Optical Properties of Solids: Lecture 4

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http://ellipsometry.nmsu.edu

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Optical Properties of Solids: Lecture 4

Electrodynamics of **continuous media**

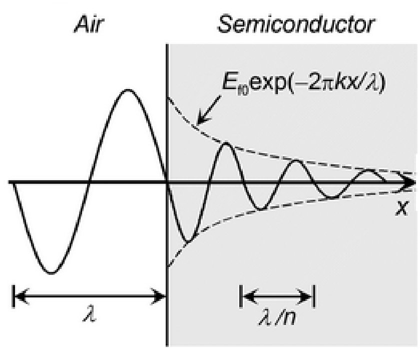
Dielectric displacement, dielectric polarization vector

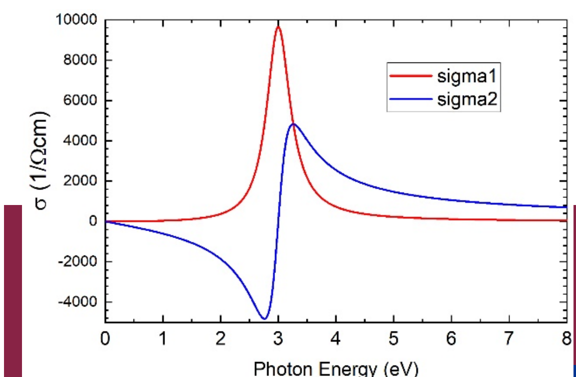
Maxwell's equations for continuous media

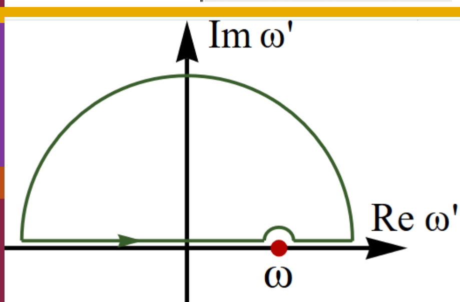
Wave equations for continuous media

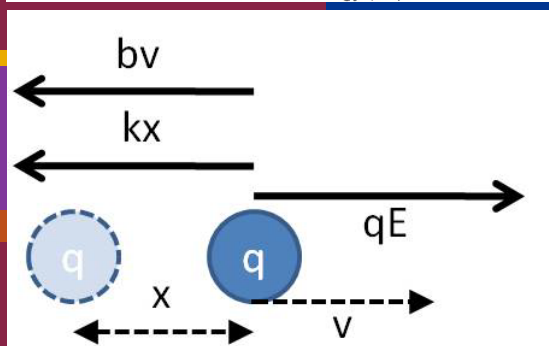
Anisotropy concerns (distorted perovskites)

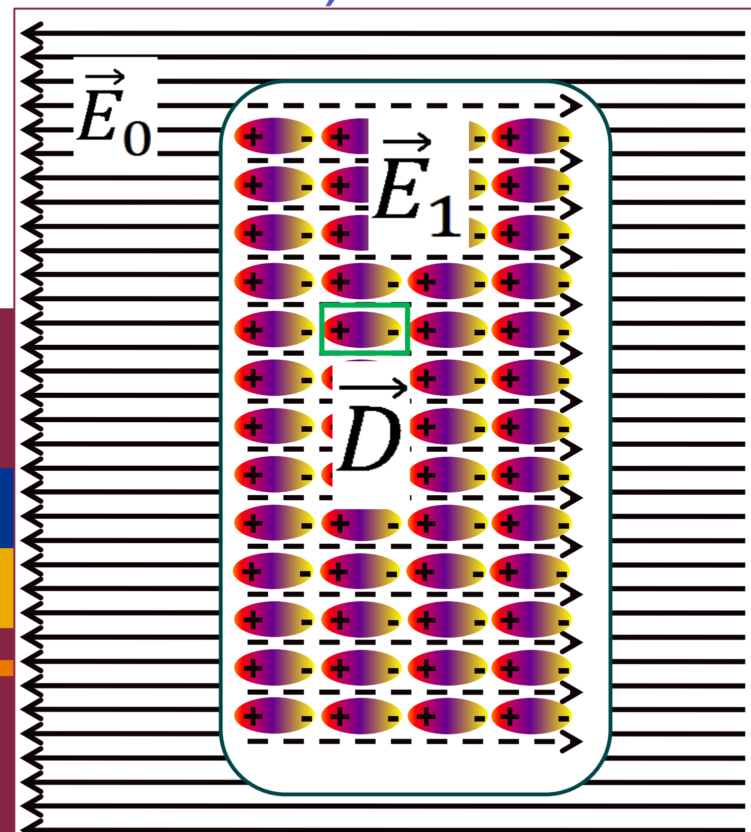
Lorentz and **Drude** model











References: Maxwell's Equations and Ellipsometry

Standard Texts on Electricity and Magnetism:

- J.D. Jackson: *Classical Electrodynamics*
- **L.D. Landau & J.M. Lifshitz, Vol. 8: *Electrodynamics of Cont. Media***
- **V.M. Agranovich & V.L. Ginzburg, *Crystal Optics with Spatial Dispersion***

Optics:

- E. Hecht: *Optics*
- M. Born, E. Wolf: *Principles of Optics*

Ellipsometry and Polarized Light:

- R.M.A. Azzam and N.M. Bashara: *Ellipsometry and Polarized Light*
- **H.G. Tompkins and E.A. Irene: *Handbook of Ellipsometry* (chapters by Josef Humlicek and Rob Collins)**
- H. Fujiwara, *Spectroscopic Ellipsometry*
- **Mark Fox, *Optical Properties of Solids***
- H. Fujiwara and R.W. Collins: *Spectroscopic Ellipsometry for PV* (Vol 1+2)
- Zollner: *Propagation of EM Waves in Continuous Media* (Lecture Notes)

Maxwell's Equations in Vacuum

$$\vec{\nabla}\cdot\vec{E}=0$$ Gauss' Law (Coulomb)

$$\vec{\nabla}\cdot\vec{H}=0$$ Gauss' Law (magnetic field)

$$\vec{\nabla}\times\vec{E}=-\mu_0\frac{\partial\vec{H}}{\partial t}$$ Faraday's Law

$$\vec{\nabla}\times\vec{H}=\varepsilon_0\frac{\partial\vec{E}}{\partial t}$$ Ampere's Law

$$\vec{E}(\vec{r},t)=\vec{E}_0\exp\left[i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right]$$
$$\vec{H}(\vec{r},t)=\vec{H}_0\exp\left[i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right]$$

Substitute plane wave solutions into differential form of Maxwell's Equations

$$\vec{k}\cdot\vec{E}_0=0$$ Gauss' Law (Coulomb)

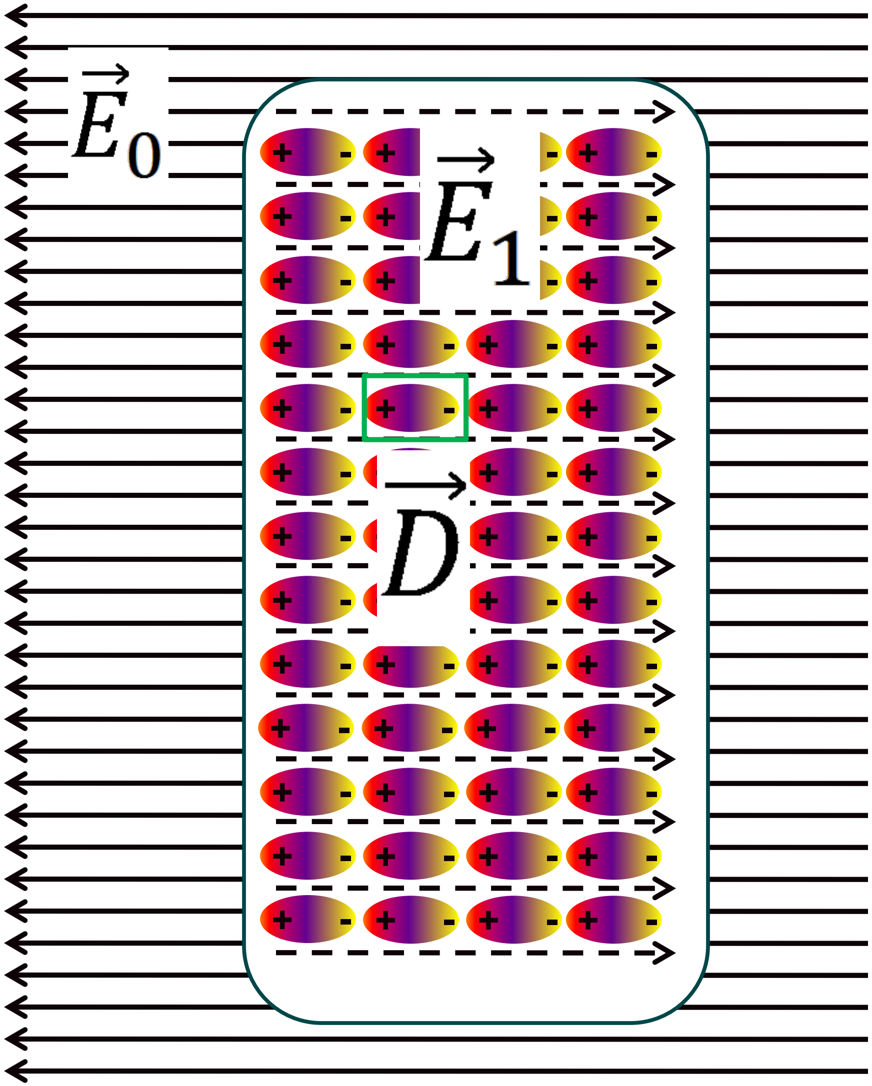
$$\vec{k}\cdot\vec{H}_0=0$$ Gauss' Law (magnetic field)

$$\vec{k}\times\vec{E}_0=\omega\mu_0\vec{H}_0$$ Faraday's Law

$$\vec{k}\times\vec{H}_0=-\omega\varepsilon_0\vec{E}_0$$ Ampere's Law

$k^2=\omega^2/c^2$; **k** $\perp$ **E,H; E** $\perp$ **H**, $E_0=Z_0H_0$, $Z_0=\sqrt{(\mu_0/\varepsilon_0)}=377\ \Omega$

Dielectric in Static Electric and Magnetic Fields



Applied external electric field $\mathbf{E}_0$
(homogeneous, constant)
Infinite dielectric
(ignore boundary effects)

Charges move in response to $\mathbf{E}_0$
Average charge density still zero
Induced (depolarizing) electric field $\mathbf{E}_1$
weakens applied field $\mathbf{E}_0$.

