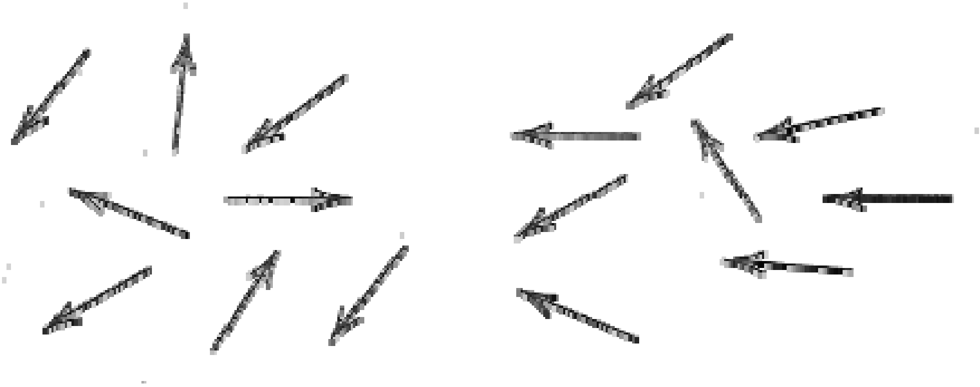
Dielectric properties of insulators and metals

Orientation (dipolar) Polarizability

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

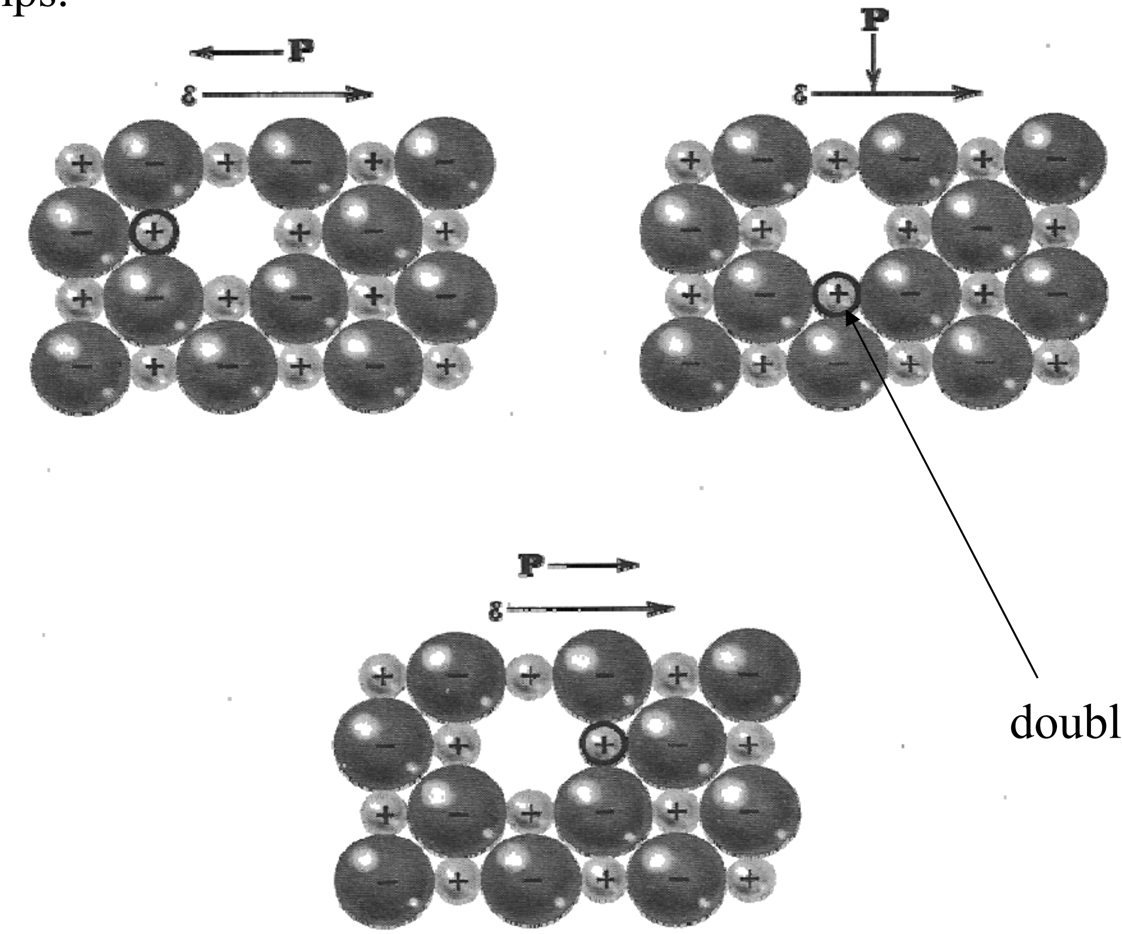
The theory is very similar to paramagnetism.



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

Orientation Polarizability

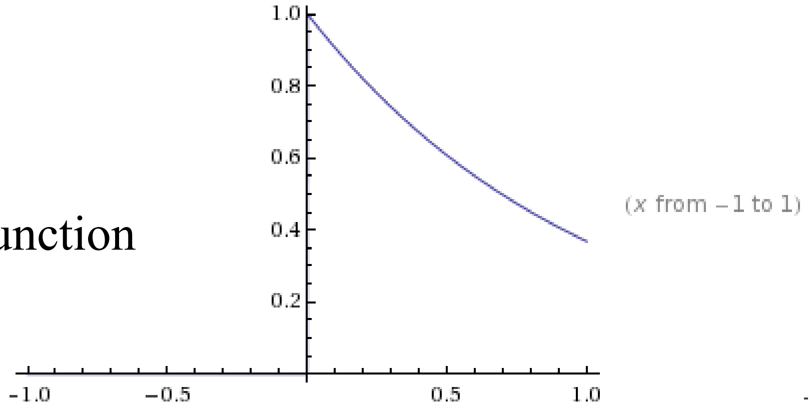
Ion jumps.



