Optical Properties of Insulators

Dielectric response of insulators

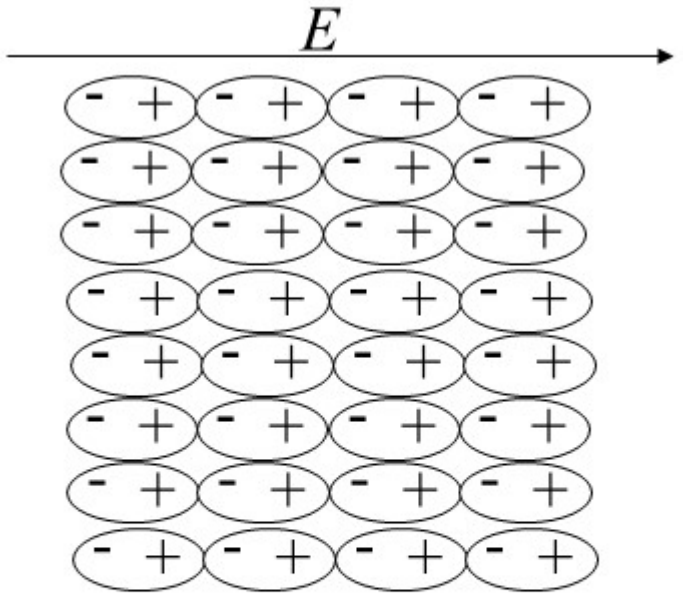
The electric polarization is related to the electric field

$$P_i = \varepsilon_0 \chi_{ij} E_j$$

The electric displacement vector D is also related to the electric field

$$D_i = P_i + \varepsilon_0 E_i = \varepsilon_0 (1 + \chi_{ij}) E_j = \varepsilon_0 \varepsilon_{ij} E_j$$

$$\varepsilon_{ij} = (1 + \chi_{ij})$$



E is decreased by a factor of the dielectric constant

Dielectric response of insulators

In an insulator, charge is bound. The response to an electric field can be modeled as a collection of damped harmonic oscillators

$$P = nex$$

Macroscopic polarization

electron density

ex = dipole moment

The core electrons of a metal respond to an electric field like this too.

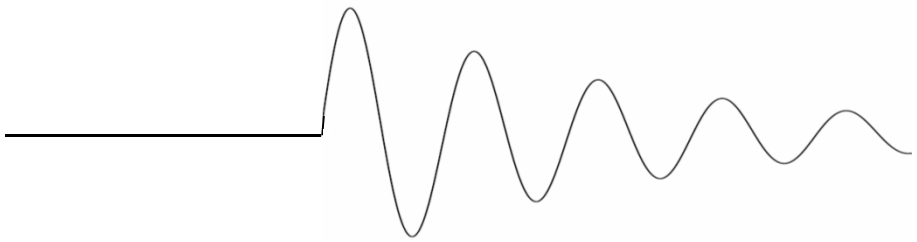
Dielectric response of insulators

The differential equation that describes how the position of the charge changes in time is:

$$m\frac{d^2x}{dt^2}+b\frac{dx}{dt}+kx=-eE(t)$$

The impulse response function is:

$$g(t)=-\frac{1}{b}\exp\left(\frac{-bt}{2m}\right)\sin\left(\frac{\sqrt{4mk-b^2}}{2m}t\right)\qquad t>0$$



Electric susceptibility

$$\vec{P} = \varepsilon_0 \chi_E \vec{E} \qquad \vec{P} = nq\vec{x}$$

$$\chi_E = \frac{P}{\varepsilon_0 E} = \frac{nqx}{\varepsilon_0 E}$$

Assume a solution of the form $x(\omega)e^{i\omega t}$, $E(\omega)e^{i\omega t}$

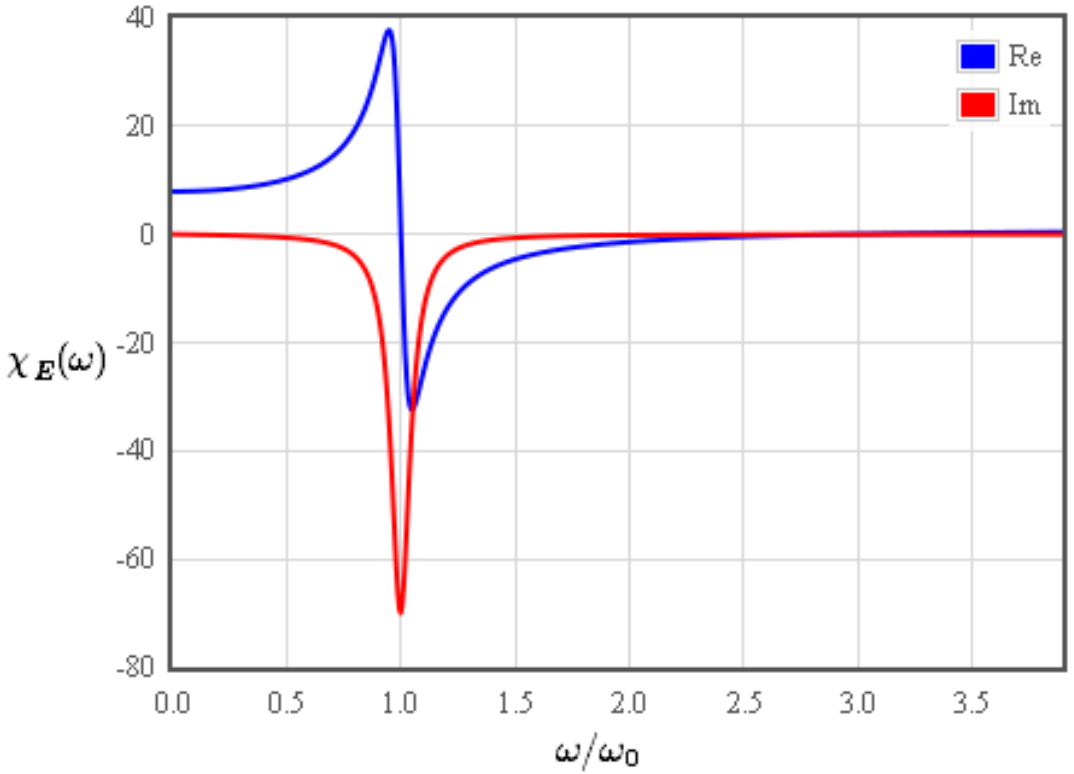
$$m\frac{d^2x}{dt^2} + b\frac{dx}{dt} + kx = qE(t)$$

$$\frac{d^2x}{dt^2} + \gamma\frac{dx}{dt} + \omega_0^2 x = -\frac{qE}{m} \qquad \omega_0 = \sqrt{\frac{k}{m}} \qquad \gamma = \frac{b}{m}$$

$$-\omega^2 x(\omega) + i\omega\gamma x(\omega) + \omega_0^2 x(\omega) = qE(\omega)$$

Electric susceptibility

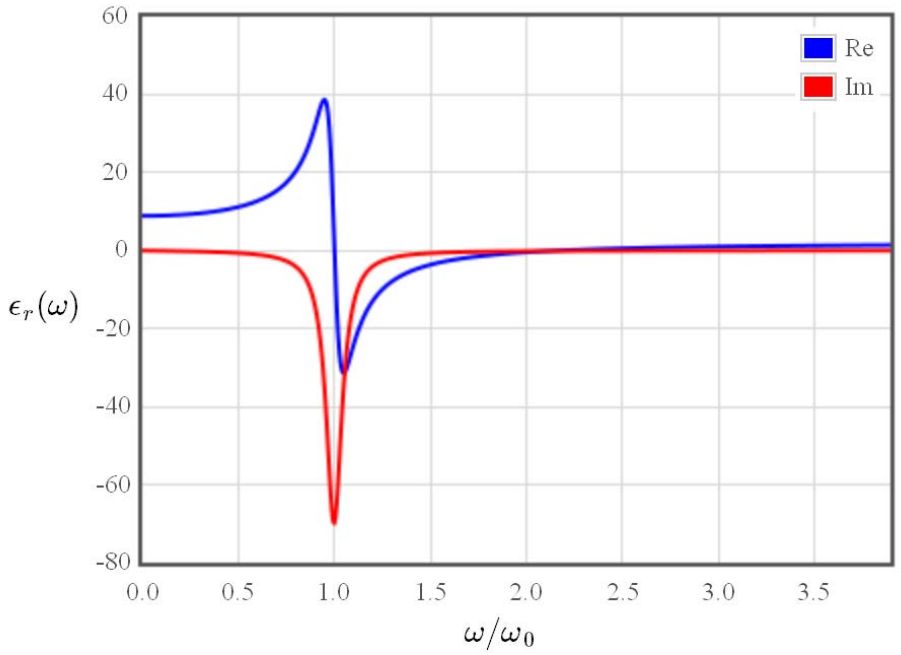
$$\chi_E(\omega) = \frac{n_{\omega_0} q^2}{\varepsilon_0 m} \frac{1}{\omega_0^2 - \omega^2 + i\gamma\omega}$$

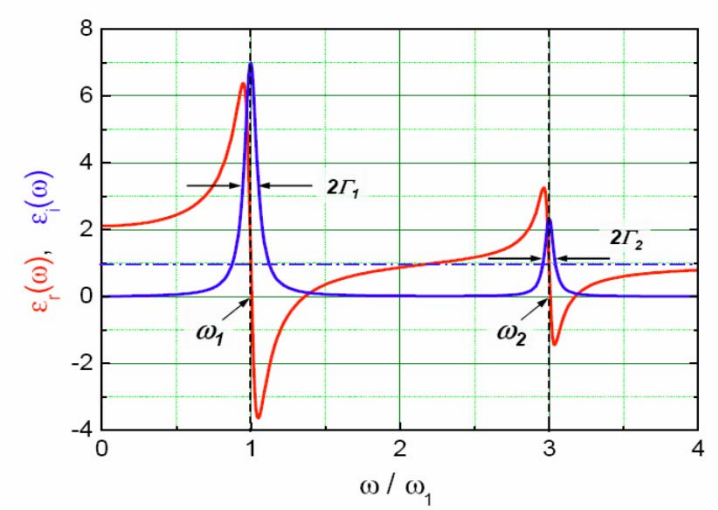


Dielectric function

$$\vec{D} = \epsilon_r \epsilon_0 \vec{E} = \vec{P} + \epsilon_0 \vec{E}$$

$$\varepsilon_r(\omega) = 1 + \chi_E(\omega) = 1 + \frac{n_{\omega_0} q^2}{\varepsilon_0 m} \frac{1}{\omega_0^2 - \omega^2 + i\gamma\omega}$$