Local electric field

$\mathbf{E}=\mathbf{E}_{local}=\mathbf{E}_0+\mathbf{E}_1$

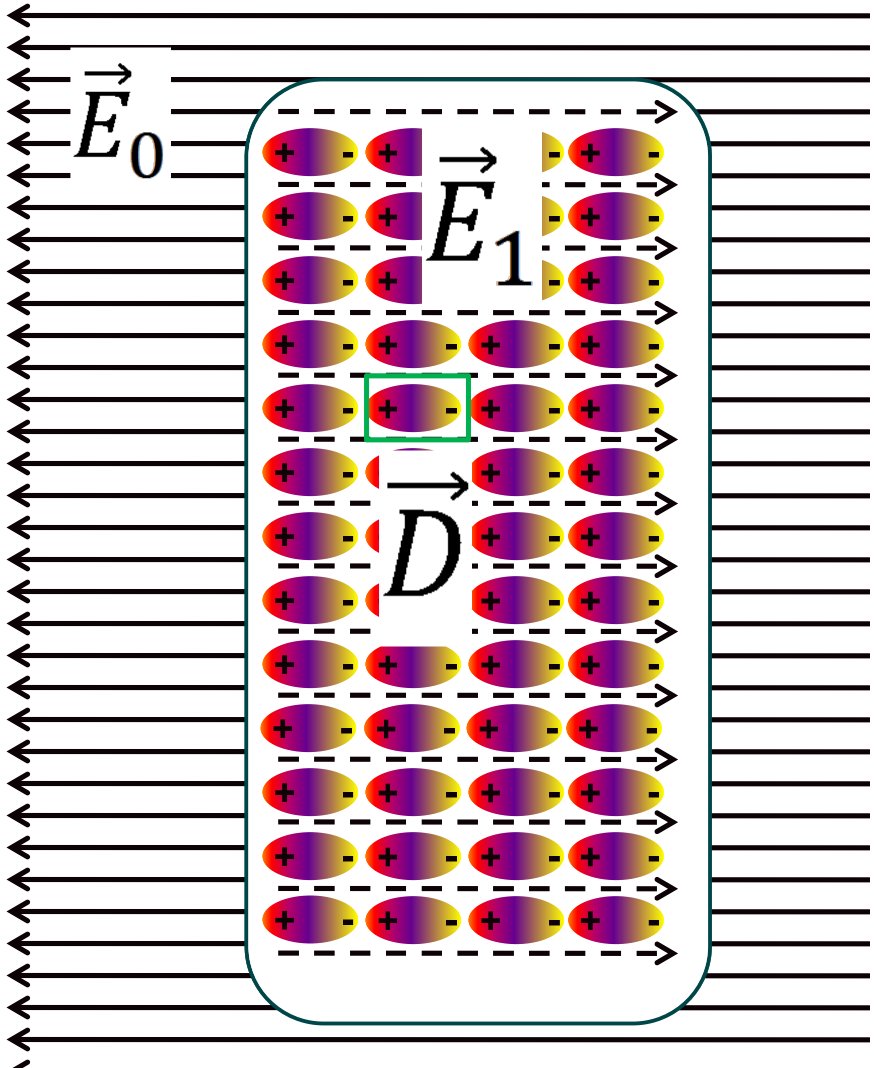
Metal: $\mathbf{E}_{local}=0$ (for $\omega=0$)

$E_{local}<E_0$ (screening)

E_{local} depends on crystal shape (boundary conditions), see Nye.

Nye, Physical Properties of Crystals

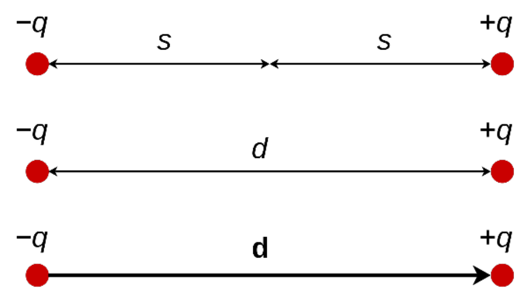
Dielectric Polarization, Dielectric Displacment



$\mathbf{E}=\mathbf{E}_{local}=\mathbf{E}_0+\mathbf{E}_1$

Applied external electric field $\mathbf{E}_0$
(homogeneous, constant)
Infinite dielectric
(ignore boundary effects)
Total electric field **E**

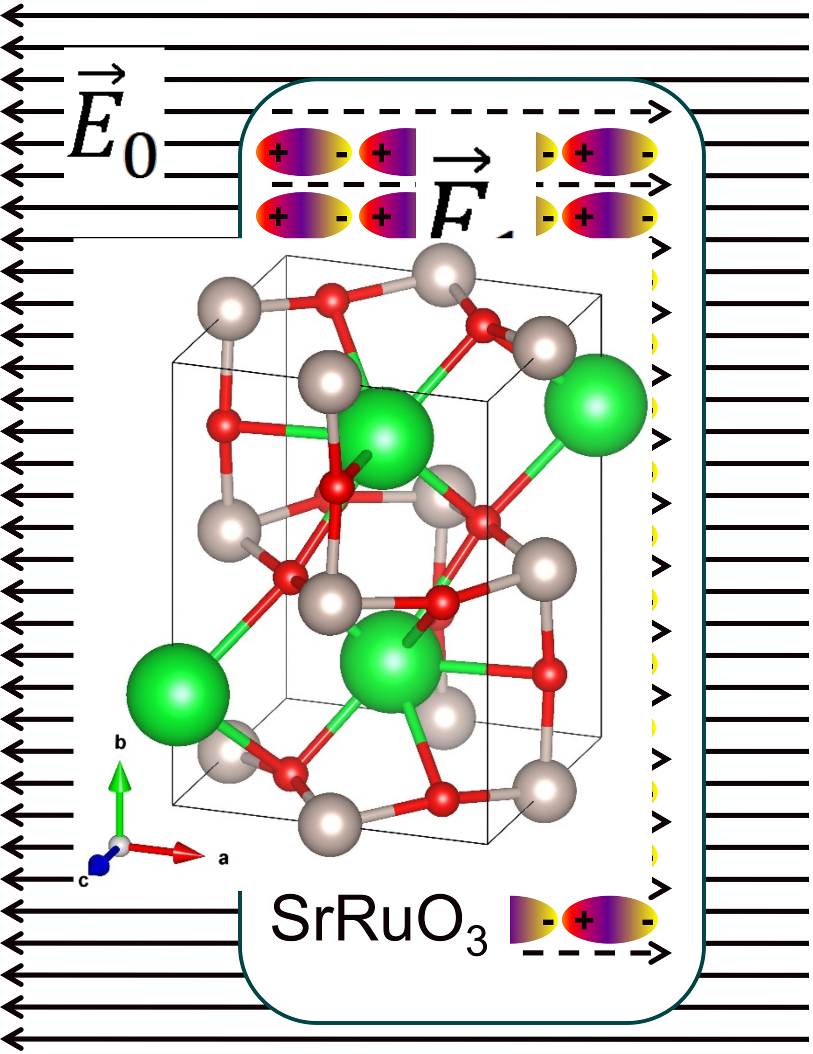
Charges move:
Dipole moment
p=q**d**
(**d** from –q to +q)



Dielectric polarization P
Dipole moment per unit volume
Dielectric Displacement: $\mathbf{D}=\varepsilon_0\mathbf{E}+\mathbf{P}$
<u>Linear dielectric susceptibility</u>
$\mathbf{P}=\varepsilon_0\chi_e\mathbf{E}$
Dielectric constant: $\varepsilon=1+\chi_e$, $\mathbf{D}=\varepsilon_0\varepsilon\mathbf{E}$

Nye, Physical Properties of Crystals

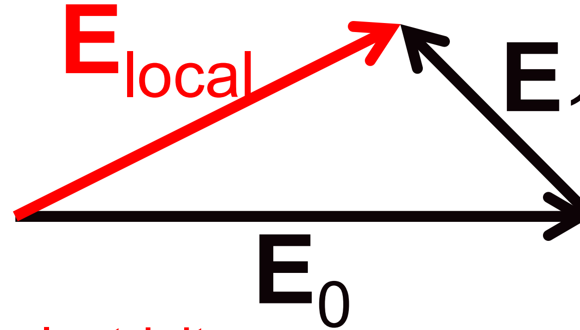
Complications



$E = E_{local} = E_0 + E_1$

<u>Anisotropy</u>

$\mathbf{E}_{local} = \mathbf{E}_0 + \mathbf{E}_1$



Tensors !!!

<u>Ferro-/Pyro-/Piezoelectricity</u>

Non-zero polarization for zero field ($\mathbf{E}_0$=0).

$\mathbf{P}(E_0=0) = \mathbf{P}_r + \mathbf{p}\Delta T + d_{ijk}X_{jk}$

$\partial \mathbf{P}_r / \partial t = 0$

<u>Nonlinear effects</u>

$\mathbf{P}(\mathbf{E}) = \mathbf{P}_r + \varepsilon_0 \chi_e \mathbf{E} + \varepsilon_0 \chi_e^{(2)} \mathbf{E} \otimes \mathbf{E} + \varepsilon_0 \chi_e^{(3)}{}_{ijkl} E_j E_k E_l + \ldots$

<u>Magneto-electric effects</u>

$\mathbf{P} = \mathbf{P}_r + \varepsilon_0 \chi_e \mathbf{E} + \varepsilon_0 \delta H$

<u>Dielectric Displacement:</u>

$\mathbf{D} = \mathbf{P}_r + \varepsilon_0 \mathbf{E} + \varepsilon_0 \chi_e \mathbf{E} + \varepsilon_0 \delta \mathbf{H}$

$\mathbf{D} = \mathbf{P}_r + \varepsilon_0 \varepsilon \mathbf{E} + \varepsilon_0 \delta \mathbf{H}$

Dielectric constant ε

Nye, Physical Properties of Crystals

Magnetostatics and Magnetization

Electric field strength **E**
Dielectric polarization **P**: electric dipole moment per unit volume
Dielectric displacement $\mathbf{D}=\varepsilon_0\mathbf{E}+\mathbf{P}=\mathbf{P}_r+\varepsilon_0\mathbf{E}+\varepsilon_0\chi_e\mathbf{E}+\varepsilon_0\delta\mathbf{H}$
Magnetic field strength **H**
Magnetization **M**: magnetic dipole moment per unit volume
$\mathbf{M}=\mathbf{M}_r+\mu_0\chi_m\mathbf{H}+\mu_0\gamma\mathbf{E}$ ($\mathbf{M}_r$ remanence, $\partial\mathbf{M}_r/\partial t=0$)
Magnetic susceptibility χ_m

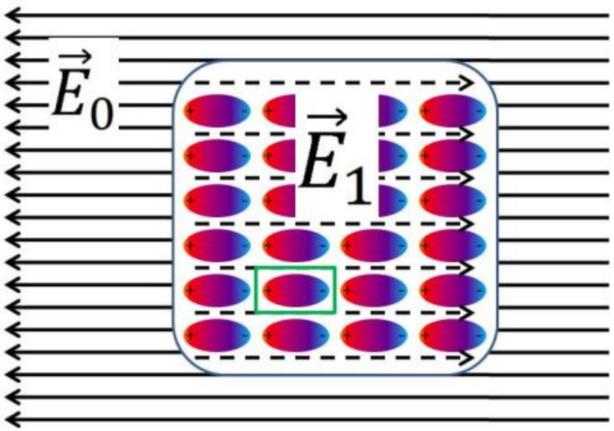
Magnetic flux density **B**
$\mathbf{B}=\mu_0\mathbf{H}+\mathbf{M}=\mathbf{M}_r+\mu_0\mu\mathbf{H}+\mu_0\gamma\mathbf{E}$
$\mu=1+\chi_m$ magnetic permeability ($\mu=1$ unless $\omega=0$)

Nye, Physical Properties of Crystals

AC Response Function: Dispersion, Nonlocality

How does a dielectric respond to an electromagnetic wave?

$$\vec{E}(\vec{r},t) = \vec{E}_0 \exp\left[i\left(\vec{k}\cdot\vec{r} - \omega t\right)\right]$$



Polarization may be delayed.
Polarization may be non-local.

$$\vec{P}(\vec{r},t) = \varepsilon_0 \int_{-\infty}^{t} \chi_e(\vec{r}',\vec{r},t',t)\vec{E}(\vec{r}',t')dt'd^3\vec{r}'$$

Time invariance
Infinite homogeneous crystal

$$\vec{P}(\vec{r},t) = \varepsilon_0 \int_{-\infty}^{t} \chi_e(\vec{r}'-\vec{r},t'-t)\vec{E}(\vec{r}',t')dt'd^3\vec{r}'$$