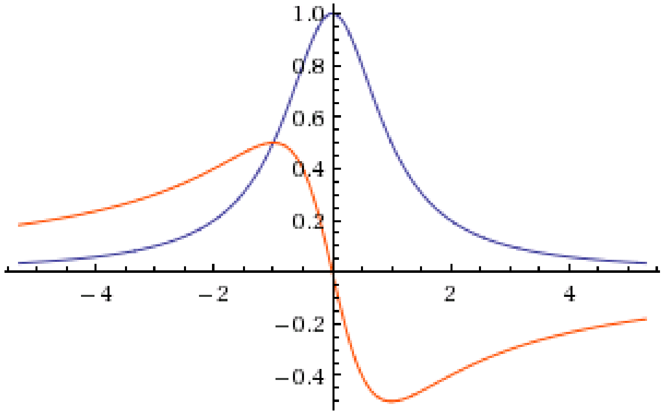
doubly ionized

Orientation (dipolar) Polarizability

Overdamped mode
Impulse response function

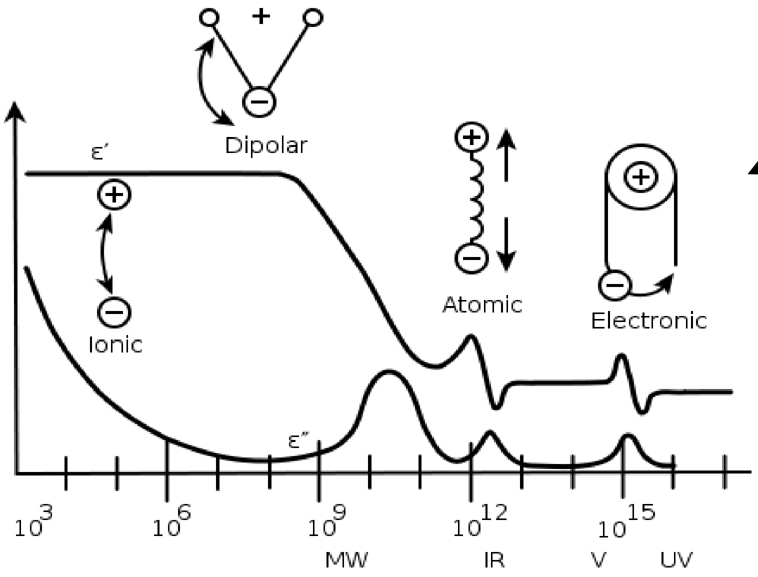


Susceptibility



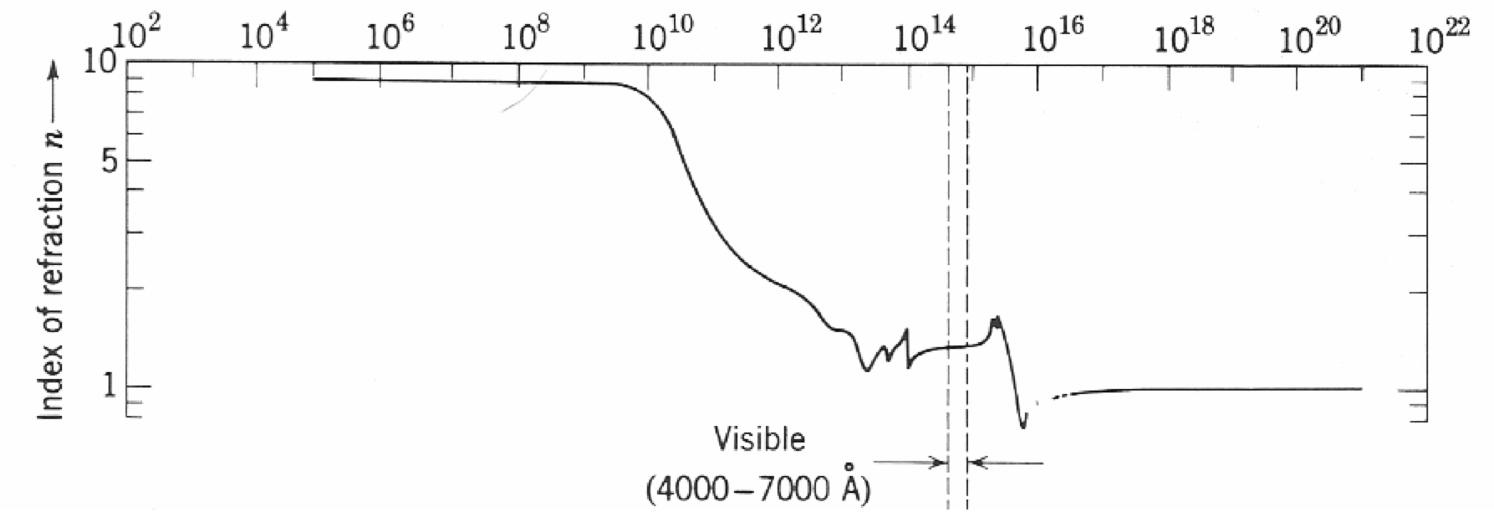
For low frequencies the dipoles can reorient with the field but at high frequencies they can't respond fast enough.

Water



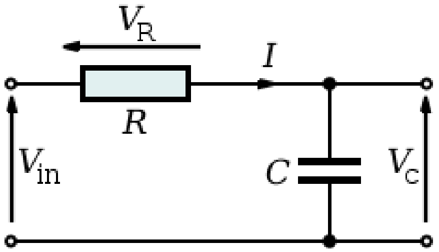
Schematic dielectric function of water from Wikipedia

Source: Classical Electrodynamics, J.D. Jackson



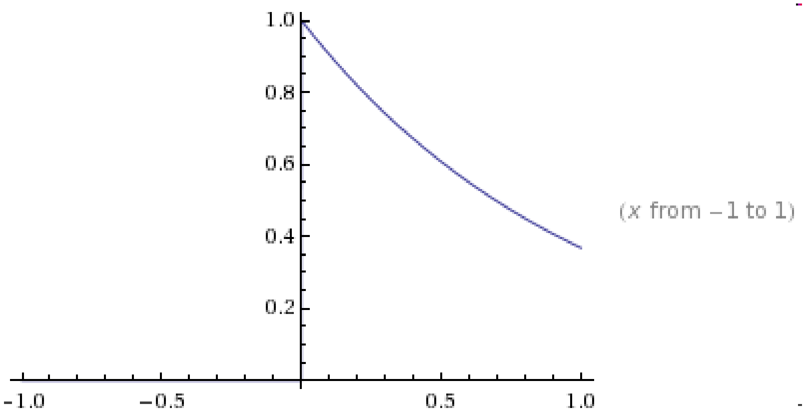
Space charge polarizability

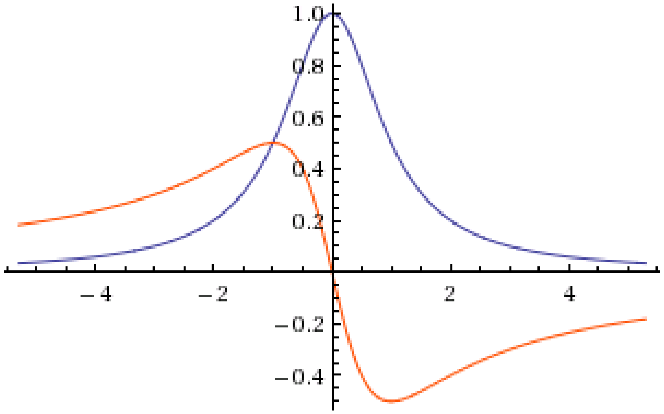
Multiple phases are present where one phase has a much higher resistivity than the other. Charge accumulates at the interfaces of the phases.