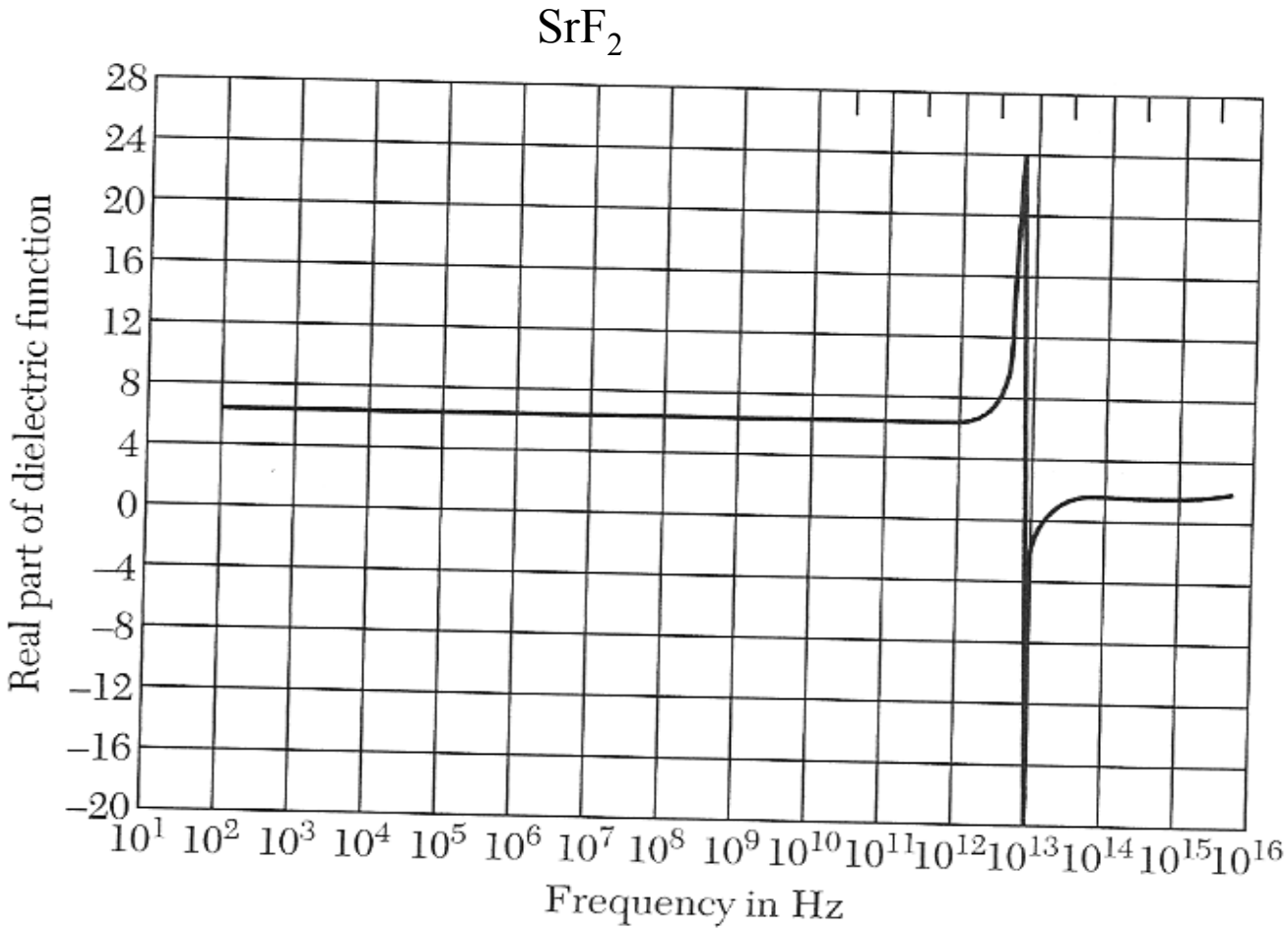




Gross and Marx

There can be more resonances.

Dielectric function of insulators



Insulators can often be modeled as a simple resonance.

Dispersion relation

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \qquad \nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t}$$

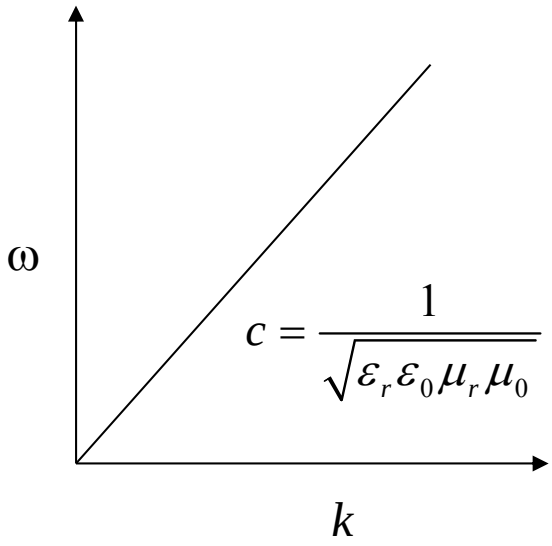
$$\vec{D} = \varepsilon \vec{E} \qquad \vec{B} = \mu \vec{H}$$

$$\nabla \times \vec{E} = -\mu \frac{\partial \vec{H}}{\partial t}$$

Take the curl $$\nabla \times \nabla \times \vec{E} = -\mu \frac{\partial \nabla \times \vec{H}}{\partial t}$$

$$\nabla \underbrace{\left(\nabla \cdot \vec{E}\right)}_{0} - \nabla^2 \vec{E} = -\mu \frac{\partial^2 \vec{D}}{\partial t^2}$$

$$\varepsilon_r \varepsilon_0 \mu_r \mu_0 \frac{\partial^2 \vec{D}}{\partial t^2} = \nabla^2 \vec{D}$$



The normal mode solutions are plane waves: $\vec{D} = \vec{D}_0 \exp\left(i\left(\vec{k} \cdot \vec{r} - \omega t\right)\right)$

$$\boxed{\varepsilon(\omega, k)\mu_0 \varepsilon_0 \omega^2 = k^2}$$

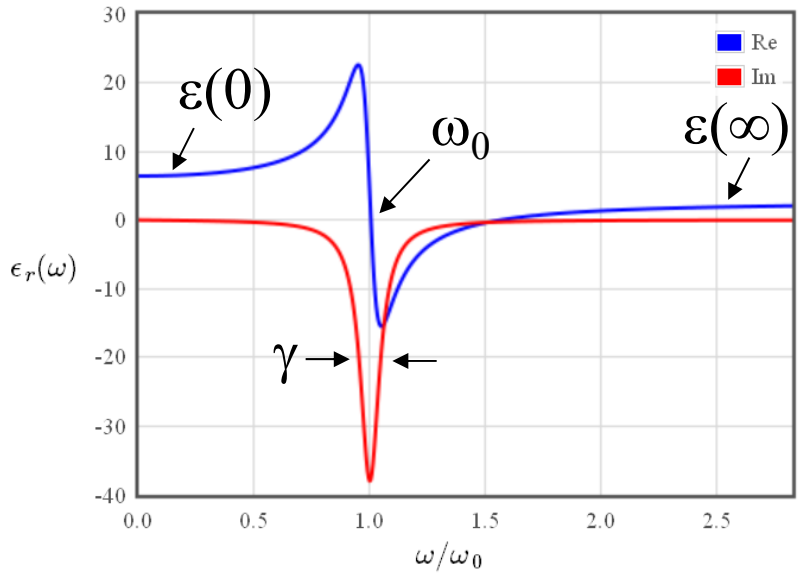
Dispersion relation

$$\varepsilon(\omega)\mu_0\varepsilon_0\omega^2 = k^2$$

If ε is real and positive: propagating electromagnetic waves $\exp\left(i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right)$

If $\varepsilon_r < 0$: decaying solutions $\exp(-\vec{k}\cdot\vec{r}-i\omega t)$

If ε is complex, $\varepsilon_r > 0$: decaying electromagnetic waves $\exp\left(i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right)\exp(-\kappa r)$



Dielectric function

Dispersion relation: $\varepsilon_r \mu_0 \varepsilon_0 \omega^2 = k^2$

$$k = \sqrt{\varepsilon_r \mu_0 \varepsilon_0}\,\omega = \frac{\sqrt{\varepsilon_r}\,\omega}{c}$$

Measurable: $\sqrt{\varepsilon} = n + iK$

refractive index

extinction coefficient

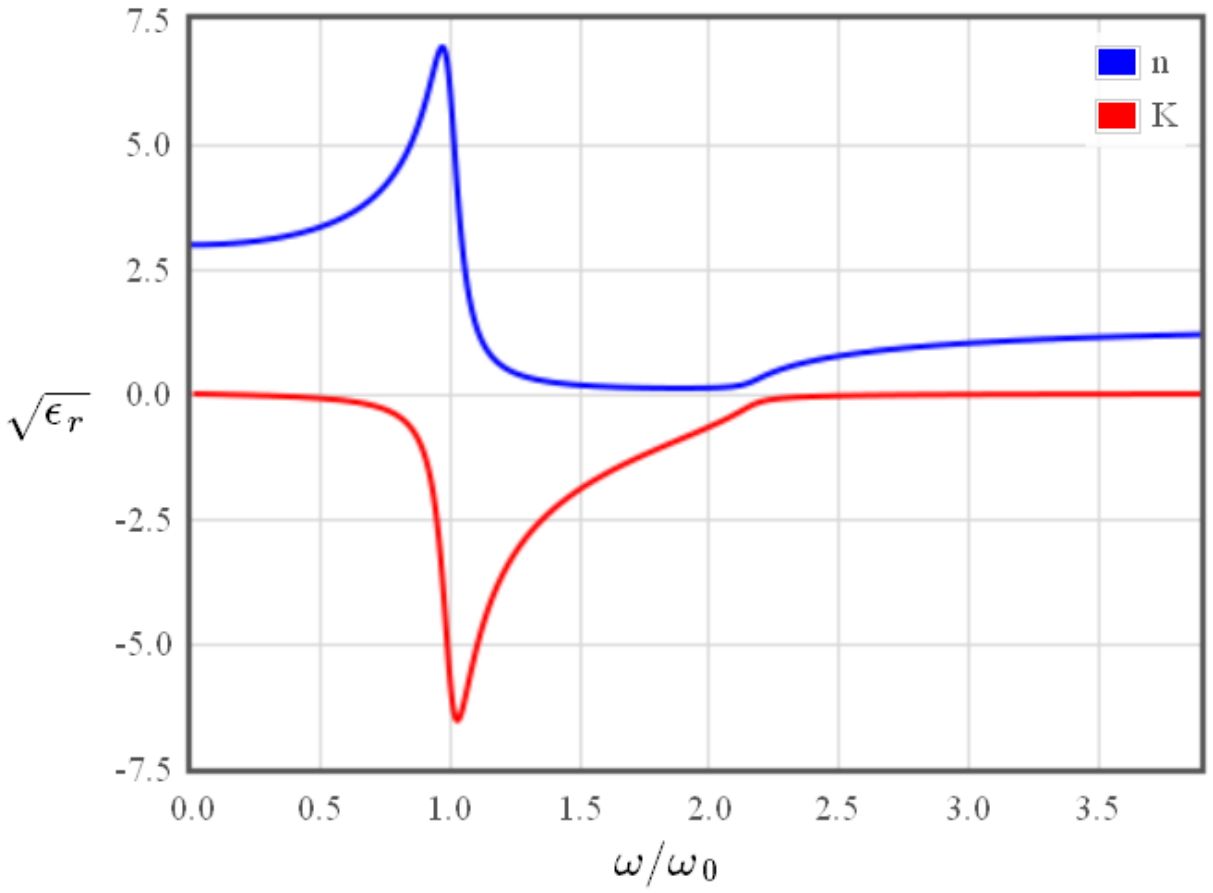
Vacuum	Dielectric
$\omega = ck$	$k = \frac{\sqrt{\varepsilon_r}\,\omega}{c}$
$\exp\left(i\left(\frac{\omega x}{c} - \omega t\right)\right)$	$\exp\left(i\left(\frac{(n+iK)\omega x}{c} - \omega t\right)\right)$
	$= \exp\left(i\left(\frac{n\omega x}{c} - \omega t\right)\right)\exp\left(-\frac{\omega K x}{c}\right)$