Use convolution theorem for Fourier transforms

$$\vec{P}(\vec{k},\omega) = \varepsilon_0\chi_e(\vec{k},\omega)\,\vec{E}(\vec{k},\omega)$$
$$\vec{D}(\vec{k},\omega) = \varepsilon_0\varepsilon(\vec{k},\omega)\,\vec{E}(\vec{k},\omega)$$

Nonlocal effects scale like 2πa/λ

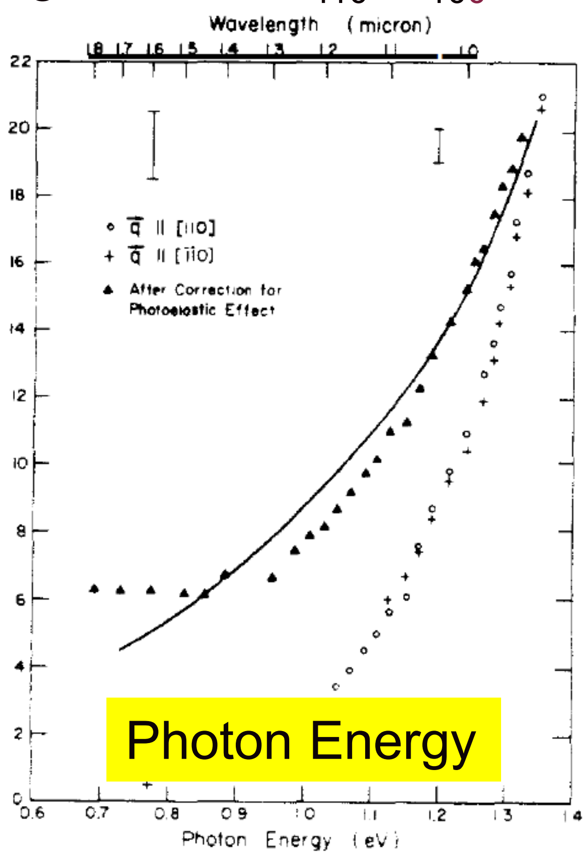
Dielectric function ε depends on frequency ω (dispersion).

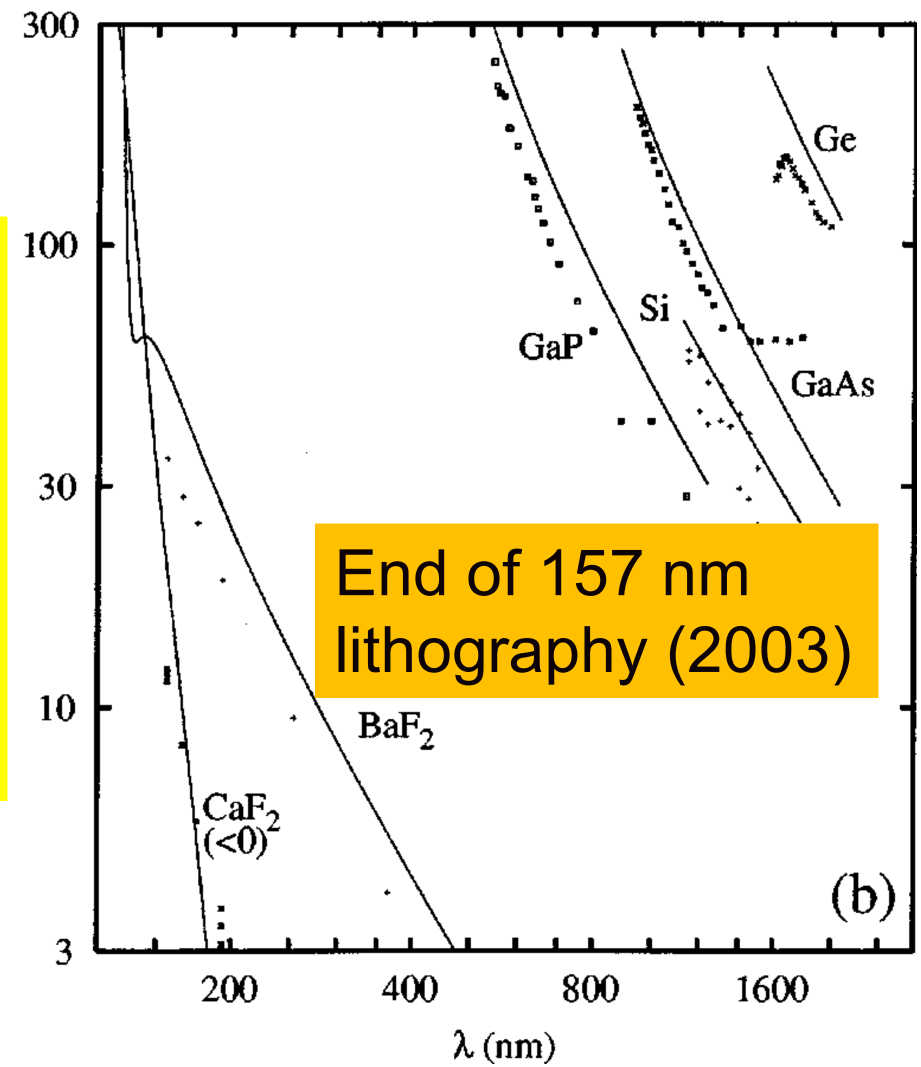
Nonlocality Example: Birefringence in Cubic Crystals

$$\Delta\varepsilon_{ij}(\vec{k}) = \alpha_{ijkl} k_k k_l$$

vanishes along [001], but not along [110]

Birefringence $\Delta n = n_{110} - n_{100}$





Birefringence in GaAs near bang gap
Model from k.p theory

Yu & Cardona, SSC **9**, 1421 (1971)

Agranovitch & Ginzburg, Crystal Optics
J.H. Burnett, PRB **64**, 241102 (2000)

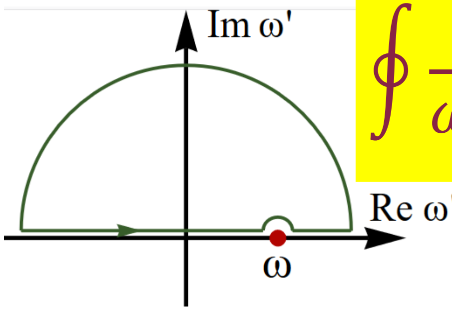
Causality: Charge Movement Follows the Field

$$\vec{P}(\vec{r},t) = \varepsilon_0 \int \chi_e(\vec{r}\,' - \vec{r}, t' - t)\vec{E}(\vec{r}\,', t')dt'd^3\vec{r}\,'$$

Response function $\chi_e(\vec{r}\,' - \vec{r}, t' - t) = 0 \text{ for } t' > t$

The charges cannot move before the field has been applied.

Kramers-Kronig relations follow:



$$\oint \frac{\chi(\omega)}{\omega' - \omega} d\omega' = 0$$

Cauchy

$$\vec{D}(\vec{k},\omega) = \varepsilon_0 \varepsilon(\vec{k},\omega)\,\vec{E}(\vec{k},\omega)$$

$$\varepsilon_1(\omega) - 1 = \frac{2}{\pi} \wp \int_0^\infty \frac{\omega' \varepsilon_2(\omega') d\omega'}{\omega'^2 - \omega^2}$$

$$\varepsilon_2(\omega) = -\frac{2\omega}{\pi} \wp \int_0^\infty \frac{\varepsilon_1(\omega') d\omega'}{\omega'^2 - \omega^2}$$

Contour integrals in complex plane:
The real part of ε can be calculated if the imaginary part is known (and vice versa).

Similar Kramers-Kronig relations for other optical constants

Maxwell's Equations for Continuous Media

$\vec{\nabla}\cdot\vec{D}=\rho=0$ Gauss' Law (Coulomb)

$\vec{\nabla}\cdot\vec{B}=0$ Gauss' Law (magnetic field)

$\vec{\nabla}\times\vec{E}=-\frac{\partial\vec{B}}{\partial t}$ Faraday's Law

$\vec{\nabla}\times\vec{H}=\vec{j}+\frac{\partial\vec{D}}{\partial t}=\frac{\partial\vec{D}}{\partial t}$ Ampere's Law

Anisotropic wave equation:

Take curl on both sides in Ampere's Law and Faraday's Law

$$\Delta\vec{E}-\vec{\nabla}\left(\vec{\nabla}\cdot\vec{E}\right)=\mu_0\frac{\partial}{\partial t}\vec{\nabla}\times\mu\vec{H}$$

$$\Delta\vec{H}-\vec{\nabla}\left(\vec{\nabla}\cdot\vec{H}\right)=-\varepsilon_0\frac{\partial}{\partial t}\vec{\nabla}\times\varepsilon\vec{E}$$

The terms in red do not vanish (cannot be simplified) in anisotropic media.

Isotropic wave equation:

$$\Delta\vec{E}=\frac{\epsilon\mu}{c^2}\frac{\partial^2}{\partial t^2}\vec{D}$$

$$v_{\text{phase}}=\frac{c}{\sqrt{\varepsilon\mu}}=\frac{c}{n}$$

Refractive index $n=\sqrt{\varepsilon}$

Assume μ=1: Crystal Optics

$\vec{\nabla} \cdot \vec{D} = \rho = 0$ Gauss' Law (Coulomb)

$\vec{\nabla} \cdot \vec{B} = 0$ Gauss' Law (magnetic field)

$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$ Faraday's Law

$\vec{\nabla} \times \vec{H} = \vec{j} + \frac{\partial \vec{D}}{\partial t} = \frac{\partial \vec{D}}{\partial t}$ Ampere's Law

Anisotropic wave equation:

Take curl on both sides in Ampere's Law and Faraday's Law

$$\Delta \vec{E} - \vec{\nabla}(\vec{\nabla} \cdot \vec{E}) = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \epsilon \vec{E}$$

$$\Delta \vec{H} = -\varepsilon_0 \frac{\partial}{\partial t} \vec{\nabla} \times \varepsilon \vec{E}$$

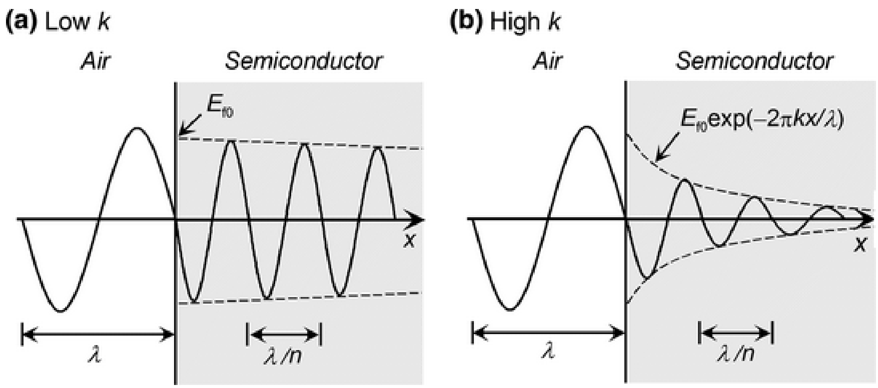
For μ=1 we get a single wave equation for **E**, from which **H** can be calculated as well.

Use Berreman / Yeh 4x4 matrix formalism for (**E**,**H**).

Agranovitch & Ginzburg, Crystal Optics

Generalized Plane Waves

Plane waves do not solve Maxwell's equations, if Im(ε)≠0.



The amplitude of the plane wave decays in the medium due to absorption.