Like a network of resistors and capacitors.

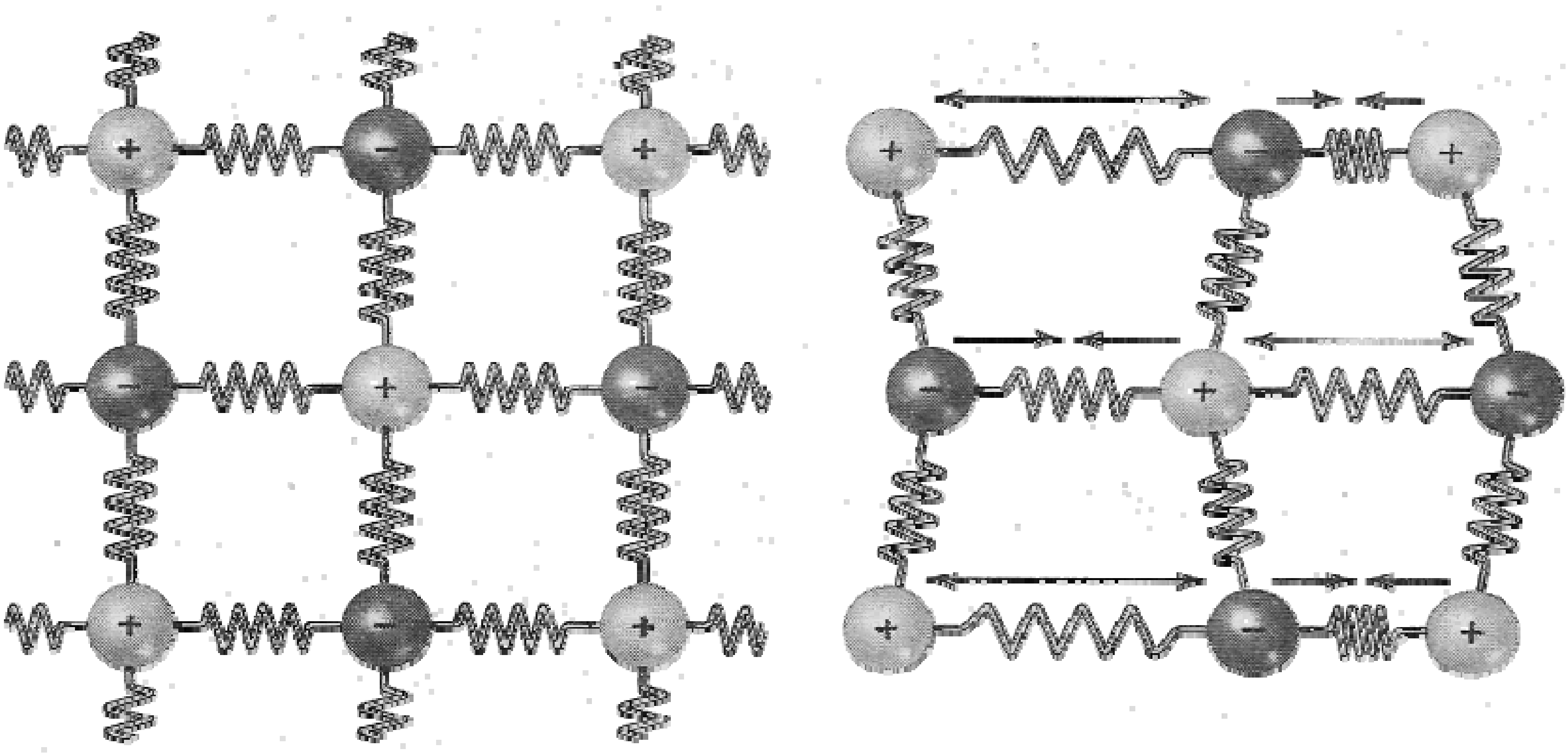
This results in an overdamped mode.





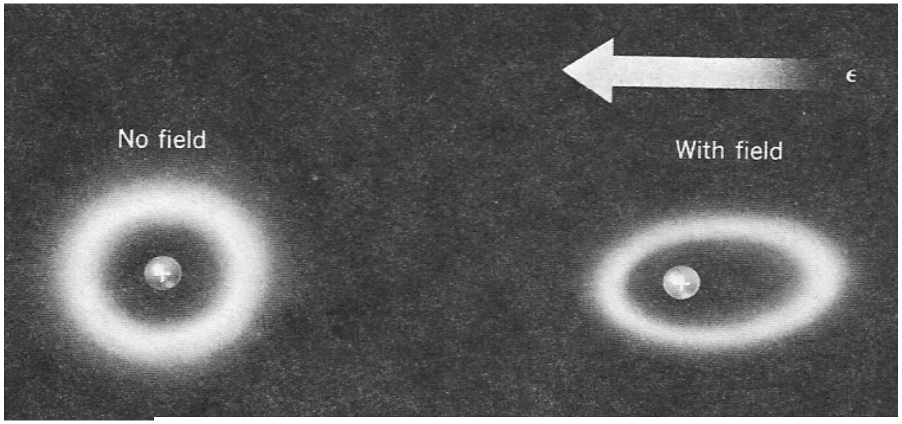
Ionic Polarizability

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



This is an underdamped mode in the infrared.

Electronic polarizability (all materials)