Intensity $I(x) = I(0)\exp(-\alpha x)$ J m^{-2} s^{-1} Beer-Lambert

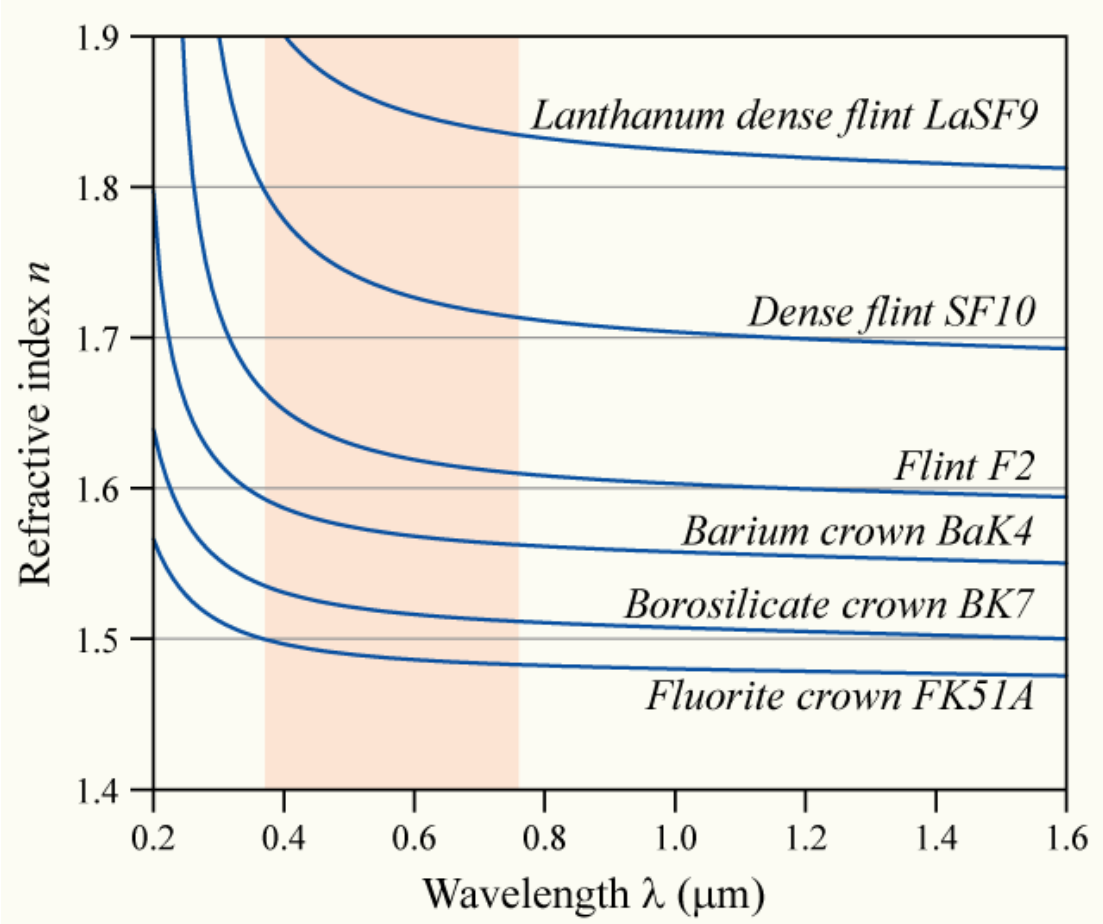
absorption coefficient $\longrightarrow \alpha = \frac{2\omega K}{c}$

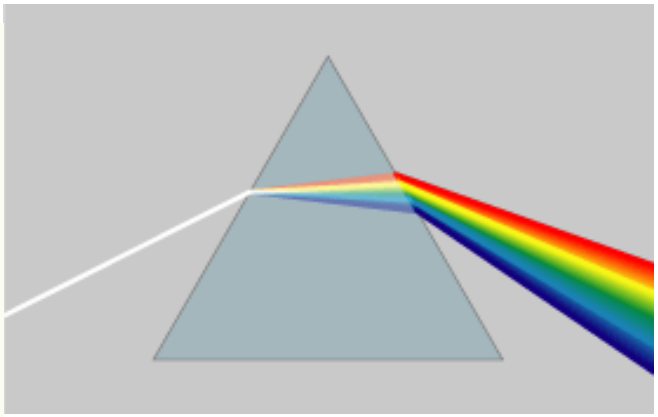
The index of refraction *n* and the extinction coefficient *K*

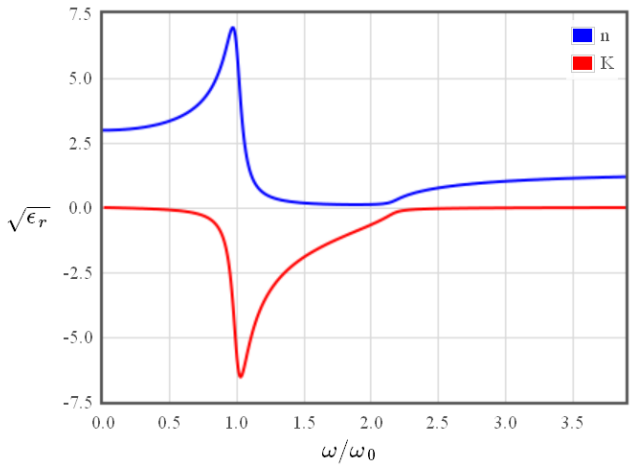
$$\sqrt{\epsilon_r} = n + iK$$



Dispersion







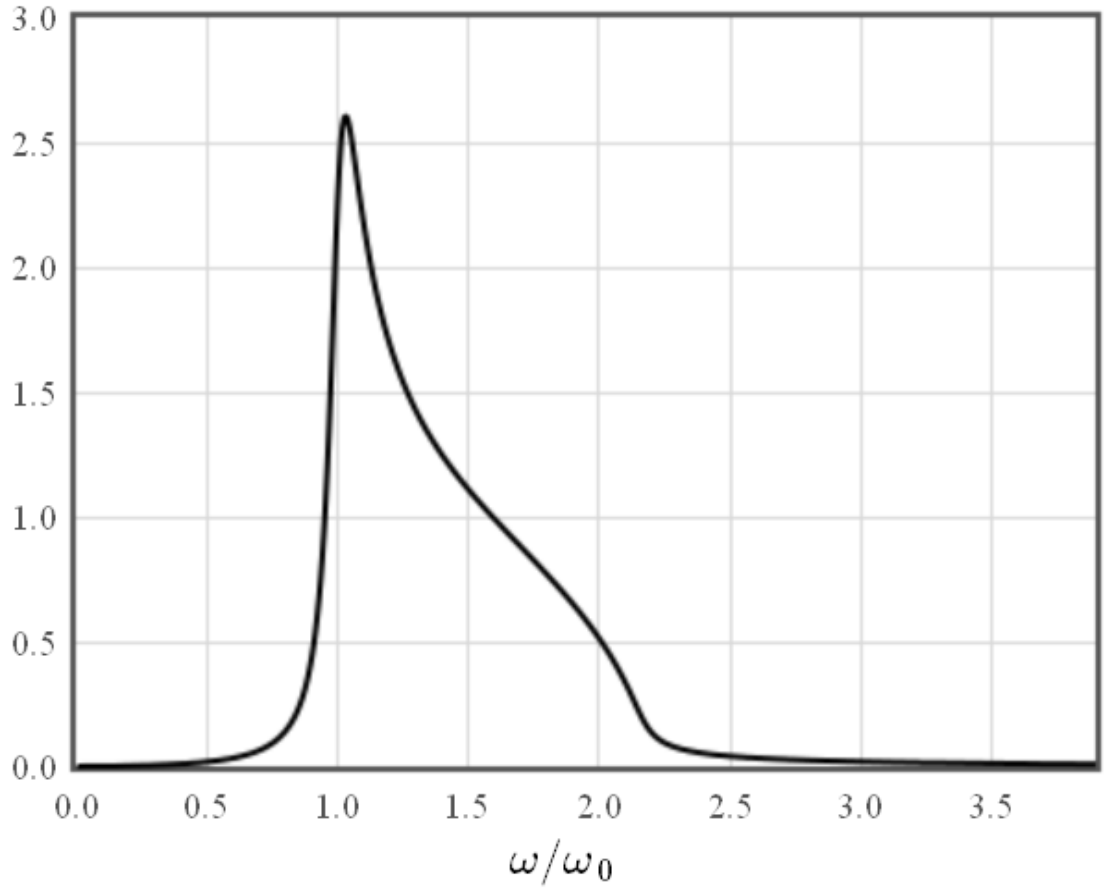
Cause of chromatic aberration in lenses.

http://en.wikipedia.org/wiki/Dispersion_%28optics%29#mediaviewer/File:Prism_rainbow_schema.png
http://en.wikipedia.org/wiki/Refractive_index

Absorption coefficient α

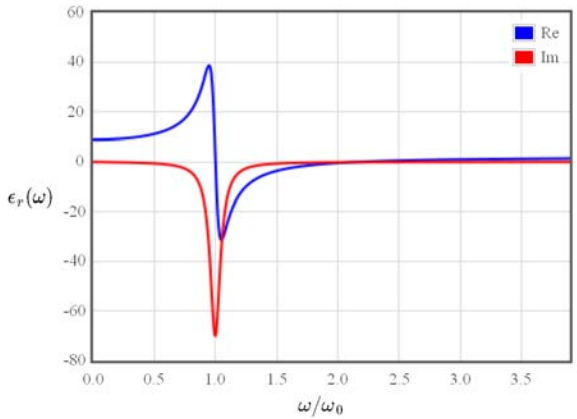
$$I = I_0 \exp(-\alpha x)$$

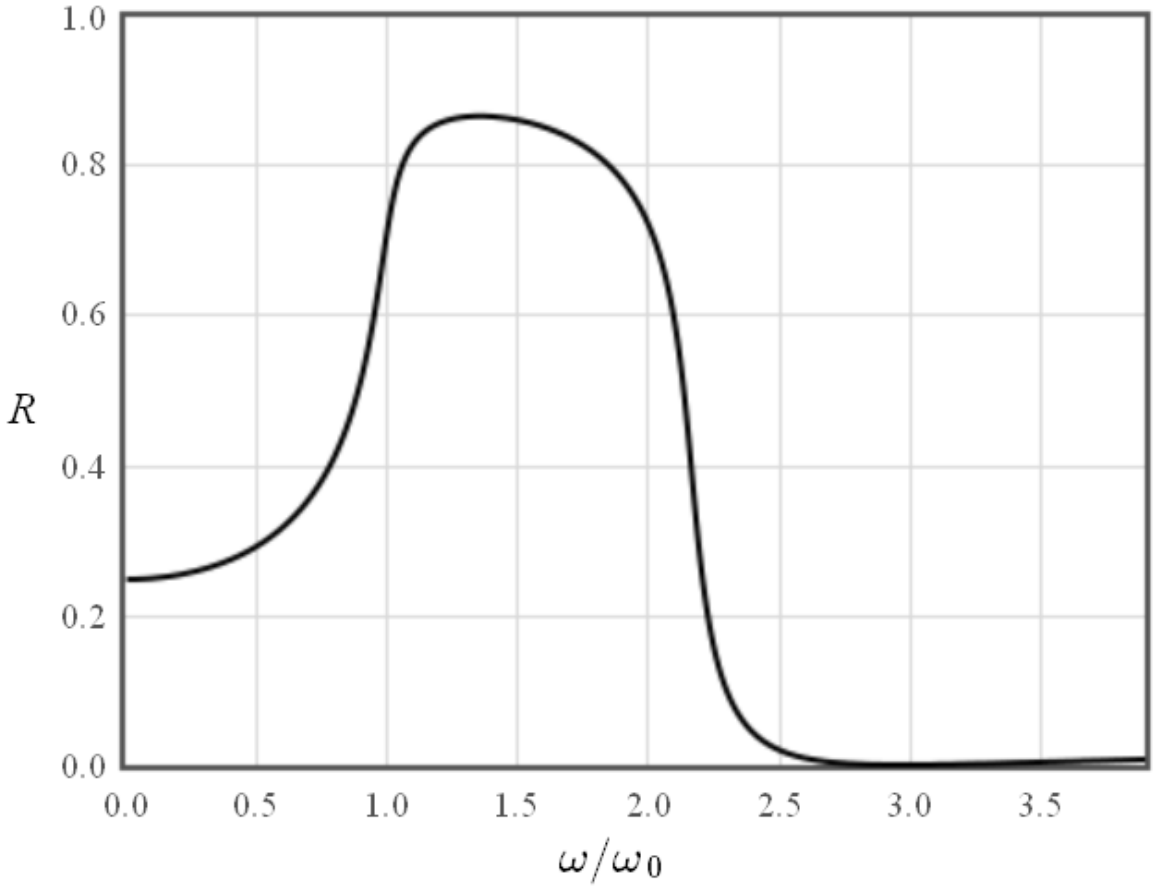
$$\alpha = \frac{2\omega K}{c}$$



Reflectance

$$R = \frac{(n-1)^2 + K^2}{(n+1)^2 + K^2}$$





Optical properties of insulators and semiconductors

In an insulator, all charges are bound. By applying an electric field, the electrons and ions can be pulled out of their equilibrium positions. When this electric field is turned off, the charges oscillate as they return to their equilibrium positions. A simple model for an insulator can be constructed by describing the motion of the charge as a damped mass-spring system. The differential equation that describes the motion of a charge is,

$$m\,\frac{d^2x}{dt^2} + b\,\frac{dx}{dt} + kx = -qE.$$

Rewriting above equation using $\omega_0 = \sqrt{\frac{k}{m}}$ and the damping constant $\gamma = \frac{b}{m}$ yields,

