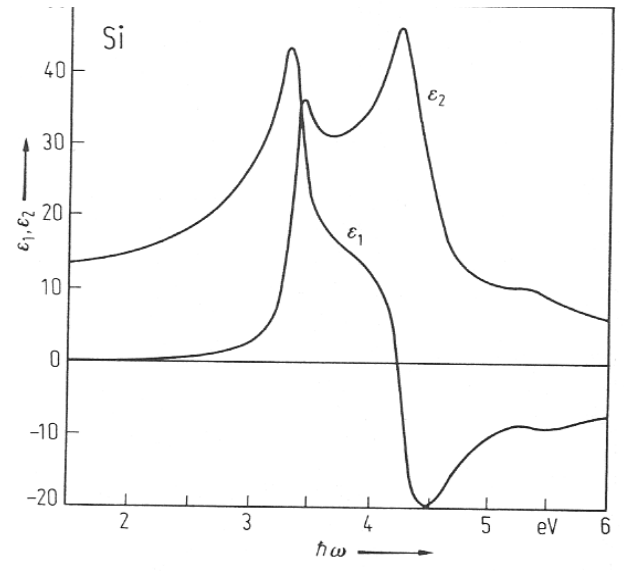
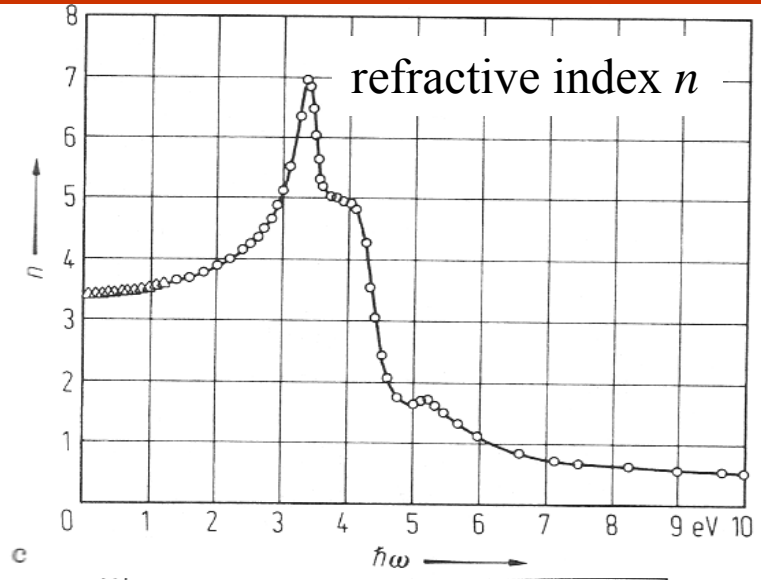
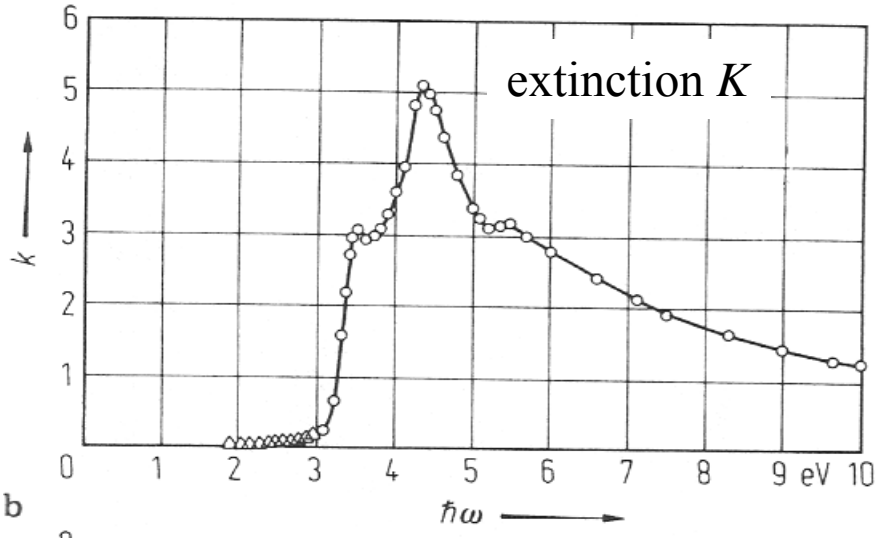
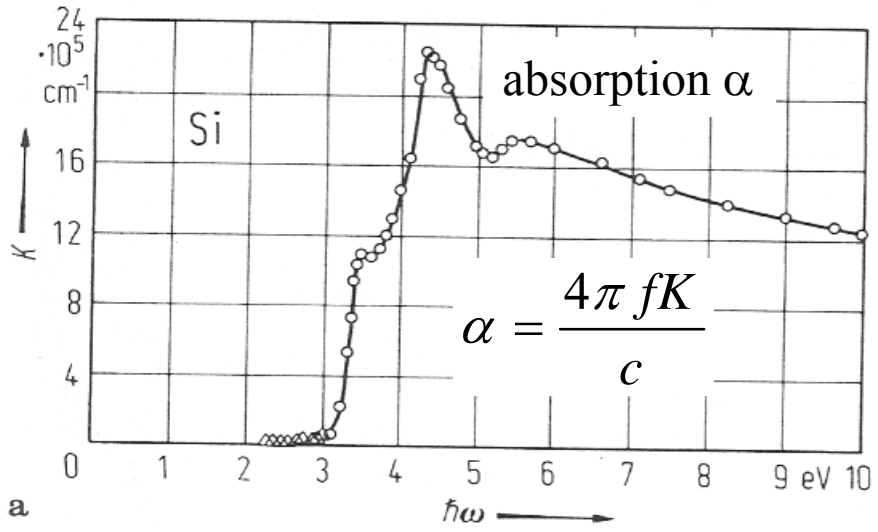


19. Optical Properties of Insulators and Metals

Dec. 9, 2019

Dielectric function of silicon $\sqrt{\epsilon(\omega)} = n(\omega) + iK(\omega)$



Optical properties of insulators and semiconductors

Outline
Quantization
Photons
Electrons
Magnetic effects and Fermi surfaces
Linear response
Transport
Crystal Physics
Electron-electron interactions
Quasiparticles
Structural phase transitions
Landau theory of second order phase transitions
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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,

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

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

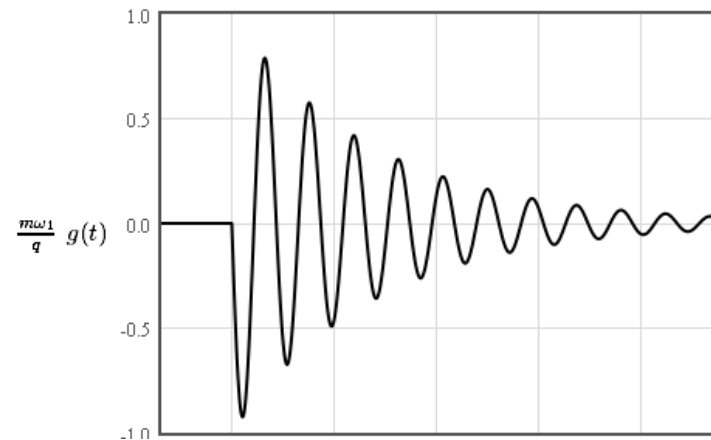
$$\frac{d^2 x}{dt^2} + \gamma \frac{dx}{dt} + \omega_0^2 x = -\frac{qE}{m}.$$

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,

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

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 $\frac{2}{\gamma}$.

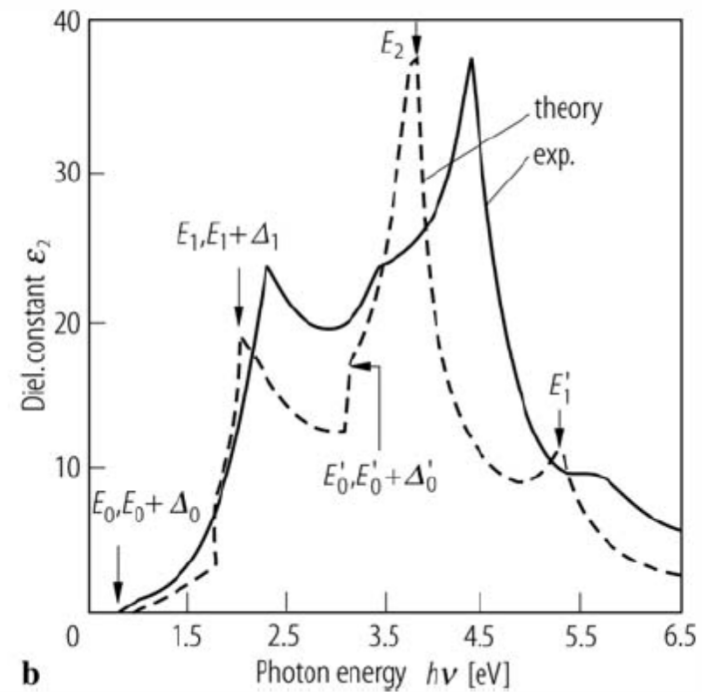
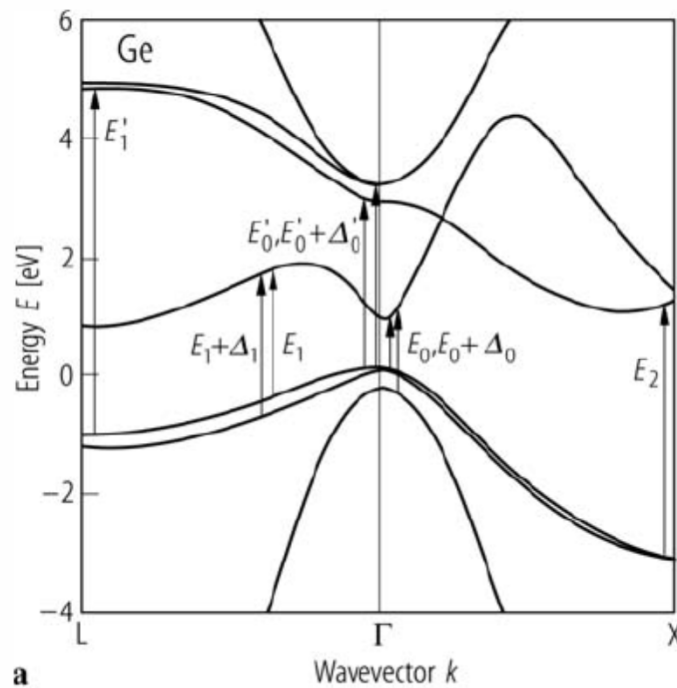
$$g(t) = -\frac{q}{m\omega_1} \exp\left(-\frac{\gamma}{2} t\right) \sin(\omega_1 t).$$