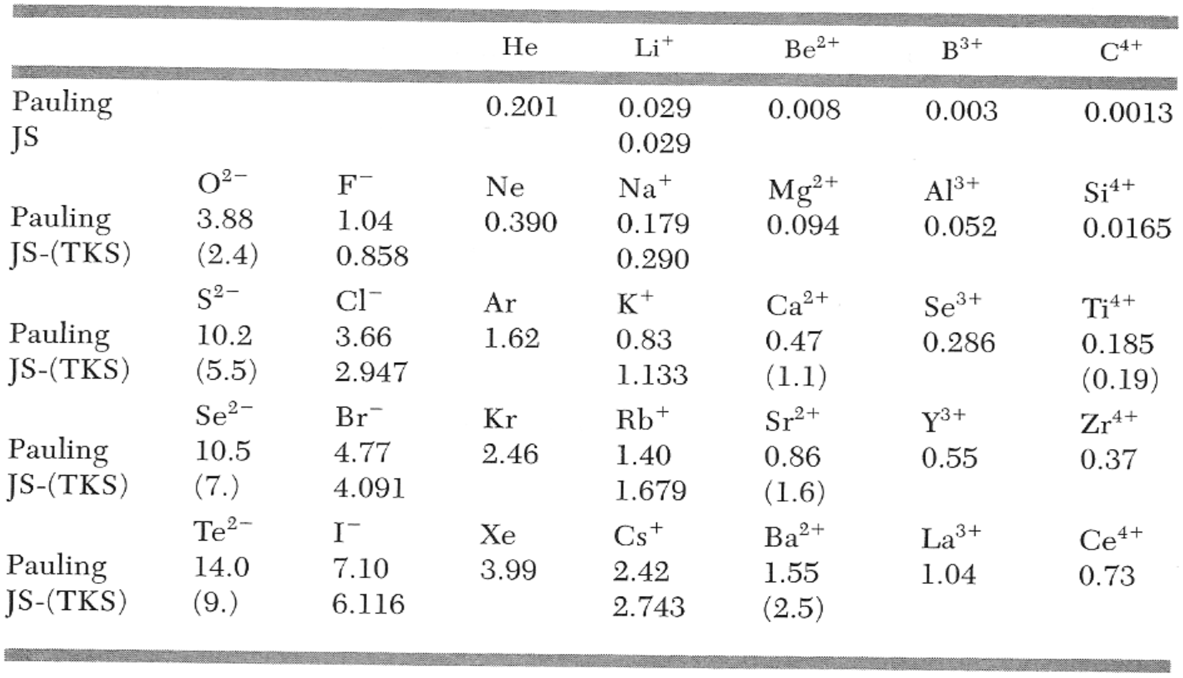
dipole moments

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

density

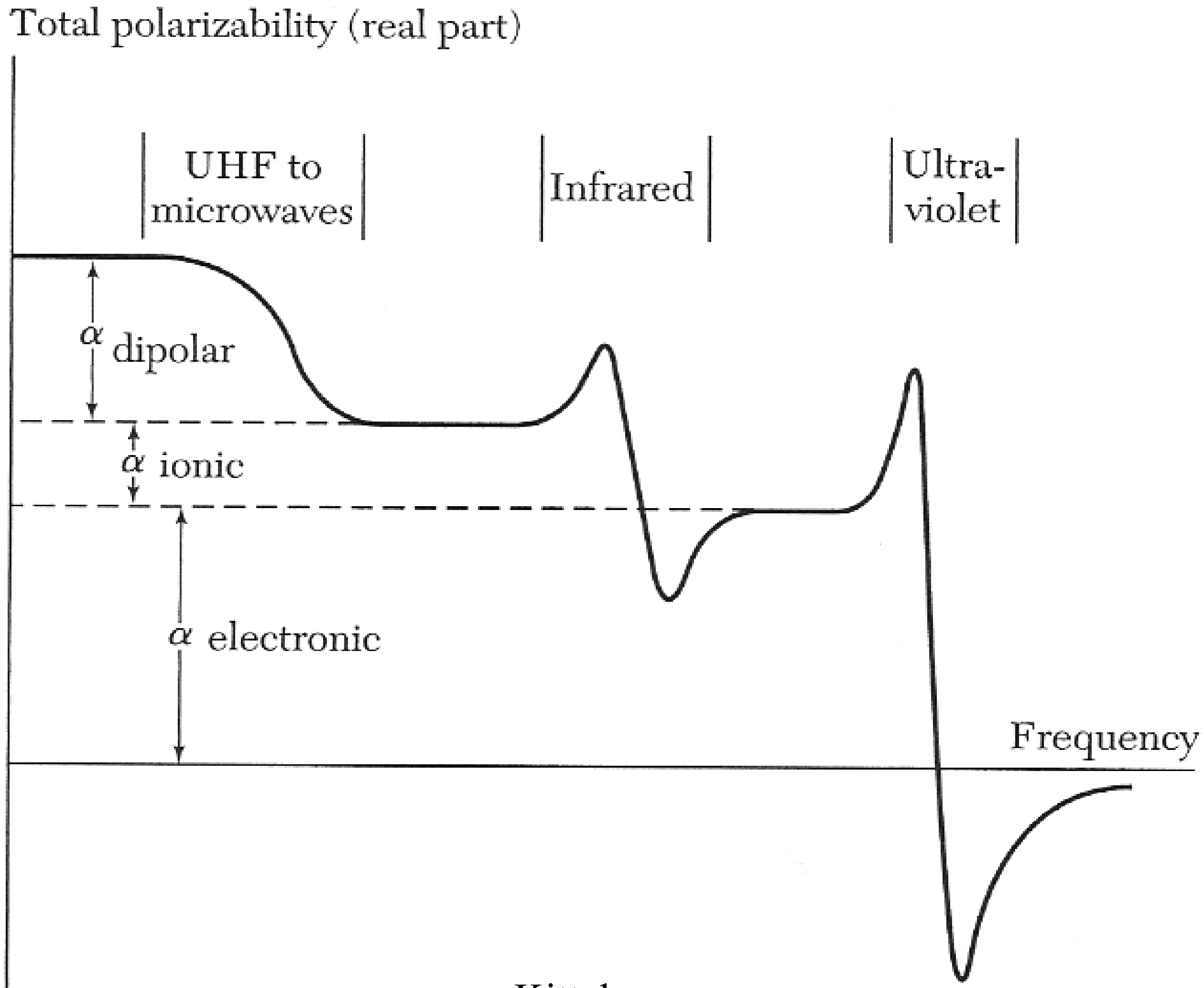
polarizability

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)		

