Introduction to infrared spectroscopy of solids

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Where to get more info?

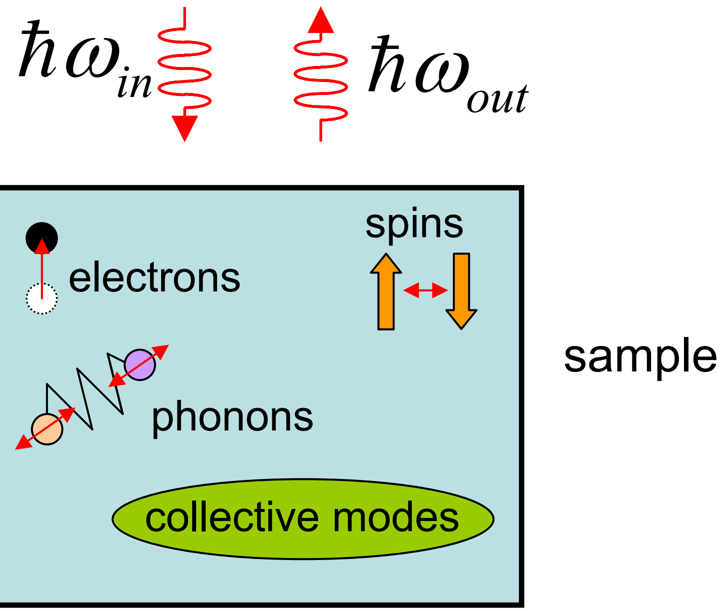
1) **F. Wooten**, « Optical Properties of Solids »,
(Academic Press, New York, 1972).

2) **M. Dressel** and **G. Grüner**, « Electrodynamics of Solids: Optical properties of Electrons in Matter »,
(Cambridge University Press, 2002).

3) **E. van Heumen** and **D. van der Marel**, « Optical probes of electron correlations in solids »,
(Lecture notes for XI Training Course of Strongly Correlated Systems, Salerno, Italy, 2006,
available at http://optics.unige.ch/vdm/marel_files/salerno_lectures.pdf).

4) **N.P. Armitage**, « Electrodynamics of correlated electron systems »
(Lecture notes for Summer School on Condensed Matter Physics, Boulder, USA, 2008,
available at http://research.yale.edu/boulder/Boulder-2008/Lectures/Armitage/NPABoulder08.pdf)

« Photons only » spectroscopies



$$\omega_{in} = \omega_{out}$$

Optical/infrared spectroscopy
X ray absorption
NMR, NQR, ESR
…

$$\omega_{in} \neq \omega_{out}$$

Raman spectroscopy
2nd (3rd etc.) harmonics generation
Inelastic X-ray scattering
Brillouin scattering
Luminescence
…

Infrared/optical spectroscopy

Photon portrait:

energy	$\hbar\omega$	0.1 meV – 10 eV
wavelength	λ	1 cm – 100 nm
momentum	$\lvert k \rvert$	10^{-7} – 10^{-3} of typical Brillouin zones in solids

Selection rules:

1. The total momentum of excitations created by a photon, is zero

$$\sum_i \vec{q}_{exc,i} = 0$$

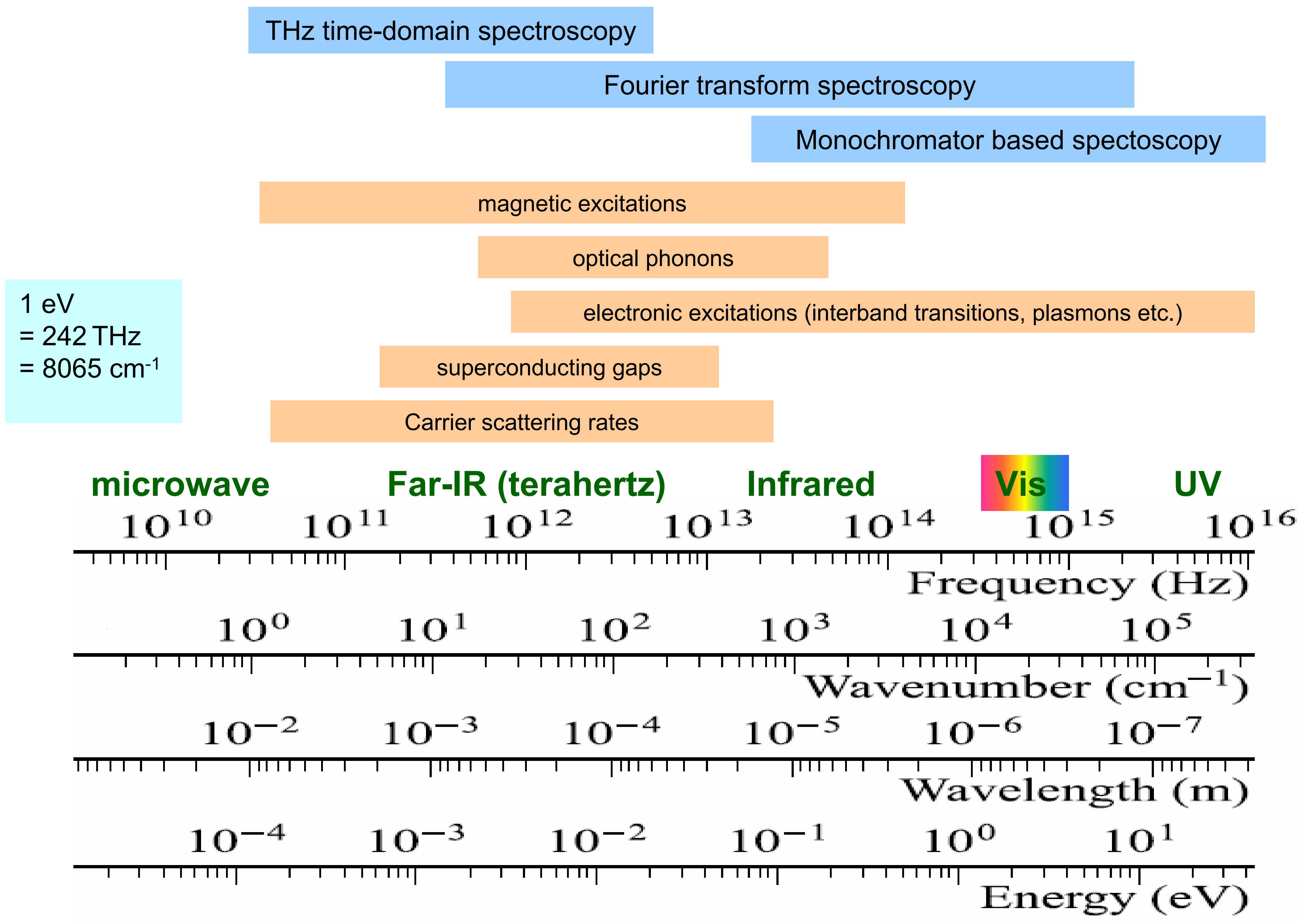
2. The total energy of excitations created by a photon is the photon energy

$$\sum_i E_{exc,i} = \hbar\omega_{photon}$$

3. In order to « couple » to photons (or to be infrared active) an excitation should posess either own electric or magnetic dipole moment, or current

$$\langle \text{initial state} | \text{Current Operator} | \text{final state} \rangle \neq 0$$

Energy scales



Optical conductivity

Ohm's law (linear response approximation): $J = \sigma E$

Generalization for non-uniform and time-dependent fields and currents:

$$J(\vec{r},t) = \int_{-\infty}^{0} dt \int d\vec{r}' \sigma(\vec{r},\vec{r}',t,t') E(\vec{r}',t')$$

Fourier transform: $J(\vec{r},t) = J_{\vec{k},\omega} e^{i(\vec{k}\vec{r}-\omega t)}, E(\vec{r},t) = E_{\vec{k},\omega} e^{i(\vec{k}\vec{r}-\omega t)}$

$$J_{\vec{k},\omega} = \sigma(\vec{k},\omega) E_{\vec{k},\omega}$$

Optical (or dynamical) conductivity

$$\sigma(\omega) \equiv \sigma(\vec{k} \to 0, \omega)$$
$$= \sigma_1(\omega) + i\sigma_2(\omega)$$

⇐ Infrared spectroscopy

Note: $\sigma_1(\omega \to 0) = \sigma_{DC}$

Optical conductivity and dielectric function

$$D = \varepsilon E \qquad J = \sigma E$$

$$\varepsilon(\omega) = 1 + \frac{4\pi i}{\omega}\sigma(\omega)$$

or

$$\varepsilon_2(\omega) = \frac{4\pi\sigma_1(\omega)}{\omega}$$

(in the CGS system)

$$\varepsilon_1(\omega) = 1 - \frac{4\pi\sigma_2(\omega)}{\omega}$$

Sometimes the total current is split in two parts: $J = J_{\text{free}} + J_{\text{bound}}$

and another definition is given: $J_{\text{free}} = \sigma E$

then $$\varepsilon(\omega) = \varepsilon_\infty + \frac{4\pi i}{\omega}\sigma(\omega)$$

ε - dimensionless (in all system units!)

σ - s^{-1} (CGS) or most often $\Omega^{-1}cm^{-1}$ (practical units)

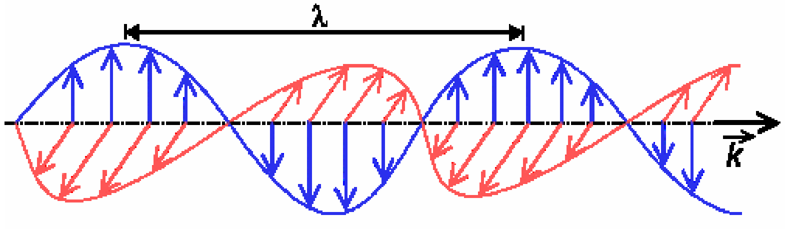
Propagation of light

Plane wave

$$\vec{E}(\vec{r},t) = \vec{E}e^{i(\vec{k}\vec{r}-\omega t)}$$

$$\vec{H}(\vec{r},t) = \vec{H}e^{i(\vec{k}\vec{r}-\omega t)}$$

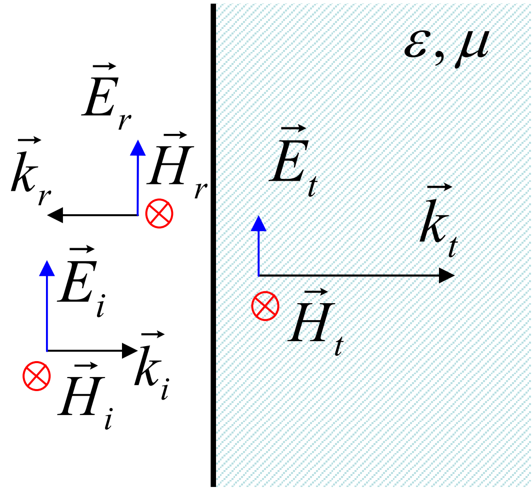
$$k = \frac{\omega}{c}\sqrt{\varepsilon\mu} \qquad \vec{H} = \vec{k}\times\vec{E}\sqrt{\frac{\varepsilon}{\mu}}$$



Boundary condtions at the interface
(normal incidence)

$$\vec{E}_i + \vec{E}_r = \vec{E}_t \qquad \Rightarrow \qquad E_i + E_r = E_t$$

$$\vec{H}_i + \vec{H}_r = \vec{H}_t \qquad \qquad E_i - E_r = \sqrt{\frac{\varepsilon}{\mu}}E_t$$



Reflection coefficient

$$r \equiv \frac{E_r}{E_i} = \frac{1-\sqrt{\varepsilon/\mu}}{1+\sqrt{\varepsilon/\mu}}$$

Transmission coefficient

$$t \equiv \frac{E_t}{E_i} = \frac{2}{1+\sqrt{\varepsilon/\mu}}$$

Fresnel equations

If $\mu = 1$

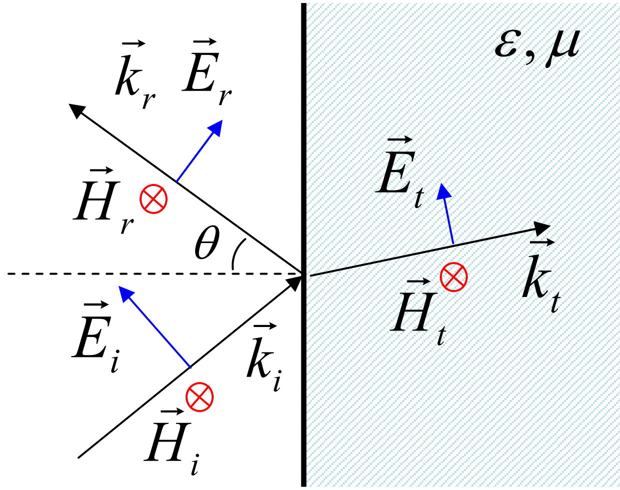
$$r = \frac{1-\sqrt{\varepsilon}}{1+\sqrt{\varepsilon}} \qquad t = \frac{2}{1+\sqrt{\varepsilon}}$$

Interface (grazing incidence)

p-polarization

$$r_p = \frac{E_r}{E_i} = \frac{\varepsilon\cos\theta - \sqrt{\mu\varepsilon - \sin^2\theta}}{\varepsilon\cos\theta + \sqrt{\mu\varepsilon - \sin^2\theta}}$$

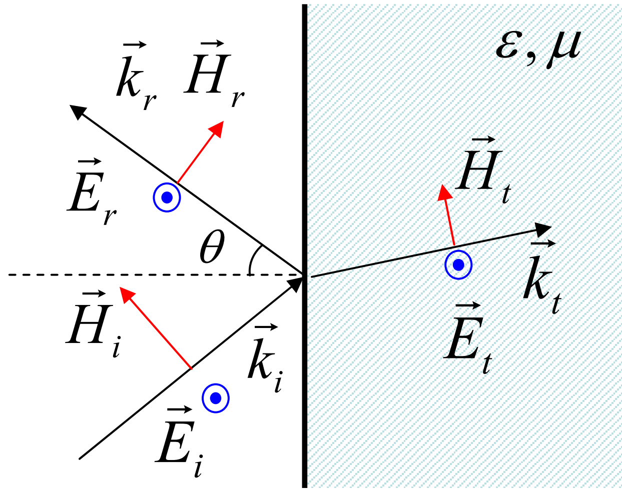
If $\mu = 1$ $\quad r_p = \frac{\varepsilon\cos\theta - \sqrt{\varepsilon - \sin^2\theta}}{\varepsilon\cos\theta + \sqrt{\varepsilon - \sin^2\theta}}$



s-polarization

$$r_s = \frac{E_r}{E_i} = \frac{\mu\cos\theta - \sqrt{\mu\varepsilon - \sin^2\theta}}{\mu\cos\theta + \sqrt{\mu\varepsilon - \sin^2\theta}}$$

If $\mu = 1$ $\quad r_s = \frac{\cos\theta - \sqrt{\varepsilon - \sin^2\theta}}{\cos\theta + \sqrt{\varepsilon - \sin^2\theta}}$