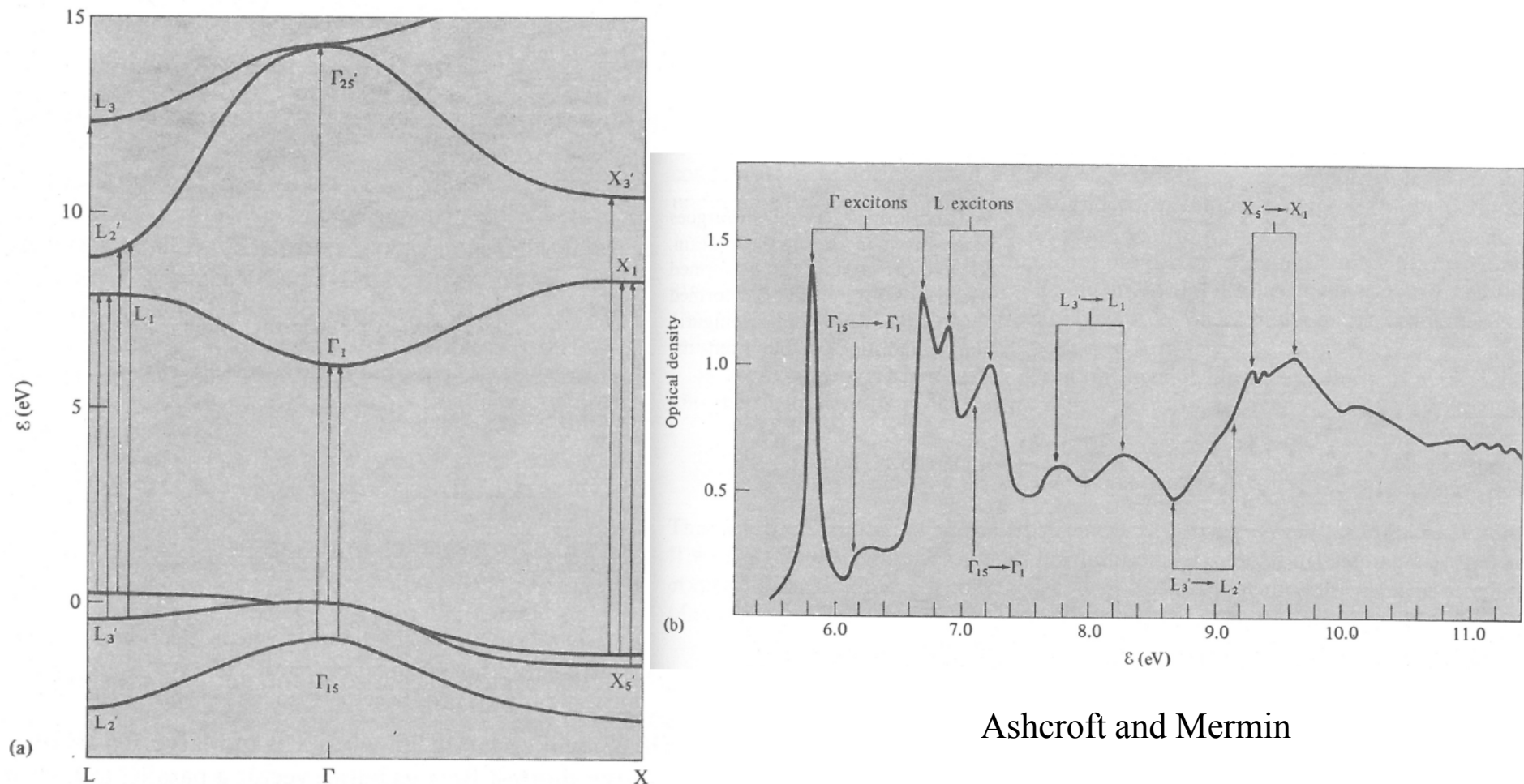
Inter- and intraband transitions

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

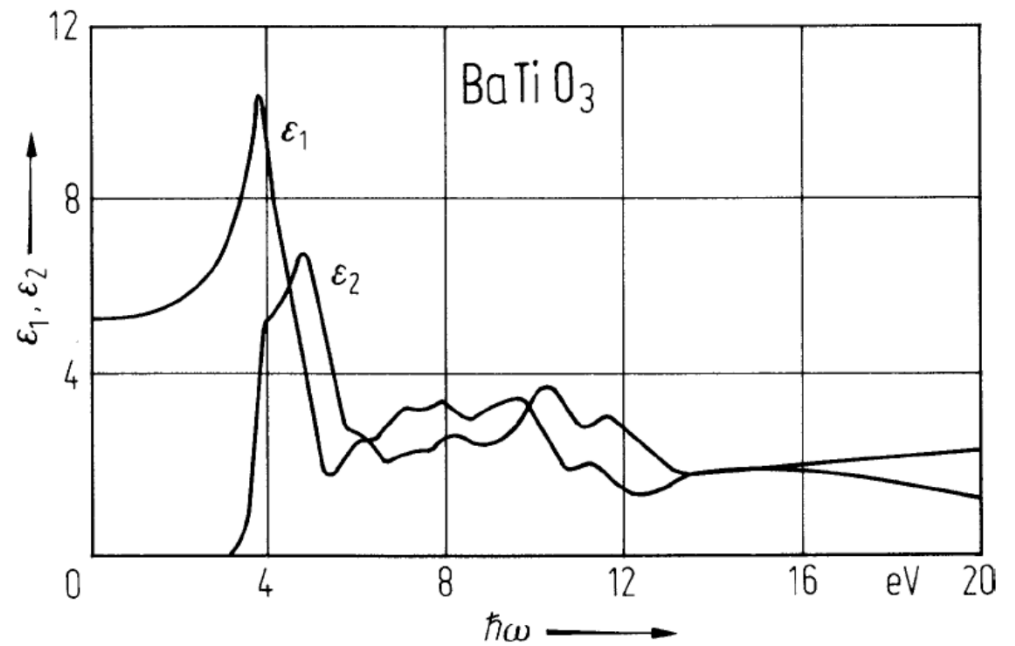
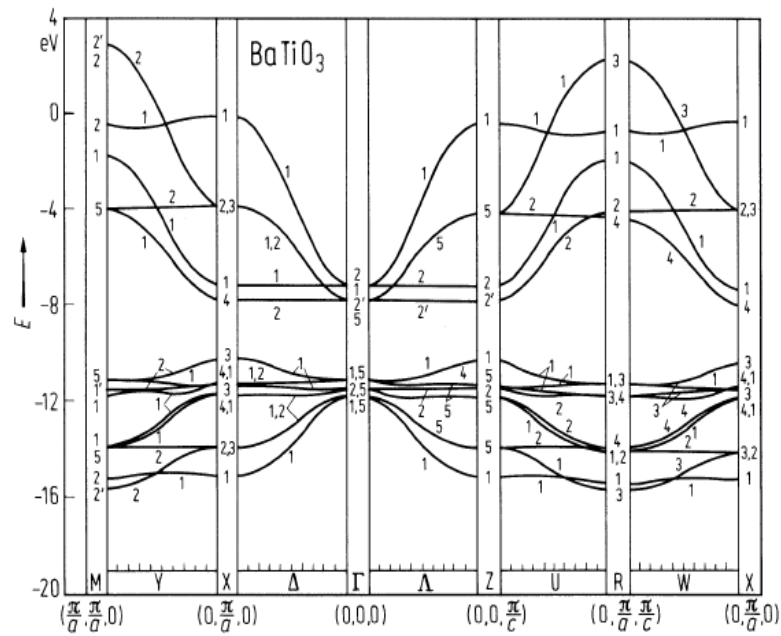


Ashcroft and Mermin

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 BaTiO₃



Dielectrics

Dielectrics used as electrical insulators should not conduct.

Large breakdown field.

Low AC losses.