Snell: $\frac{\sin\theta_1}{\sin\theta_2}=\frac{n_1}{n_2}$

Generalized plane wave:

$$\vec{E}(\vec{r},t)=\vec{E}_0\exp\left[i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right]$$

Allow complex wave vector: $\vec{k}=\vec{k}_1+i\vec{k}_2=k_1\vec{u}+ik_2\vec{v}$

$$\vec{E}(\vec{r},t)=\vec{E}_0\exp\left[-\vec{k}_2\cdot\vec{r}\right]\exp\left[i\left(\vec{k}_1\cdot\vec{r}-\omega t\right)\right]$$

Attenuation Propagation

Mansuripur, *Magneto-Optical Recording*, 1995

Maxwell's Equations in Continuous Media

$\vec{\nabla} \cdot \vec{D} = 0$ Gauss' Law (Coulomb)

$\vec{\nabla} \cdot \vec{B} = 0$ Gauss' Law (magnetic field)

$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$ Faraday's Law

$\vec{\nabla} \times \vec{H} = \frac{\partial \vec{D}}{\partial t}$ Ampere's Law

$$\vec{E}(\vec{r},t) = \vec{E}_0 \exp\left[i\left(\vec{k} \cdot \vec{r} - \omega t\right)\right]$$

etc. for other fields

Generalized plane waves with complex wave vectors

$\vec{k} \cdot \vec{D}_0 = 0$ Gauss' Law (Coulomb)

$\vec{k} \cdot \vec{B}_0 = 0$ Gauss' Law (magnetic field)

$\vec{k} \times \vec{E}_0 = \omega \vec{B}_0$ Faraday's Law

$\vec{k} \times \vec{H}_0 = -\omega \vec{D}_0$ Ampere's Law

Anisotropic Wave Equations in Continuous Media

$$\vec{k}\cdot\vec{D}_0=0$$ Gauss' Law (Coulomb)

$$\vec{k}\cdot\vec{B}_0=0$$ Gauss' Law (magnetic field)

$$\vec{k}\times\vec{E}_0=\omega\vec{B}_0$$ Faraday's Law

$$\vec{k}\times\vec{H}_0=-\omega\vec{D}_0$$ Ampere's Law

$$\vec{D}_0(\vec{k},\omega)=\varepsilon_0\varepsilon(\vec{k},\omega)\vec{E}_0(\vec{k},\omega)$$
$$\vec{B}_0(\vec{k},\omega)=\mu_0\mu(\vec{k},\omega)\vec{H}_0(\vec{k},\omega)$$

Constitutive Relations

Anisotropic wave equation:

$$\left|\vec{k}\right|^2\vec{E}_0-\left(\vec{k}\cdot\vec{E}_0\right)\vec{k}=-\mu_0\omega\vec{k}\times\mu\vec{H}_0$$
$$\left|\vec{k}\right|^2\vec{H}_0-\left(\vec{k}\cdot\vec{H}_0\right)\vec{k}=-\varepsilon_0\omega\vec{k}\times\varepsilon\vec{E}_0$$

D and **B** are transverse, but **E** and **H** are not.

Isotropic wave equation:

$$\left|\vec{k}\right|^2=\varepsilon\mu\frac{\omega^2}{c^2}$$

$$v_{\text{phase}}=\frac{c}{\sqrt{\varepsilon\mu}}=\frac{c}{n}$$

Refractive index n=√ε

Assume μ=1: Crystal Optics

$\vec{k}\cdot\vec{D}_0 = 0$ Gauss' Law (Coulomb)

$\vec{k}\cdot\vec{B}_0 = 0$ Gauss' Law (magnetic field)

$\vec{k}\times\vec{E}_0 = \omega\vec{B}_0$ Faraday's Law

$\vec{k}\times\vec{H}_0 = -\omega\vec{D}_0$ Ampere's Law

$$\vec{D}_0(\vec{k},\omega) = \varepsilon_0\varepsilon(\vec{k},\omega)\vec{E}_0(\vec{k},\omega)$$
$$\vec{B}_0(\vec{k},\omega) = \mu_0\mu(\vec{k},\omega)\vec{H}_0(\vec{k},\omega)$$

Constitutive Relations

Anisotropic wave equation:

$$|\vec{k}|^2\vec{E}_0 - (\vec{k}\cdot\vec{E}_0)\vec{k} = \frac{\omega^2}{c^2}\varepsilon\vec{E}_0$$
$$|\vec{k}|^2\vec{H}_0 = -\varepsilon_0\omega\vec{k}\times\varepsilon\vec{E}_0$$

Algebraic equation for **E**, from which **H** can be calculated.

Isotropic wave equation:

$$|\vec{k}|^2 = \varepsilon\frac{\omega^2}{c^2}$$

$$v_{\text{phase}} = \frac{c}{\sqrt{\varepsilon}} = \frac{c}{n}$$

Refractive index $n=\sqrt{\varepsilon}$

Agranovitch & Ginzburg, Crystal Optics

Longitudinal Solutions to Maxwell's Equations

$\vec{k} \cdot \varepsilon\vec{E}_0 = 0$ Gauss' Law (Coulomb)

$\vec{k} \cdot \vec{B}_0 = 0$ Gauss' Law (magnetic field)

$\vec{k} \times \vec{E}_0 = \omega\vec{B}_0$ Faraday's Law

$\vec{k} \times \vec{H}_0 = -\omega\varepsilon\vec{E}_0$ Ampere's Law

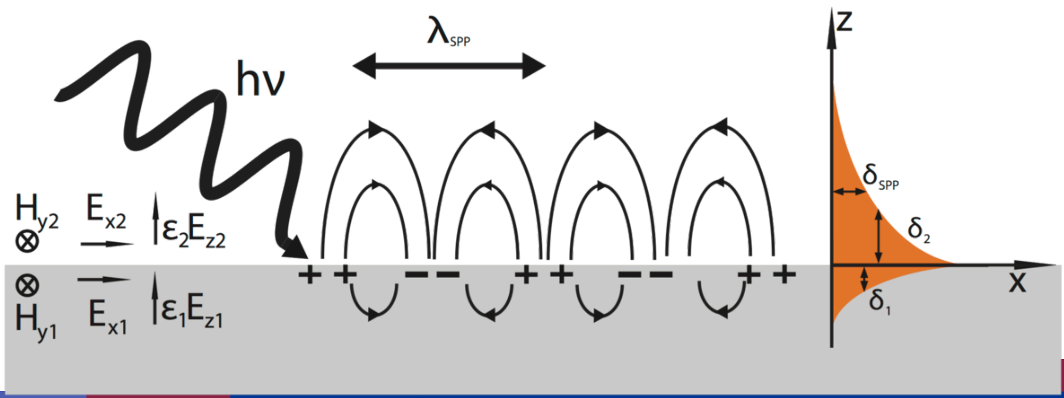
Transverse solution: D is transverse

□ 0 and $|\vec{k}|^2\vec{E}_0 - (\vec{k}\cdot\vec{E}_0)\vec{k} = \frac{\omega^2}{c^2}\varepsilon\vec{E}_0$ and $|\vec{k}|^2\vec{H}_0 = -\varepsilon_0\omega\vec{k} \times \varepsilon\vec{E}_0$

Longitudinal solution:

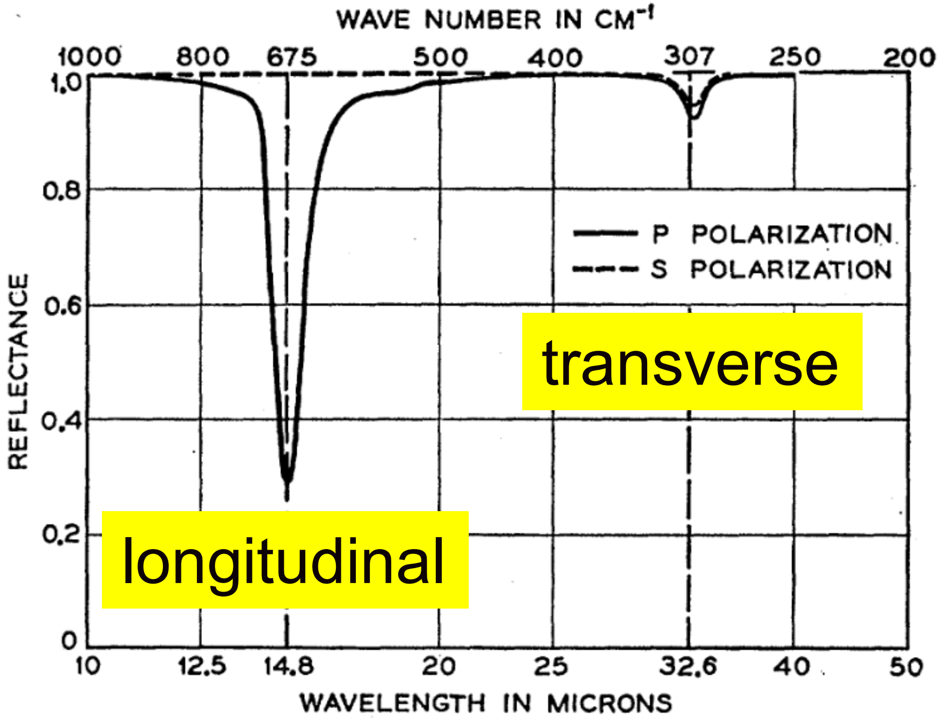
$\varepsilon=0$ and $\vec{E}_0 \parallel \vec{k}$ and $\vec{H}_0 = 0$

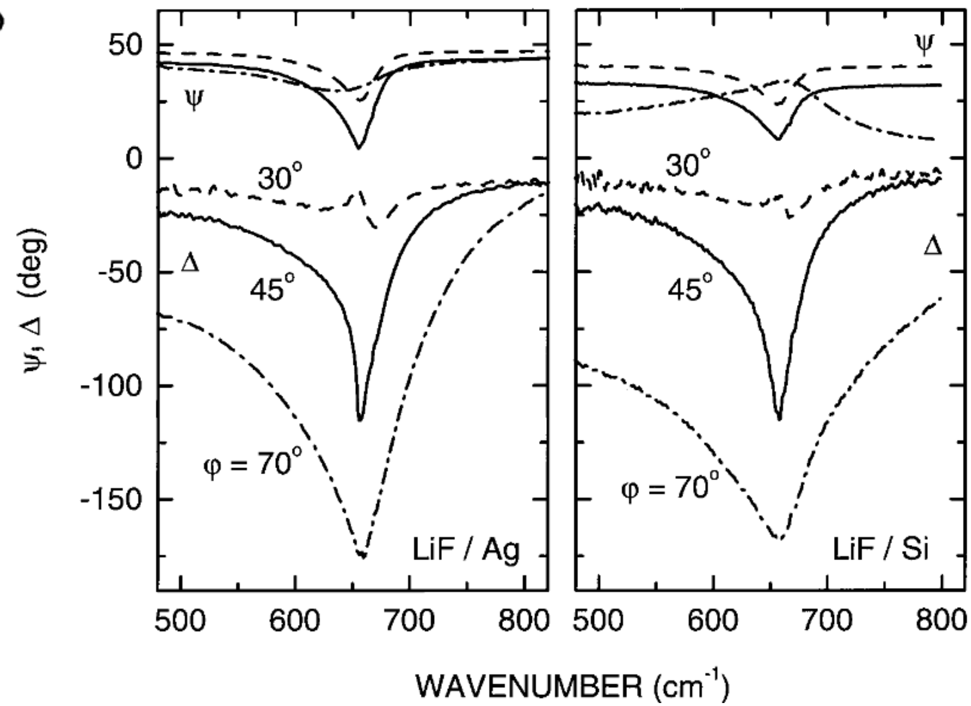
Longitudinal solutions are also called plasmons.



Agranovitch & Ginzburg, Crystal Optics

Berreman Modes: Insulator (LiF) on Metal (Ag)





350 nm LiF on Ag

LiF on Ag

LiF on Si

Humlicek: The Berreman mode is an interference effect, which occurs when $\varepsilon_{film}=0$. It is not a longitudinal mode.