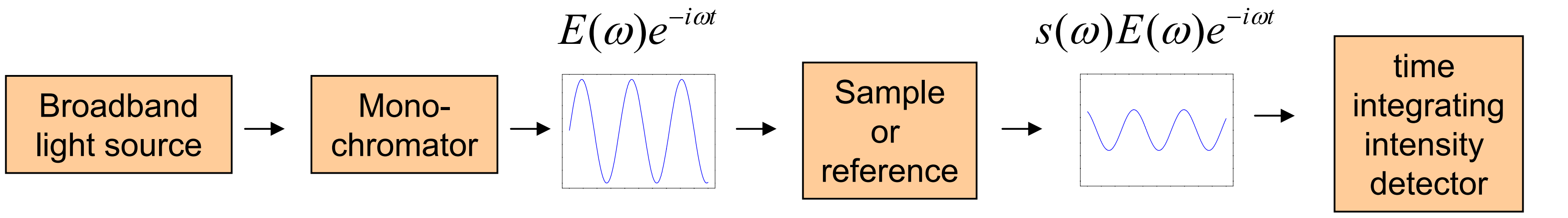
Spectroscopic approaches

- Frequency domain spectroscopy

- Fourier transform spectroscopy

- Time domain spectroscopy

Frequency domain spectroscopy



$$I(\omega) \propto |s(\omega)|^2 |E(\omega)|^2$$

referencing

$$|s(\omega)|^2$$

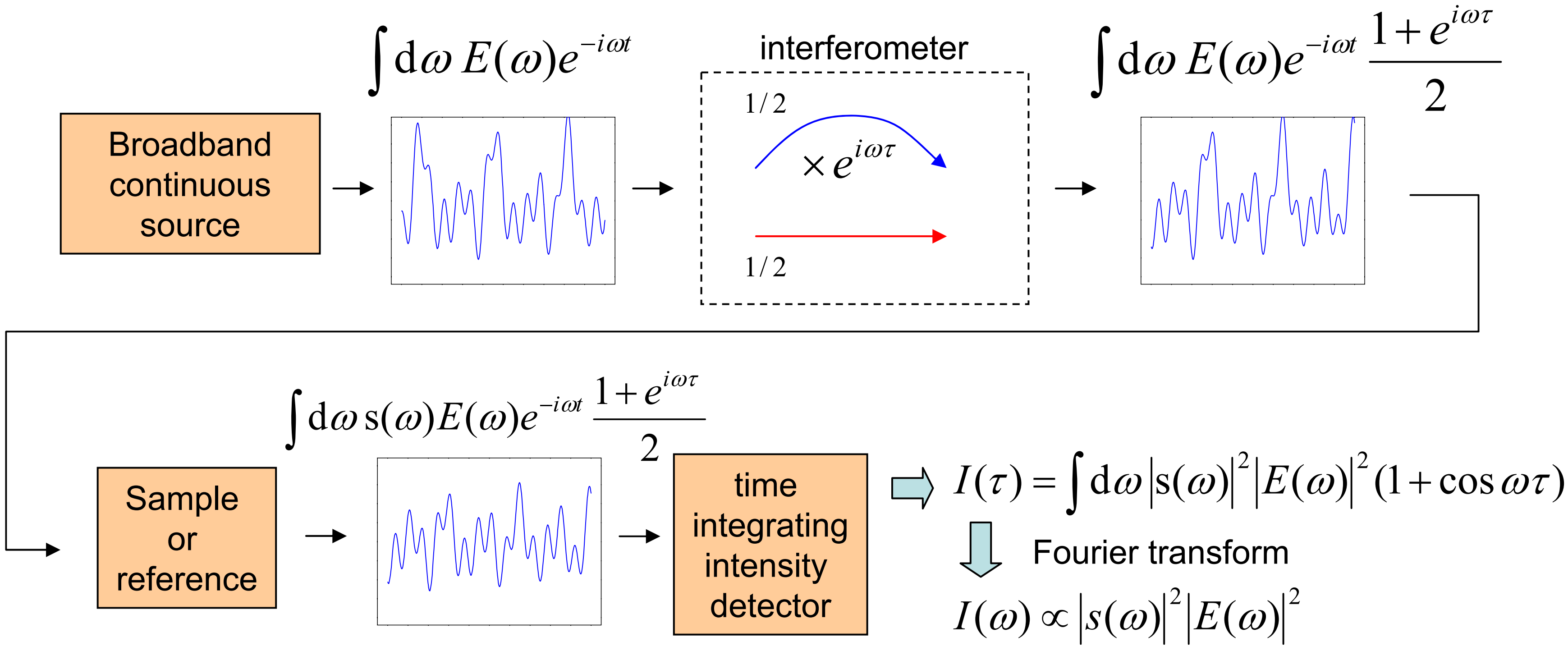
$s(\omega)$ - complex transmission/reflection coefficient of the sample (= 1 for the reference)

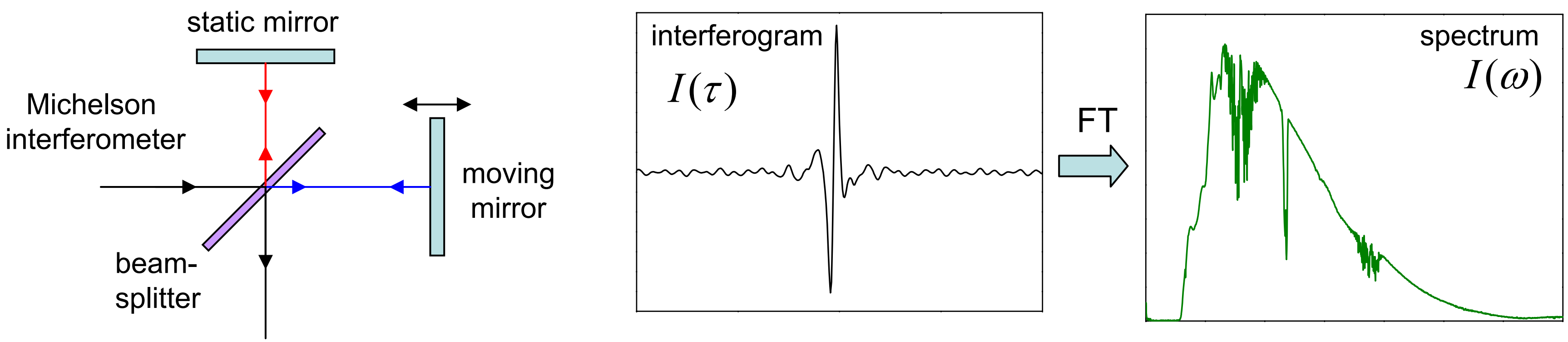
Other configurations:

-a monochromatic (tunable) source

-a broadband source and a CCD detector (without a monochromator)