Polarizability

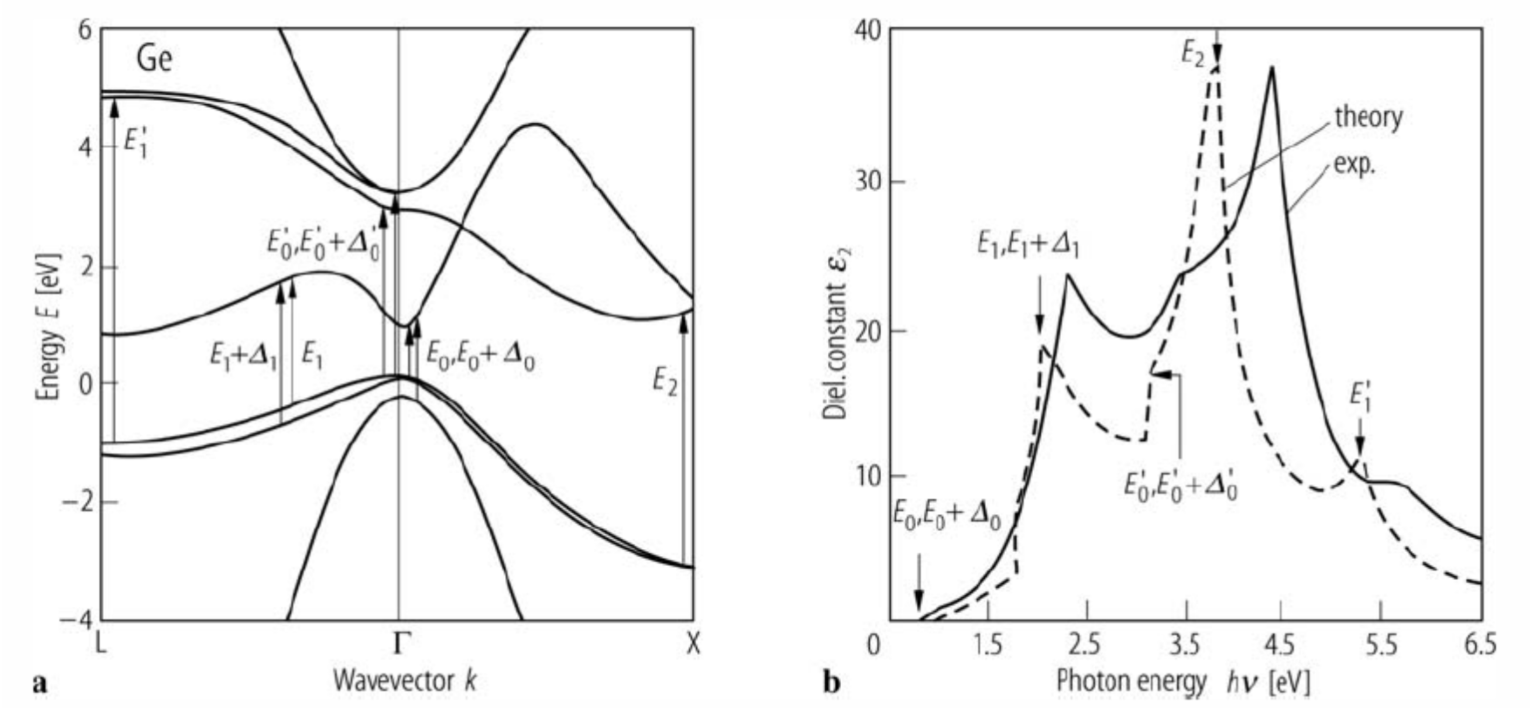


Kittel

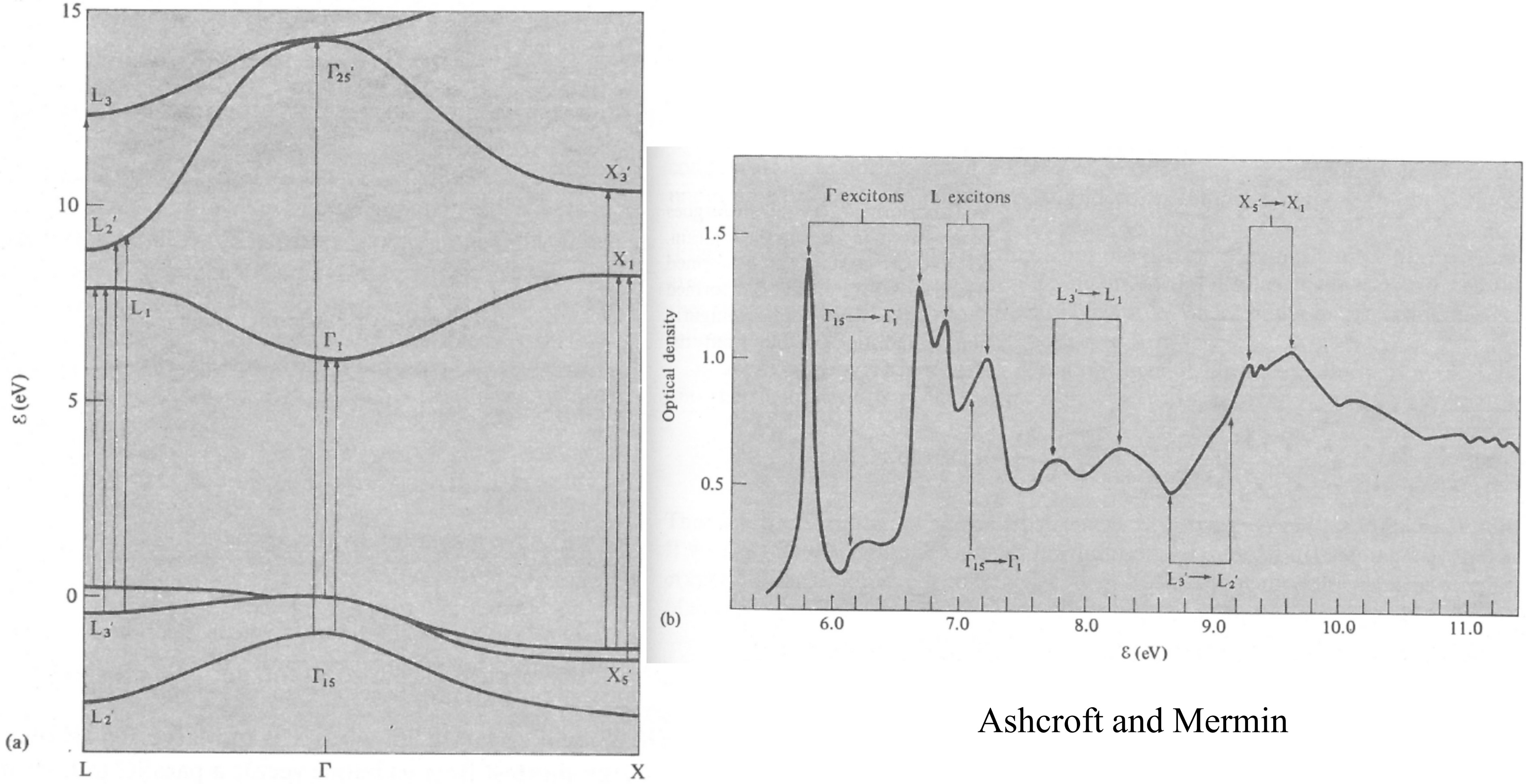
Inter- and intraband transitions

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

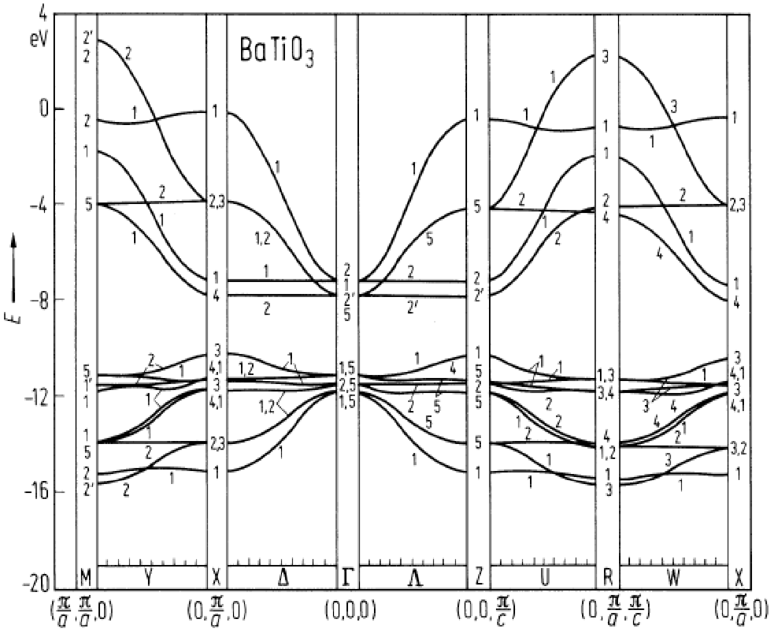


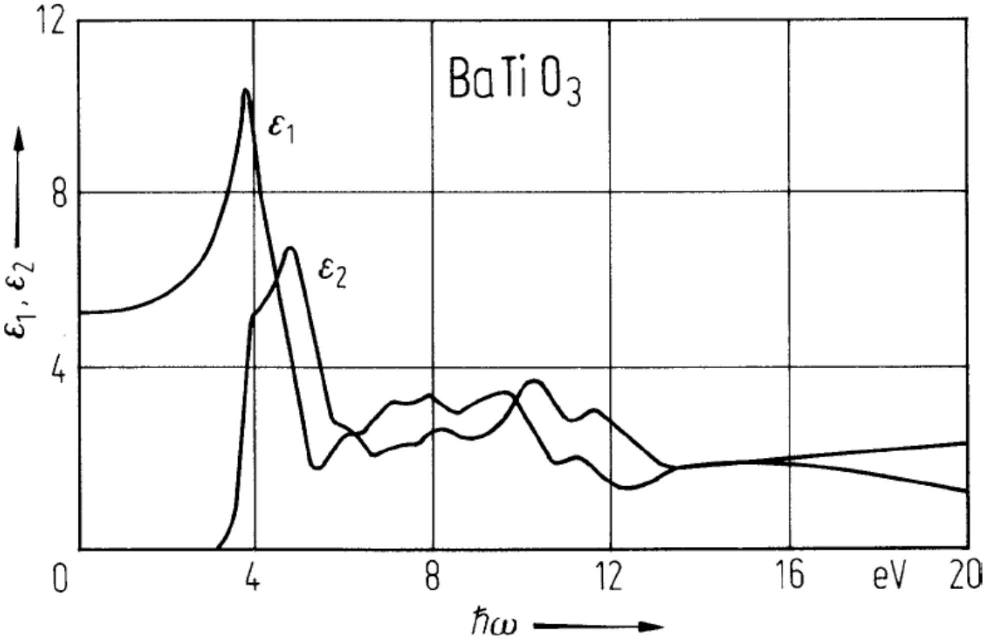