D.W. Berreman, Phys. Rev. **130**, 2193 (1963)

J. Humlicek, phys. stat. sol. (b) **215**, 155 (1999)

Energy density, Poynting Vector

Energy density:

$$u = \frac{1}{2}\left(\vec{E}\cdot\vec{D} + \vec{H}\cdot\vec{B}\right) = \frac{1}{2}\left(\vec{E}\cdot\varepsilon_0\epsilon\vec{E} + \vec{H}\cdot\mu_0\mu\vec{H}\right)$$

$$\frac{\partial^2 u}{\partial E_i \partial E_j} = \frac{\varepsilon_0}{2}\varepsilon_{ij}$$

Implies ε_{ij} symmetric tensor (B=0).

Onsager relation

in isotropic medium: $u = \frac{\epsilon\epsilon_0}{2}\left|\vec{E}\right|^2$

Poynting's theorem (energy flow):

$$\frac{\partial u}{\partial t} = -\vec{\nabla}\cdot\vec{S} - \vec{j}\cdot\vec{E}$$

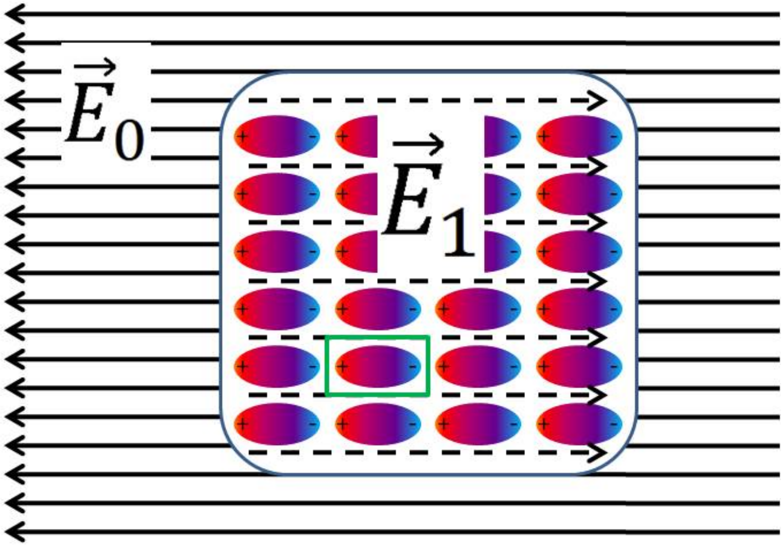
EM wave has no Ohmic power **j·E**

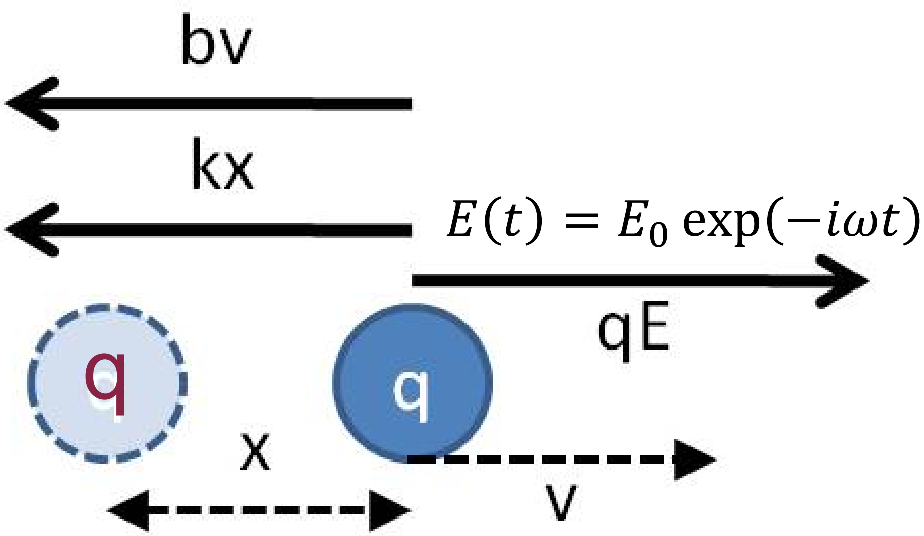
$$\frac{\partial u}{\partial t} = -\vec{\nabla}\cdot\vec{S} = -\vec{\nabla}\cdot\frac{1}{\mu_0}\left(\vec{E}\times\vec{B}\right) = \frac{1}{\mu_0}\left(\vec{B}\cdot\vec{\nabla}\times\vec{E} - \vec{E}\cdot\vec{\nabla}\times\vec{B}\right)$$

Longitudinal modes carry no energy.

Agranovitch & Ginzburg, Crystal Optics

Lorentz Model for Oscillating Charges



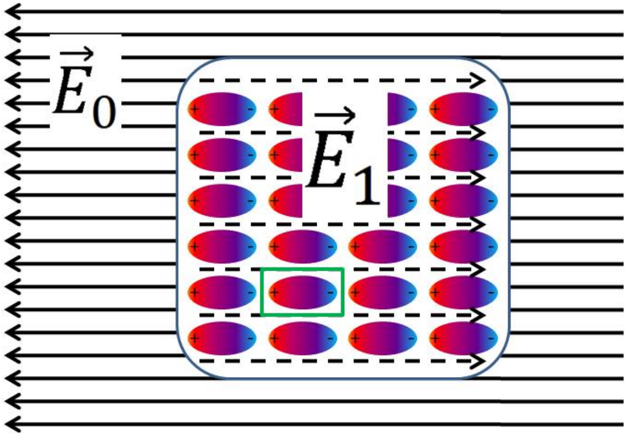


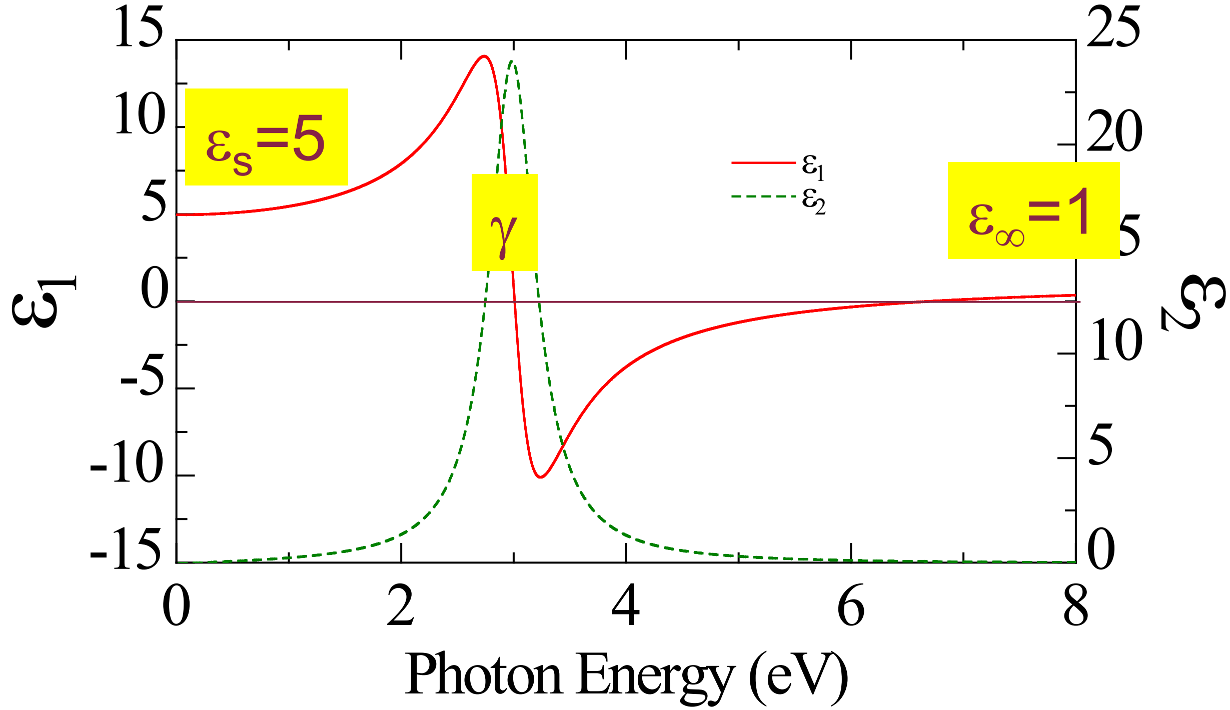
$$F = ma$$
$$qE - b\dot{x} - kx = m\ddot{x}$$
$$\text{Try } x(t) = x_0 \exp(-i\omega t)$$
$$x(t) = \frac{-qE_0}{m\omega^2 + ib\omega - k} \exp(-i\omega t)$$
$$P_0 = \chi_e E_0 = \frac{qx(t)}{V} E_0$$
$$\varepsilon = 1 + \chi_e$$

$$\varepsilon(\omega) = 1 + \frac{\omega_P^2}{\omega_0^2 - \omega^2 - i\gamma\omega}$$
$$\omega_P^2 = \frac{nq^2}{m\varepsilon_0}$$
Charge density
$$\omega_0^2 = \frac{k}{m}$$
Resonance frequency

H. Helmholtz, Ann. Phys **230**, 582 (1875)

Lorentz Model (Dielectric Function)





Peak of ε_2 at ω_0

Broadening γ

Amplitude $\omega_P{}^2=A\omega_0{}^2$

Dimensionless $A=\varepsilon_s-\varepsilon_\infty$

ε_2 is never negative

ε_1 has a wiggle at ω_0

Longitudinal solution for

$$\omega_L=\sqrt{\omega_0^2+\omega_P^2-i\gamma}\approx 6.7\text{ eV}$$

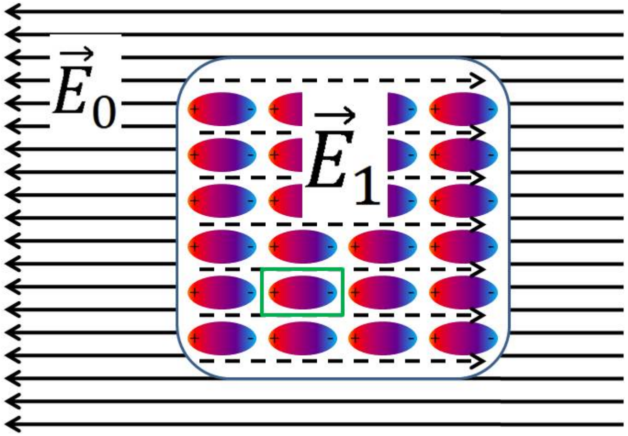
ε_1 negative from ω_0 to ω_L

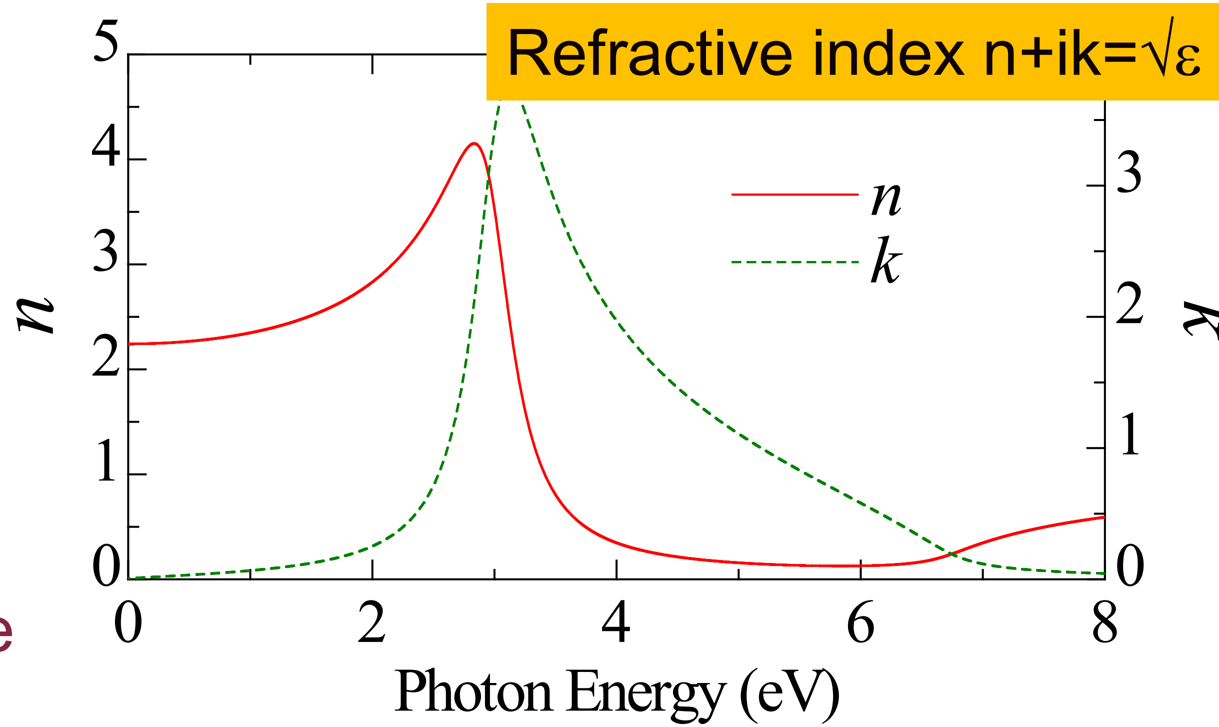
$$\varepsilon(\omega)=1+\frac{\omega_P^2}{\omega_0^2-\omega^2-i\gamma\omega}$$