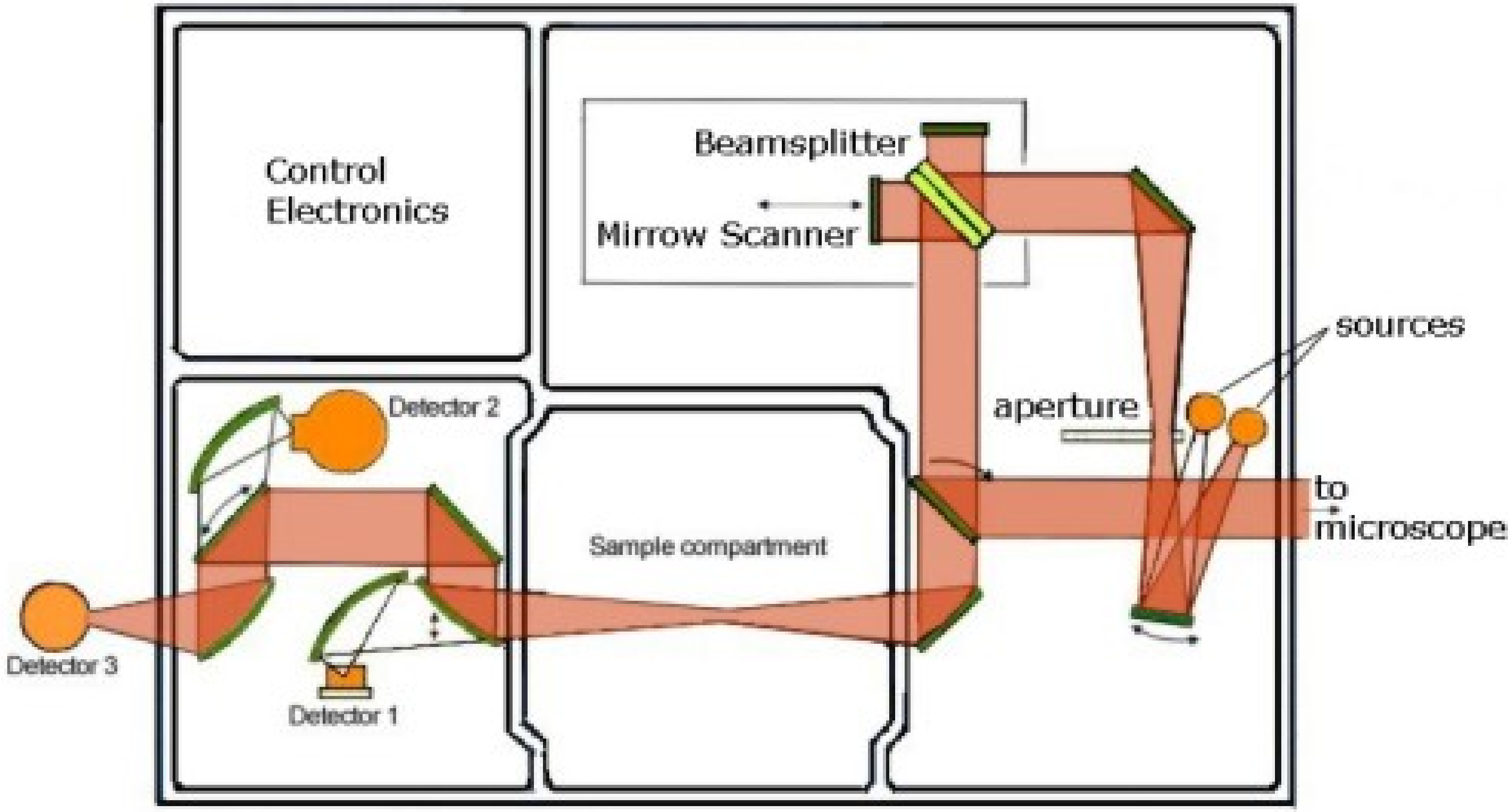
Fourier transform spectroscopy





Fourier transform spectroscopy

An example of FTIR spectrometer: Bruker 66 v



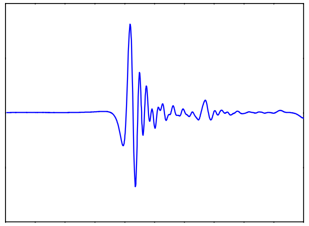
Time domain spectroscopy

$$\int \mathrm{d}\omega\, E(\omega) e^{-i\omega t}$$

$$E(t) = \int \mathrm{d}\omega\, s(\omega) E(\omega) e^{-i\omega t}$$

Short pulse generator (Femtosecond laser + semiconducting switch) →

→ Sample or reference →



→ time resolved electric field detector

⇩

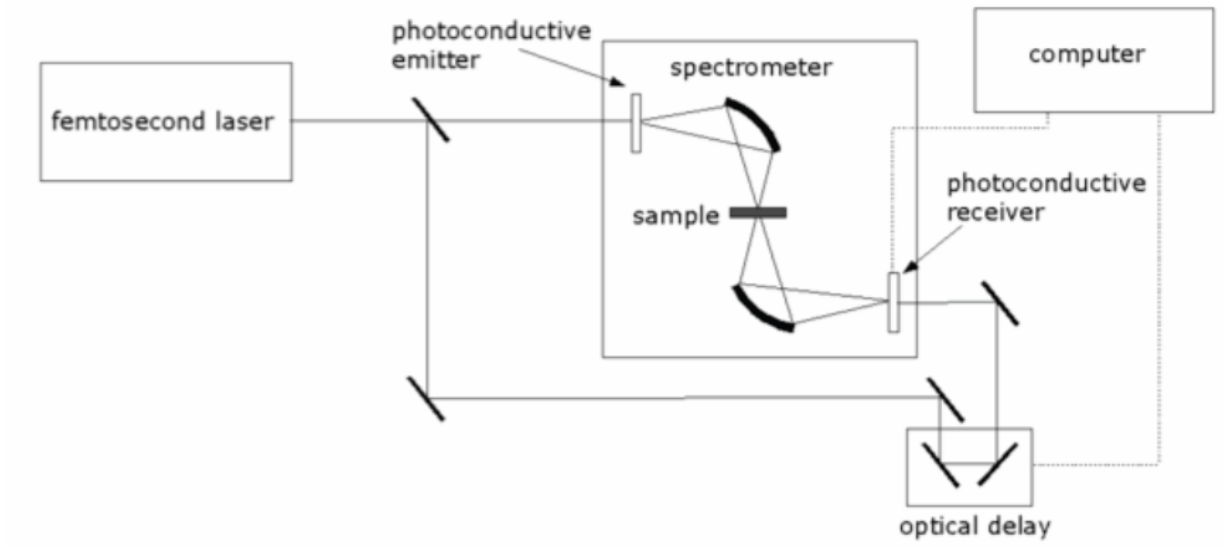
$E(t)$

⇩ Fourier transform

$s(\omega)E(\omega)$

⇩ referencing

$s(\omega)$



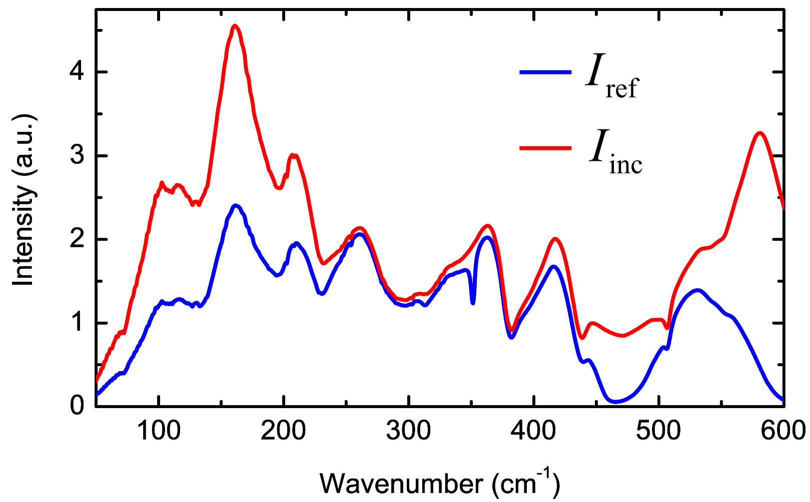
Most typical infrared techniques

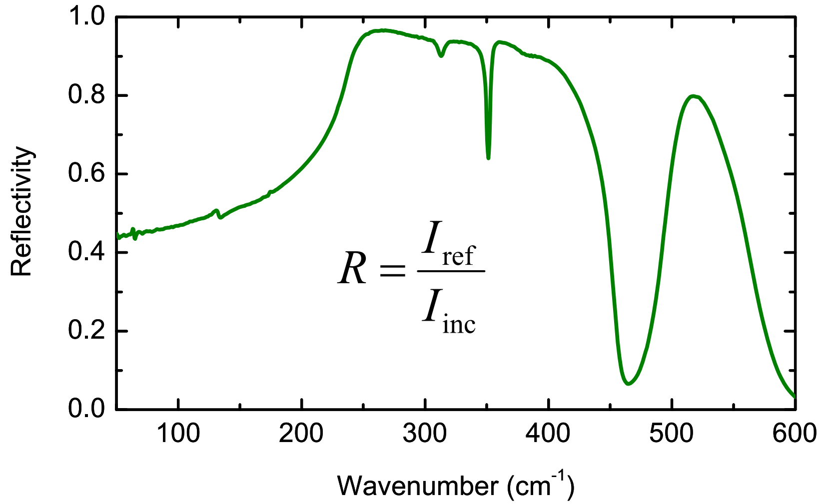
- Normal-incidence reflection

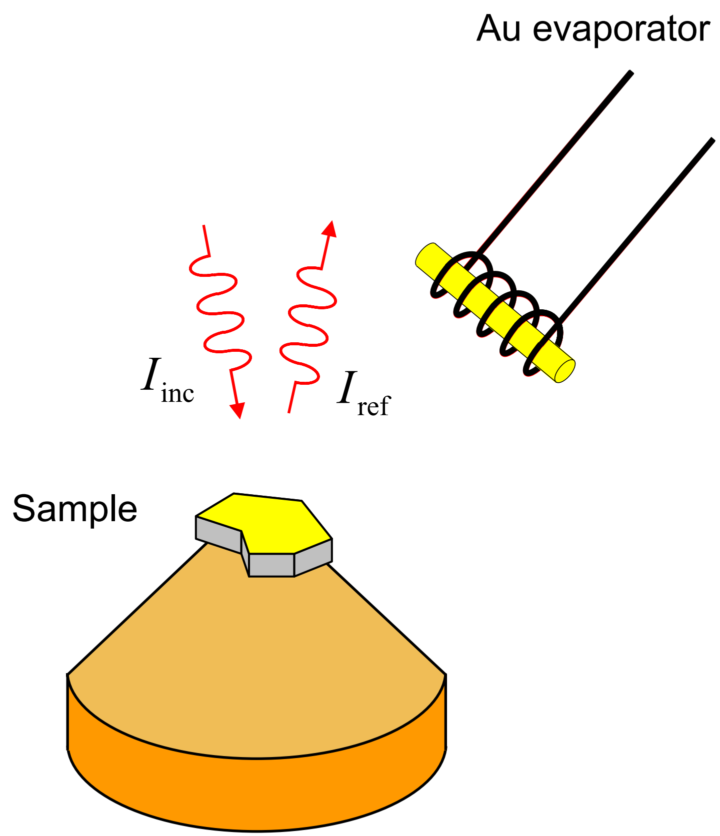
- Normal-incidence transmission

- Ellipsometry

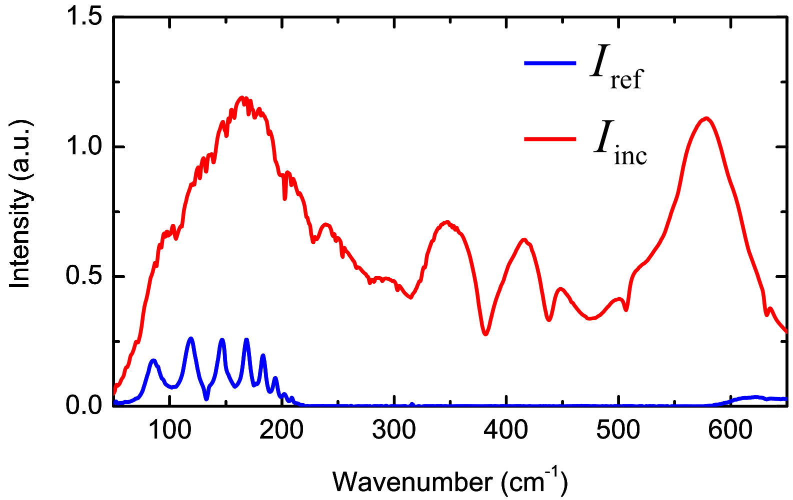
Normal-incidence reflection

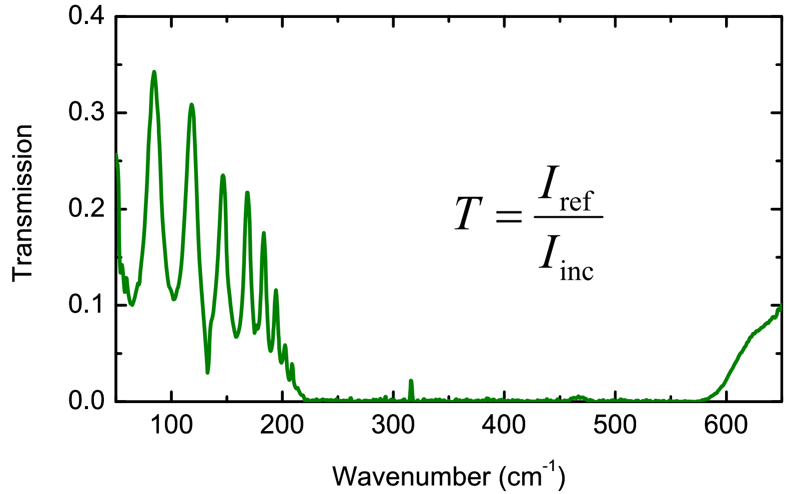


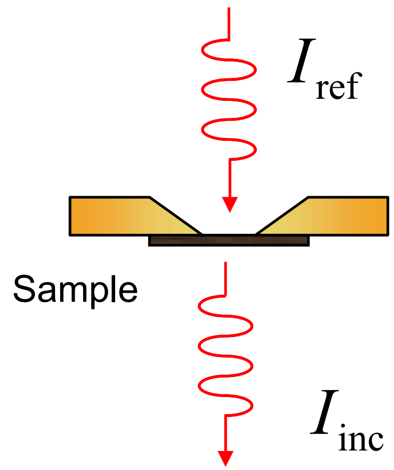




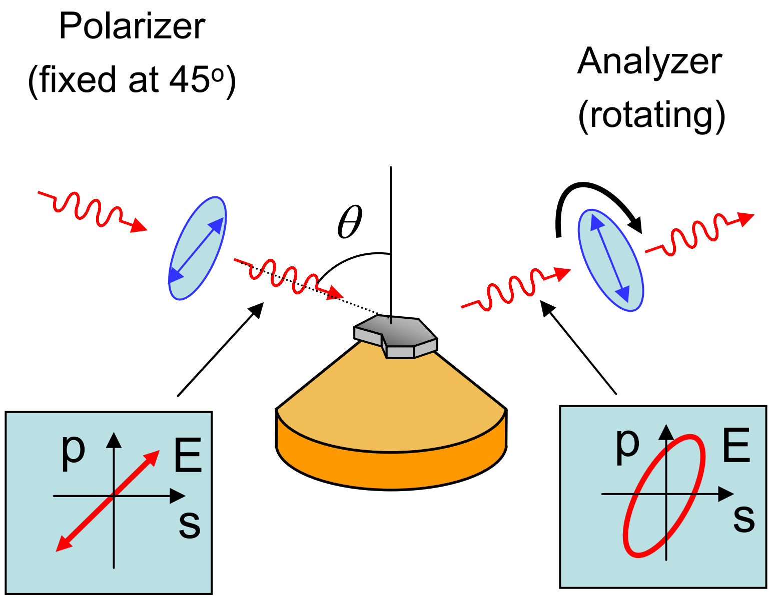
Normal-incidence transmission







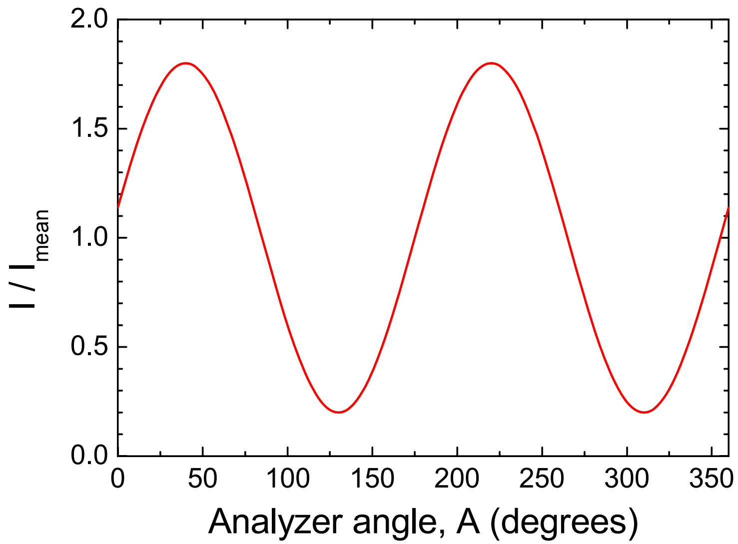
Ellipsometry



$$r_p = \frac{\varepsilon\cos\theta - \sqrt{\varepsilon - \sin^2\theta}}{\varepsilon\cos\theta + \sqrt{\varepsilon - \sin^2\theta}}$$

$$r_s = \frac{\cos\theta - \sqrt{\varepsilon - \sin^2\theta}}{\cos\theta + \sqrt{\varepsilon - \sin^2\theta}}$$

$$\rho = \frac{r_p}{r_s}$$



$$\frac{I(A)}{I_{mean}} = 1 + \frac{|\rho|^2 - 1}{|\rho|^2 + 1}\cos 2A + \frac{2\,\mathrm{Re}\,\rho}{|\rho|^2 + 1}\sin 2A$$

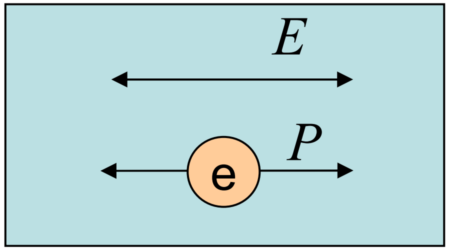
⇩

$$\rho$$

⇩

$$\varepsilon = \sin^2\theta \cdot \left[1 + \tan^2\theta \cdot \left(\frac{1-\rho}{1+\rho}\right)^2\right]$$

Drude-Lorentz model (classical derivation)



$$\frac{d^2x}{dt^2} = \frac{eE}{m}e^{-i\omega t} - \gamma\frac{dx}{dt} - \omega_0^2 x$$

« driving » force — friction (scattering) — restoring force

$$x(t) = \frac{eE}{m}\frac{e^{-i\omega t}}{\omega_0^2 - \omega^2 - i\gamma\omega} \qquad P(t) = enx(t)$$

$$\varepsilon(\omega) = \varepsilon_\infty + 4\pi\frac{P}{E} = \varepsilon_\infty + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

Quantum-mechanical derivation leads to the same result !

Model parameters

oscillator frequency	ω_0
plasma frequency	$\omega_p = \sqrt{\frac{4\pi n e^2}{m}}$
damping	$\gamma = \tau^{-1}$
« background » contribution	ε_∞

Free charges (Drude): $\omega_0 = 0$

Bound charges (Lorentz): $\omega_0 \neq 0$

Drude model

$$\varepsilon(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\gamma\omega}$$

$$\varepsilon_1(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + \gamma^2} \qquad \sigma_1(\omega) = \frac{\omega_p^2}{4\pi}\frac{\gamma}{\omega^2 + \gamma^2}$$

$\varepsilon_1(\omega)$ crosses zero at $\omega = \omega_p^* \approx \dfrac{\omega_p}{\sqrt{\varepsilon_\infty}}$

↑ screened plasma frequency

A: $\omega << \gamma$ (Hagen-Rubens regime)

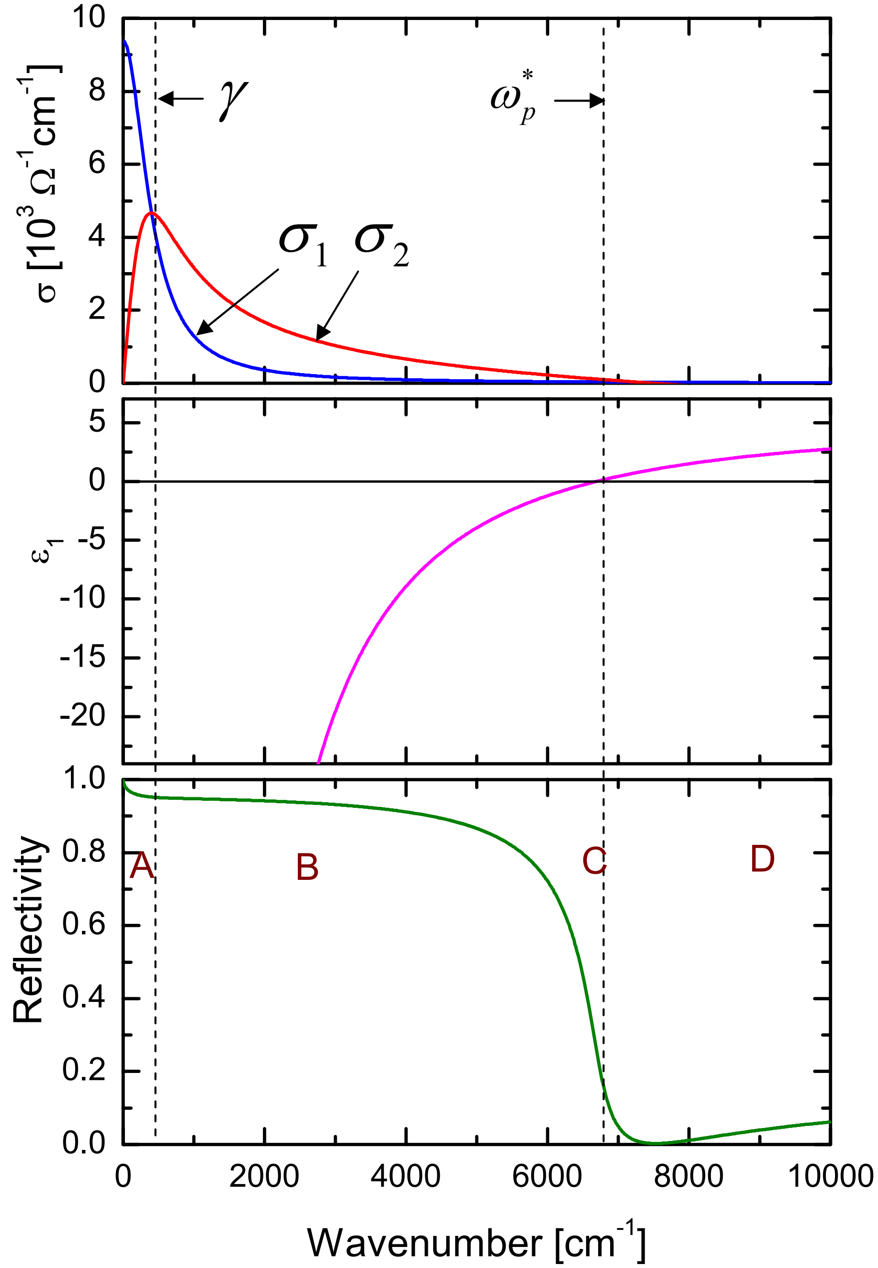
$R = 1 - (2\omega/\pi\sigma_{DC})^{1/2}$

B: $\gamma << \omega << \omega_p^*$ (relaxation regime)

$R \approx 1 - 2\gamma/\omega_p$

C: $\omega \sim \omega_p^*$ (plasma edge)

D: $\omega >> \omega_p^*$ (transparency regime)



Lorentz model

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

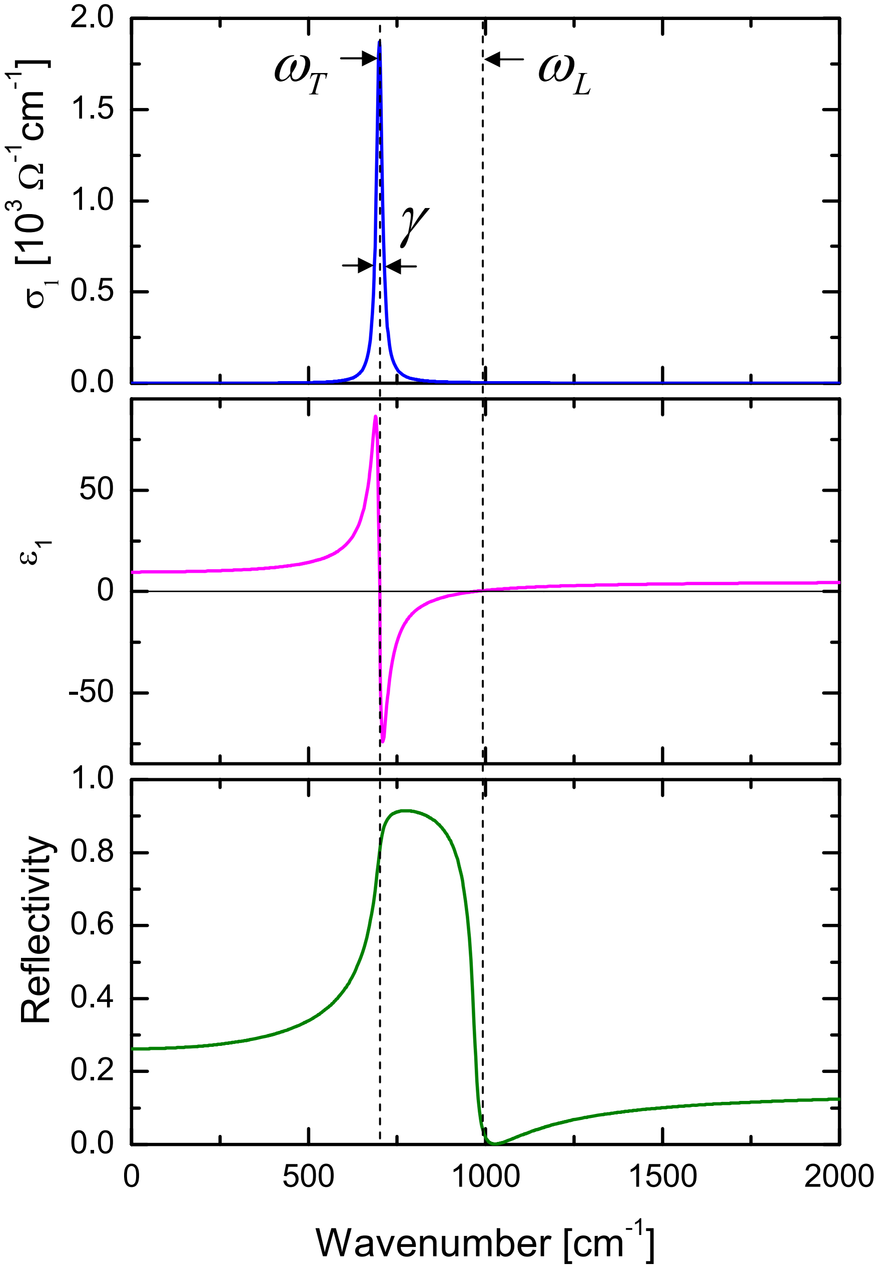
$\omega_T = \omega_0$ « transverse » frequency

$\omega_L = \sqrt{\frac{\omega_p^2}{\varepsilon_\infty} + \omega_0^2}$ « longitudinal» frequency $\varepsilon(\omega_L) = 0$

$$\varepsilon(0) = \varepsilon_\infty + \frac{\omega_p^2}{\omega_0^2}$$

oscillator strength (S)