Ashcroft and Mermin

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.)

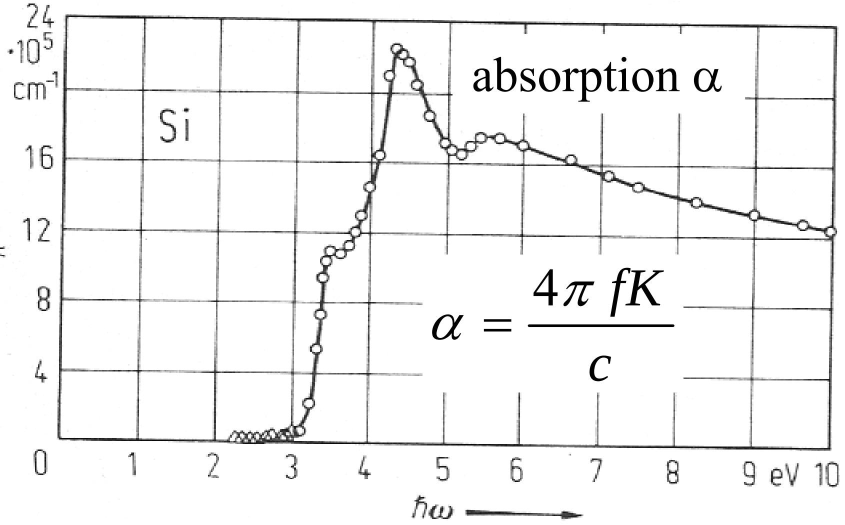
Dielectric function of $BaTiO_3$





Dielectric function of silicon

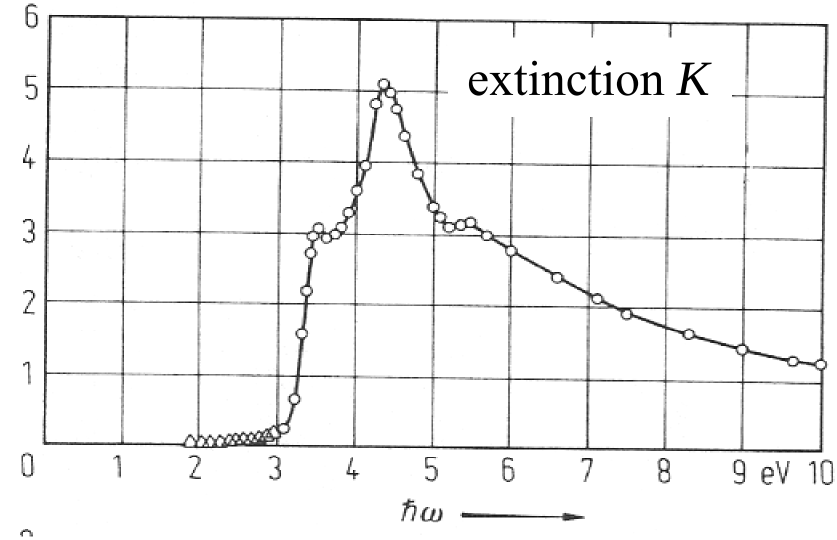
$$\sqrt{\varepsilon(\omega)} = n(\omega) + iK(\omega)$$