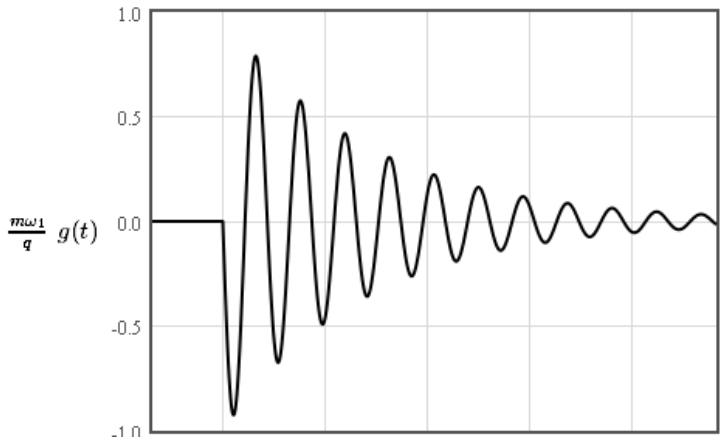
$$\frac{d^2x}{dt^2} + \gamma\,\frac{dx}{dt} + \omega_0^2 x = -\,\frac{qE}{m}\,.$$

If the electric field is pulsed on, the response of the charges is described by the **impulse response function** $g(t)$. The impulse response function satisfies the equation,

$$\frac{d^2g}{dt^2} + \gamma\,\frac{dg}{dt} + \omega_0^2 g = -\,\frac{q}{m}\,\delta(t).$$

The solution to this equation is zero before the electric field is pulsed on and at the time of the pulse the charges suddenly start oscillating with the frequency $\omega_1 = \sqrt{\omega_0^2 - \frac{\gamma^2}{4}}$. The amplitude of the oscillation decays exponentially to zero in a characteristic time $\frac{2}{\gamma}$.

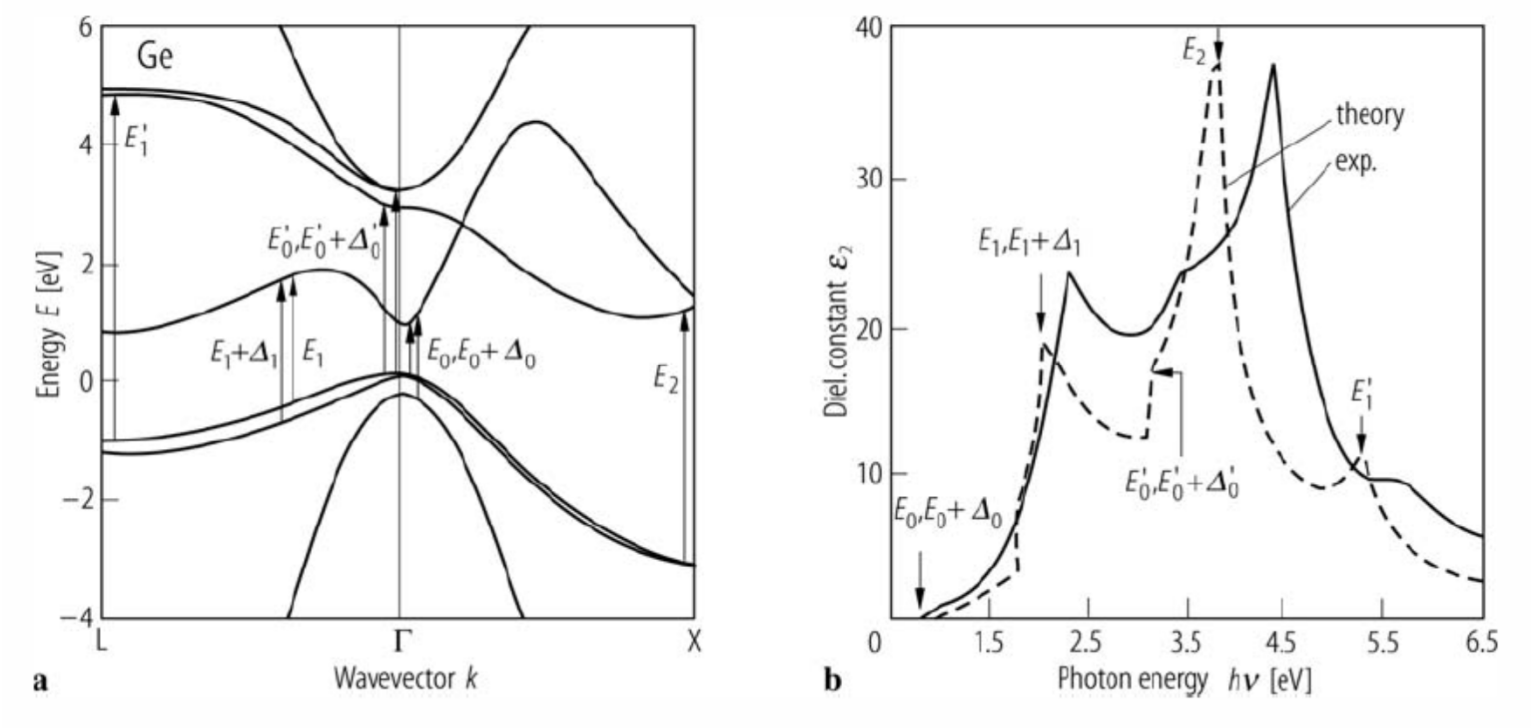
$$g(t) = -\,\frac{q}{m\omega_1}\exp(-\,\frac{\gamma}{2}\,t)\sin(\omega_1 t).$$



Inter- and intraband transitions

When the bands are parallel, there is a peak in the absorption (ε")

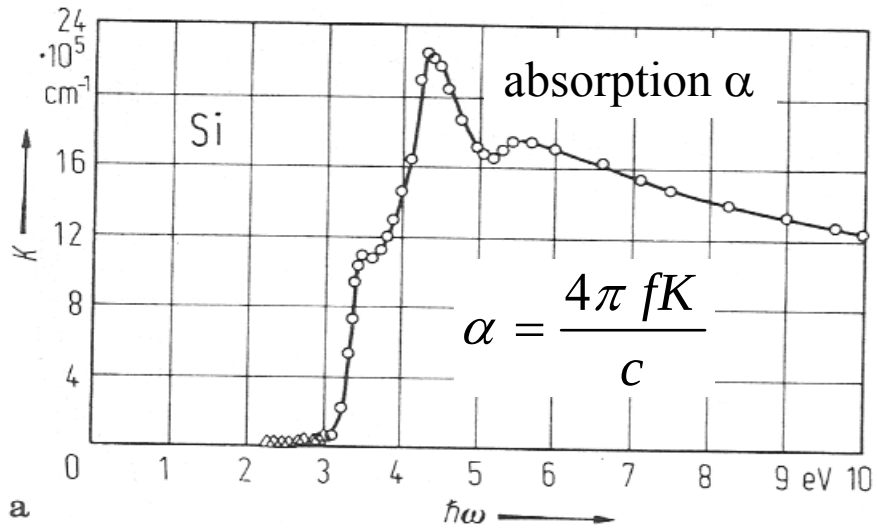
$$\hbar\omega = E_c(\vec{k}) - E_v(\vec{k})$$

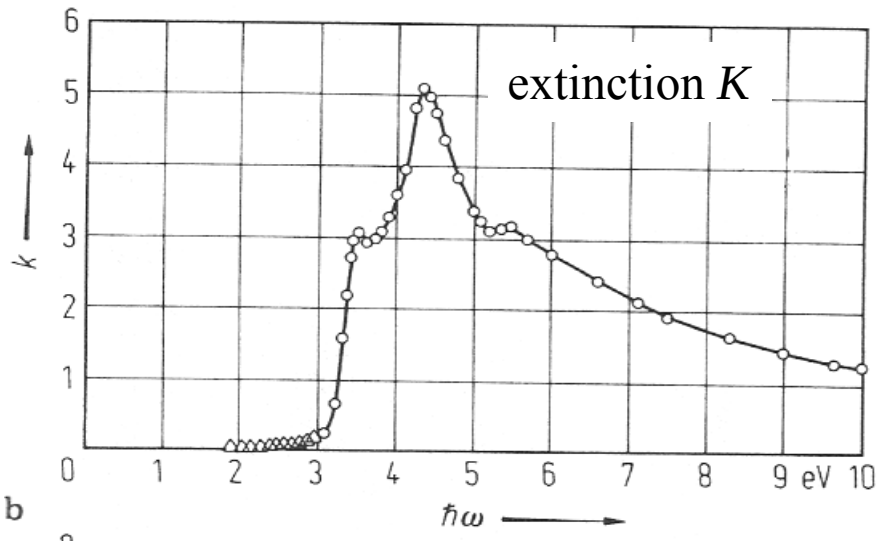


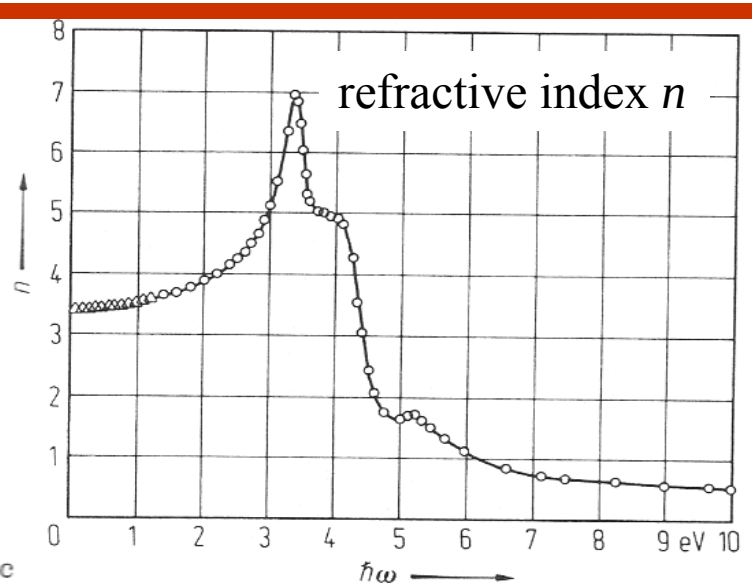
Optical spectroscopy has developed into the most important experimental tool for band structure determination. - Kittel