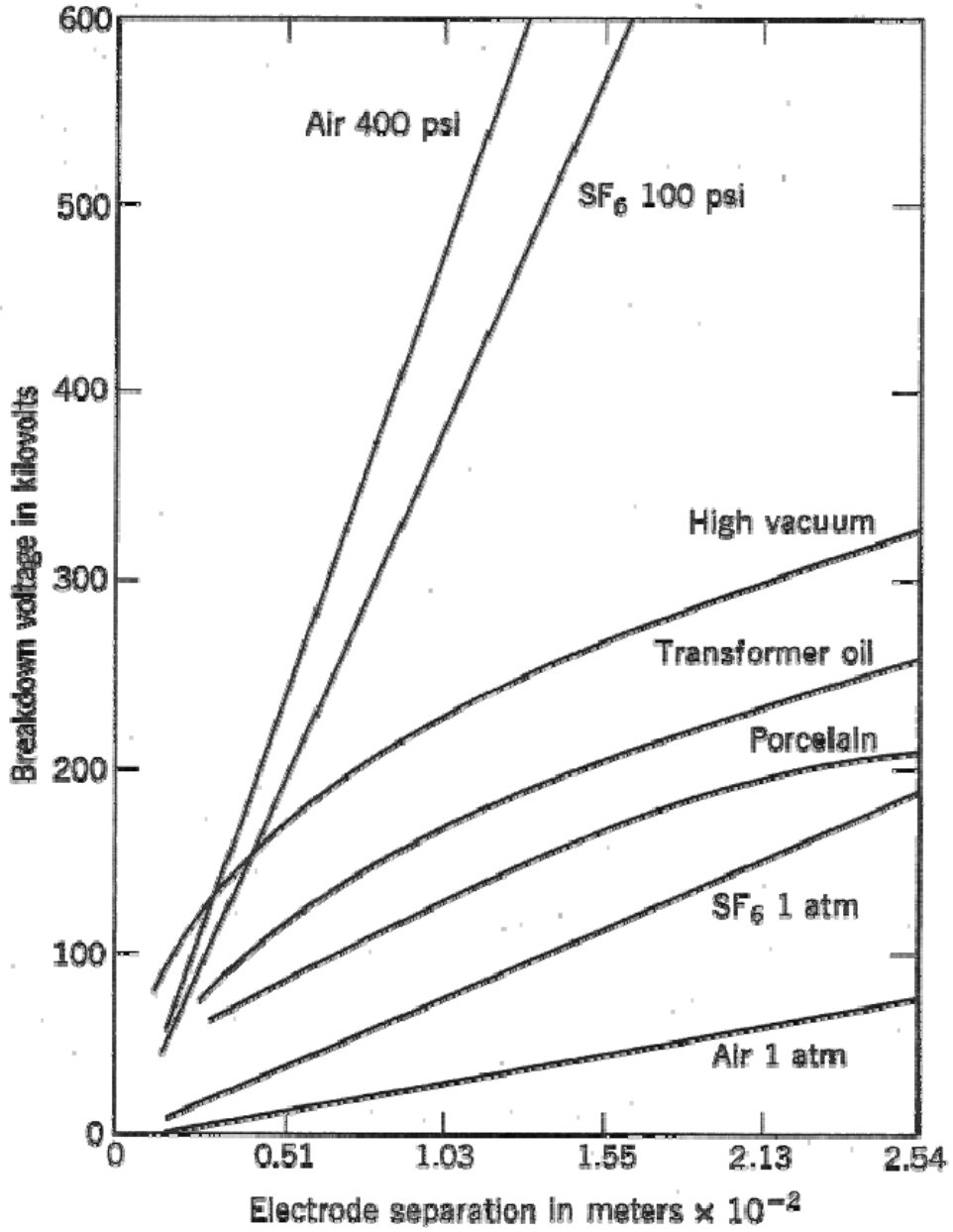
Sometimes a low dielectric constant is desired (CMOS interconnects)

Sometimes a high dielectric constant is desired (supercapacitors).

Breakdown field



Typically 10^5 - 10^6 V/cm



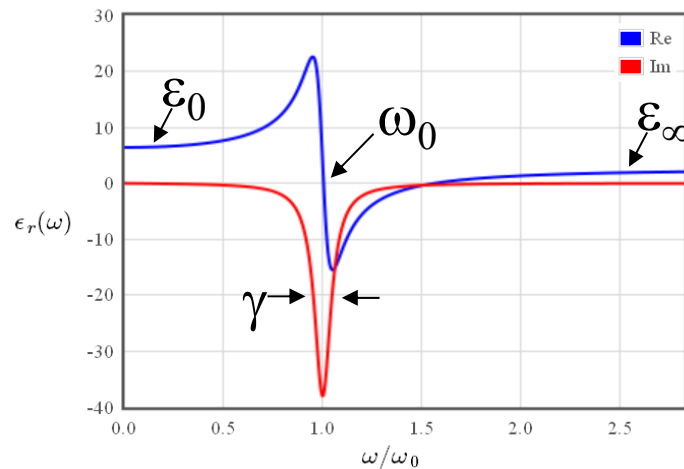
AC losses - loss tangent

In an ideal capacitor, current leads voltage by 90° .

Because the dielectric constant is complex, in real materials current leads voltage by $90^\circ - \delta$.

$$\text{Power loss} = \frac{\omega \epsilon_1 V_0^2}{2} \tan \delta$$

Becomes more of an issue at high frequencies (microwaves)



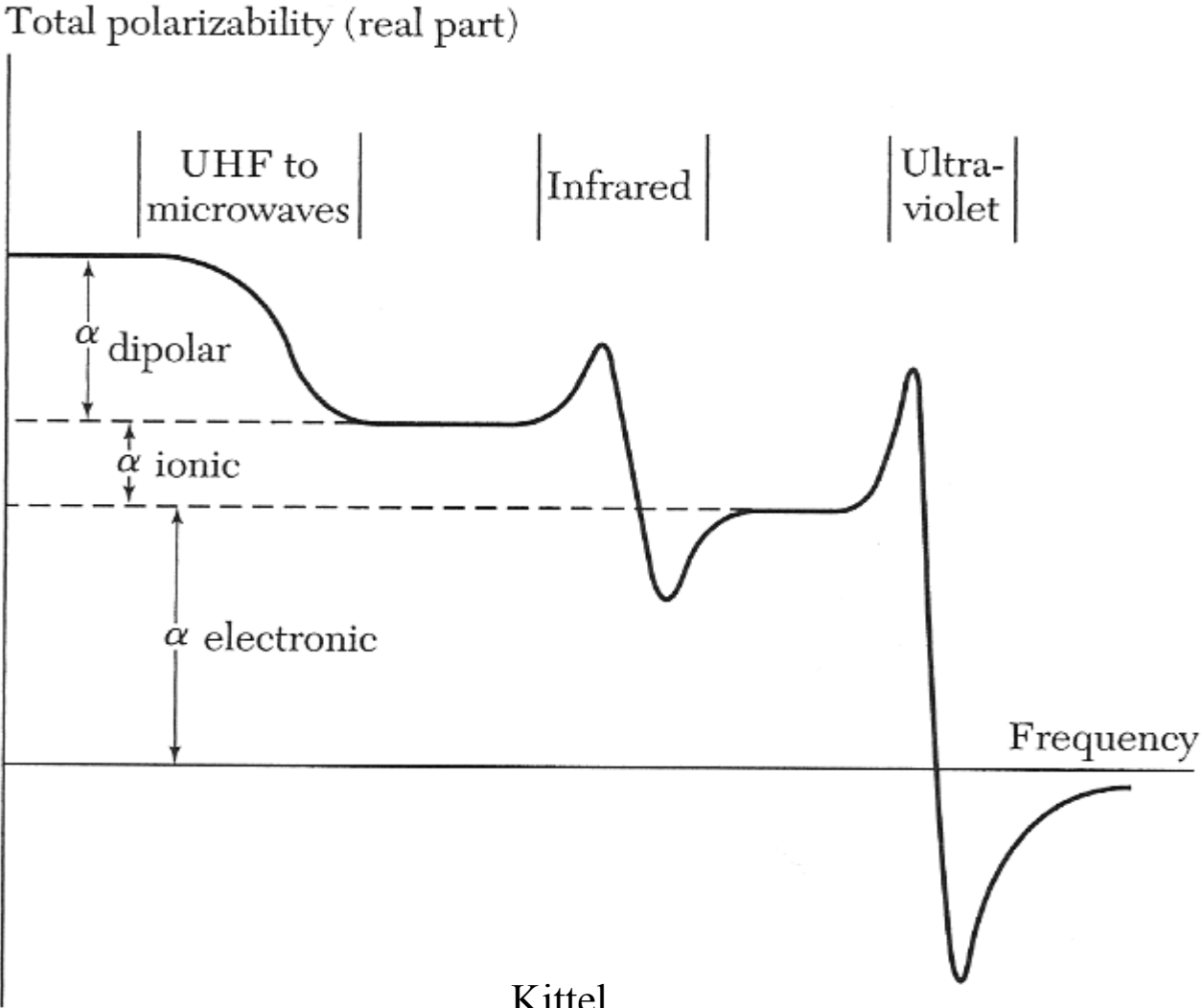
Loss tangent

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

Polarizability

- Overdamped modes
- Orientation polarizability
 - Space charge polarizability
- Underdamped modes
- Ionic polarizability
 - Electronic polarizability

