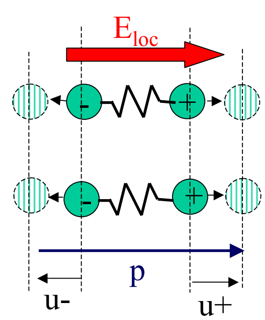
Parabolic at bottom near R_o

$$E = \frac{k(R-R_o)^2}{2}$$

$$F = \frac{\partial E}{\partial R} = k(R-R_o)$$

$$F = kx \Rightarrow \sigma_{ij} = C_{ijkl}\varepsilon_{kl}$$

Ionic Polarizability



- 2 coupled differential eqn's
  - 1 for + ions
  - 1 for - ions

$$w = u_+ - u_-, \ \ddot{w} = \ddot{u}_+ - \ddot{u}_-$$

$$M = \frac{1}{\frac{1}{M_+} + \frac{1}{M_-}}$$

$$M\ddot{w} = -2Kw + eE_{loc}$$

$$E_{loc} = E_o e^{-i\omega t}, w = w_o e^{-i\omega t}$$

$$w_o = \frac{eE_o}{M\left(\omega_{oi}^2 - \omega^2\right)}, \ \omega_{oi} = \sqrt{\frac{2K}{M}}$$

$$p_o = ew_o = \alpha_i E_o$$

$$\alpha_i = \frac{e^2}{M\left(\omega_{oi}^2 - \omega^2\right)}$$

Ionic materials always have ionic and electronic polarization, so:

$$\alpha_{tot} = \alpha_i + \alpha_e = \alpha_+ + \alpha_- + \frac{e^2}{M\left(\omega_{oi}^2 - \omega^2\right)}$$

Ionic Polarizability

- Usually Clausius-Mosotti necessary due to high density of dipoles

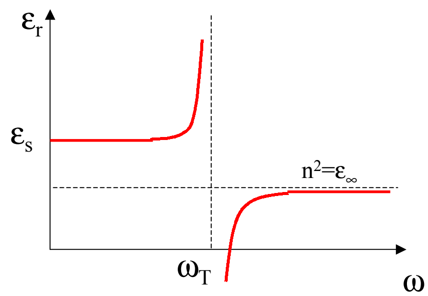
$$\frac{\varepsilon_r-1}{\varepsilon_r+2}=\frac{N\alpha_{tot}}{3\varepsilon_o}=\frac{1}{3\varepsilon_o v}\left[\alpha_+ +\alpha_- +\frac{e^2}{M\left(\omega_{oi}^2-\omega^2\right)}\right]$$

By convention, things are abbreviated by using ε_s and ε_∞:

$$\omega \ll \omega_{oi},\quad \frac{\varepsilon_s-1}{\varepsilon_s+2}=\frac{1}{3\varepsilon_o v}\left[\alpha_+ +\alpha_- +\frac{e^2}{M\left(\omega_{oi}^2\right)}\right]$$

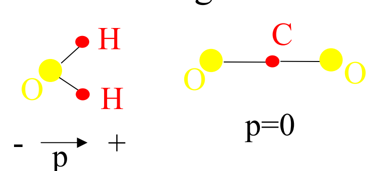
$$\omega \gg \omega_{oi},\quad \frac{\varepsilon_\infty-1}{\varepsilon_\infty+2}=\frac{n^2-1}{n^2+2}=\frac{1}{3\varepsilon_o v}\left[\alpha_+ +\alpha_-\right]$$

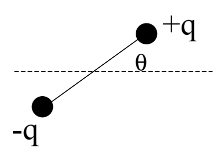
$$\therefore\ \varepsilon_r=\varepsilon_\infty+\frac{\varepsilon_\infty-\varepsilon_s}{\frac{\omega^2}{\omega_T^2}-1},\quad \omega_T^2=\omega_{oi}^2\left(\frac{\varepsilon_\infty+2}{\varepsilon_s+2}\right)$$