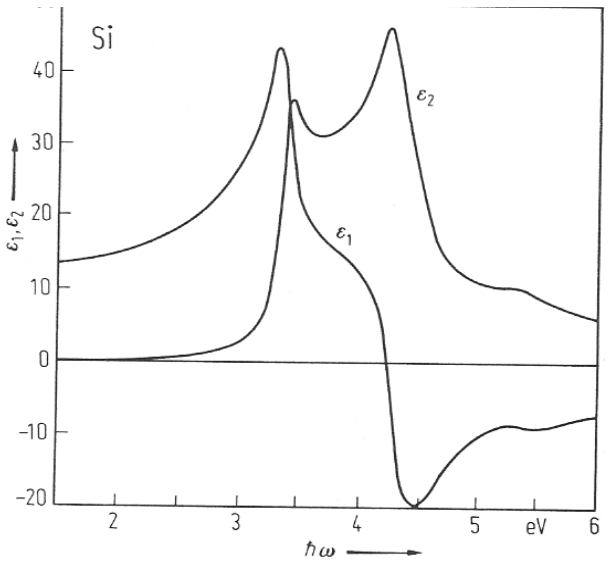
Dielectric function of silicon

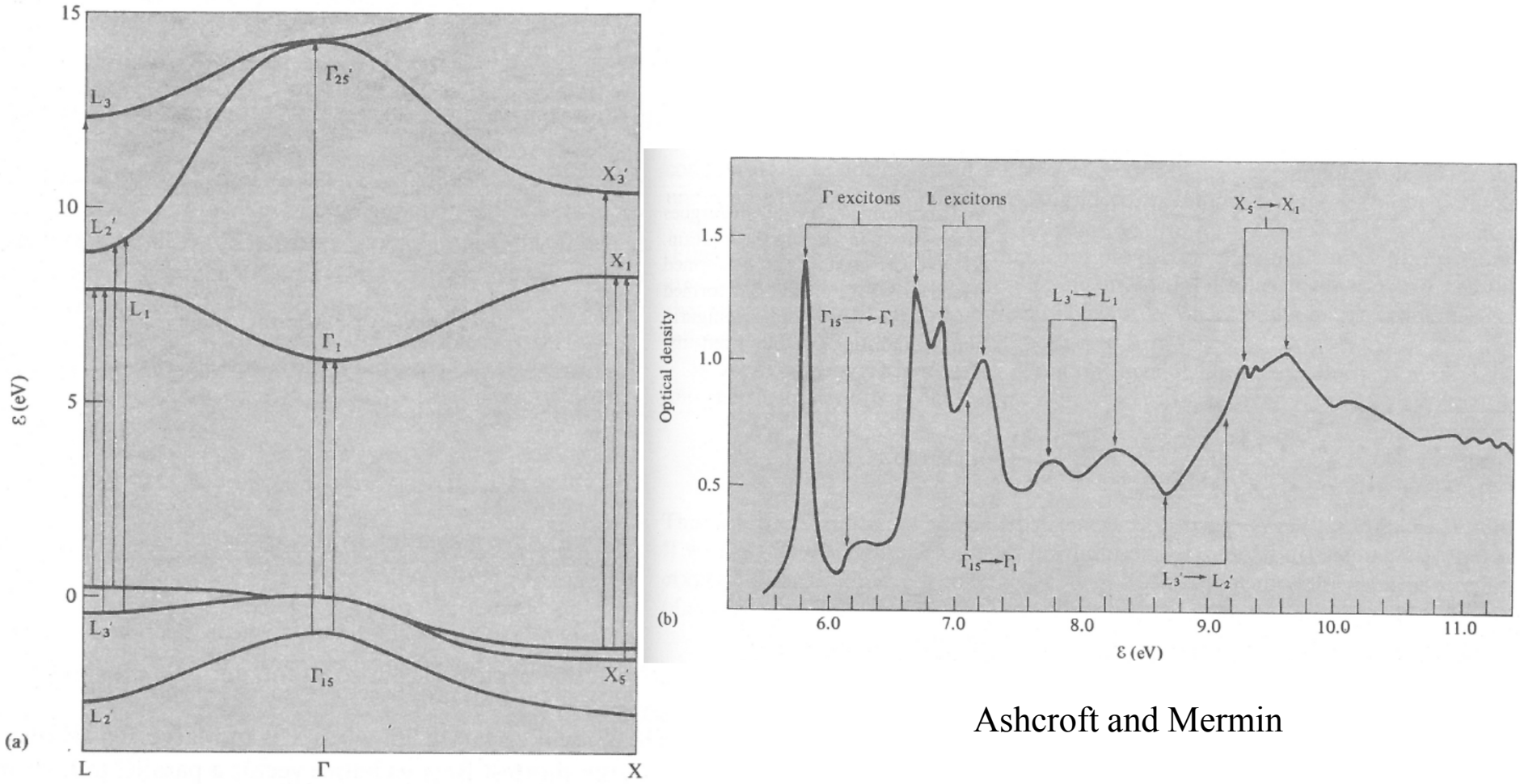
$$\sqrt{\varepsilon(\omega)} = n(\omega) + iK(\omega)$$









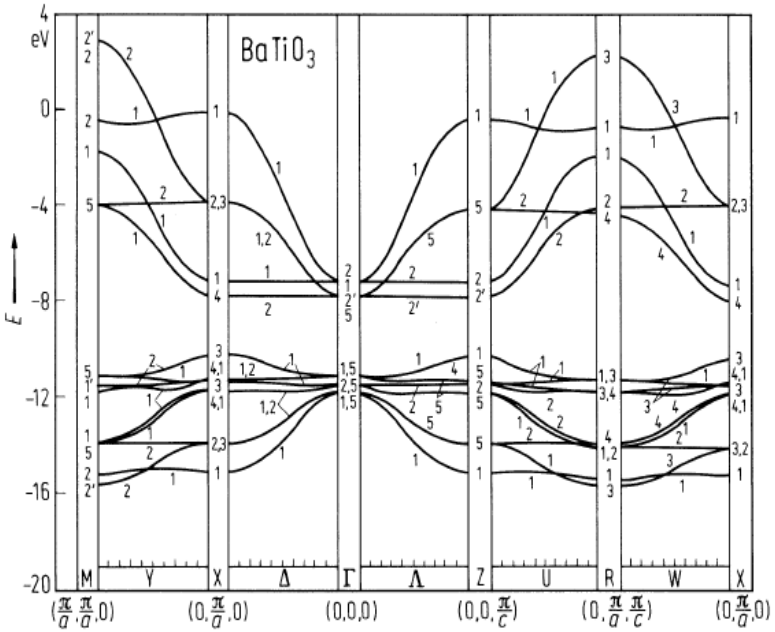


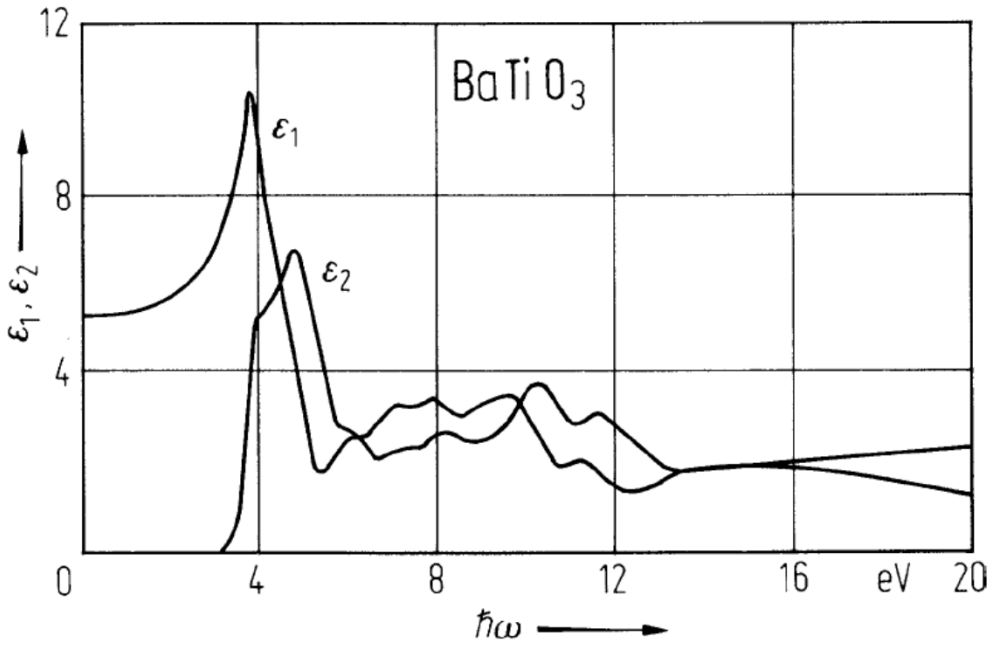
Ashcroft and Mermin

Figure 30.11

(a) The band structure of KI as inferred by J. C. Phillips (*Phys. Rev.* **136**, A1705 (1964) from its optical absorption spectrum. (b) The exciton spectrum associated with the various valence and conduction band maxima and minima. (After J. E. Eby, K. J. Teegarden, and D. B. Dutton, *Phys. Rev.* **116**, 1099 (1959), as summarized by J. C. Phillips, "Fundamental Optical Spectra of Solids," in *Solid State Physics*, vol. 18, Academic Press, New York, 1966.)

Dielectric function of $BaTiO_3$





Dielectrics

Dielectrics used as electrical insulators should not conduct.

Large breakdown field.

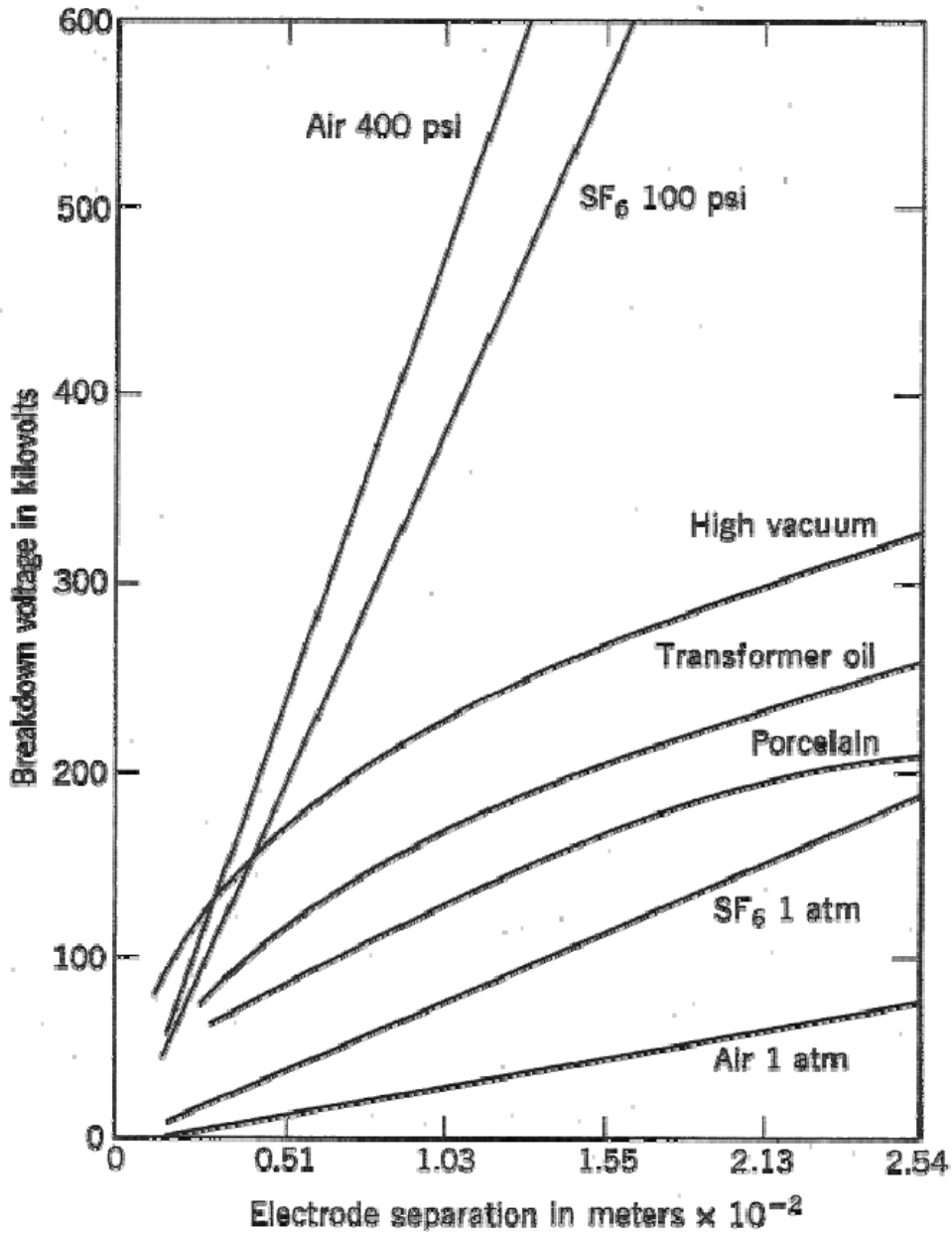
Low AC losses.