ε_∞ oscillator strength of resonances at much higher frequencies

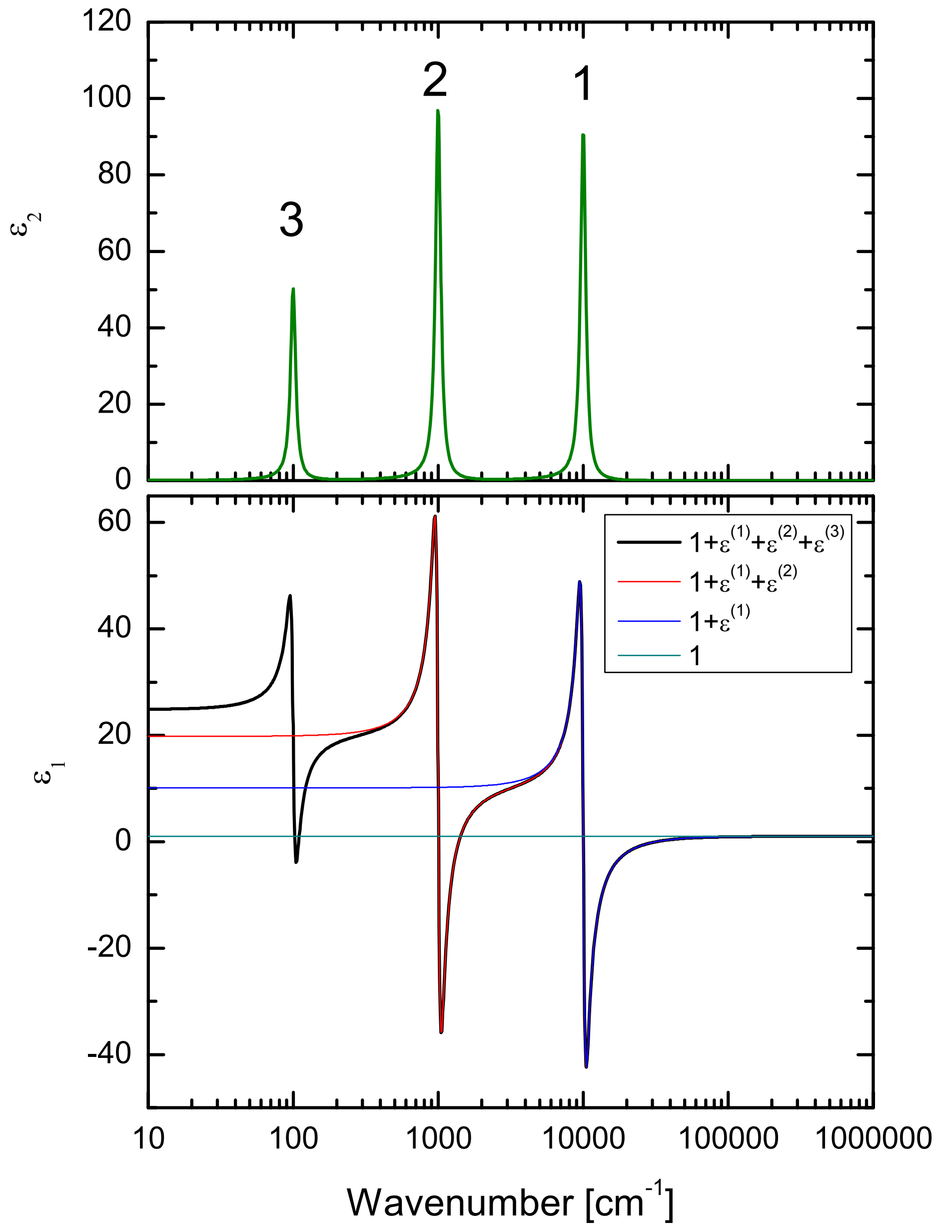


Adding Lorentz oscillators together

An example (3 oscillators)

$$\varepsilon(\omega) = 1 + \sum_{i=1}^{3} \frac{\omega_{p,i}^2}{\omega_{0,i}^2 - \omega^2 - i\gamma_i\omega}$$

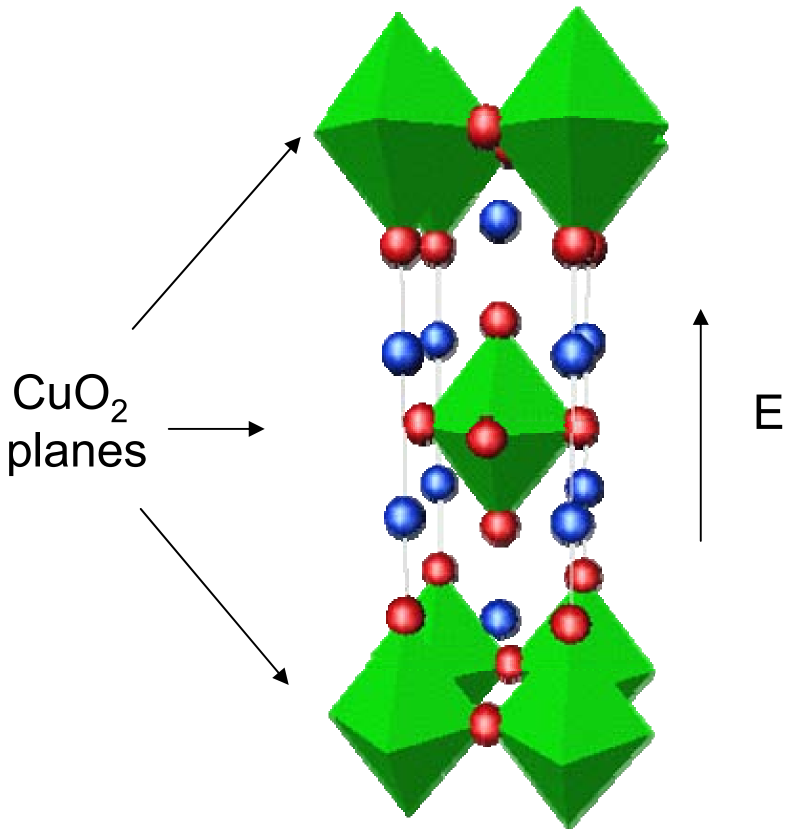
$$\varepsilon(0) = 1 + \sum_{i=1}^{3} \frac{\omega_{p,i}^2}{\omega_{0,i}^2} = 1 + \sum_{i=1}^{3} S_i$$

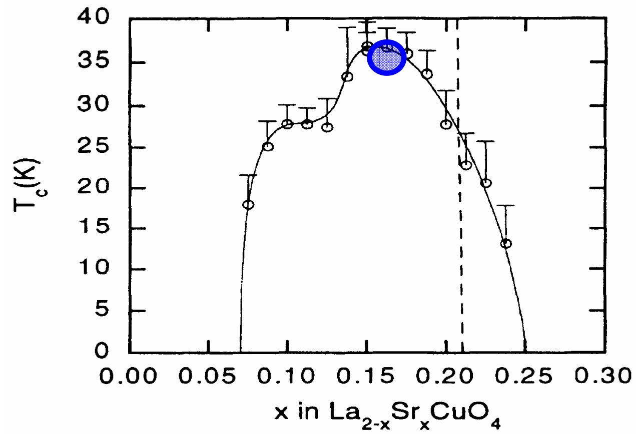


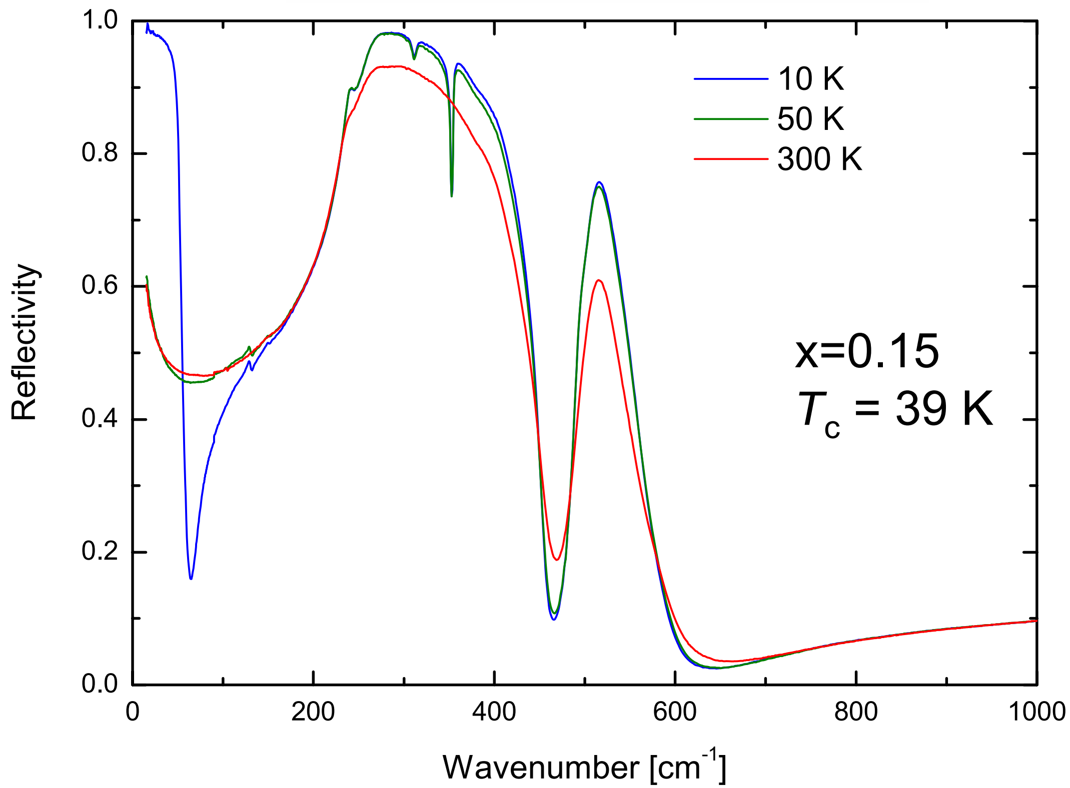
Typical contributions to ε(0):

vacuum	= 1
core electrons:	~ 1 - 2
valence electrons:	~ 1-5 (dielectrics)
	~ 10 (semiconductors)
	~ 100 (semimetals, e.g. Bi)
optical phonons:	<<1 (elemental compounds)
	~ 10 (multiatomic compounds)
	∞ (ferroelectrics)

c-axis optical reflectivity of $La_{2-x}Sr_xCuO_4$







In the normal state,
the electronic transport
along the c-axis is incoherent
In the SC state, a sharp plasma edge
Due to the Josephson tunneling
of the Cooper pairsshows up

Drude-Lorentz fitting of reflectivity

Model: $R(\omega) = \left|\frac{1-\sqrt{\varepsilon}}{1-\sqrt{\varepsilon}}\right|^2$ $\quad \varepsilon(\omega) = \varepsilon_\infty + \sum_{i=1}^{3} \frac{\omega_{p,i}^2}{\omega_{0,i}^2 - \omega^2 - i\gamma_i\omega}$

Dataset: $(\omega_1, R_1 \pm \delta R_1), (\omega_2, R_2 \pm \delta R_2) \dots (\omega_N, R_N \pm \delta R_N)$

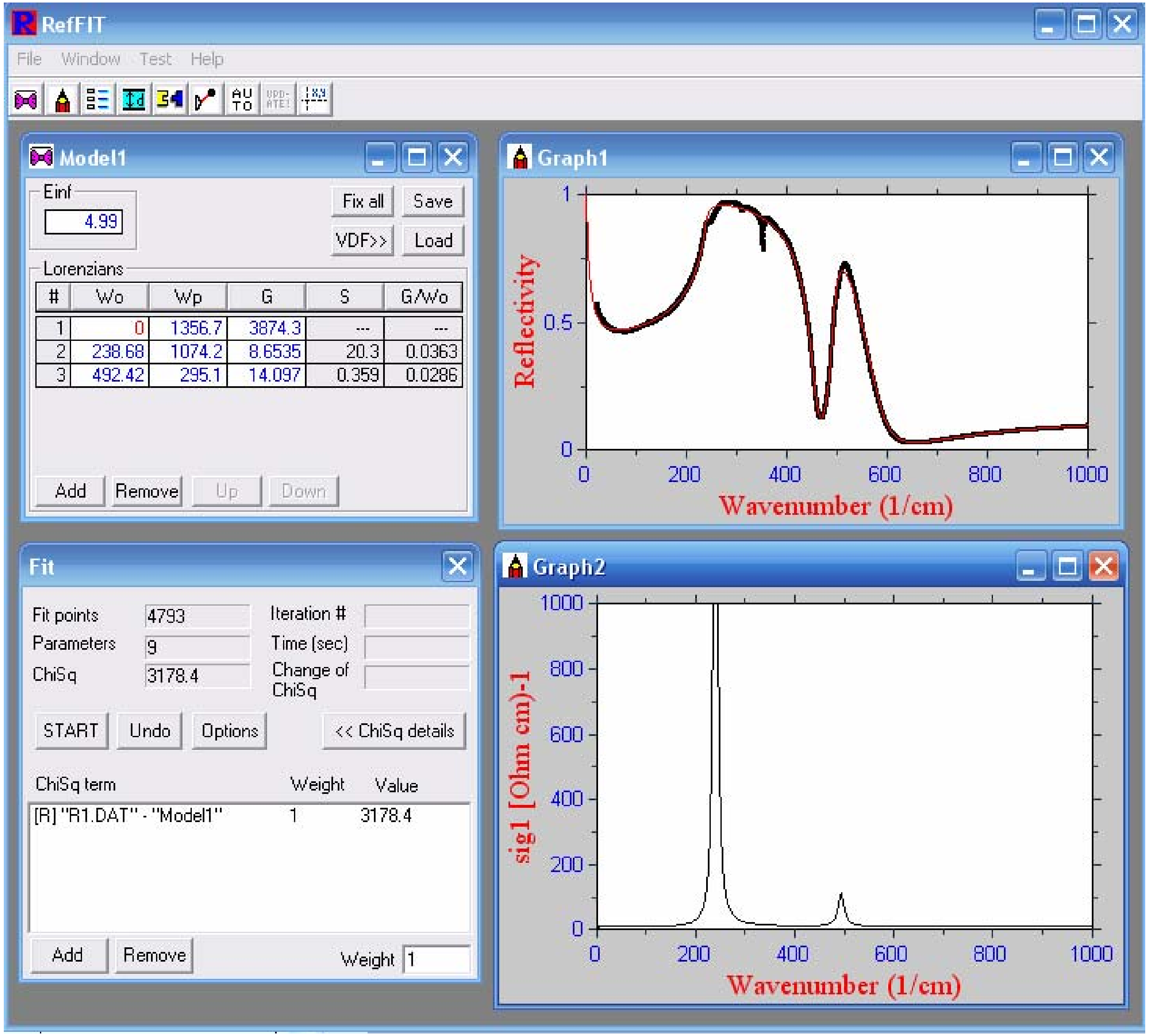
Least-square method: $\chi^2 = \sum_{k=1}^{N} \left(\frac{R_k - R(\omega_k)}{\delta R_k} \right)^2 \to \min$

An effiecient technique for minimization:
Levenberg-Marquardt method

(requires analytical calculation of derivatives $\frac{\partial \chi^2}{\partial [parameters]}$

Numerical recipes,
W.H.Press, B.P.Flannery, S.A.Teukolsky and W.T.Vetterling,
Cambridge Univ. Press (1986).