ω_0=3 eV, γ=0.5 eV, ω_p=6 eV

H. Helmholtz, Ann. Phys **230**, 582 (1875)

Lorentz Model (Complex Refractive Index)



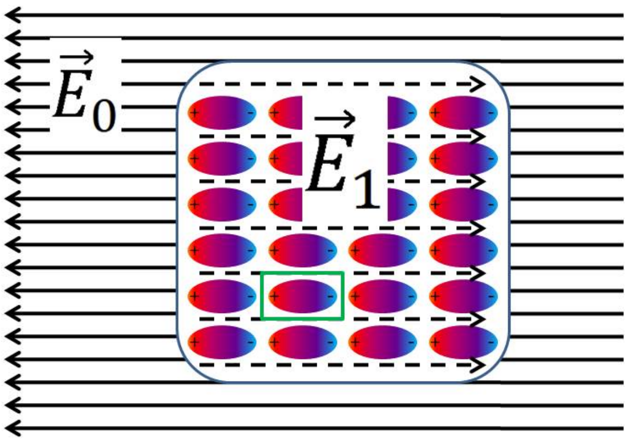


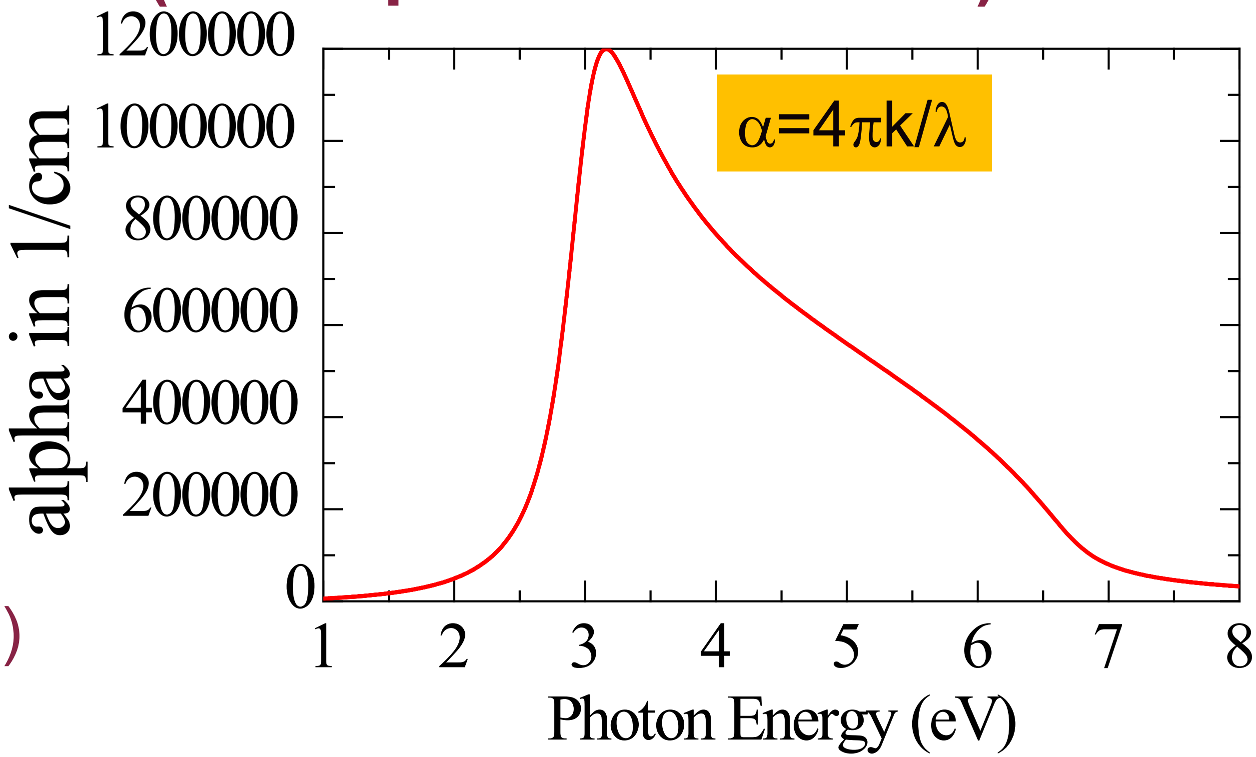
Peak of k shifted (>ω_0)
k is asymmetric
n and k always positive
n→1 at large energies
n<1 above ω_0, below ω_L
(Reststrahlen band,
high reflectance)
Normal dispersion: dn/dE>0
Anomalous dispersion

$$\varepsilon(\omega) = 1 + \frac{\omega_P^2}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

ω_0=3 eV, γ=0.5 eV, ω_p=6 eV

Lorentz Model (Absorption Coefficient)



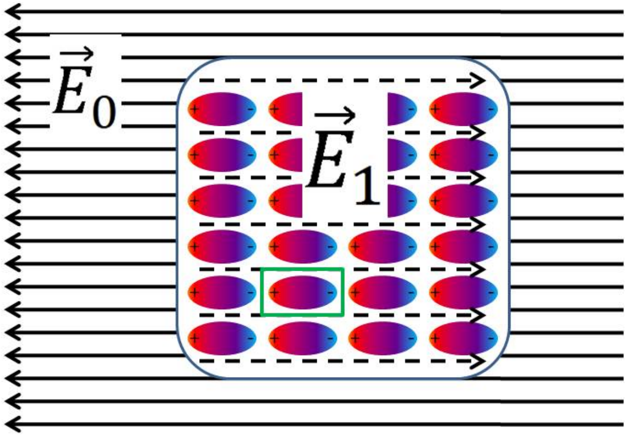


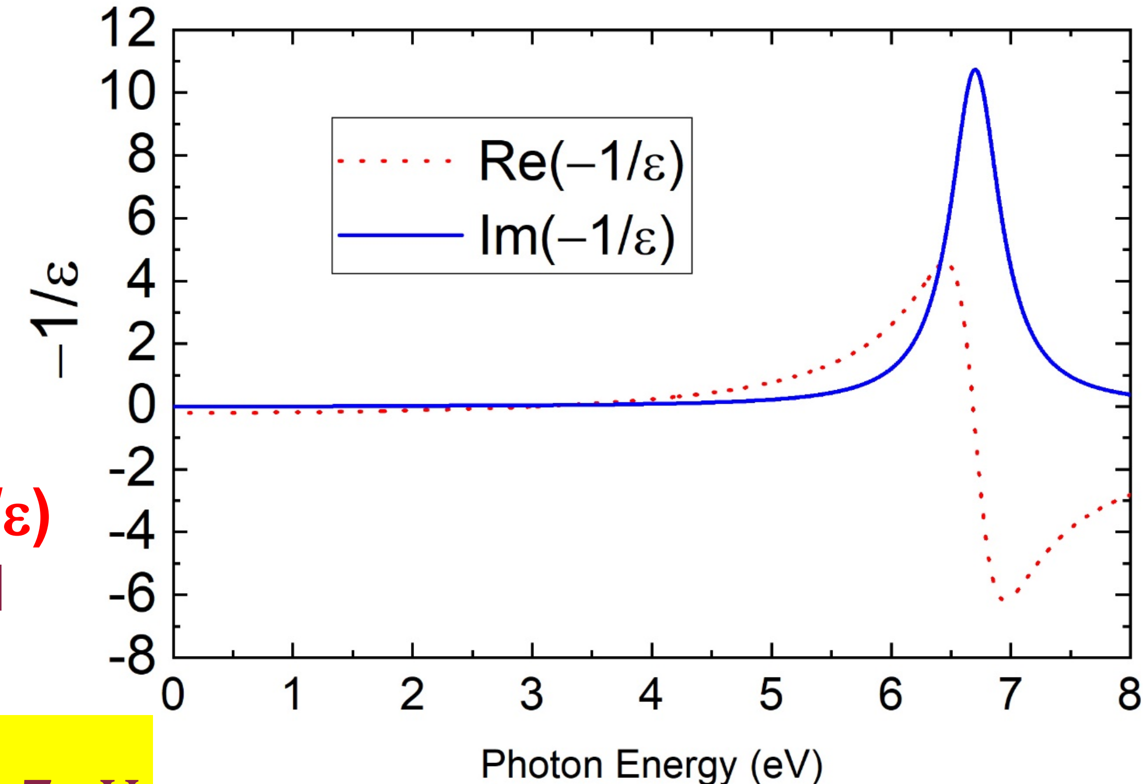
Peak of α shifted (>ω_0)
α is asymmetric
α Is always positive
Fast rise, slow drop

$$\varepsilon(\omega) = 1 + \frac{\omega_P^2}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

ω_0=3 eV, γ=0.5 eV, ω_p=6 eV

Lorentz Model (Loss function)





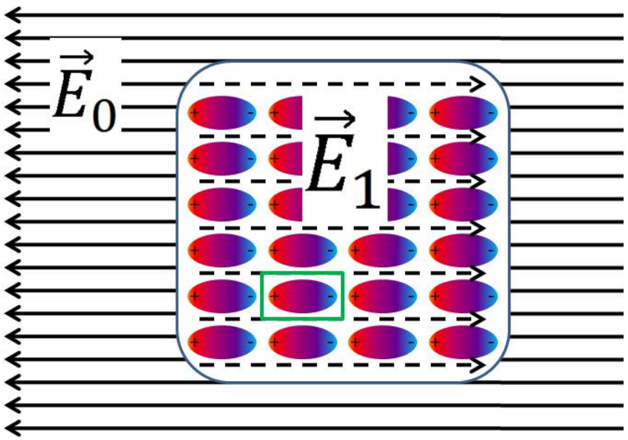
The loss function **Im(–1/ε)** peaks at the longitudinal frequency