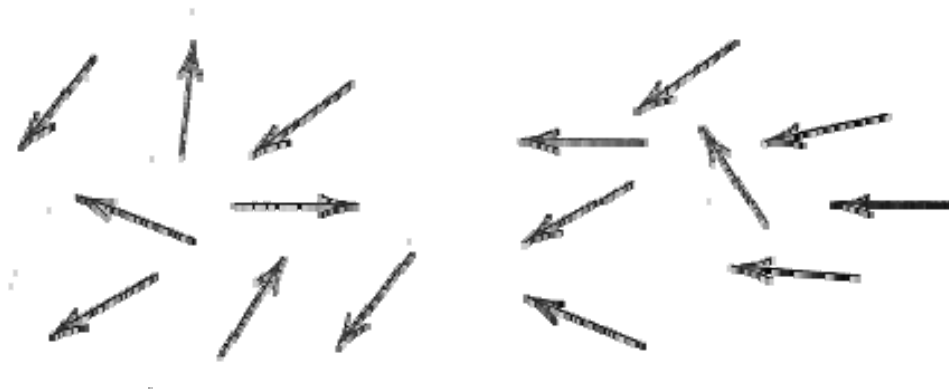
Polarizability



Orientation (dipolar) Polarizability

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

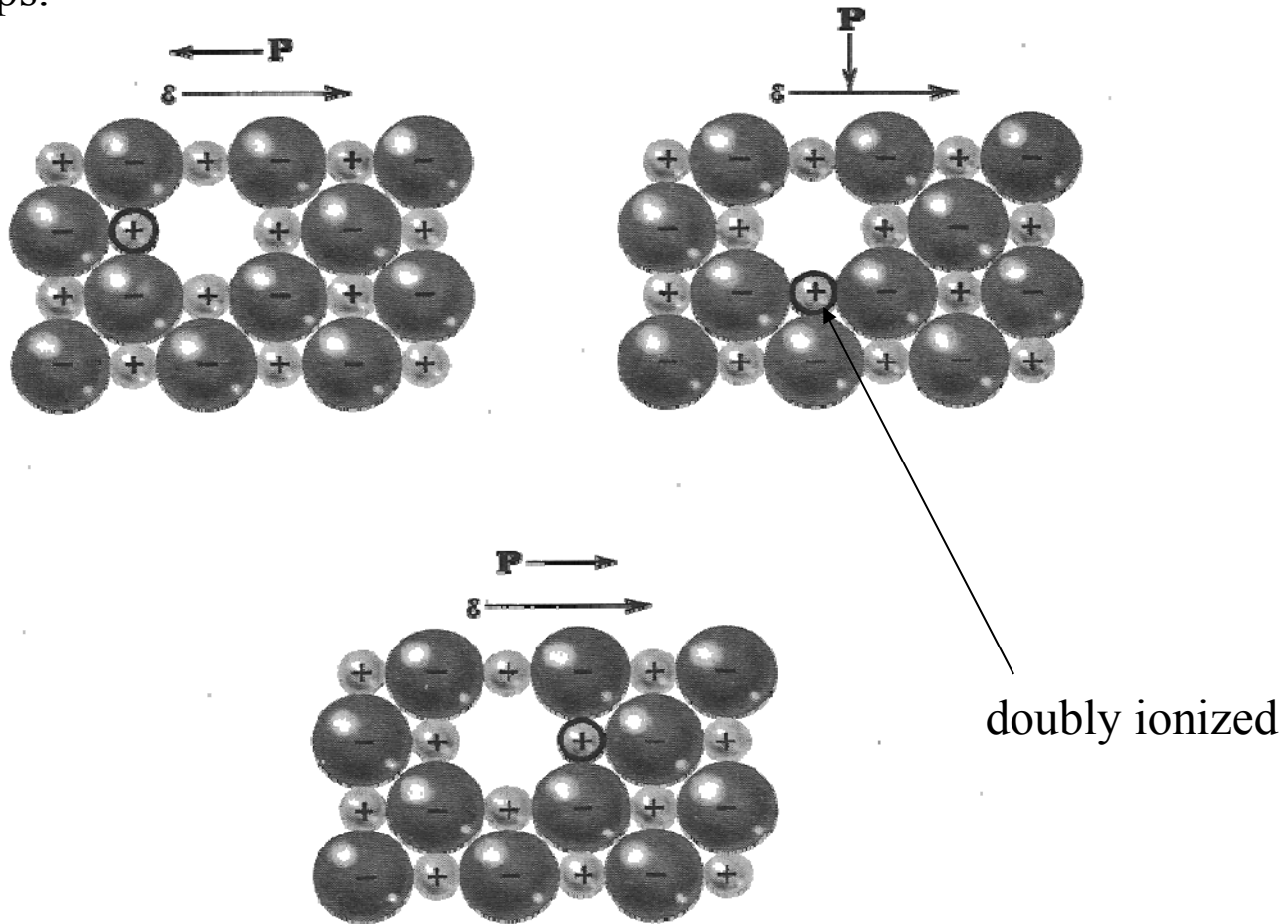
The theory is very similar to paramagnetism.



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

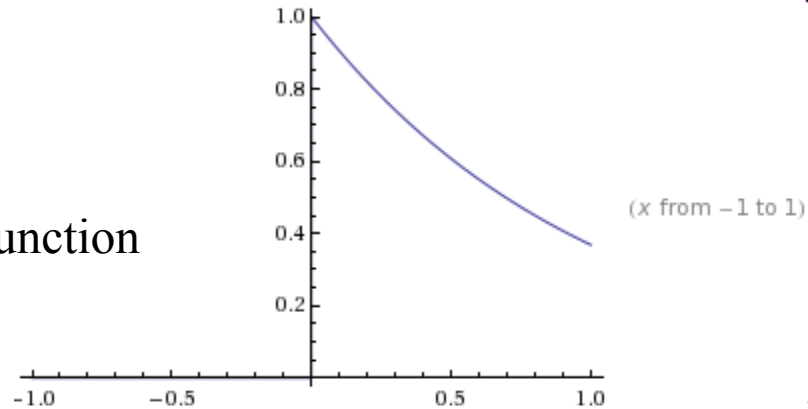
Orientation Polarizability

Ion jumps.

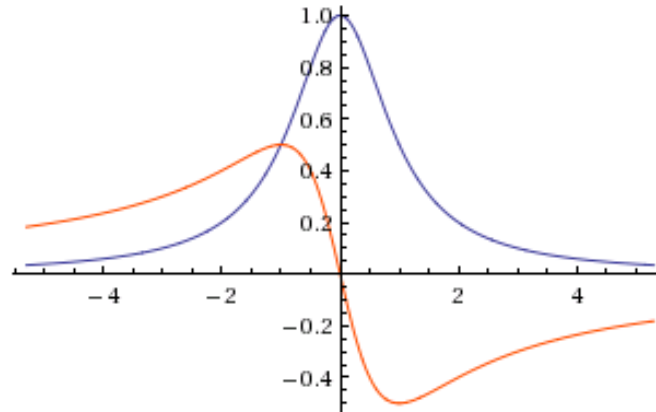


Orientation (dipolar) Polarizability

Overdamped mode
Impulse response function



Susceptibility



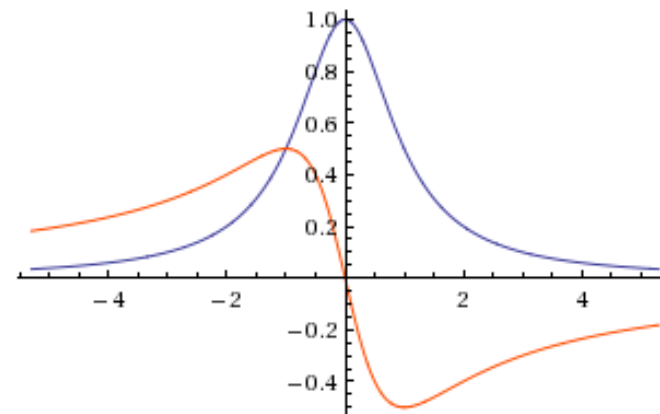
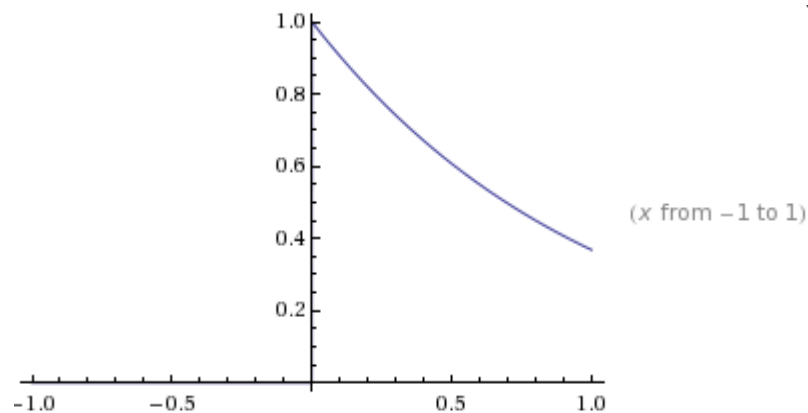
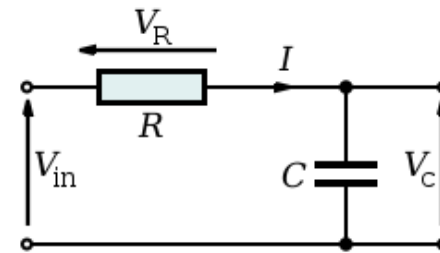
For low frequencies the dipoles can reorient with the field but at high frequencies they can't respond fast enough.

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.

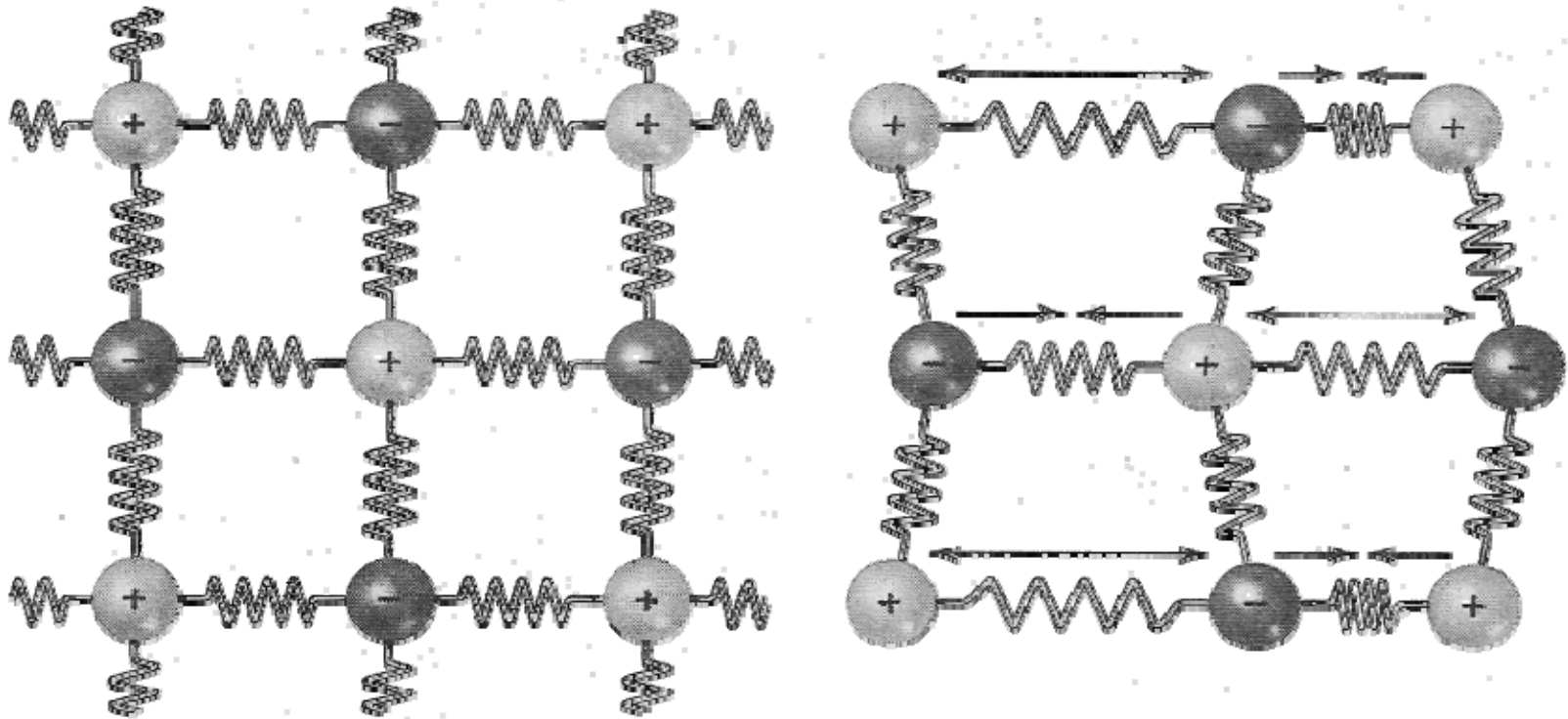
Like a network of resistors and capacitors.