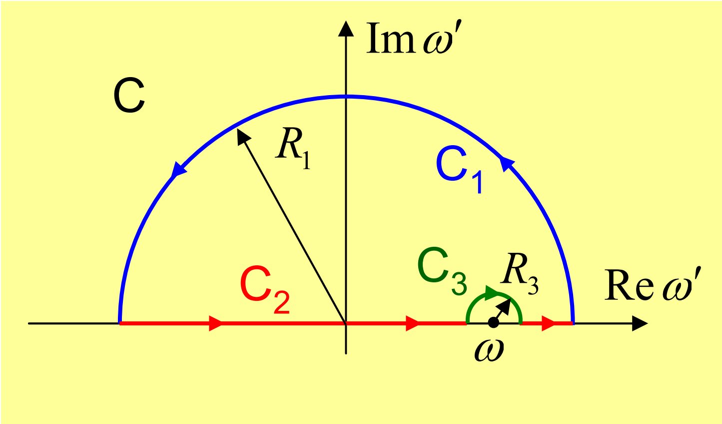
Fitting in practice (RefFIT program)



available online at:http://optics.unige.ch/alexey/reffit.html

Kramers-Kronig relations

$\sigma(\omega)$ is analytical (has no poles) in the upper complex semiplane of ω as follows from the causality principle



Cauchy's theorem $\oint_C \frac{\sigma(\omega')}{\omega'-\omega}d\omega' = 0$

$R_1 \to \infty; R_3 \to 0$

$\oint_{C_1} \to 0 \qquad \oint_{C_2} \to \mathcal{P}\int_{-\infty}^{\infty}\frac{\sigma(\omega')}{\omega'-\omega}d\omega' \qquad \oint_{C_3} \to -i\pi\sigma(\omega)$

$$i\pi\sigma(\omega) = \mathcal{P}\int_{-\infty}^{\infty}\frac{\sigma(\omega')}{\omega'-\omega}d\omega'$$

$$\sigma_1(\omega) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{\sigma_2(\omega')}{\omega'-\omega}d\omega'$$

$$\sigma_2(\omega) = -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{\sigma_1(\omega')}{\omega'-\omega}d\omega'$$

Using symmetry

$$\sigma_1(-\omega) = \sigma_1(\omega)$$

$$\sigma_2(-\omega) = -\sigma_2(\omega)$$

$$\sigma_1(\omega) = \frac{2}{\pi}\mathcal{P}\int_0^{\infty}\omega'\frac{\sigma_2(\omega')}{\omega'^2-\omega^2}d\omega'$$

$$\sigma_2(\omega) = \frac{2\omega}{\pi}\mathcal{P}\int_0^{\infty}\frac{\sigma_1(\omega')}{\omega^2-\omega'^2}d\omega'$$

KK relations and Lorentz oscillators

KK relations

$$\sigma_1(\omega) = \frac{2}{\pi}\mathcal{P}\int_0^\infty \omega' \frac{\sigma_2(\omega')}{\omega'^2 - \omega^2} d\omega'$$

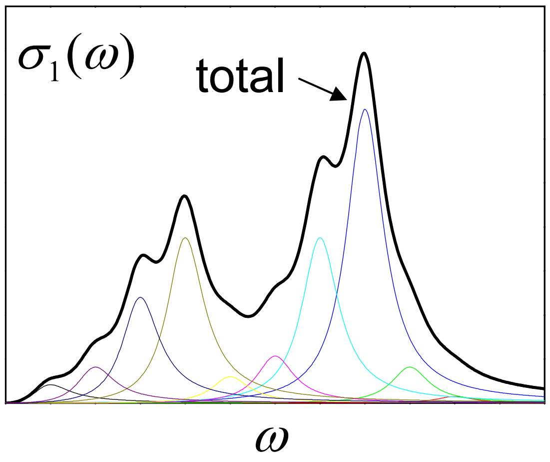
$$\sigma_2(\omega) = \frac{2\omega}{\pi}\mathcal{P}\int_0^\infty \frac{\sigma_1(\omega')}{\omega^2 - \omega'^2} d\omega'$$

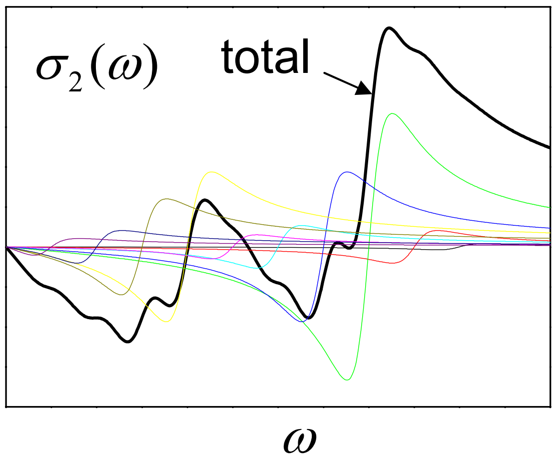
$$\sigma(\omega) = \mathcal{P}\int_0^\infty \sigma_1(\omega')\left[\delta(\omega-\omega') + \frac{i}{\pi}\frac{2\omega}{\omega^2 - \omega'^2}\right] d\omega'$$

Lorentzian

$$\sigma_L(\omega) = \frac{\omega}{4\pi i}\frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\gamma\omega} \xrightarrow[\gamma \to 0]{} \frac{\omega_p^2}{8}\left[\delta(\omega-\omega_0) + \frac{i}{\pi}\frac{2\omega}{\omega^2 - \omega_0^2}\right]$$

Any KK consistent function can be decomposed into a sum of (a large number of) narrow Lorentzians





KK transformation for reflectivity

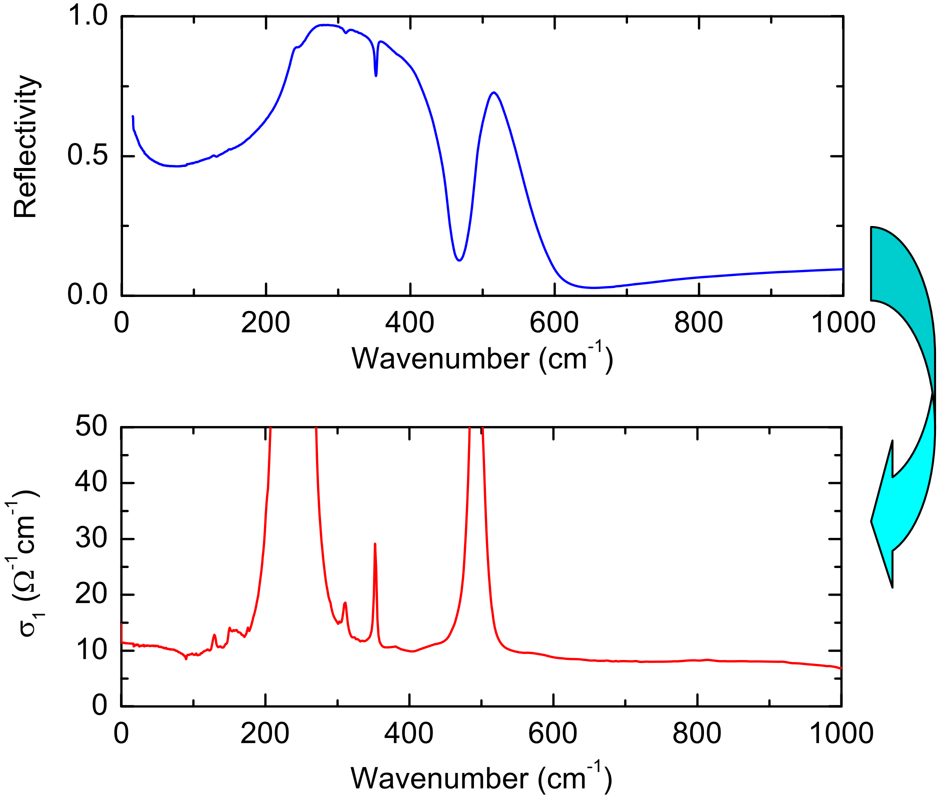
Normal incidence; bulk sample $r = \dfrac{1-\sqrt{\varepsilon}}{1+\sqrt{\varepsilon}}$

$$r(\omega) = \sqrt{R(\omega)}\, e^{i\varphi(\omega)}$$

real reflectivity (measured) — complex phase (usually not measured)

$$\ln r(\omega) = \frac{1}{2}\ln R(\omega) + i\varphi(\omega)$$

KK related



1. Restore the phase numerically

$$\varphi(\omega) = -\frac{2\omega}{\pi}\mathcal{P}\int_0^\infty \frac{\ln R(\omega')}{\omega'^2-\omega^2}d\omega'$$

(need extrapolations at low and high energies!)

2. Obtain ε and σ

$$\varepsilon(\omega) = \left[\frac{1-r(\omega)}{1+r(\omega)}\right]^2$$

$$\sigma(\omega) = \frac{\omega}{4\pi i}\left[\varepsilon(\omega)-1\right]$$

This trick is first used in:

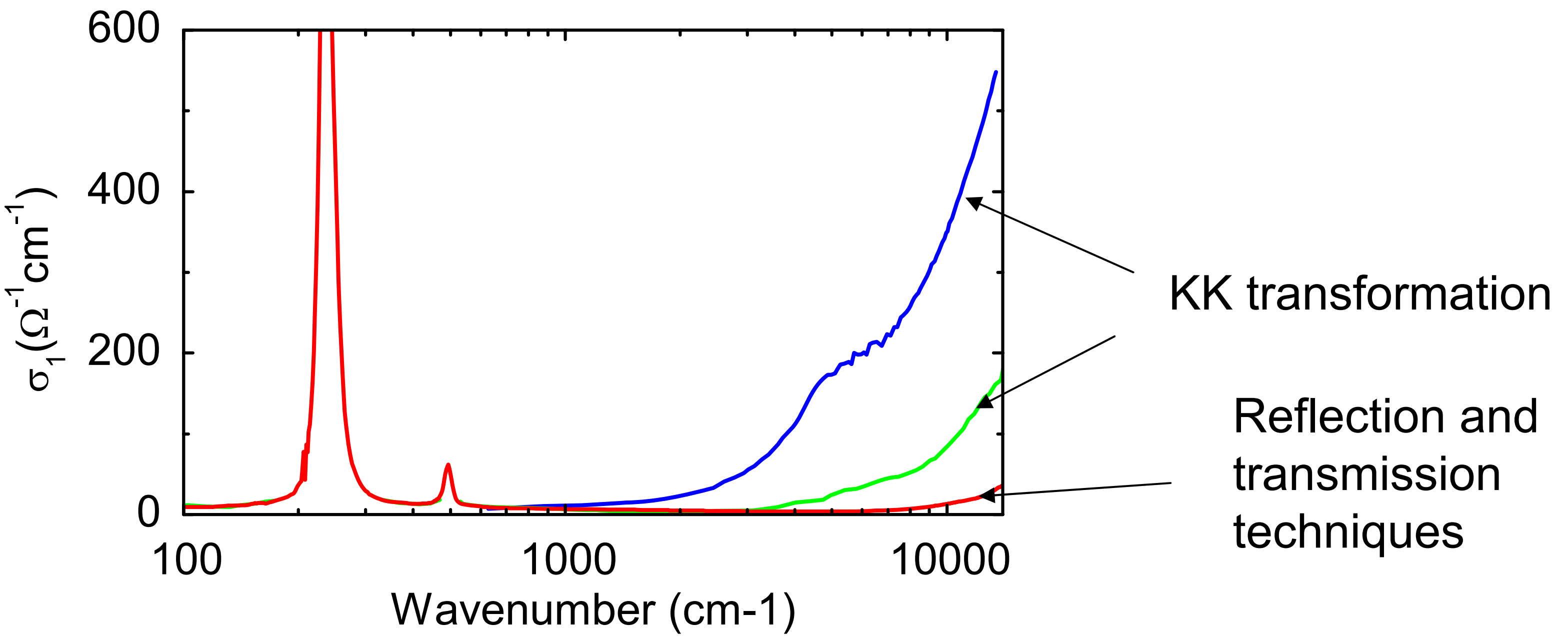
F. C. Jahoda, Phys. Rev. **107**, 1261 (1957)

Followed by thousands of papers !

Be careful with the KK transformation !

$$\varphi(\omega) = -\frac{2\omega}{\pi}\mathcal{P}\int_0^\infty \frac{\ln R(\omega')}{\omega'^2 - \omega^2}d\omega'$$

Extrapolations may introduce significant errors !



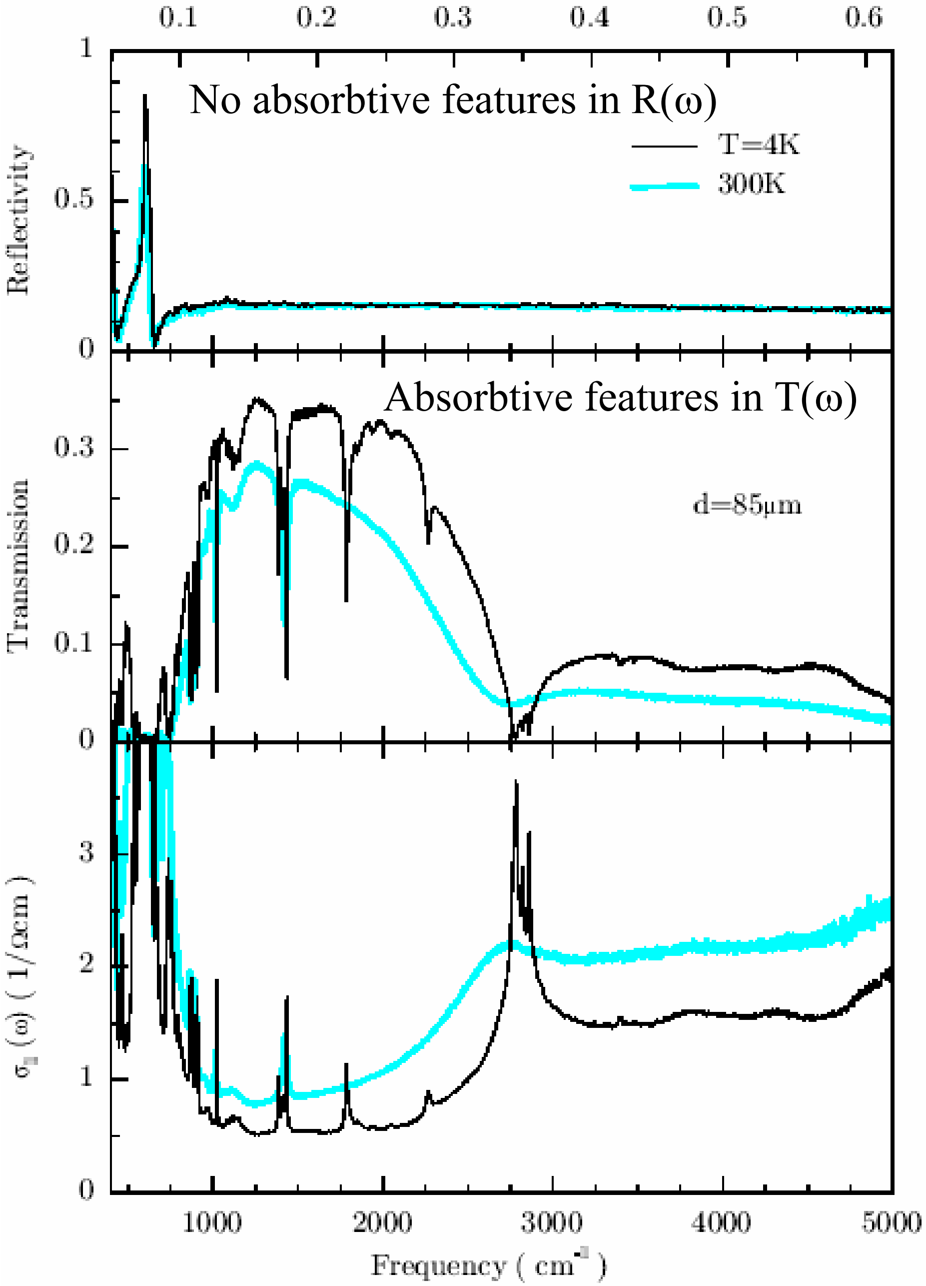
Probing weak excitations with transmission

Weakly absorbing magnetic excitations in insulating $YBa_2Cu_3O_6$

Transmission is much more sensitive to weak excitations than reflectivity

$$\sigma_1(\omega) \sim -\ln T(\omega)$$

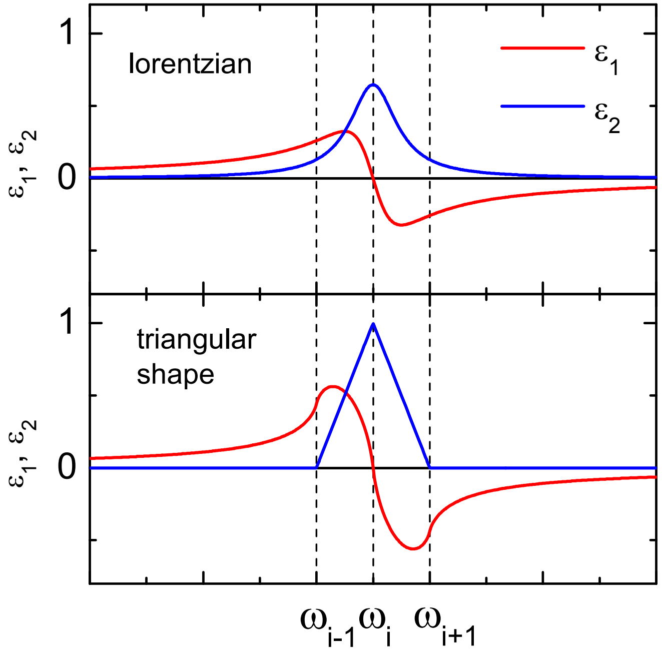
M.Gruninger, 1999, PhD Thesis

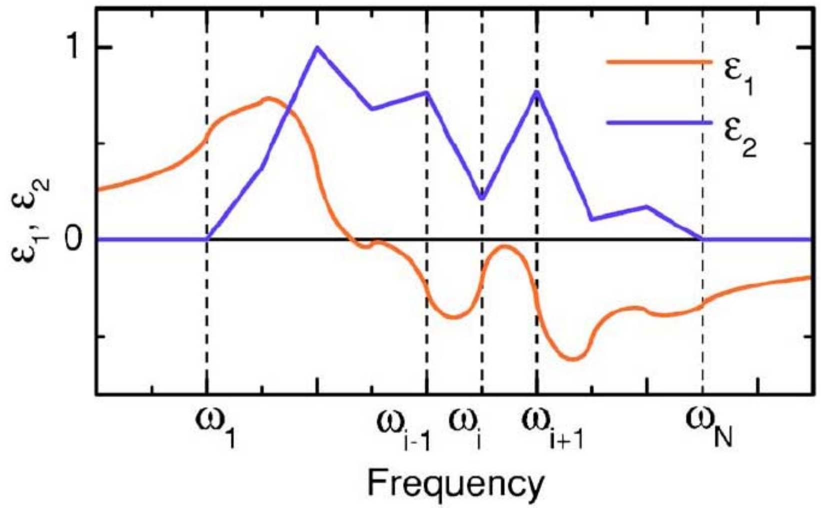


Kramers-Kronig constrained variational fitting

$\varepsilon_2(\omega)$ - « flexible », parametrized independently at every frequency