Sometimes a low dielectric constant is desired (CMOS interconnects)

Sometimes a high dielectric constant is desired (supercapacitors).

Breakdown field

Typically 10^5-10^6 V/cm



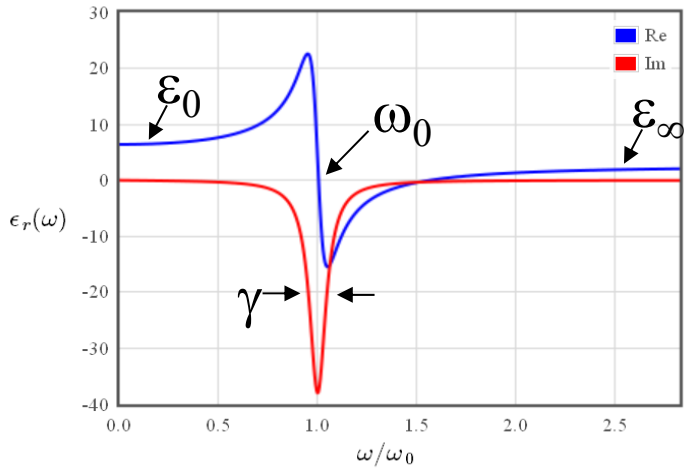
AC losses - loss tangent

In an ideal capacitor, current leads voltage by 90^o.

Because the dielectric constant is complex, in real materials current leads voltage by 90^o - δ.

$$\text{Power loss} = \frac{\omega \varepsilon_1 V_0^2}{2} \tan \delta$$

Becomes more of an issue at high frequencies (microwaves)



Loss tangent

Substance	Dielectric Constant (relative to air)	Dielectric Strength (V/mil)	Loss Tangent	Max Temp (°F)
ABS (plastic), Molded	2.0 - 3.5	400 - 1350	0.00500 - 0.0190	171 - 228
Air	1.00054	30 - 70		
Alumina - 96% - 99.5%	10.0 9.6		0.0002 @ 1 GHz 0.0002 @ 100 MHz 0.0003 @ 10 GHz	
Aluminum Silicate	5.3 - 5.5			
Bakelite	3.7			
Bakelite (mica filled)	4.7	325 - 375		
Balsa Wood	1.37 @ 1 MHz 1.22 @ 3 GHz		0.012 @ 1 MHz 0.100 @ 3 GHz	
Beeswax (yellow)	2.53 @ 1 MHz 2.39 @ 3 GHz		0.0092 @ 1 MHz 0.0075 @ 3 GHz	
Beryllium oxide	6.7		0.006 @ 10 GHz	
Butyl Rubber	2.35 @ 1 MHz 2.35 @ 3 GHz		0.001 @ 1 MHz 0.0009 @ 3 GHz	
Carbon Tetrachloride	2.17 @ 1 MHz 2.17 @ 3 GHz		<0.0004 @ 1 MHz 0.0004 @ 3 GHz	
Diamond	5.5 - 10			
Delrin (acetyl resin)	3.7	500		180
Douglas Fir	1.9 @ 1 MHz		0.023 @ 1 MHz	
Douglas Fir Plywood	1.93 @ 1 MHz 1.82 @ 3 GHz		0.026 @ 1 MHz 0.027 @ 3 GHz	
Enamel	5.1	450		
Epoxy glass PCB	5.2	700		
Ethyl Alcohol (absolute)	24.5 @ 1 MHz 6.5 @ 3 GHz		0.09 @ 1 MHz 0.25 @ 3 GHz	
Ethylene Glycol	41 @ 1 MHz 12 @ 3 GHz		-0.03 @ 1 MHz 1 @ 3 GHz	
Formica XX	4.00			
FR-4 (G-10) - low resin - high resin	4.9 4.2		0.008 @ 100 MHz 0.008 @ 3 GHz	
Fused quartz	3.8		0.0002 @ 100 MHz 0.00006 @ 3 GHz	
Fused silica (glass)	3.8			
Gallium Arsenide (GaAs)	13.1		0.0016 @ 10 GHz	
Germanium	16			
Glass	4 - 10			
Glass (Corning 7059)	5.75		0.0036 @ 10 GHz	
Gutta-percha	2.6			
Halowax oil	4.8			
High Density Polyethylene (HDPE), Molded	1.0 - 5.0	475 - 3810	0.0000400 - 0.00100	158 - 248
Ice (pure distilled water)	4.15 @ 1 MHz 3.2 @ 3 GHz		0.12 @ 1 MHz 0.0009 @ 3 GHz	
Kapton® Type 100 Type 150	3.9 2.9	7400 4400		500

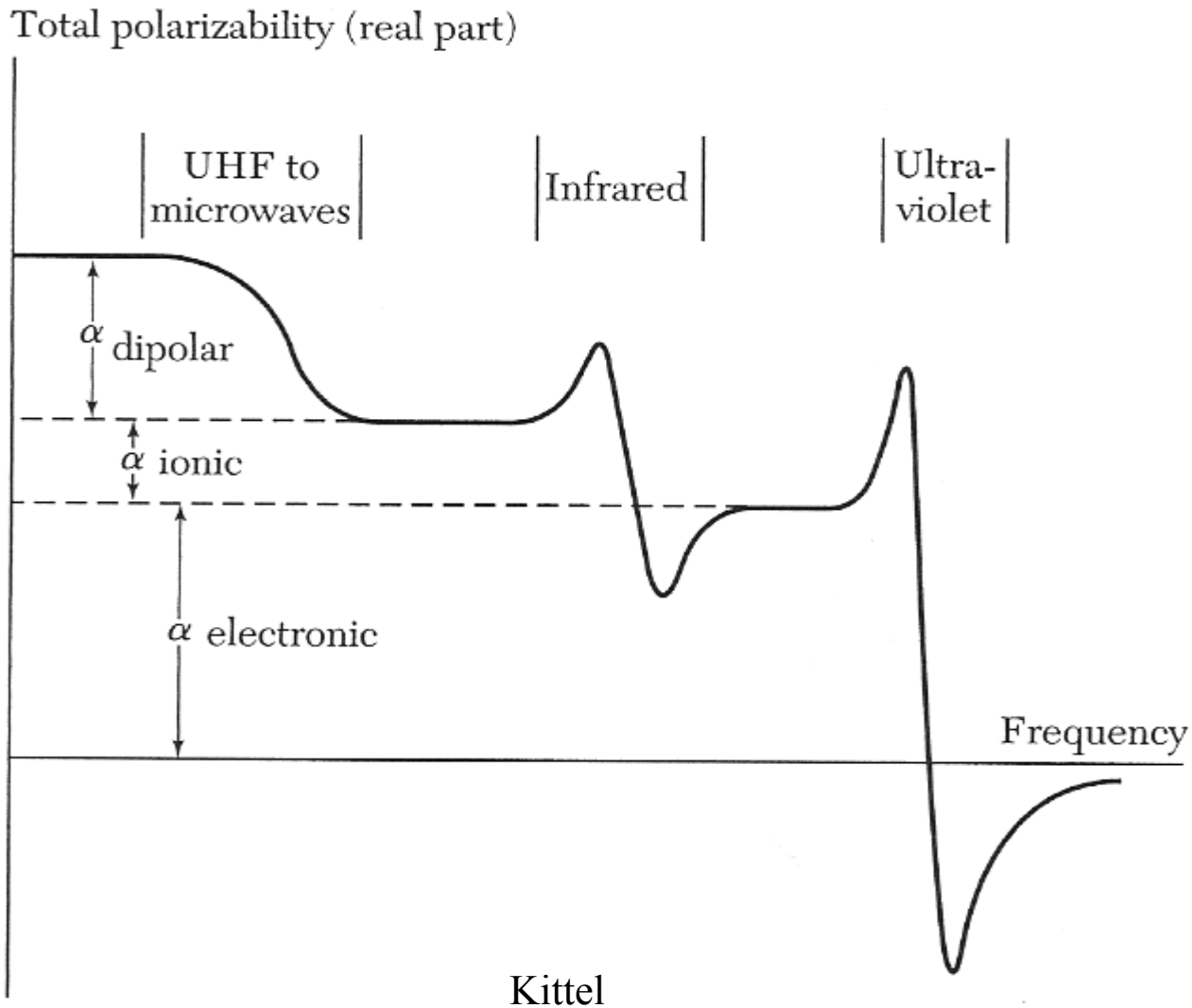
http://www.rfcafe.com/references/electrical/dielectric-constants-strengths.htm

Polarizability

Overdamped modes
- Orientation polarizability
- Space charge polarizability

Underdamped modes
- Ionic polarizability
- Electronic polarizability

Polarizability

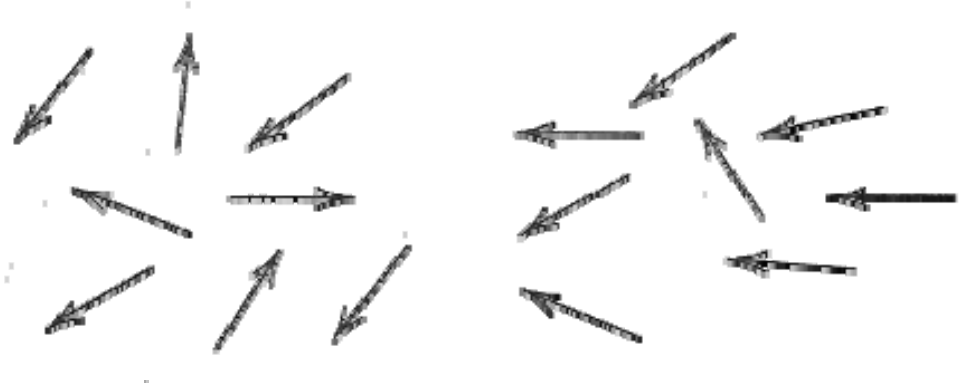


Kittel

Orientation (dipolar) Polarizability

For materials (gases, liquids, solids) with a permanent dipole moment.

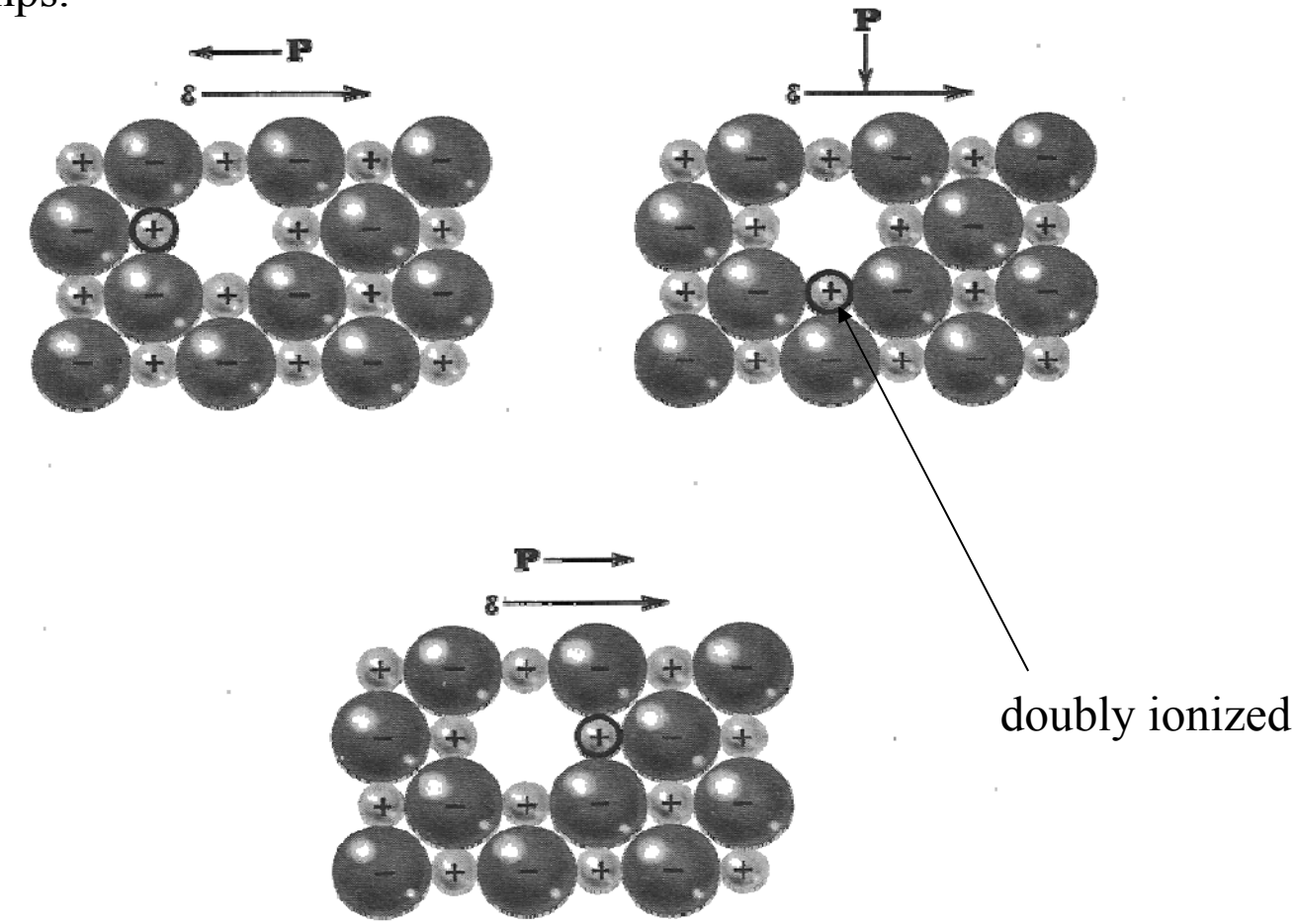
The theory is very similar to paramagnetism.