absorption α

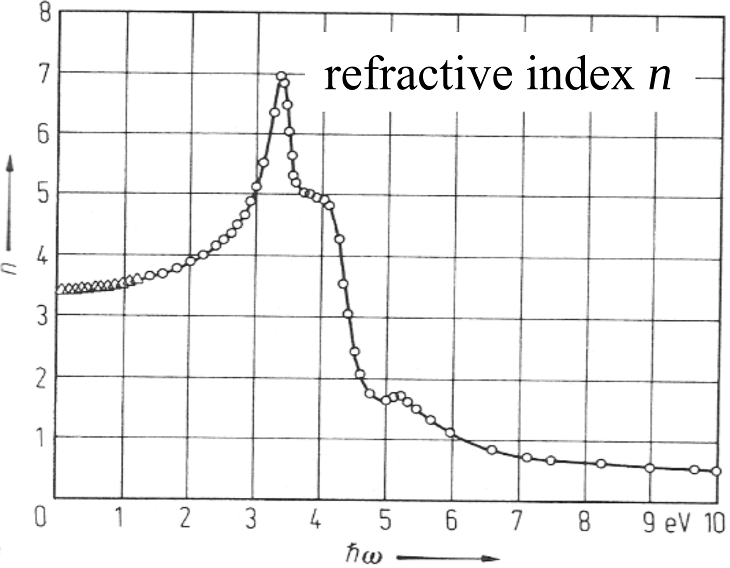
$$\alpha = \frac{4\pi fK}{c}$$

a



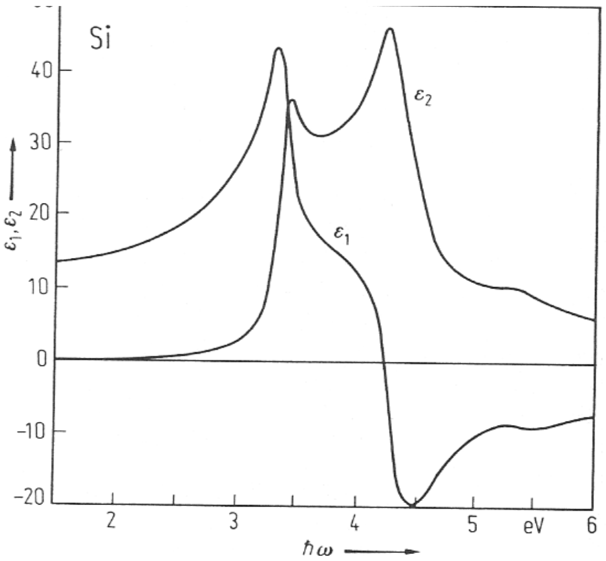
extinction *K*

b



refractive index *n*

c



AC Conductivity

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

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

For low ac voltages 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 $v = v(\omega)e^{i\omega t}, \quad x = x(\omega)e^{i\omega t}, \quad E = E(\omega)e^{i\omega t}$

$$\chi(\omega) = \frac{P(\omega)}{\varepsilon_0 E(\omega)} = \frac{-nex(\omega)}{\varepsilon_0 E(\omega)} \qquad v(\omega) = i\omega x(\omega)$$

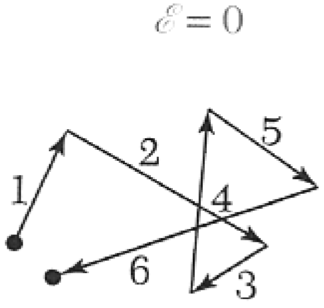
$$\sigma(\omega) = \frac{j(\omega)}{E(\omega)} = \frac{-nev(\omega)}{E(\omega)} = \frac{-i\omega nex(\omega)}{E(\omega)}$$

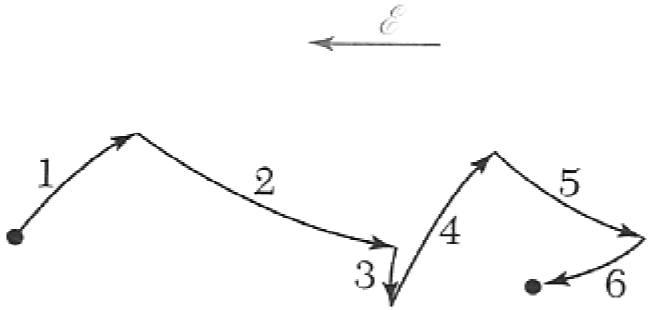
$$\chi(\omega) = \frac{\sigma(\omega)}{i\omega\varepsilon_0}$$

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

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)





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

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

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

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

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

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

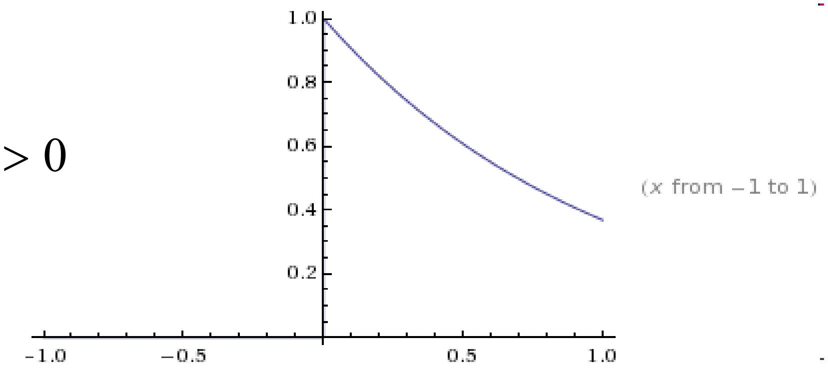
The differential equation that describes how the velocity changes in time is:

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

Inertial term

The impulse response function :

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



Diffusive metal

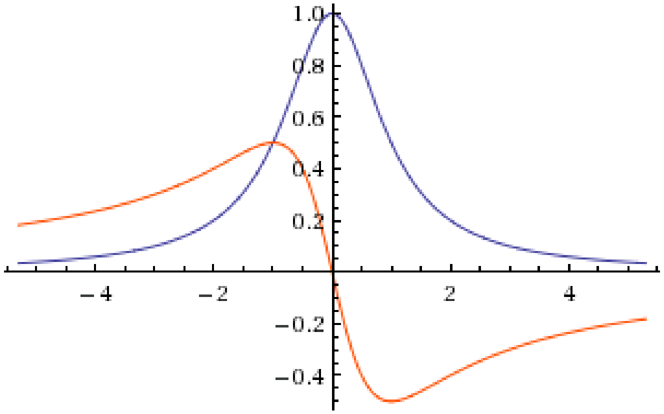
The differential equation is:

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

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

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

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



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

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

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

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

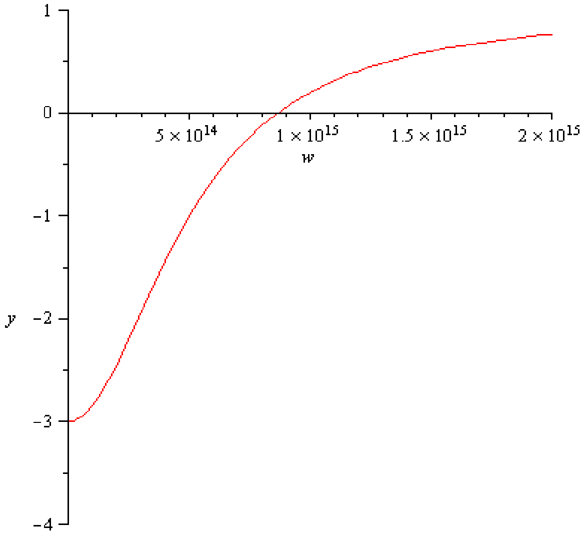
Diffusive metal

$$\chi(\omega)=\frac{P(\omega)}{\varepsilon_0 E(\omega)}=\frac{-nex(\omega)}{\varepsilon_0 E(\omega)}=\frac{-nev(\omega)}{i\omega\varepsilon_0 E(\omega)}=\frac{\sigma(\omega)}{i\omega\varepsilon_0}=\frac{ne\mu}{i\omega\varepsilon_0}\left(\frac{1-i\omega\tau}{1+\omega^2\tau^2}\right)$$

$$\varepsilon(\omega)=1+\chi=1-\frac{ne\mu}{\omega\varepsilon_0}\left(\frac{\omega\tau+i}{1+\omega^2\tau^2}\right)$$