$\varepsilon_1(\omega)$ - KK transform of $\varepsilon_2(\omega)$



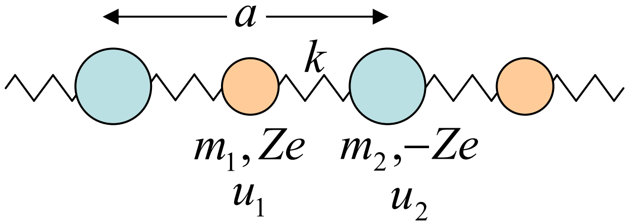


Generalization of the KK method to virtually any type of optical data

A.B.K., Rev. Sci. Instrum.**76**, 083108 (2005)

Optical phonons

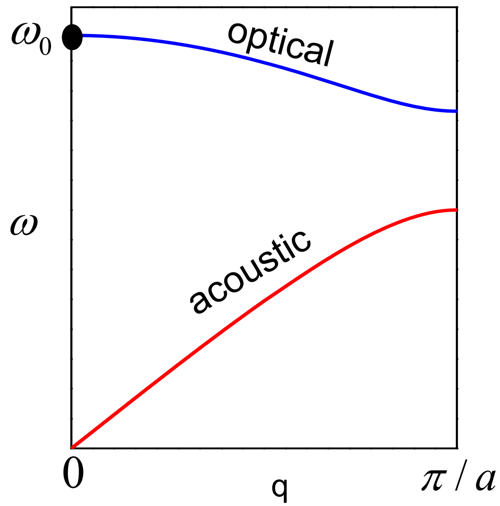
Toy model of a crystal: a chain of alternating « rigid » ions connected by « spring » forces



$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

$$u = u_1 - u_2$$

$$\omega_0 = \left(\frac{k}{\mu}\right)^{1/2}$$



Optical branch, q=0

$$\begin{cases} m_1 \ddot{u}_1 = ZeE - k(u_1 - u_2) \\ m_2 \ddot{u}_2 = -ZeE - k(u_2 - u_1) \end{cases}$$

$$\mu \ddot{u} = (Ze)Ee^{-i\omega t} - ku \quad \Rightarrow \quad u(t) = \frac{Ze/\mu}{\omega_0^2 - \omega^2} e^{-i\omega t}$$

$$P = \frac{u(Ze)}{V_c}$$

$$\varepsilon_1(\omega) = \varepsilon_\infty + \frac{4\pi}{V_c} \frac{(Ze)^2}{\mu} \frac{1}{\omega_0^2 - \omega^2} \qquad \sigma_1(\omega) = \frac{\pi (Ze)^2}{2V_c \mu} \delta(\omega - \omega_0)$$

V_c - unit cell volume

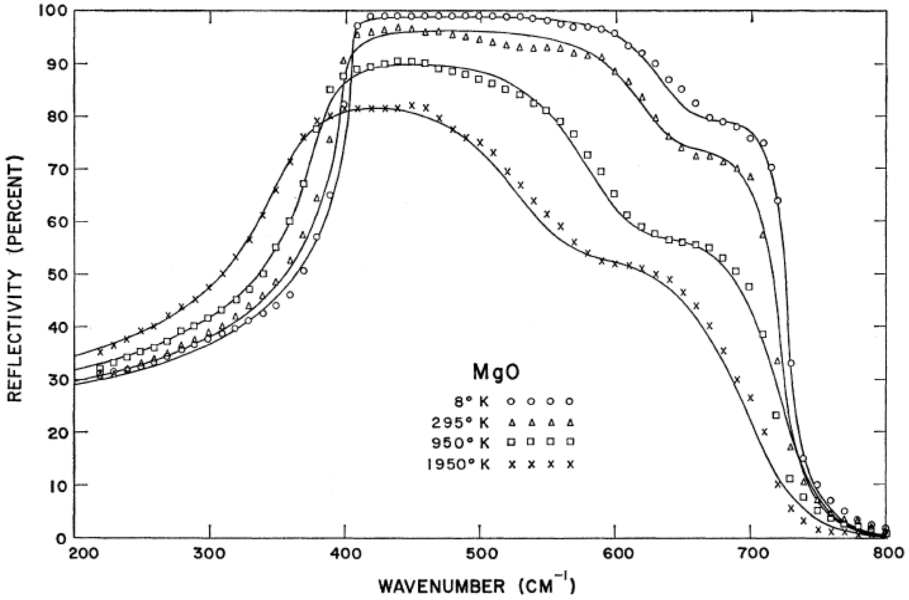
sum rule:

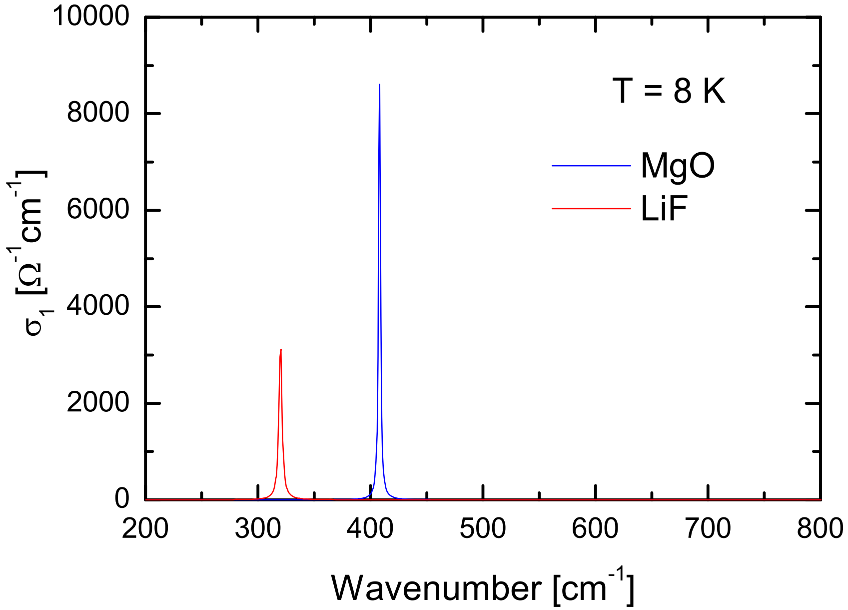
$$\int_0^\infty \sigma_1(\omega) d\omega = \frac{\pi (Ze)^2}{2V_c} \left[\frac{1}{m_1} + \frac{1}{m_2}\right]$$

For arbitrary number of atoms per unit cell

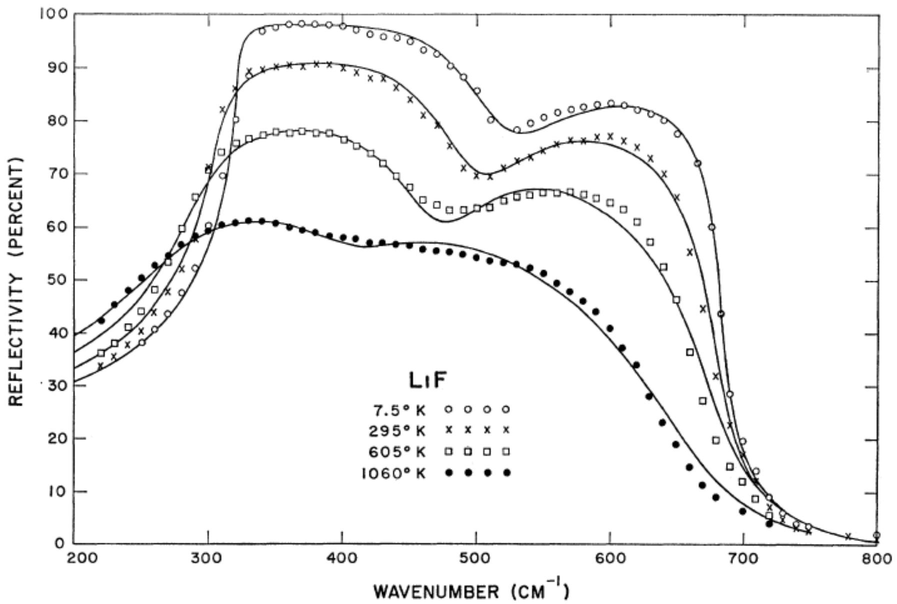
$$\int_0^\infty \sigma_1(\omega) d\omega = \frac{\pi e^2}{2V_c} \sum_i \frac{Z_i^2}{m_i}$$

Optical phonons in ionic crystals





$$\int_0^\infty \sigma_1(\omega)d\omega = \frac{\pi(Ze)^2}{2V_c\mu}$$



Effective charges:

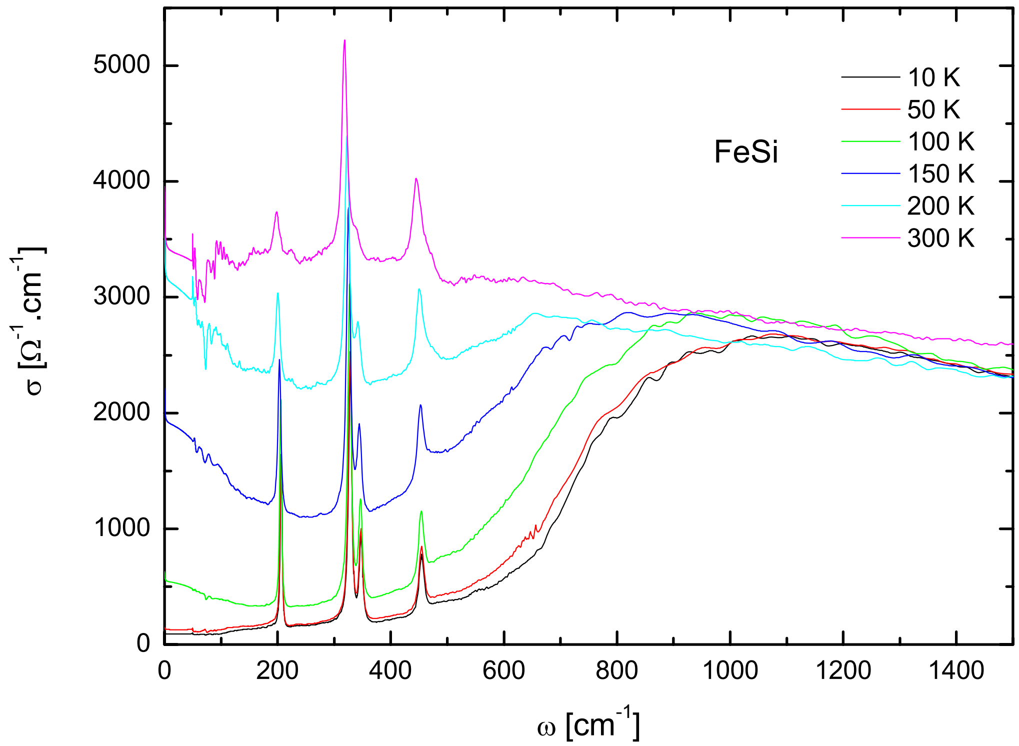
$Z_{MgO} = 1.96$

$Z_{LiF} = 1.03$

} match almost exactly the valence charges

J.R. Jasperse et al. Phys. Rev. 146, 526 (1965)

Optical phonons in FeSi



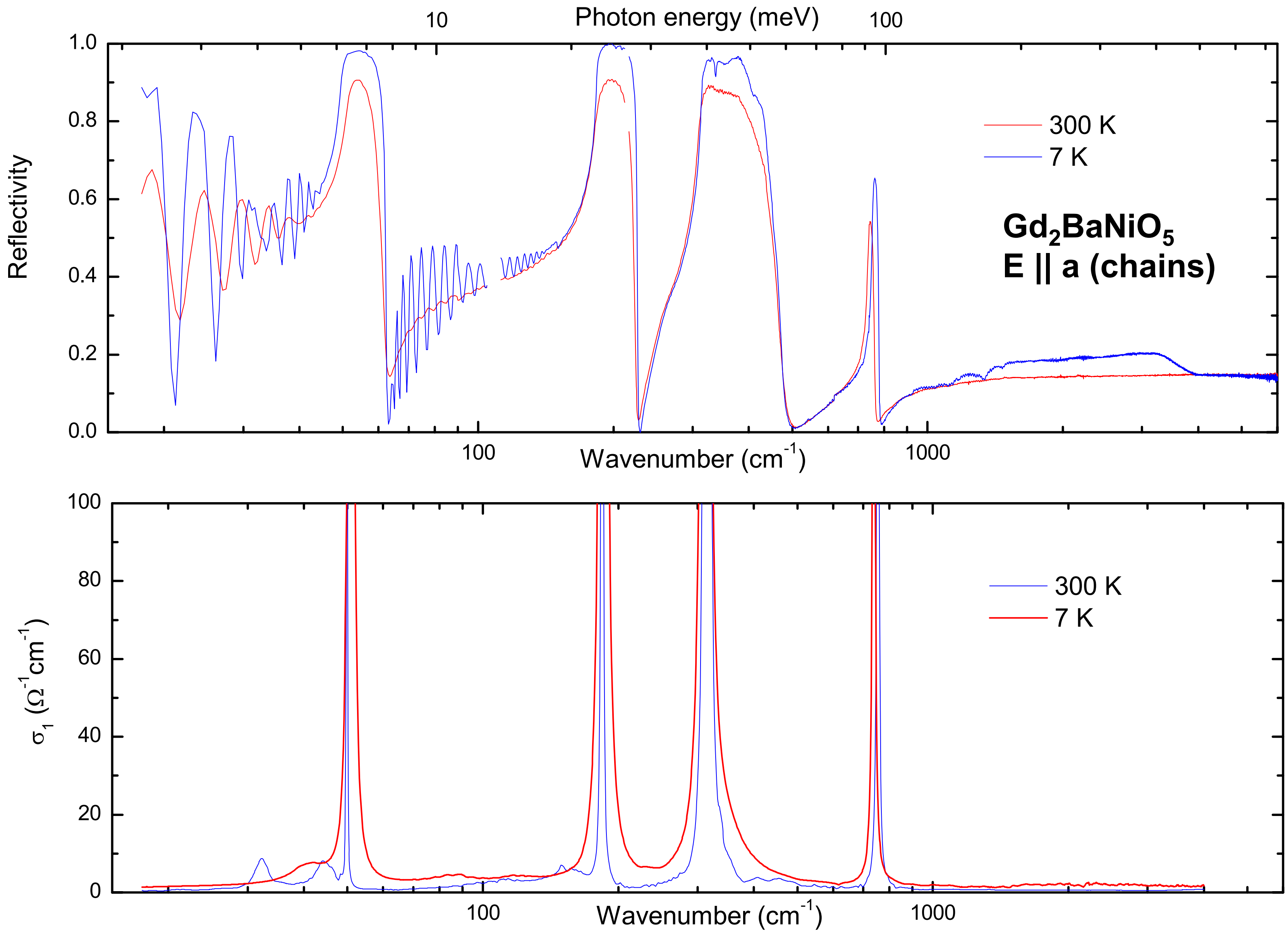
A. Damascelli et al.
Phys. Rev. B 55, R4863 (1997)

Effective charge: $Z_{FeSi} \approx 4$

much larger than the nominal valence charge

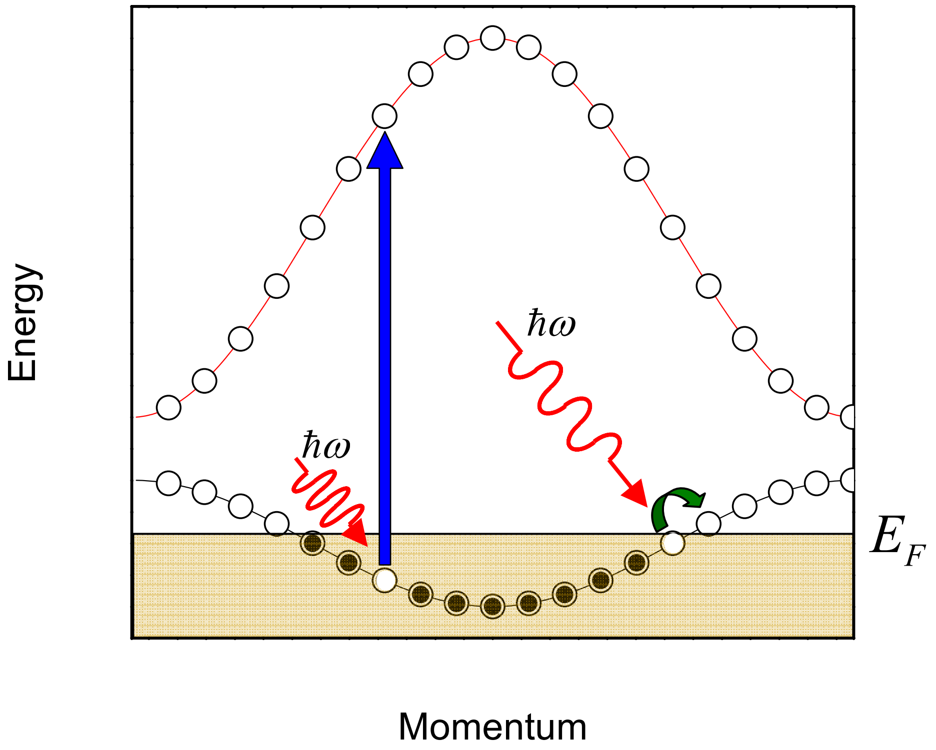
Evidence for strong coupling of lattice vibrations to electron-hole excitations