Orientational Polarizability

- No restoring force: analogous to conductivity





For a group of many molecules at some temperature:

$$f=e^{\frac{-U}{k_bT}}=e^{\frac{pE\cos\theta}{k_bT}}$$

After averaging over the polarization of the ensemble molecules (valid for low E-fields):

$$\alpha_{DC}\sim\frac{p^2}{3k_bT}$$

Analogous to conductivity, the molecules collide after a certain time t, giving:

$$\alpha_o=\frac{\alpha_{DC}}{1-i\omega\tau}$$

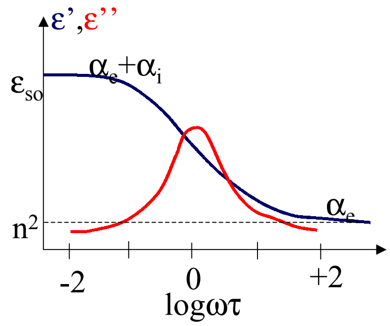
Dielectric Loss

- For convenience, imagine a low density of molecules in the gas phase
- C-M can be ignored for simplicity
- There will be only electronic and orientational polarizability

$$\varepsilon_r = 1 + \chi_e + \chi_o = n^2 + \frac{N\alpha_{DC}}{3\varepsilon_o(1 - i\omega\tau)}$$

$$\omega\tau << 1, \ , \ \varepsilon_r = \varepsilon_{so} = n^2 + \frac{N\alpha_{DC}}{3\varepsilon_o}$$

$$\therefore \ \varepsilon_r = n^2 + \frac{\varepsilon_{so} - n^2}{1 - i\omega\tau}$$



We can write this in terms of a real and imaginary dielectric constant if we choose:

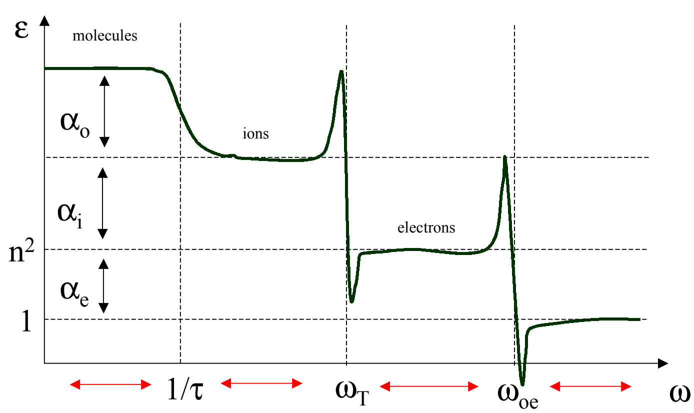
$$\varepsilon_r = \varepsilon' + i\varepsilon''$$

$$\varepsilon' = n^2 + \frac{\varepsilon_{so} - n^2}{1 + \omega^2\tau^2}; \ \varepsilon'' = \frac{\varepsilon_{so} - n^2}{1 + \omega^2\tau^2}\omega\tau$$

Water molecule: $\tau = 9.5\text{x}10^{-11}$ sec, $\omega \sim 10^{10}$
microwave oven, transmission of E-M waves

Dielectric Constant vs. Frequency

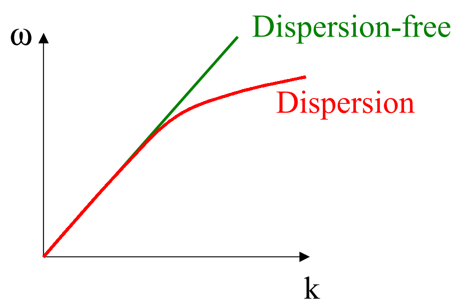
- Completely general ε due to the *localized* charge in materials



Dispersion-free regions, $v_g = v_p$

Dispersion

- Dispersion can be defined a couple of ways (same, just different way)
  - when the group velocity ceases to be equal to the phase velocity
  - when the dielectric constant has a frequency dependence (i.e. when $d\varepsilon/d\omega$ not 0)



$$\omega = \frac{c}{\sqrt{\varepsilon_r}} k$$

$$v_p = \frac{\omega}{k} = \frac{c}{\sqrt{\varepsilon_r}} = \frac{\partial \omega}{\partial k} = v_g$$

$$v_p = \frac{\omega}{k} = \frac{c}{\sqrt{\varepsilon_r(\omega)}} \neq \frac{\partial \omega}{\partial k} = v_g$$