This results in an overdamped mode.



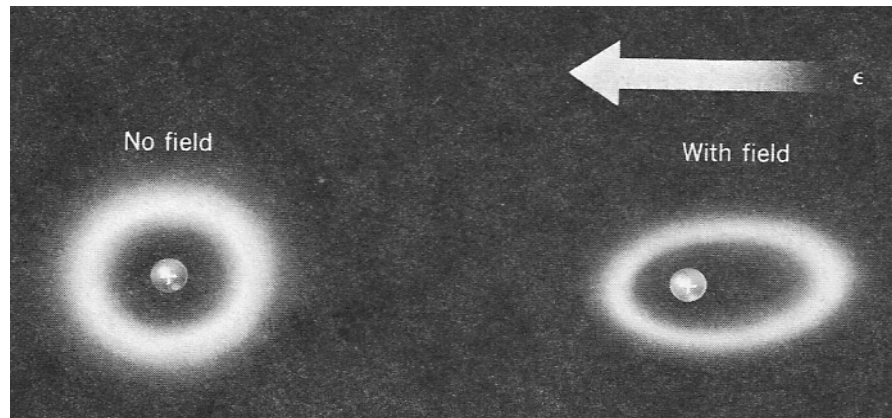
Ionic Polarizability

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



This is an underdamped mode in the infrared.

Electronic polarizability (all materials)



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

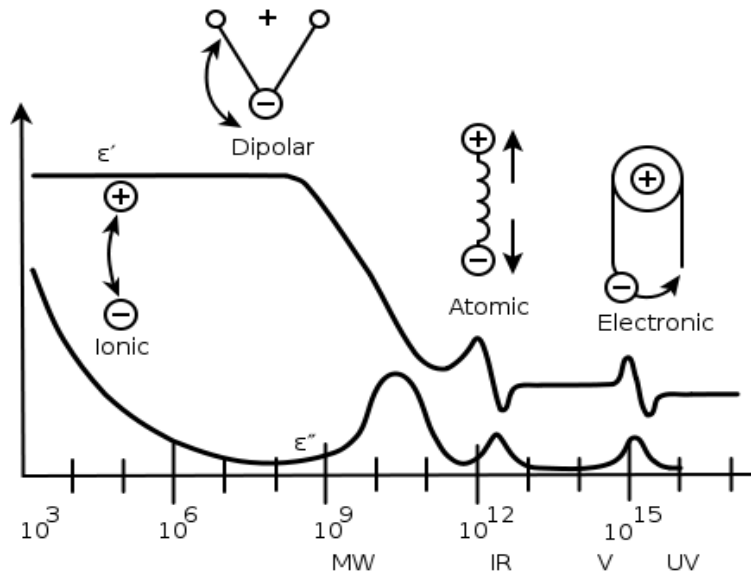
↑ dipole moments
↑ polarizability

↑ density

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

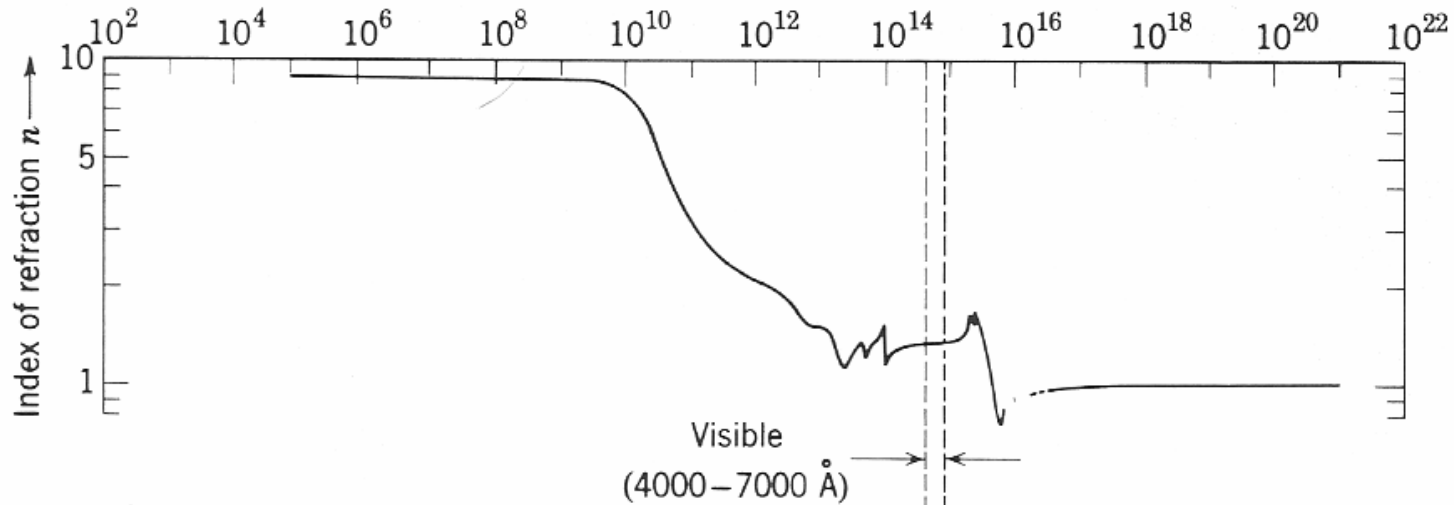
		He	Li ⁺	Be ²⁺	B ³⁺	C ⁴⁺	
Pauling		0.201	0.029	0.008	0.003	0.0013	
JS			0.029				
Pauling	O ²⁻	F ⁻	Ne	Na ⁺	Mg ²⁺	Al ³⁺	Si ⁴⁺
JS-(TKS)	3.88 (2.4)	1.04 0.858	0.390	0.179 0.290	0.094	0.052	0.0165
Pauling	S ²⁻	Cl ⁻	Ar	K ⁺	Ca ²⁺	Se ³⁺	Ti ⁴⁺
JS-(TKS)	10.2 (5.5)	3.66 2.947	1.62	0.83 1.133	0.47 (1.1)	0.286	0.185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

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

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

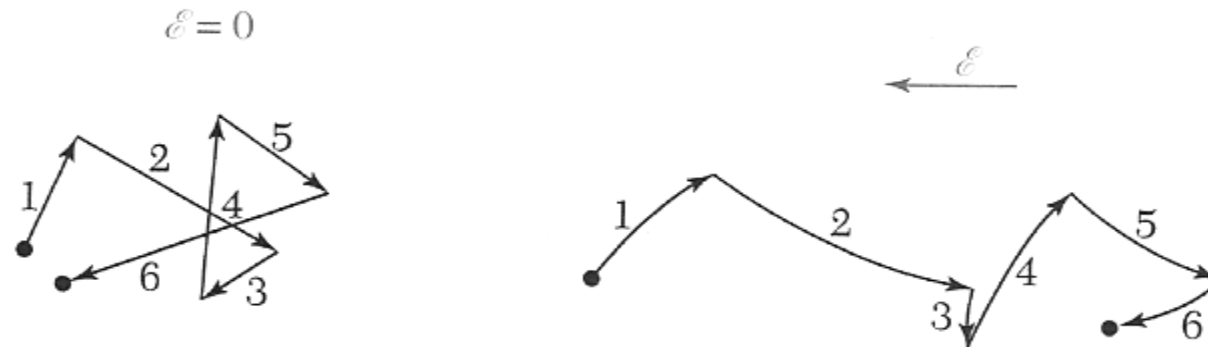
$$\chi(\omega) = \frac{P(\omega)}{\varepsilon_0 E(\omega)} = \frac{-nex(\omega)}{\varepsilon_0 E(\omega)} \quad \sigma(\omega) = \frac{j(\omega)}{E(\omega)} = \frac{-nev(\omega)}{E(\omega)} = \frac{-i\omega nex(\omega)}{E(\omega)}$$

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

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

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)



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

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

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

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

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

Diffusive metal

The current is related to the electric field

$$j_n = \sigma_{nm} E_m \quad v_n = -\mu_{nm} E_m \leftarrow \text{Steady state solution}$$

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

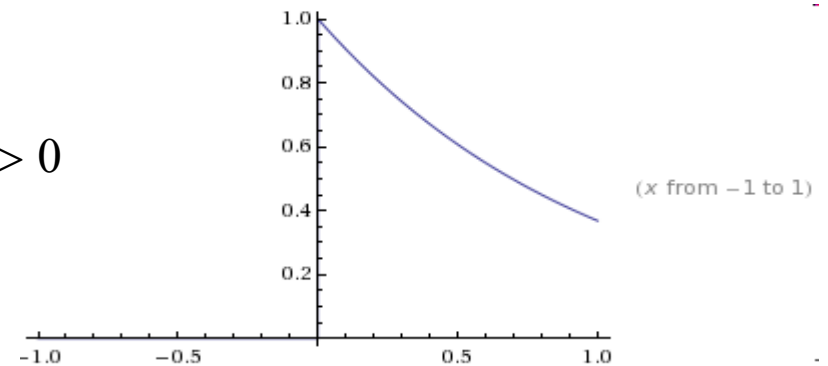
$$m \frac{dv(t)}{dt} + \frac{ev(t)}{\mu} = -eE(t)$$