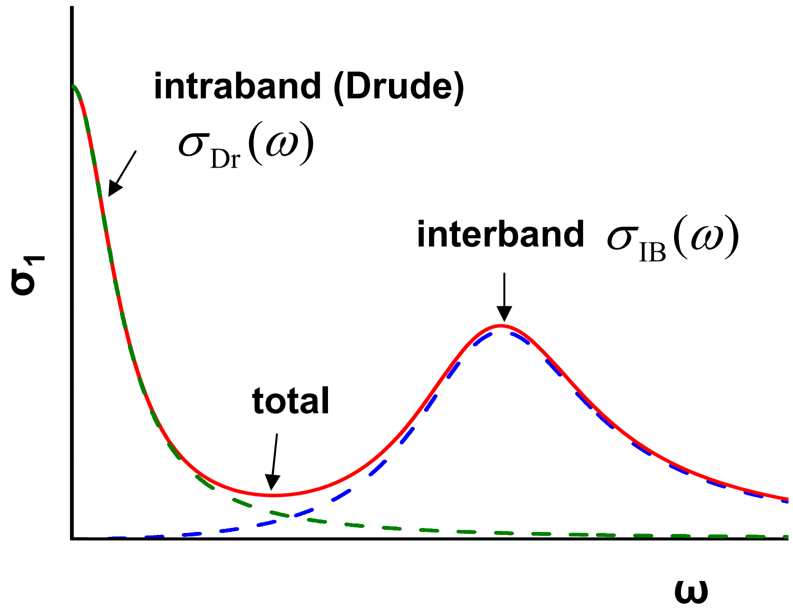
An example: multiple optical phonons



to be published

Intraband and interband transitions





$$\mathrm{Re}\,\sigma_{\mathrm{Dr}}(\omega) = \frac{e^2}{8\pi^2} \sum_{\substack{i \\ \text{(bands)}}} \int_{\substack{\text{Brillouin} \\ \text{Zone}}} d\mathbf{k}\ \left|v_{\mathbf{k},ii}\right|^2 \left[-\frac{\partial f}{\partial \varepsilon}(\varepsilon_{\mathbf{k},i})\right] \delta(\omega)$$

$$\mathrm{Re}\,\sigma_{\mathrm{IB}}(\omega) = \frac{e^2}{4\pi^2} \sum_{\substack{i,j\neq i \\ \text{(bands)}}} \int_{\substack{\text{Brillouin} \\ \text{Zone}}} d\mathbf{k}\ \left|v_{\mathbf{k},ij}\right|^2 \frac{f(\varepsilon_{\mathbf{k},i}) - f(\varepsilon_{\mathbf{k},j})}{\hbar\omega} \delta\left(\omega - \frac{\varepsilon_{\mathbf{k},j} - \varepsilon_{\mathbf{k},i}}{\hbar}\right)$$

$$f(\varepsilon) = \left(\exp\frac{\varepsilon\text{-}E_F}{T} + 1\right)^{-1}$$

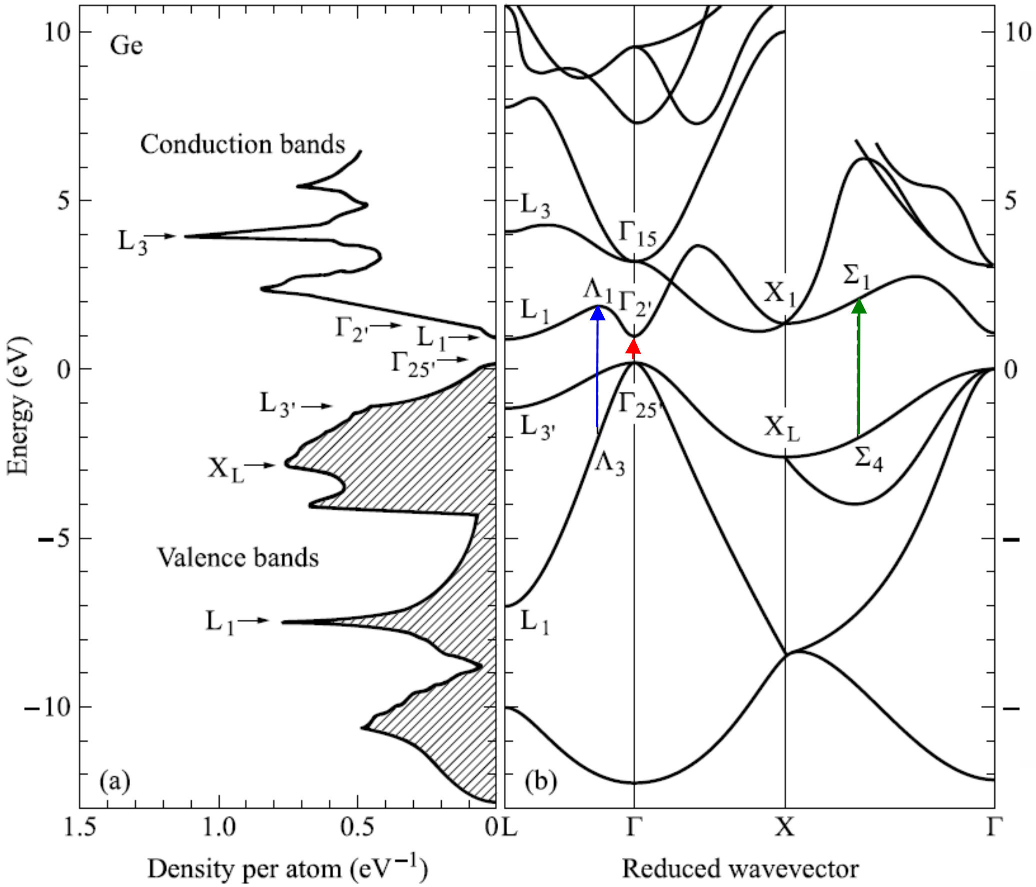
– Fermi – Dirac distribution

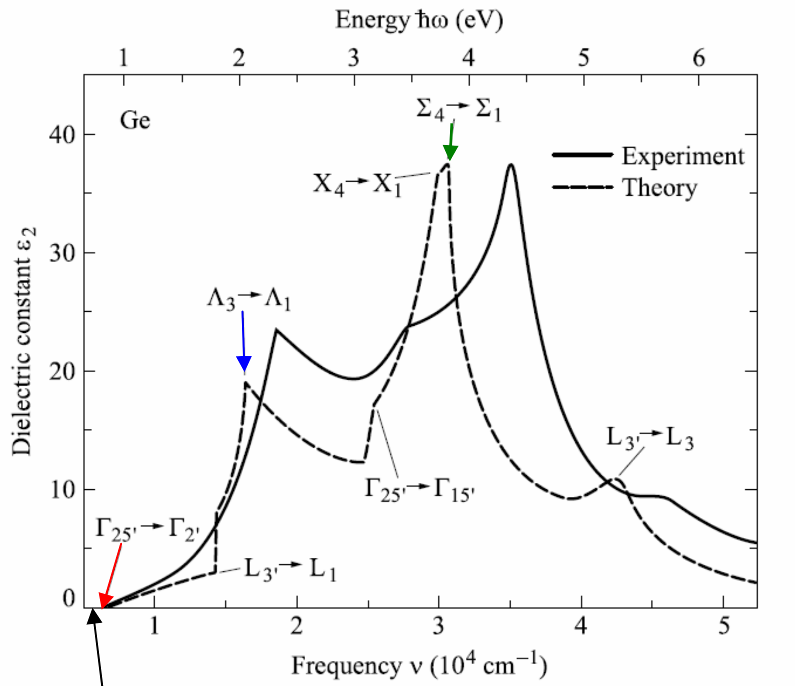
$$v_{\mathbf{k},ij} \equiv -\frac{i\hbar}{m}\left\langle \psi_{\mathbf{k}i}\left|\frac{\partial}{\partial x}\right|\psi_{\mathbf{k}j}\right\rangle$$

- velocity matrix element

δ-functions are broadened due to scattering and many-body effects !

Optical spectra of germanium





below the bandgap

$$\varepsilon_2(\omega) = 0$$

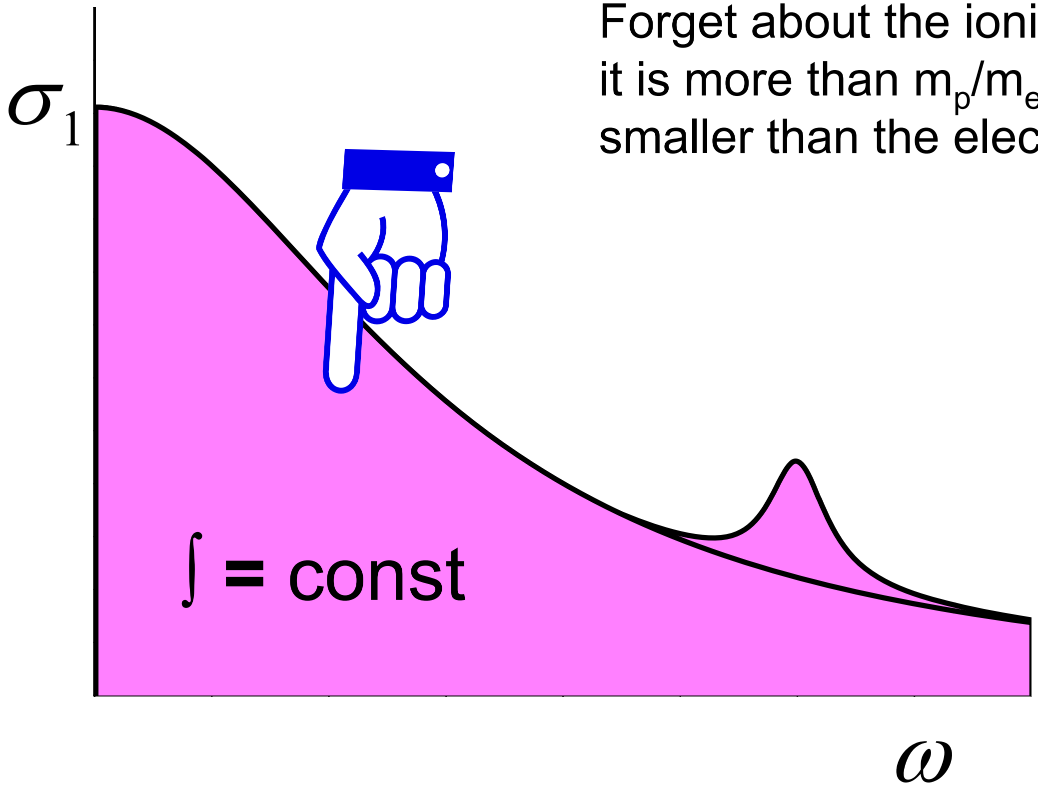
H.R. Philipp and H. Ehrenreich,
Phys. Rev. B **129**, 1550 (1963)

Optical conductivity sum rule

$$\int_0^\infty \sigma_1(\omega)d\omega = \frac{\pi e^2 n}{2m_e}$$

total density of electrons (n)

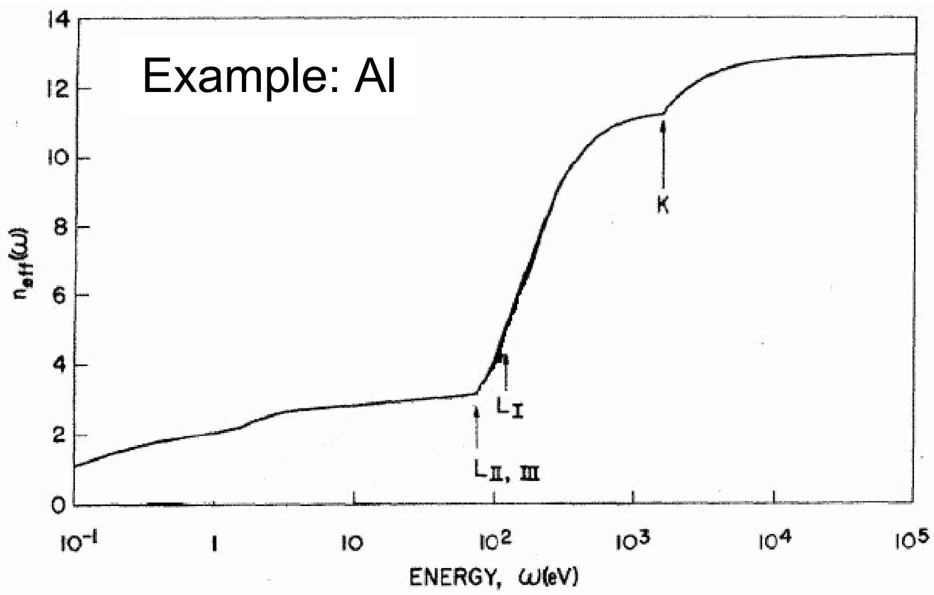
bare electron mass (m_e)



Forget about the ionic contribution here: it is more than m_p/m_e=2000 times smaller than the electronic one

Partial sum rule

$$N_{eff}(\omega) \equiv \frac{2m_e V_c}{\pi e^2} \int_0^{\omega} \sigma_1(\omega')d\omega'$$

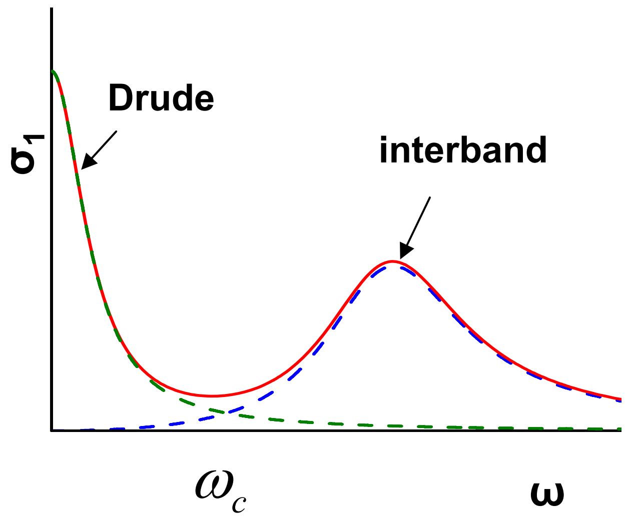


D.Y.Smith and E. Shiles, Phys. Rev. B, **17**, 4689 (1978)

Drude spectral weight:

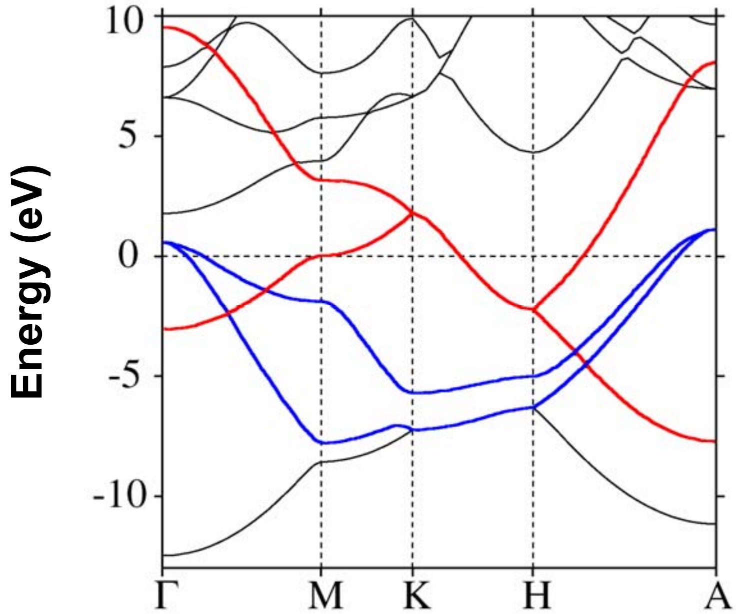
$$\int_0^{\omega_c} \sigma_1(\omega')d\omega' = \frac{\omega_p^2}{8} = \frac{\pi n e^2}{2m_{band}}$$