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

$$\omega_p^2=\frac{ne^2}{m\varepsilon_0}$$

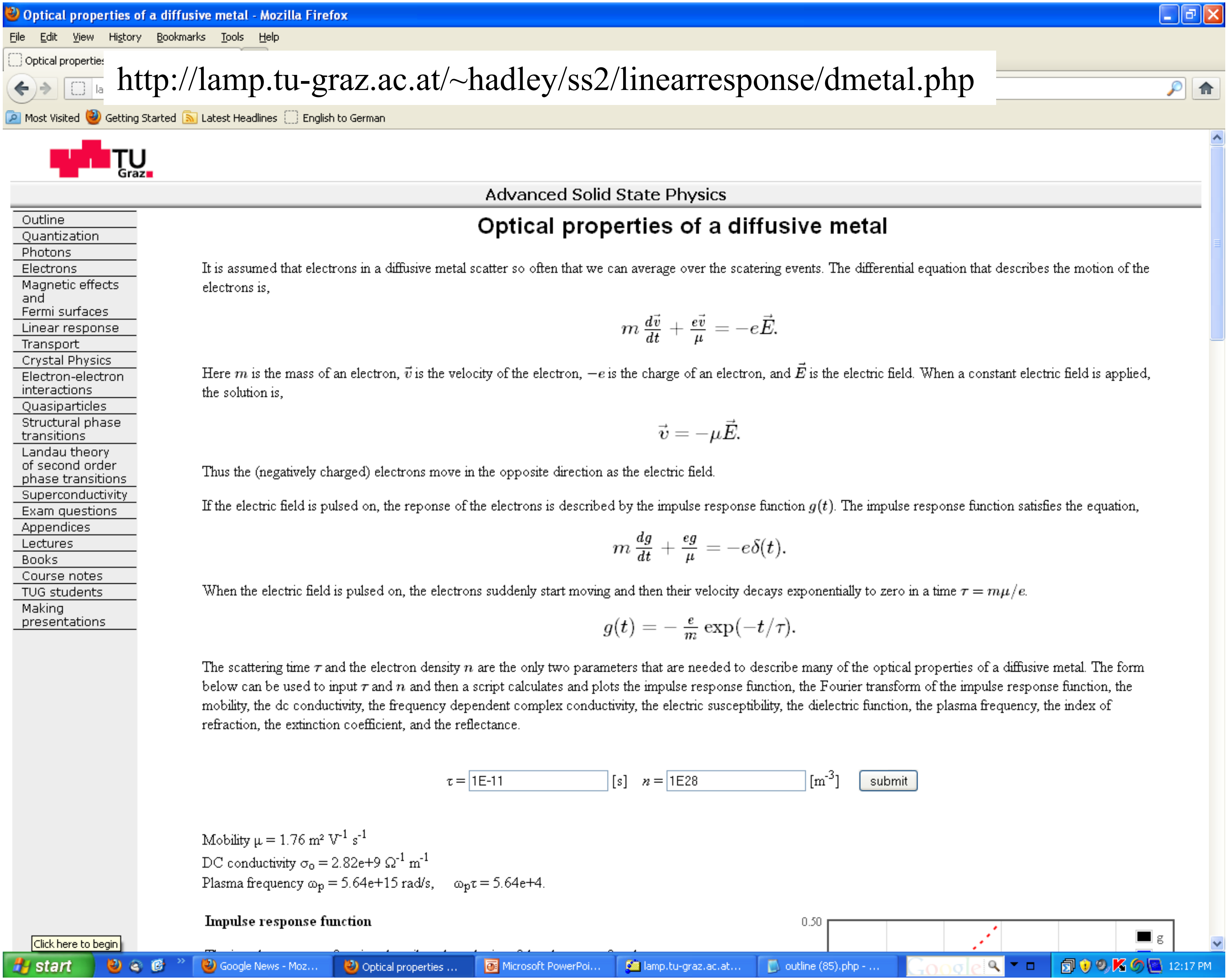


Take the limit as τ goes to infinity

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

$$\varepsilon''(\omega)=\begin{matrix}0 & \text{for} & \omega>0\\ \infty & \text{for} & \omega=0\end{matrix}$$

http://lamp.tu-graz.ac.at/~hadley/ss2/linearresponse/dmetal.php



Optical properties of a diffusive metal

It is assumed that electrons in a diffusive metal scatter so often that we can average over the scatering events. The differential equation that describes the motion of the electrons is,

$$m\frac{d\vec{v}}{dt}+\frac{e\vec{v}}{\mu}=-e\vec{E}.$$

Here m is the mass of an electron, $\vec{v}$ is the velocity of the electron, $-e$ is the charge of an electron, and $\vec{E}$ is the electric field. When a constant electric field is applied, the solution is,

$$\vec{v}=-\mu\vec{E}.$$

Thus the (negatively charged) electrons move in the opposite direction as the electric field.

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

$$m\frac{dg}{dt}+\frac{eg}{\mu}=-e\delta(t).$$

When the electric field is pulsed on, the electrons suddenly start moving and then their velocity decays exponentially to zero in a time $\tau = m\mu/e$.

$$g(t)=-\frac{e}{m}\exp(-t/\tau).$$

The scattering time τ and the electron density n are the only two parameters that are needed to describe many of the optical properties of a diffusive metal. The form below can be used to input τ and n and then a script calculates and plots the impulse response function, the Fourier transform of the impulse response function, the mobility, the dc conductivity, the frequency dependent complex conductivity, the electric susceptibility, the dielectric function, the plasma frequency, the index of refraction, the extinction coefficient, and the reflectance.

$\tau =$ 1E-11 [s] $n =$ 1E28 [$\mathrm{m^{-3}}$] submit

Mobility $\mu = 1.76\ \mathrm{m^2\,V^{-1}\,s^{-1}}$
DC conductivity $\sigma_0 = 2.82\mathrm{e}{+}9\ \Omega^{-1}\,\mathrm{m}^{-1}$
Plasma frequency $\omega_p = 5.64\mathrm{e}{+}15$ rad/s, $\omega_p\tau = 5.64\mathrm{e}{+}4$.

Impulse response function