Inertial term \rightarrow

The impulse response function :

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

$$t > 0$$



Diffusive metal

The differential equation is:

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

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

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

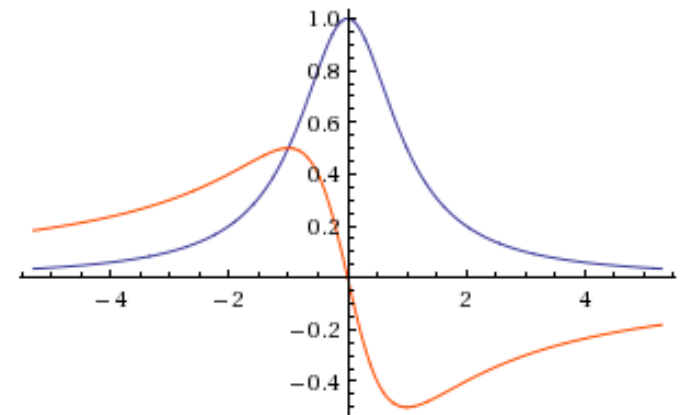
$$\frac{v(\omega)}{E(\omega)} = \left(-\frac{i\omega m}{e} - \frac{1}{\mu} \right)^{-1} = -\mu(1 + i\omega\tau)^{-1} = \frac{-\mu(1 - i\omega\tau)}{1 + \omega^2\tau^2}$$

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

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

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

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



Diffusive metal

$$\chi(\omega) = \frac{\sigma(\omega)}{i\omega\epsilon_0} = \frac{ne\mu}{i\omega\epsilon_0} \left(\frac{1-i\omega\tau}{1+\omega^2\tau^2} \right)$$

$$\epsilon(\omega) = 1 + \chi = 1 - \frac{ne\mu}{\omega\epsilon_0} \left(\frac{\omega\tau + i}{1 + \omega^2\tau^2} \right)$$

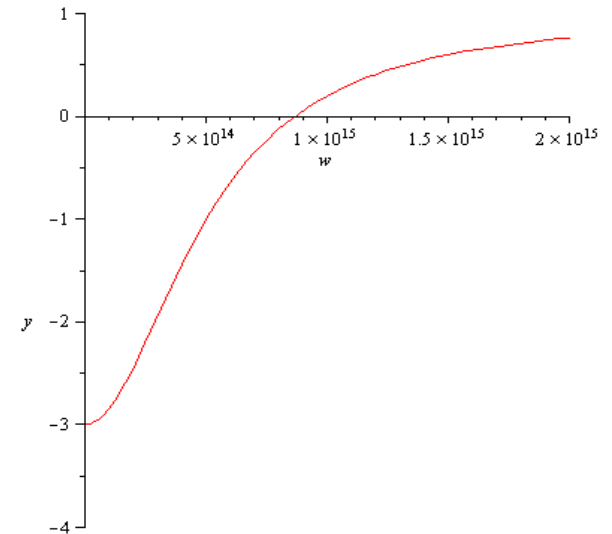
$$\epsilon(\omega) = 1 - \omega_p^2 \left(\frac{\omega\tau^2 + i\tau}{\omega + \omega^3\tau^2} \right)$$

$$\omega_p^2 = \frac{ne^2}{m\epsilon_0}$$

Take the limit as τ goes to infinity

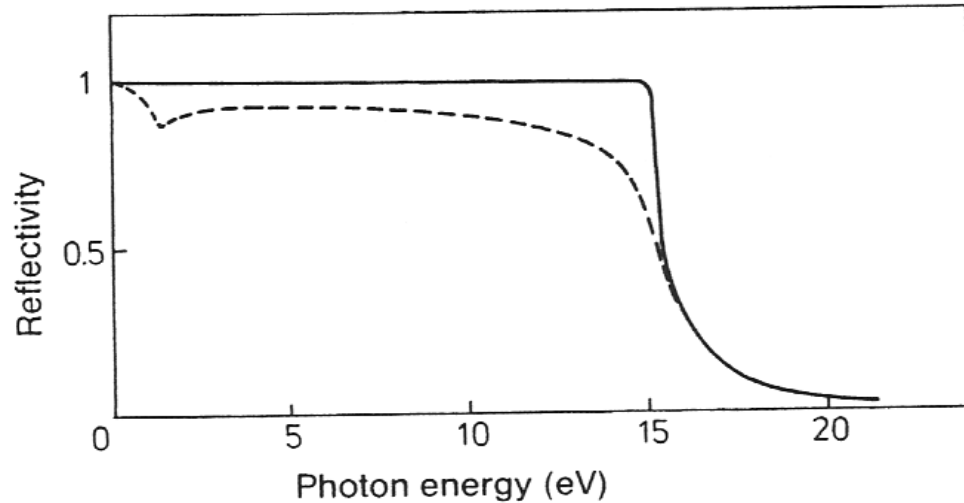
$$\epsilon'(\omega) = 1 - \frac{\omega_p^2}{\omega^2}$$

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

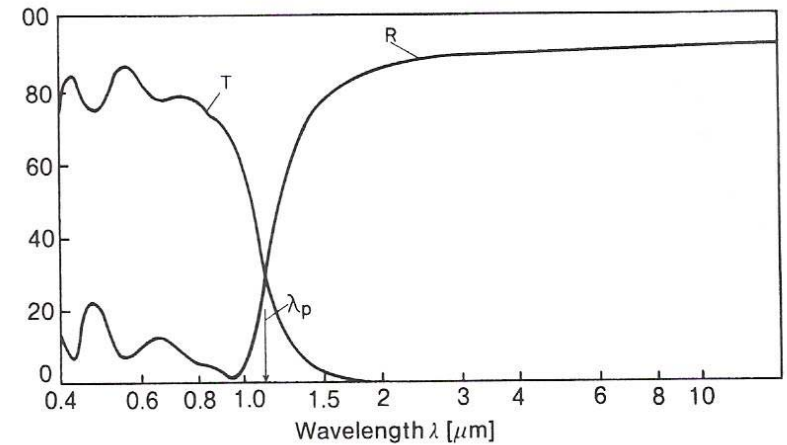


low frequency metal / high frequency insulator

Ibach & Lueth



Aluminum



ITO

Conducting transparent contacts for LEDs and Solar cells

Windows that reflect infrared

Reflection of radio waves from ionosphere

$$\omega_p^2 \approx \frac{ne^2}{\epsilon_0 m}$$



Advanced Solid State Physics

Optical properties of a diffusive metal

- Outline
- Quantization
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It is assumed that electrons in a diffusive metal scatter so often that we can average over the scattering 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 response 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.

$\tau =$ [s] $n =$ [m^{-3}]

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

Impulse response function



[Click here to begin](#)

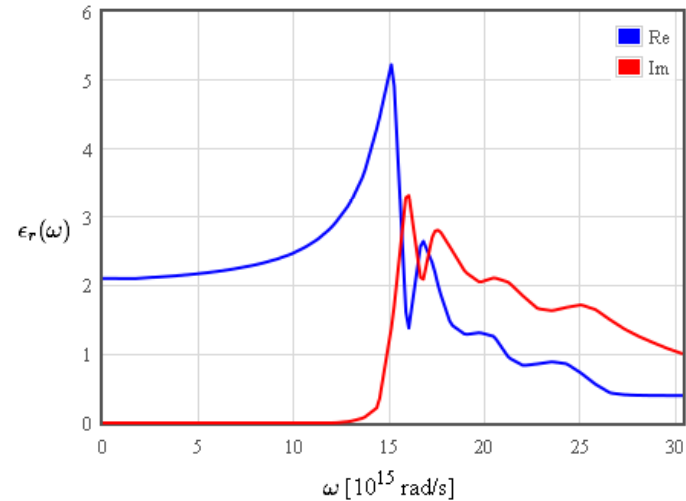
- Outline
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The optical properties of SiO₂ (glass)

nanophotonics.csic.es

Dielectric function

The relative dielectric constant describes the relationship between the electric displacement \vec{D} and the electric field \vec{E} , $\vec{D} = \epsilon_r \epsilon_0 \vec{E} = \vec{P} + \epsilon_0 \vec{E}$.



There are two conventions for dielectric function. Either it is assumed that the time dependence of \vec{D} , \vec{P} , and \vec{E} is $\exp(-i\omega t)$ and the plot of the dielectric function looks as it is shown above, or it is assumed that the time dependence of \vec{D} , \vec{P} , and \vec{E} is $\exp(i\omega t)$ and the imaginary part of the has the opposite sign as in the plot above. Here we will assume a time dependence of $\exp(-i\omega t)$.