$$\chi \propto \frac{1}{T}$$ Curie law

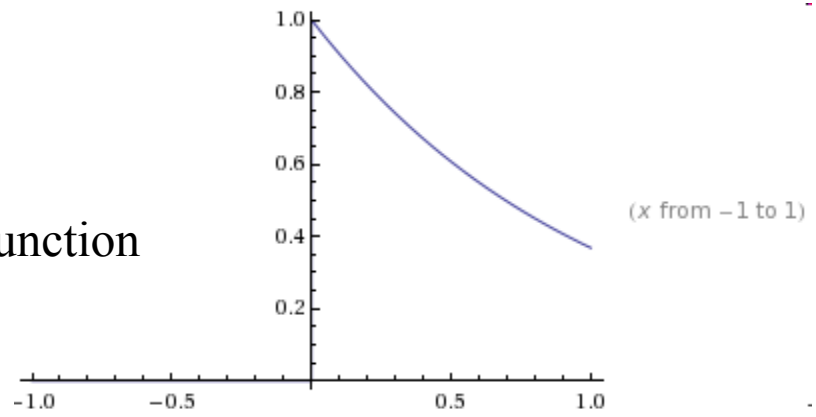
Orientation Polarizability

Ion jumps.

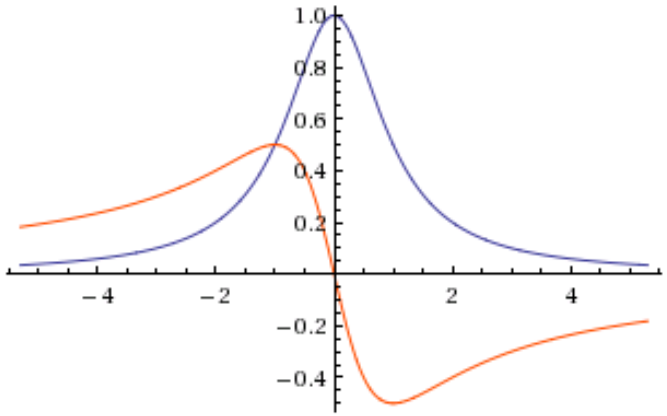


Orientation (dipolar) Polarizability

Overdamped mode
Impulse response function



Susceptibility



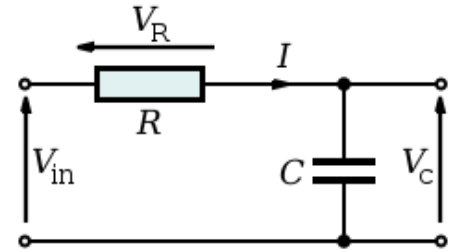
For low frequencies the dipoles can reorient with the field but at high frequencies they can't respond fast enough.

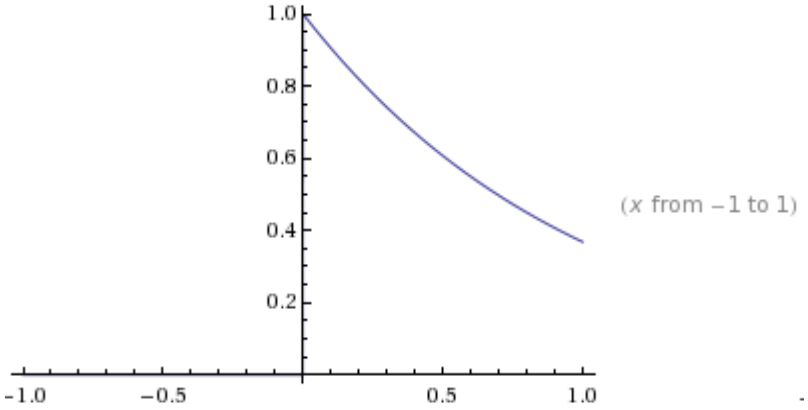
Space charge polarizability

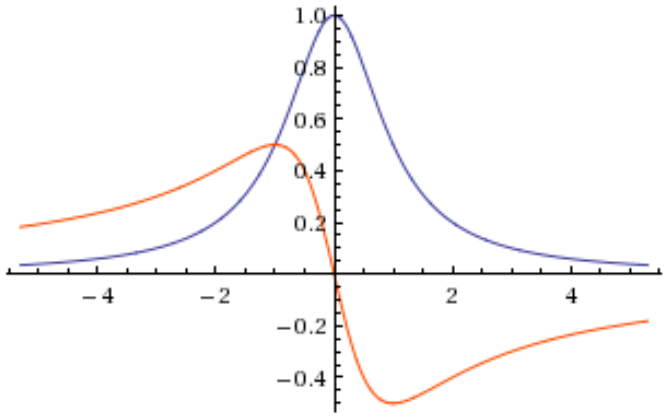
Multiple phases are present where one phase has a much higher resistivity than the other. Charge accumulates at the interfaces of the phases.

Like a network of resistors and capacitors.

This results in an overdamped mode.

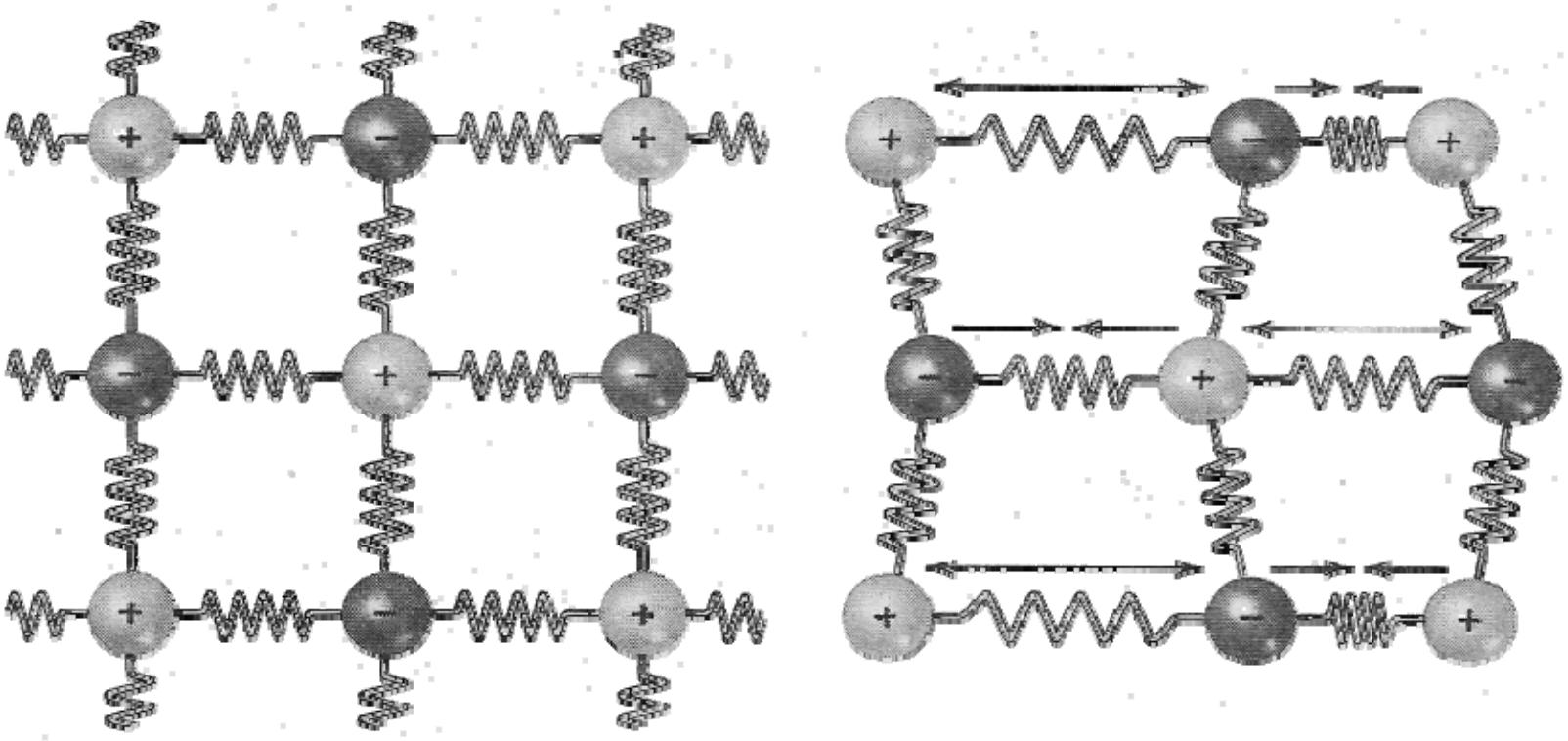






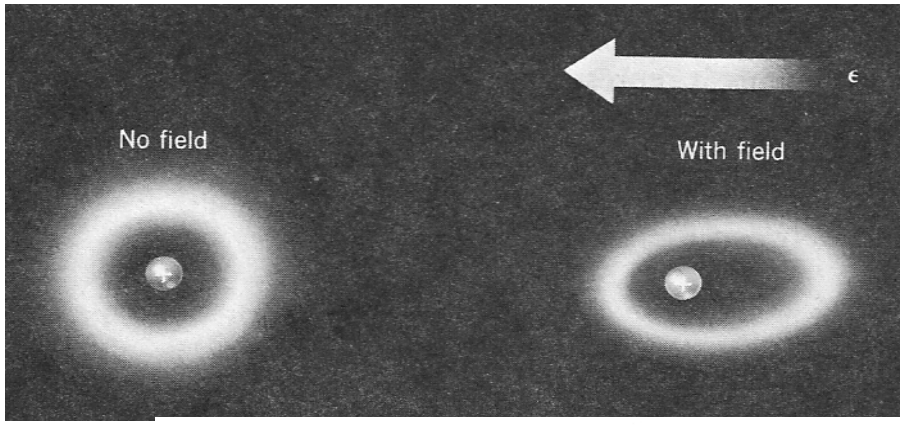
Ionic Polarizability

Displacement of ions of opposite sign. Only in ionic substances.



This is an underdamped mode in the infrared.