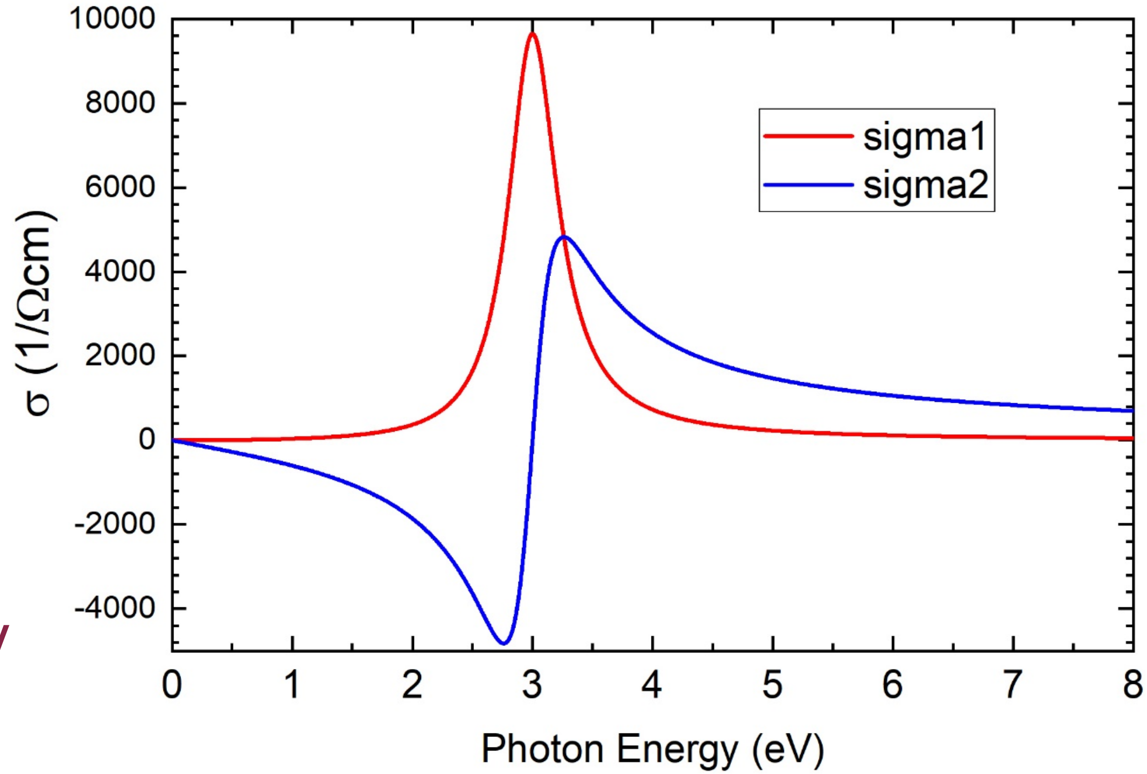
$$\omega_L = \sqrt{\omega_0^2 + \omega_P^2 - i\gamma} \approx 6.7 \text{ eV}$$

$$\varepsilon(\omega) = 1 + \frac{\omega_P^2}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

ω_0=3 eV, γ=0.5 eV, ω_p=6 eV

Lorentz Model (Optical Conductivity)





$$\sigma(\omega) = -i\omega(\varepsilon - 1)$$

The optical conductivity has a peak at the resonance frequency.

$$\varepsilon(\omega) = 1 + \frac{\omega_P^2}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

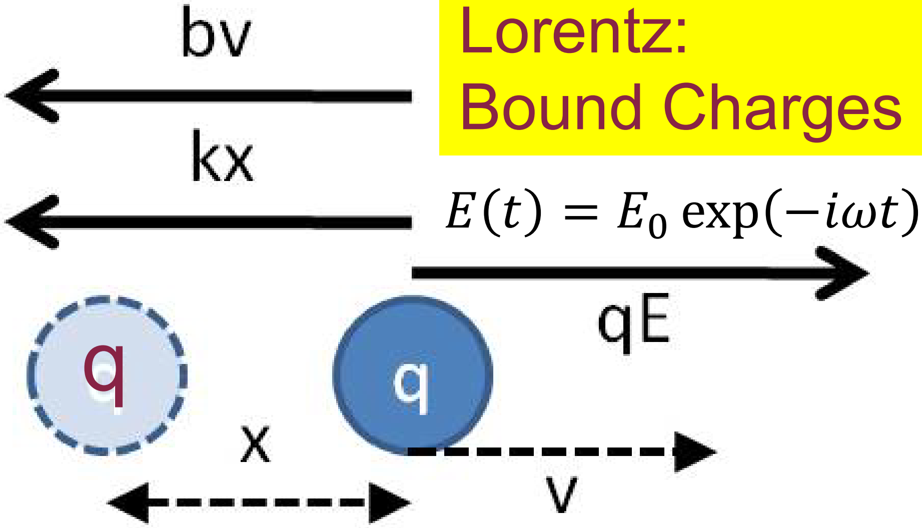
ω_0=3 eV, γ=0.5 eV, ω_p=6 eV

Re(σ), Im(ε): Dissipation
Im(σ), Re(ε): Dispersion
j=σE
Absorption is a resonant current.

NM STATE

Drude Model for Free Carriers

Lorentz: Bound Charges

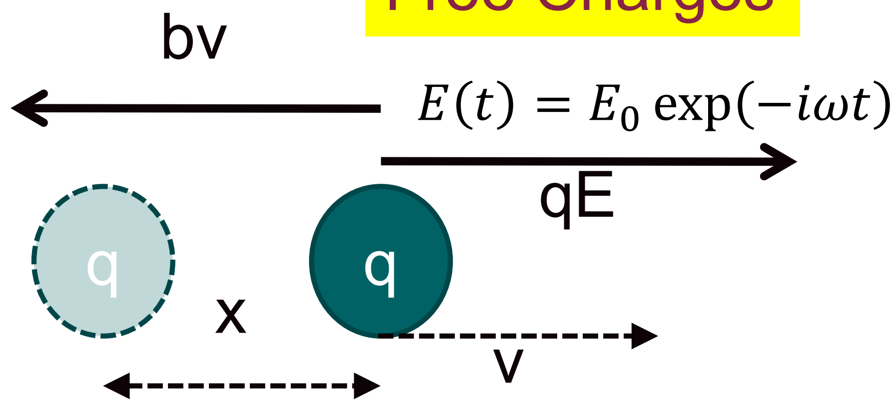


$$\varepsilon(\omega) = 1 + \frac{\omega_P^2}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

$$\omega_P^2 = \frac{nq^2}{m\varepsilon_0}$$ Charge density

$$\omega_0^2 = \frac{k}{m}$$ Resonance frequency

Drude: Free Charges



$$\varepsilon(\omega) = 1 - \frac{\omega_P^2}{\omega^2 + i\gamma\omega}$$

$$\omega_P^2 = \frac{nq^2}{m\varepsilon_0}$$ Charge density

$$\omega_0^2 = 0$$ Resonance frequency

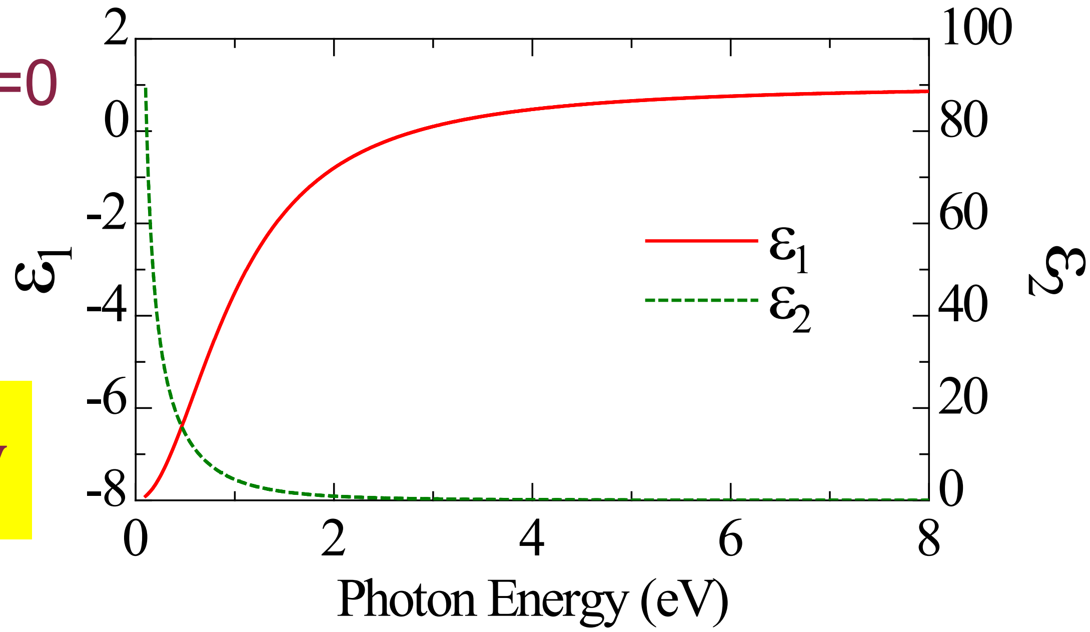
H. Helmholtz, Ann. Phys **230**, 582 (1875).

P. Drude, Phys. Z. **1**, 161 (1900).

Drude Model for Free Carriers (Dielectric Function)

Both ε_1 and ε_2 **diverge** at $\omega=0$
Broadening γ
$\varepsilon_1 \rightarrow 1$ at large energies
$\varepsilon_2 \rightarrow 0$ at large energies

$$\omega_L = \sqrt{\omega_P^2 - i\gamma} \approx \omega_P = 3\ \text{eV}$$



ε_1 negative from ω_0 to ω_L
Real/imaginary part has factor γ/ω

$$\varepsilon(\omega) = 1 - \frac{\omega_P^2}{\omega^2 + i\gamma\omega} = 1 - \frac{\omega_P^2}{\omega^2 + \gamma^2} + i\frac{\omega_P^2}{\omega^2 + \gamma^2} \times \frac{\gamma}{\omega}$$

ω_p=3 eV, γ=1 eV, $\tau=1/\gamma$=0.6 fs

$$n = \frac{\omega_P^2 \epsilon_0 m_0}{\hbar^2 e^2} = 6.5 \times 10^{21}\text{cm}^{-3}$$

Bad metal

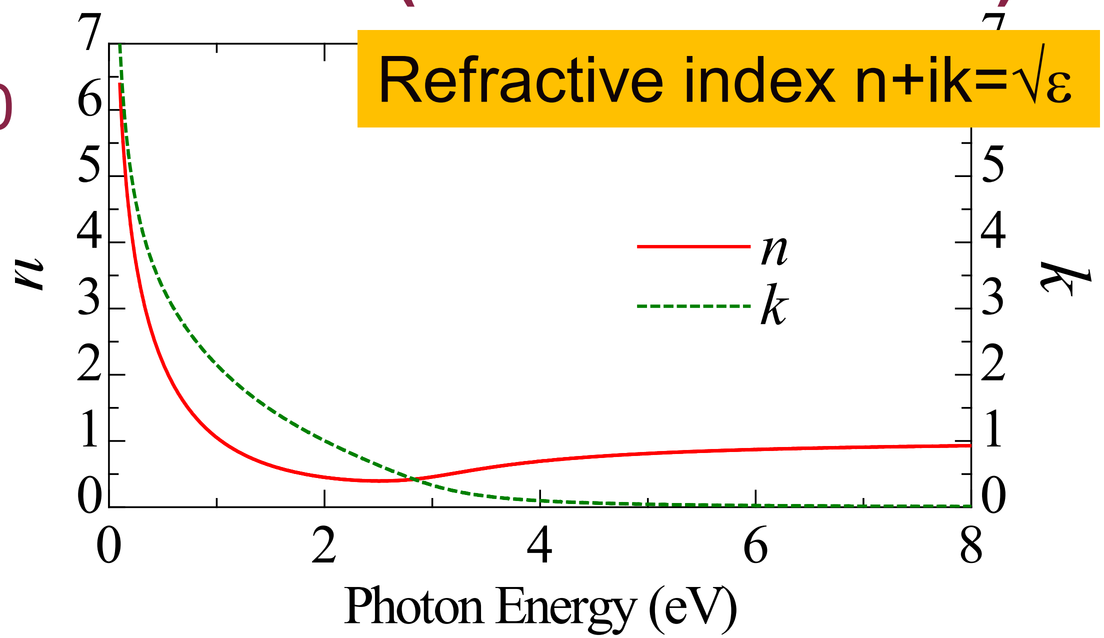
Dresselhaus, *Solid-State Properties*

Drude Model for Free Carriers (Refractive Index)

Both n and k diverge at $\omega=0$
Broadening γ
n drops off faster than k
n,k always positive

$n \rightarrow 1$ at large energies
$n<1$ at large energies
(important for XRR)
$v_{phase}>c$ if $n<1$
n drops up to ω_P, then rises.