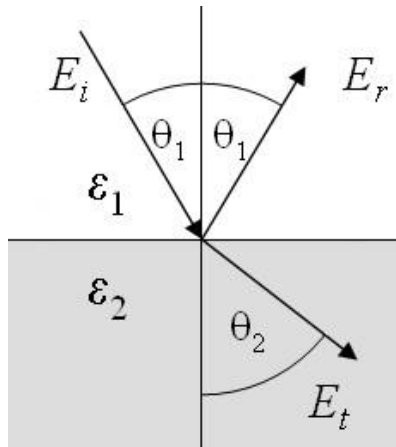
Electric susceptibility

The electric susceptibility χ_E describes the relationship between the polarization \vec{P} and the electric field \vec{E} , $\vec{P} = \epsilon_0 \chi_E \vec{E}$.

$$\chi_E = \epsilon_r - 1$$



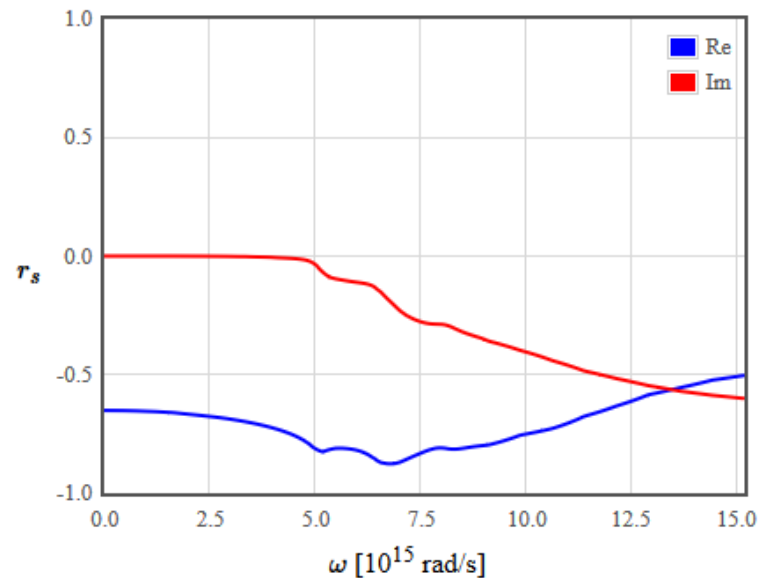
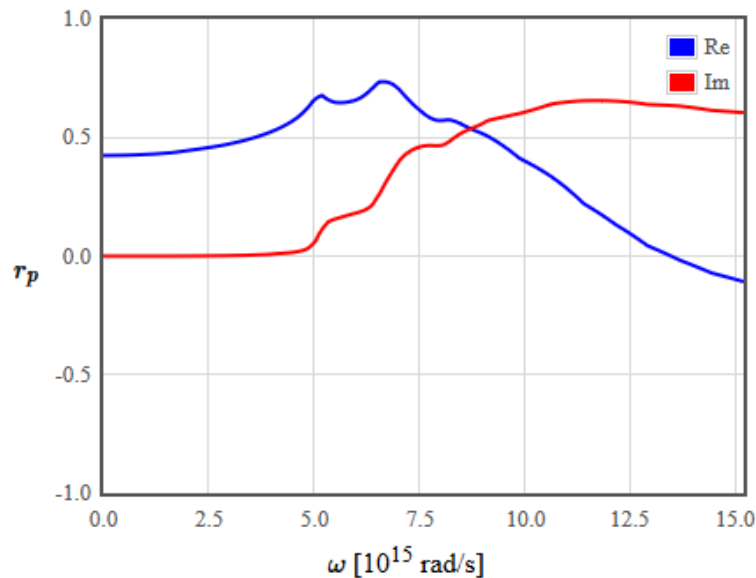
Ellipsometry



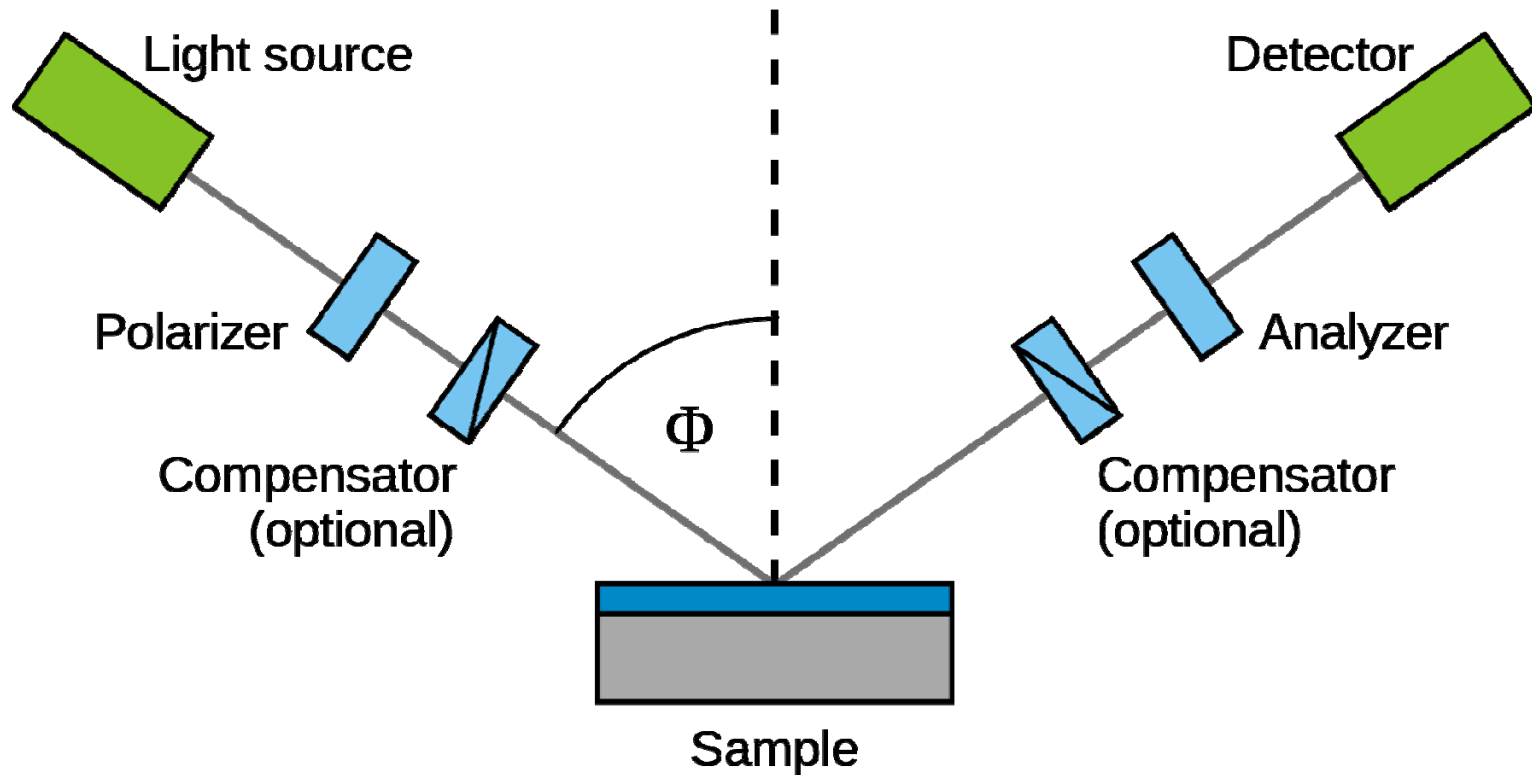
$$r_p = \frac{E_{rp}}{E_{ip}} = \frac{\sqrt{\epsilon_2} \cos \theta_1 - \sqrt{\epsilon_1} \cos \theta_2}{\sqrt{\epsilon_2} \cos \theta_1 + \sqrt{\epsilon_1} \cos \theta_2}$$

$$r_s = \frac{E_{sr}}{E_{si}} = \frac{\sqrt{\epsilon_2} \cos \theta_2 - \sqrt{\epsilon_1} \cos \theta_1}{\sqrt{\epsilon_1} \cos \theta_1 + \sqrt{\epsilon_2} \cos \theta_2}$$

$$n_1 \sin \theta_1 = n_2 \sin \theta_2$$



Ellipsometry

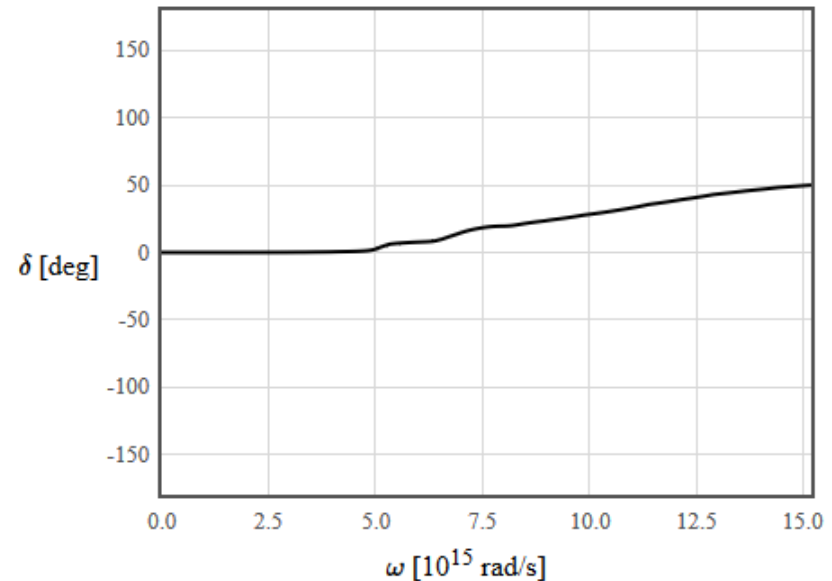
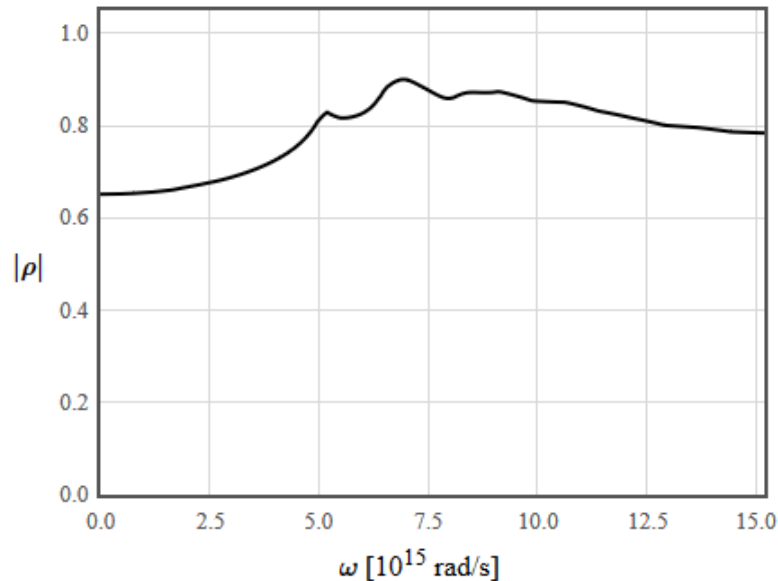


Ellipsometry measures the change of polarization upon reflection. The measured signal depends on the thickness and the dielectric constant.