Electronic polarizability (all materials)



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

dipole moments

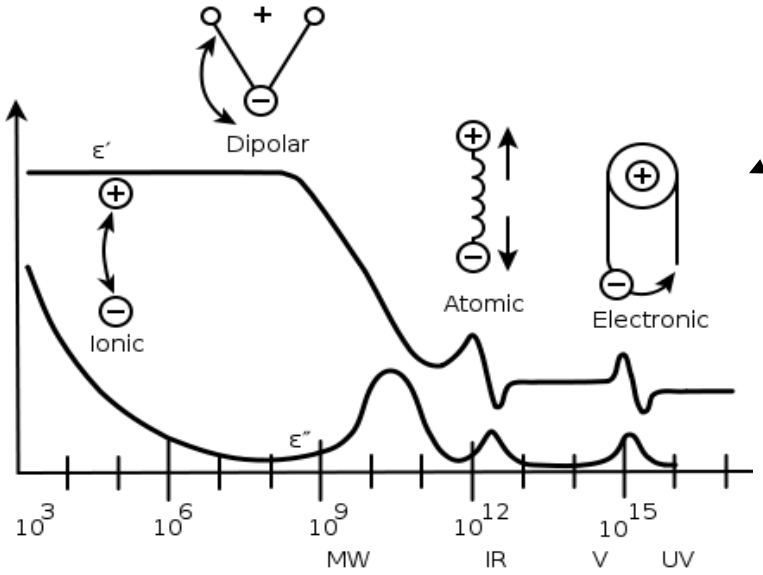
density

polarizability

Table 1 Electronic polarizabilities of atoms and ions, in 10^{-24} cm^3

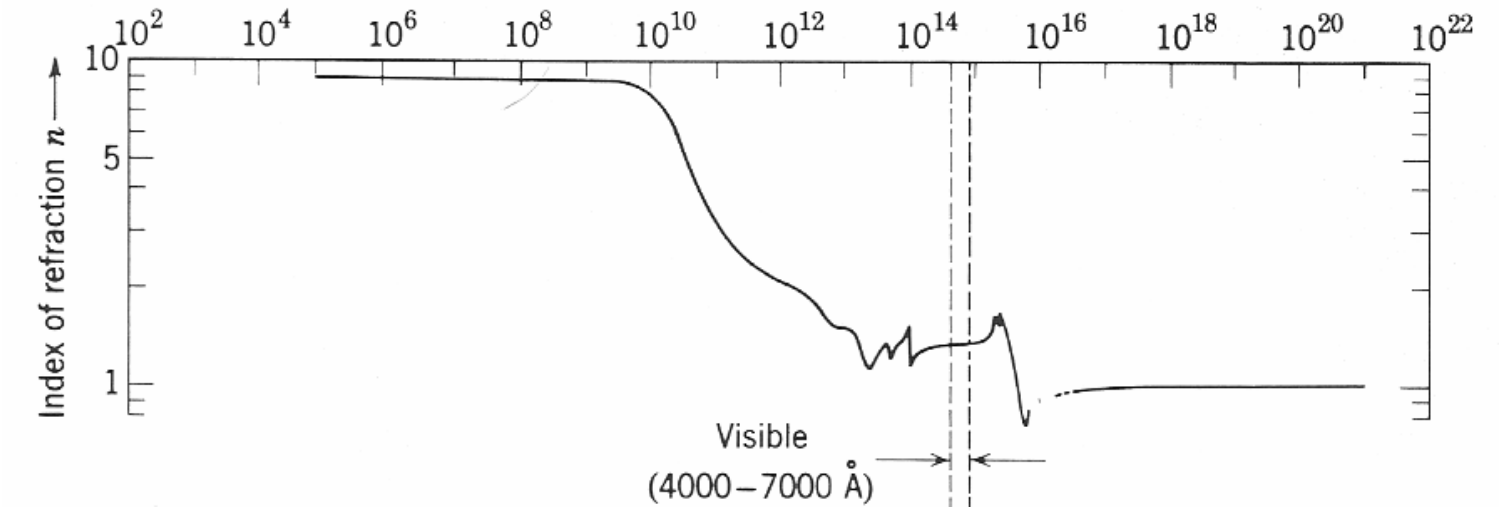
			He	Li^+	Be^{2+}	B^{3+}	C^{4+}
Pauling			0.201	0.029	0.008	0.003	0.0013
JS				0.029			
	O^{2-}	F^-	Ne	Na^+	Mg^{2+}	Al^{3+}	Si^{4+}
Pauling	3.88	1.04	0.390	0.179	0.094	0.052	0.0165
JS-(TKS)	(2.4)	0.858		0.290			
	S^{2-}	Cl^-	Ar	K^+	Ca^{2+}	Se^{3+}	Ti^{4+}
Pauling	10.2	3.66	1.62	0.83	0.47	0.286	0.185
JS-(TKS)	(5.5)	2.947		1.133	(1.1)		(0.19)
	Se^{2-}	Br^-	Kr	Rb^+	Sr^{2+}	Y^{3+}	Zr^{4+}
Pauling	10.5	4.77	2.46	1.40	0.86	0.55	0.37
JS-(TKS)	(7.)	4.091		1.679	(1.6)		
	Te^{2-}	I^-	Xe	Cs^+	Ba^{2+}	La^{3+}	Ce^{4+}
Pauling	14.0	7.10	3.99	2.42	1.55	1.04	0.73
JS-(TKS)	(9.)	6.116		2.743	(2.5)		

Water



Schematic dielectric function of water from Wikipedia

Source: Classical Electrodynamics, J.D. Jackson



AC Conductivity

For constant voltage, conductors conduct and insulators don't.

For low ac frequencies in a conductor, electric field and the electron velocity are in-phase, electric field and electron position are out-of-phase.

For low ac frequencies in an insulator, electric field and the electron position are in-phase, electric field and electron velocity are out-of-phase.

At high (optical) frequencies the in-phase and out-of-phase component of the response is described by the dielectric function.

Conductivity / Dielectric function

Harmonic dependence $v = v(\omega)e^{i\omega t}, \quad x = x(\omega)e^{i\omega t}, \quad E = E(\omega)e^{i\omega t}$

$$v(\omega) = i\omega x(\omega)$$

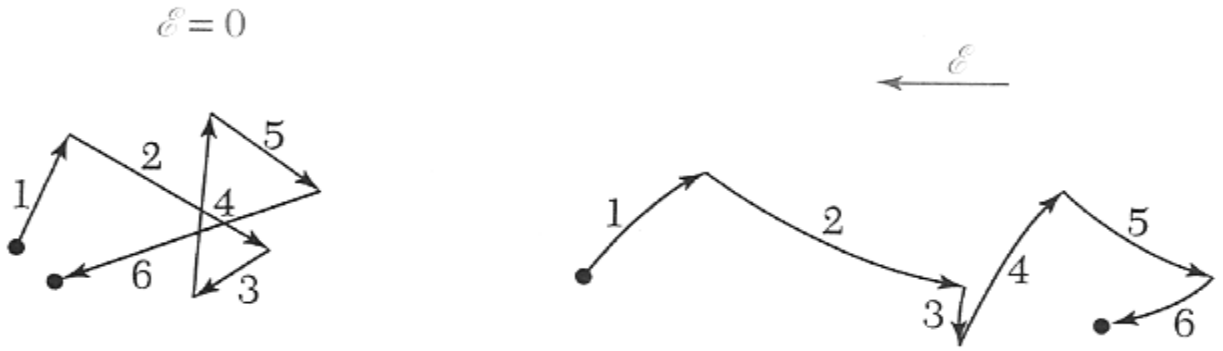
$$\chi(\omega) = \frac{P(\omega)}{\varepsilon_0 E(\omega)} = \frac{-nex(\omega)}{\varepsilon_0 E(\omega)} \qquad \sigma(\omega) = \frac{j(\omega)}{E(\omega)} = \frac{-nev(\omega)}{E(\omega)} = \frac{-i\omega nex(\omega)}{E(\omega)}$$

$$\chi(\omega) = \frac{\sigma(\omega)}{i\omega\varepsilon_0}$$

$$\boxed{\varepsilon(\omega) = 1 + \chi = 1 + \frac{\sigma(\omega)}{i\omega\varepsilon_0}}$$

Below about 100 GHz the frequency dependent conductivity is normally used.
Above about 100 GHz the dielectric function is used (optical experiments).

Diffusive transport (low frequencies)



$$\vec{F} = m\vec{a} = -e\vec{E} = m\frac{\vec{v}_d}{\tau_{\text{sc}}}$$

$$-\frac{e\tau_{\text{sc}}}{m}\vec{E} = \vec{v}_d$$

$$-\mu_e\vec{E} = \vec{v}_d$$

$$\tau_{\text{sc}} = \frac{\mu m}{e}$$

$$\sigma = ne\mu = \frac{ne^2\tau}{m}$$

Diffusive metal

The current is related to the electric field

$$j_n = \sigma_{nm} E_m \qquad v_n = -\mu_{nm} E_m$$ ← Steady state solution

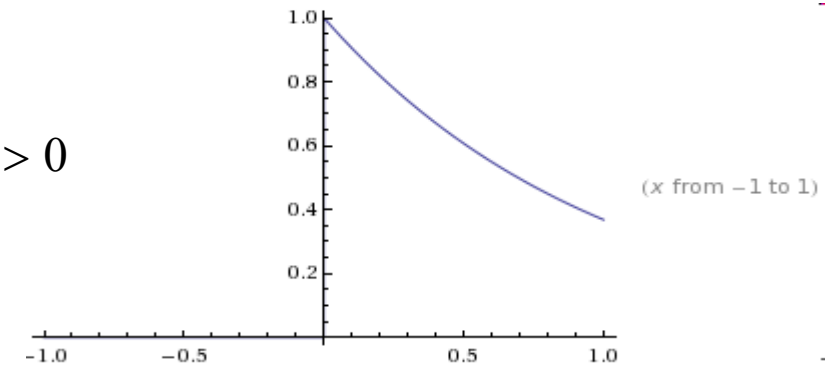
The differential equation that describes how the velocity changes in time is:

$$m\frac{dv(t)}{dt} + \frac{ev(t)}{\mu} = -eE(t)$$

Inertial term

The impulse response function :

$$g(t) = \frac{1}{m}\exp\left(\frac{-et}{\mu m}\right) \qquad t > 0$$



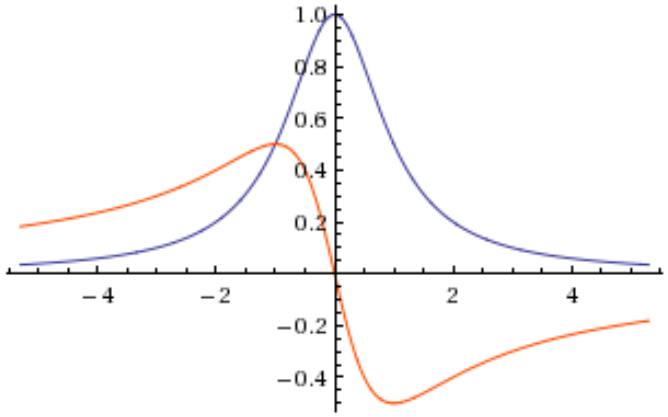
Diffusive metal

The differential equation is:

$$m\frac{dv(t)}{dt}+\frac{ev(t)}{\mu}=-eE(t)$$

Assume a harmonic solution $E(\omega)e^{i\omega t}$, $v(\omega)e^{i\omega t}$

$$\left(-\frac{i\omega m}{e}-\frac{1}{\mu}\right)v(\omega)=E(\omega)$$



$$\frac{v(\omega)}{E(\omega)}=\left(-\frac{i\omega m}{e}-\frac{1}{\mu}\right)^{-1}=-\mu\left(1+i\omega\tau\right)^{-1}=\frac{-\mu\left(1-i\omega\tau\right)}{1+\omega^2\tau^2}$$

$$\sigma(\omega)=\frac{j(\omega)}{E(\omega)}=-ne\frac{v(\omega)}{E(\omega)}=ne\mu\left(\frac{1-i\omega\tau}{1+\omega^2\tau^2}\right)$$

$$\tau=\frac{\mu m}{e}$$ ← Scattering time

$$\sigma(\text{low }\omega)=ne\mu$$

$$\sigma(\text{high }\omega)=\frac{-ine^2}{\omega m}$$