$k \rightarrow 0$ at large energies



$$\varepsilon(\omega) = 1 - \frac{\omega_P^2}{\omega^2 + i\gamma\omega}$$

$\omega_p=3$ eV, $\gamma=1$ eV

Drude Model (Absorption Coefficient)

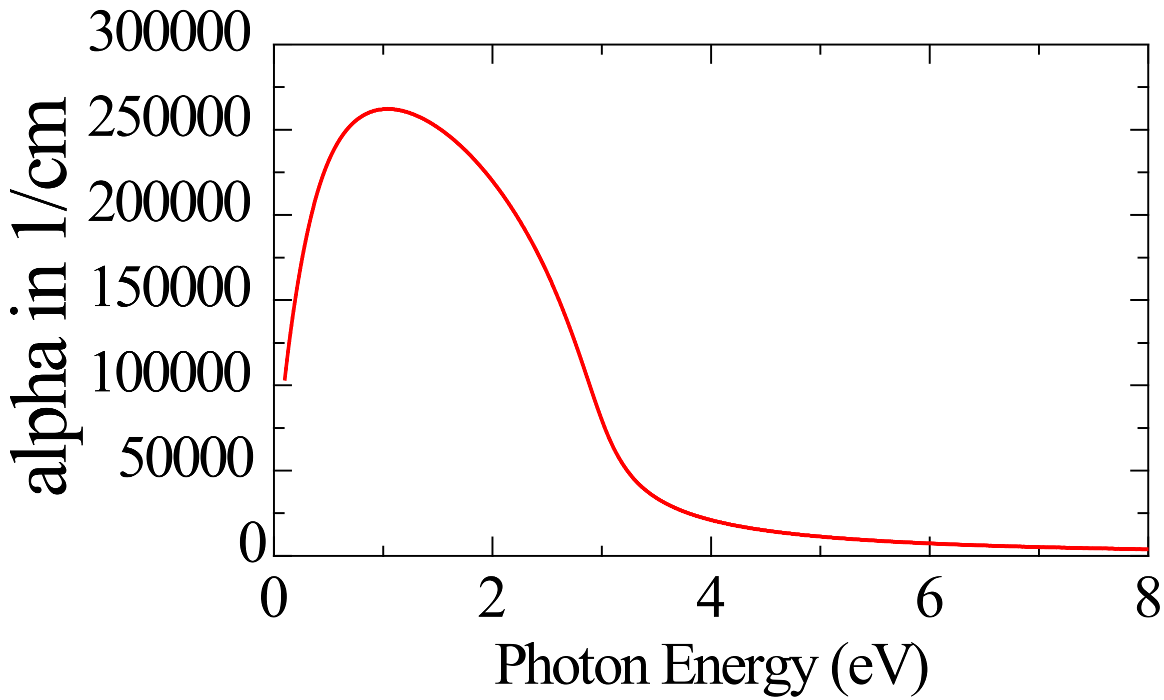
$\alpha \to 0$ as $E \to 0$.

Peak around $\omega_p/2$

Small α above ω_P.
$\alpha \to 0$ as $E \to \infty$

Metals become nearly transparent above the plasma frequency.

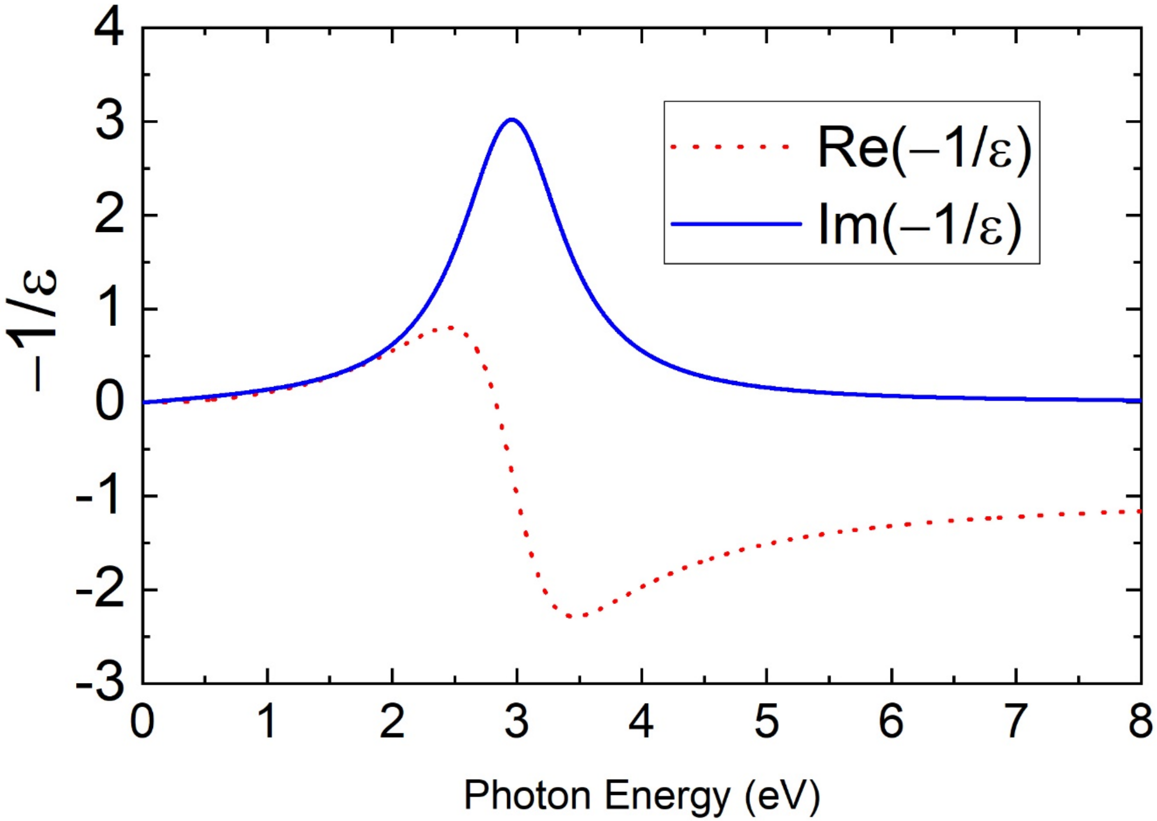
Reflectance minimum at ω_P.



$$\varepsilon(\omega) = 1 - \frac{\omega_P^2}{\omega^2 + i\gamma\omega}$$

ω_p=3 eV, γ=1 eV

Drude Model for Free Carriers (Loss Function)



ε peak:
Dissipation (TO)

Im(–1/ε) peak:
Plasmon solution (LO)

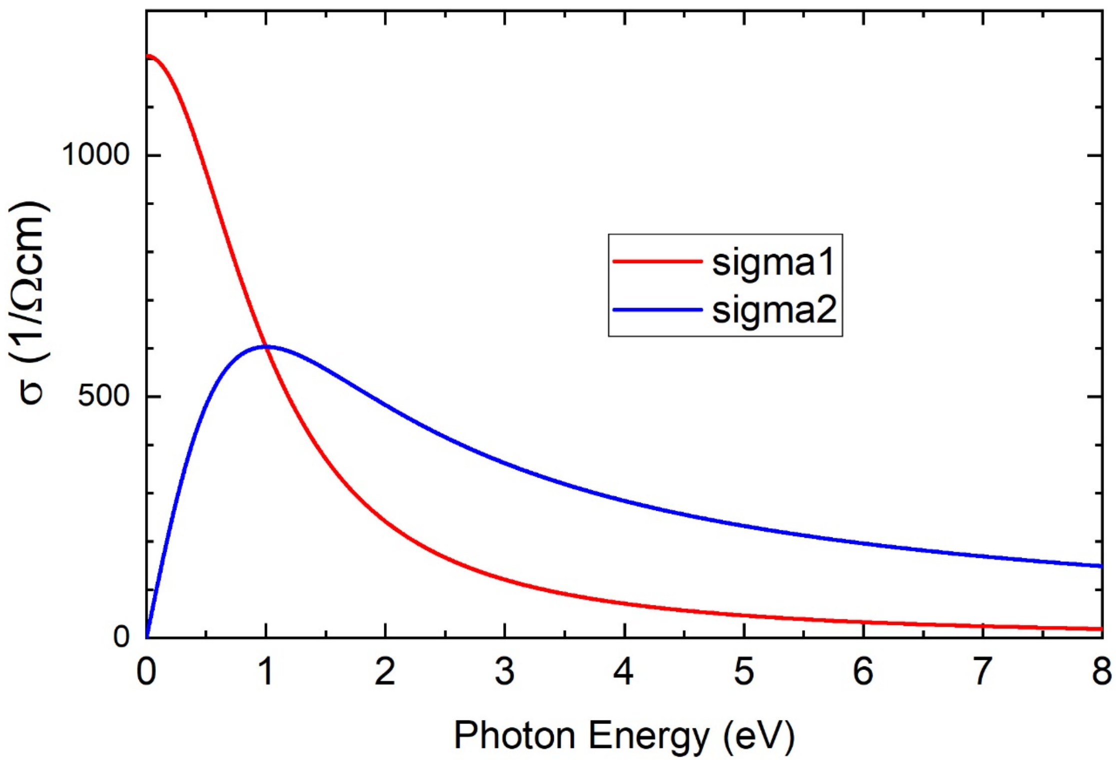
ω_p=3 eV, γ=1 eV

$$\varepsilon(\omega) = 1 - \frac{\omega_P^2}{\omega^2 + i\gamma\omega}$$

The loss function **Im(–1/ε)** peaks at the longitudinal frequency

$$\omega_L = \sqrt{\omega_P^2 - i\gamma} \approx \omega_P = 3 \text{ eV}$$

Drude Model (Optical Conductivity)



$$\sigma(\omega) = -i\omega(\varepsilon - 1)$$

Multiplying by ω cancels the divergence at E=0.

$\sigma_2 \to 0$ as $E \to 0$

σ_2 peaks at $\omega=\gamma$

Finite $\sigma_{DC}=\sigma_1(\omega=0)$

$\sigma_{DC}=ne\mu=e\tau/m_0m^*$

$\tau=1/\gamma$ scattering time

$\omega_p=3$ eV, $\gamma=1$ eV,
$\mu_0=1.1$ cm^2/Vs

Re(σ), Im(ε): Dissipation
Im(σ), Re(ε): Dispersion
j=σE

$\sigma_{DC}=1000$ 1/Ωcm

$$\varepsilon(\omega) = 1 - \frac{\omega_P^2}{\omega^2 + i\gamma\omega}$$

Bad metal

Dresselhaus, *Solid-State Properties*

Summary

- Electrodynamics of **continuous media**
- Dielectric displacement, dielectric polarization vector
- **Maxwell's equations** for continuous media
- **Wave equations** for continuous media
- Anisotropy concerns (distorted perovskites)
- **Lorentz** and **Drude** model