<http://en.wikipedia.org/wiki/Ellipsometry>

Ellipsometry

$$\rho = \frac{r_p}{r_s} = |\rho|e^{i\delta}$$



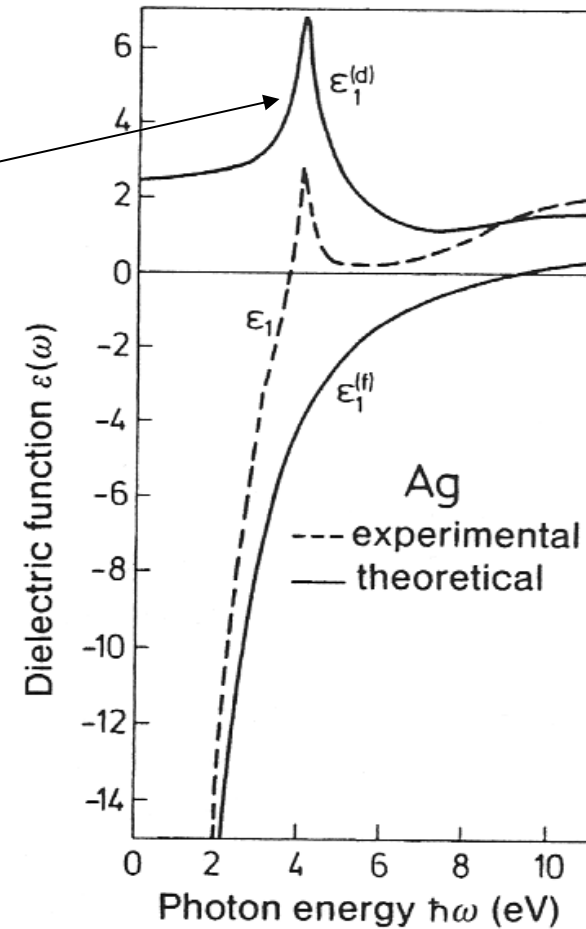
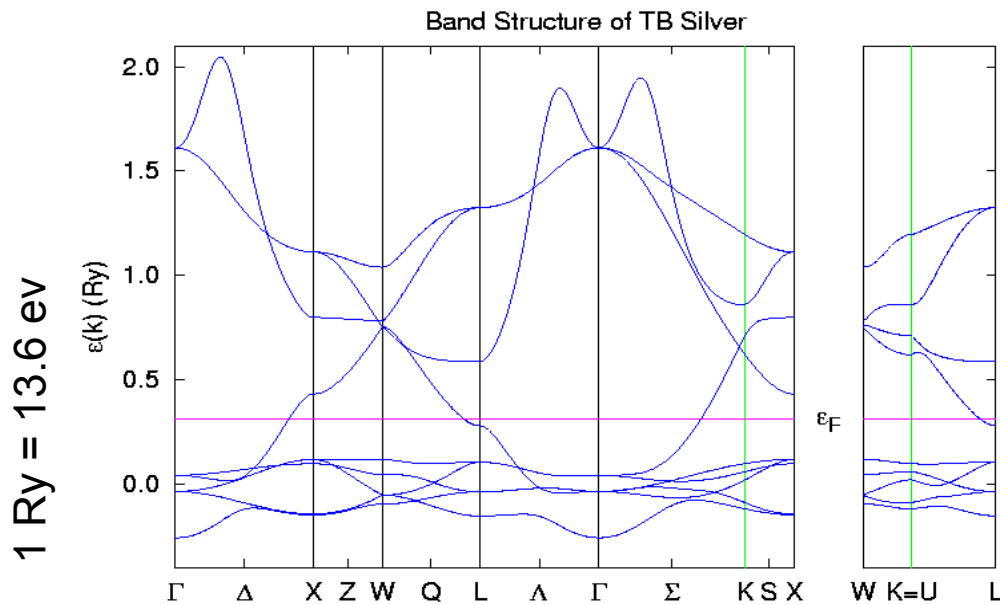
The ratio of the two reflected polarizations is insensitive to instabilities of light source or atmospheric absorption.

Intraband transitions

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

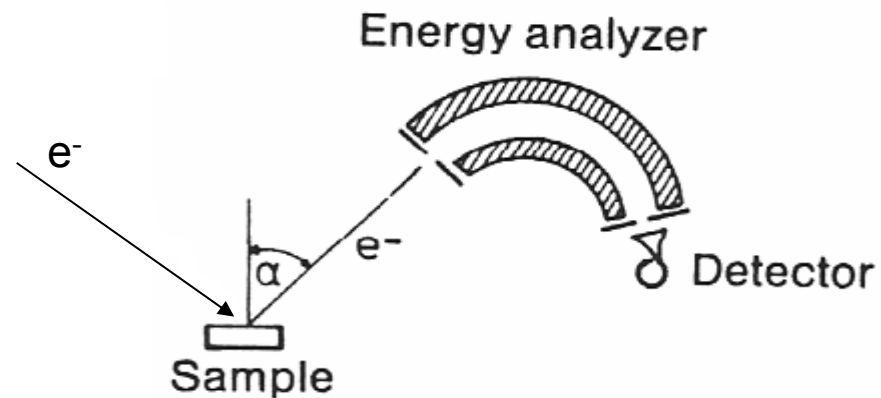
$$\hbar\omega = E_c(\vec{k}) - E_v(\vec{k})$$

Intraband (d-band) absorption



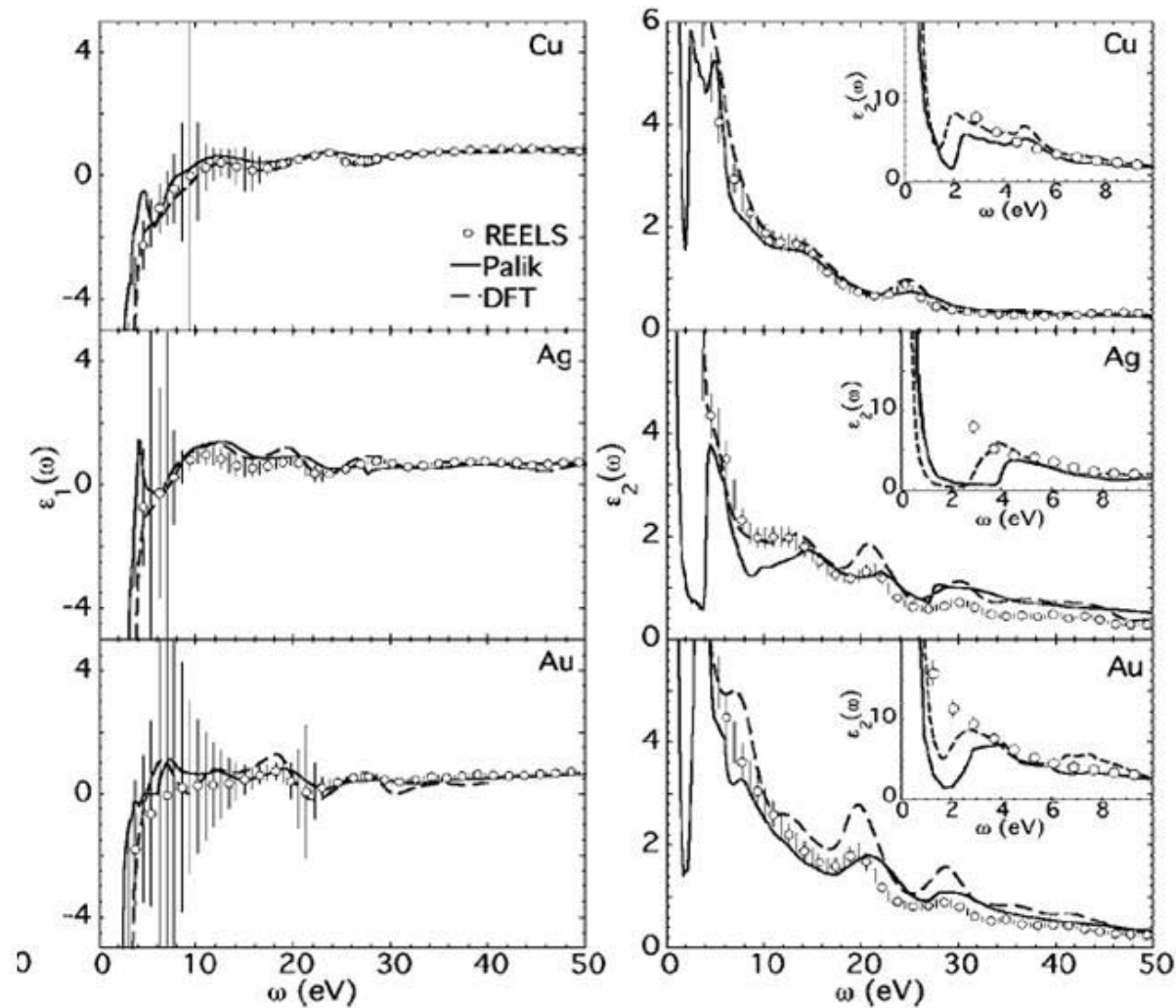
Ibach & Lueeth

Reflection Electron Energy Loss Spectroscopy



Fast electrons moving through the solid generate a time dependent electric field. If the polarization moves out of phase with this field, energy will be lost. This is detected in the reflected electrons.

Dielectric function of Cu, Ag, and Au obtained from reflection electron energy loss spectra, optical measurements, and density functional theory



Werner (TU Vienna) APL 89 213106 (2006)

Microwave engineering

Microwave frequencies are a few GHz

The wavelength is smaller than the circuit

Losses in metals increase with increasing frequency

Losses in dielectrics increase with increasing frequency

There is a characteristic length scale called the skin depth which tells us how far into a metal fields penetrate before they are reflected out.