ω_c -separates Drude and interband transitions

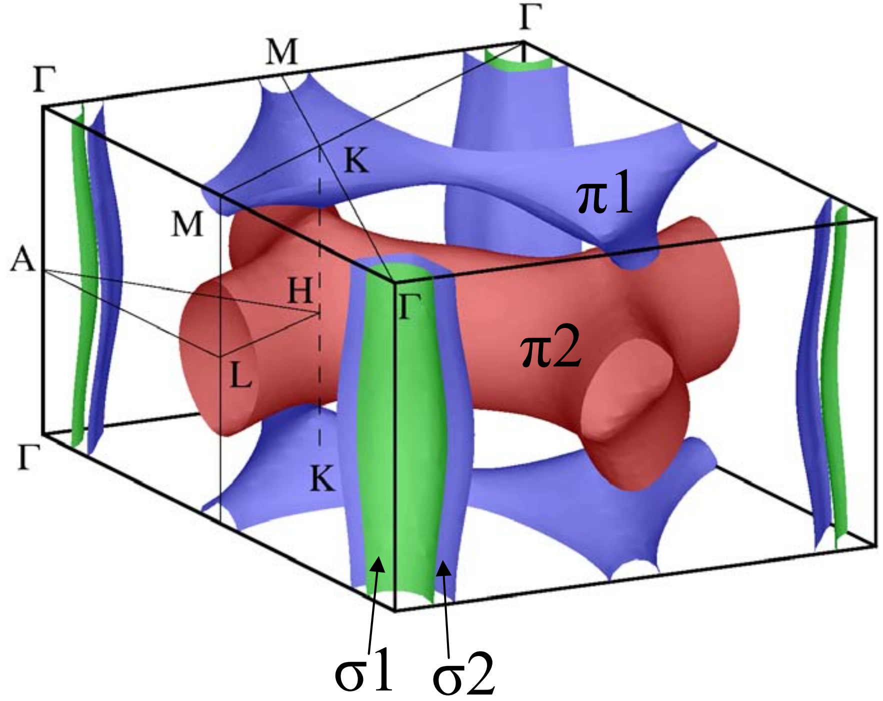


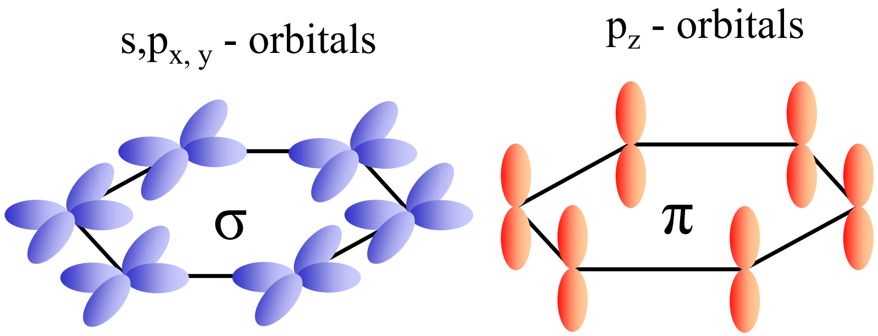
Band structure of MgB_2

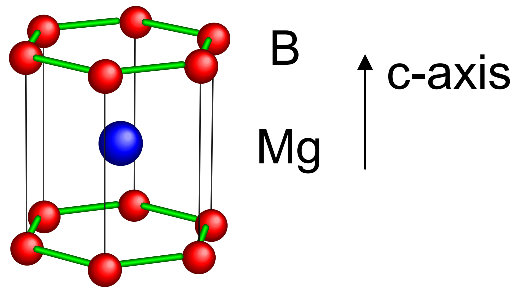
Band structure



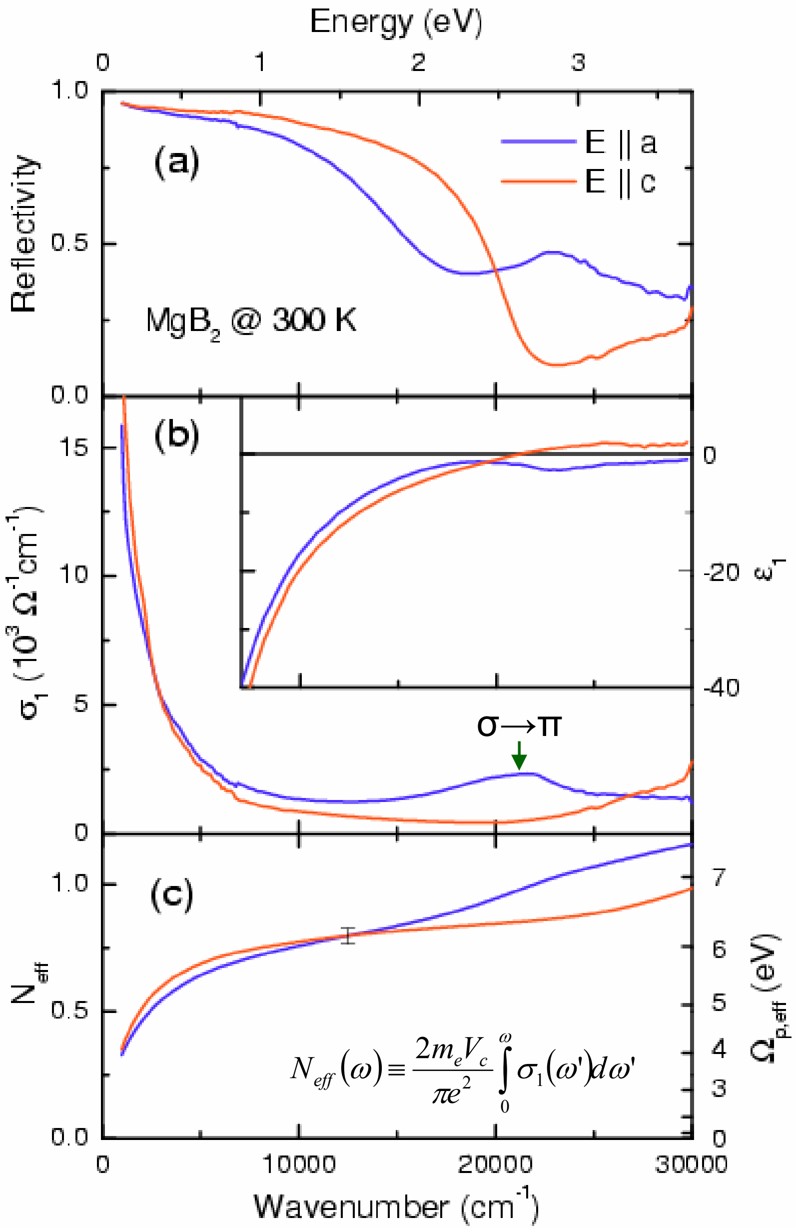
Fermi surface



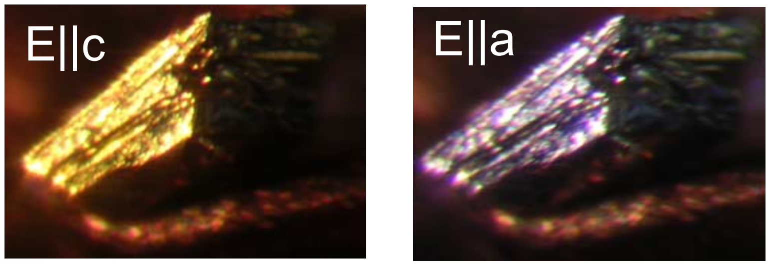


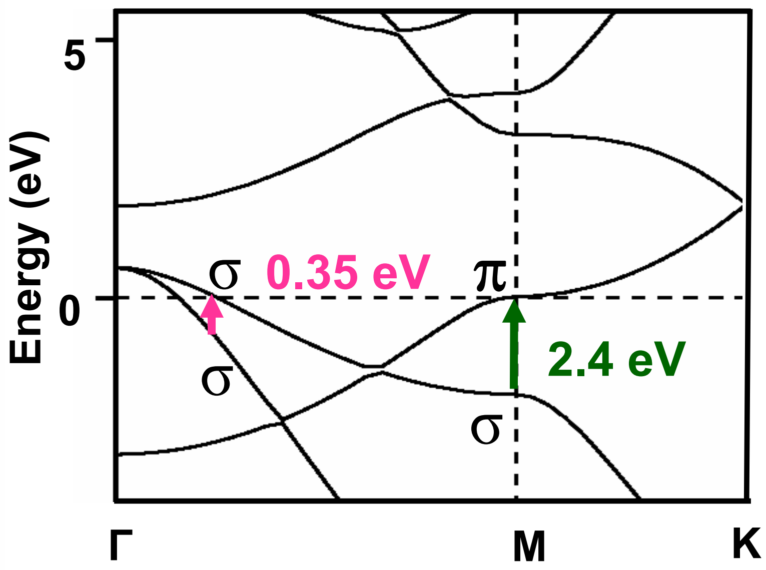


Optical spectra of in MgB_2



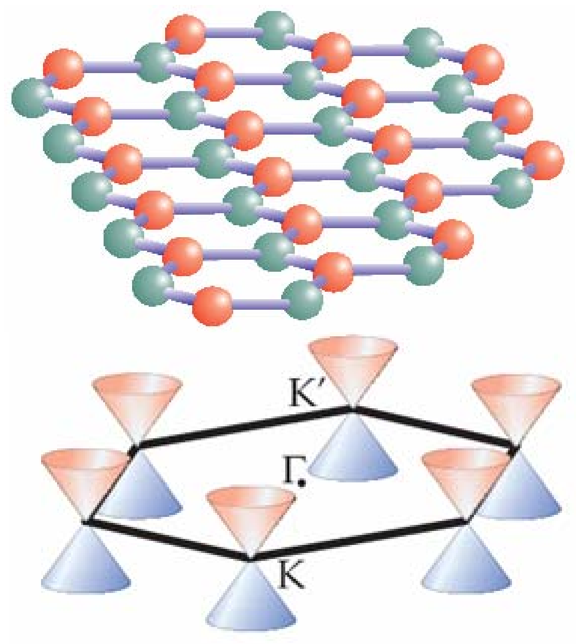
Two colors of MgB_2

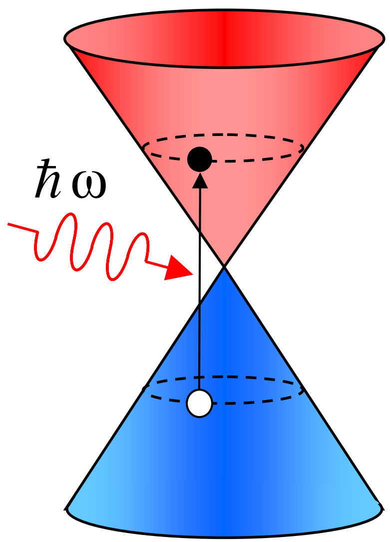




V. Guritanu *et al.* PRB **73**, 104509 (2006)

Monolayer graphene





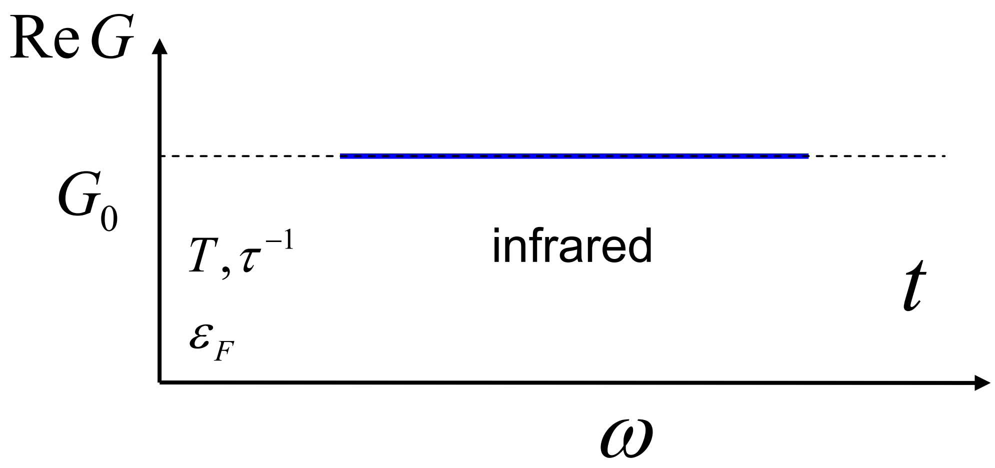
Joint density of states $\mathrm{JDOS}(\omega) \propto \dfrac{\hbar\omega}{t^2 a^2}$

Velocity matrix element $v_{h\to e}(\omega) \propto \dfrac{ta}{\hbar}$

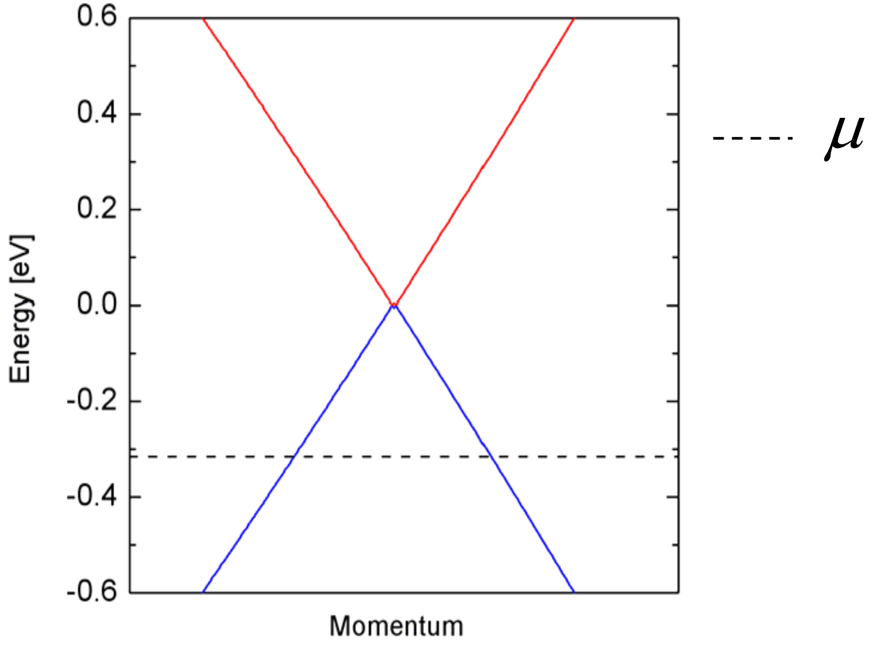
t – C-C hopping
a – C-C distance

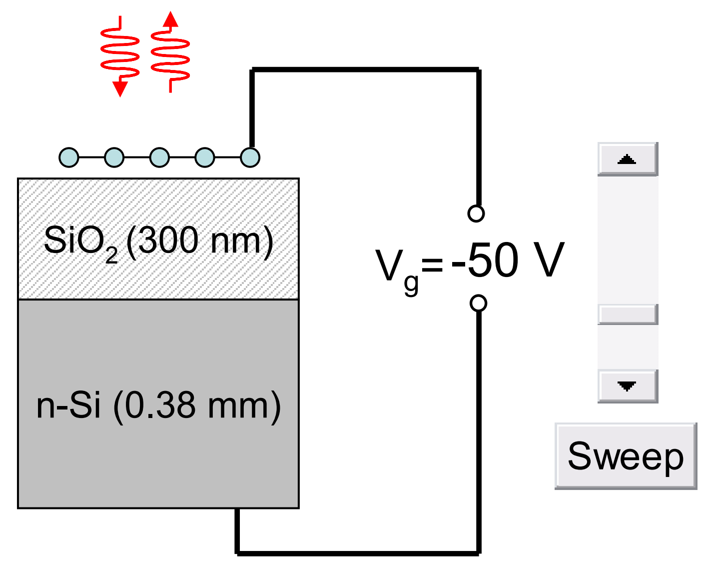
Sheet conductance:

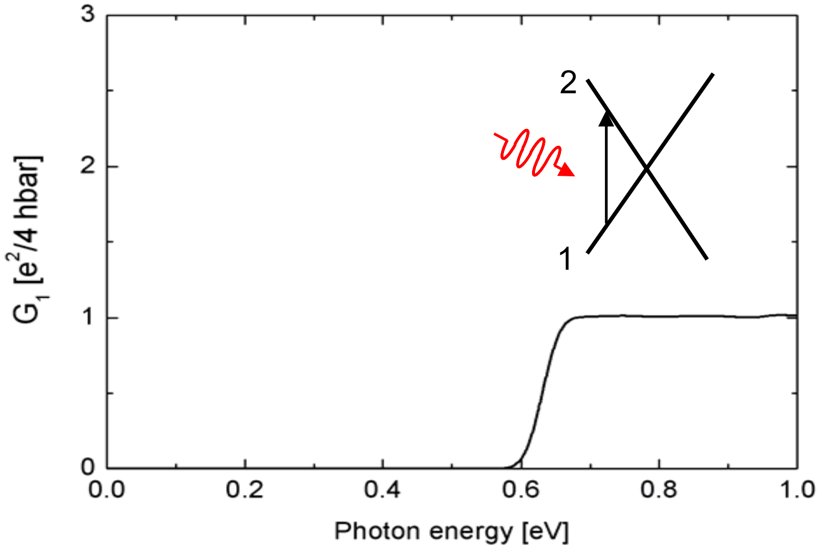
$$\mathrm{Re}\, G(\omega) = \frac{\pi e^2}{\omega} \left| v_{h\to e}(\omega) \right|^2 \mathrm{JDOS}(\omega) = \frac{e^2}{4\hbar} = G_0$$

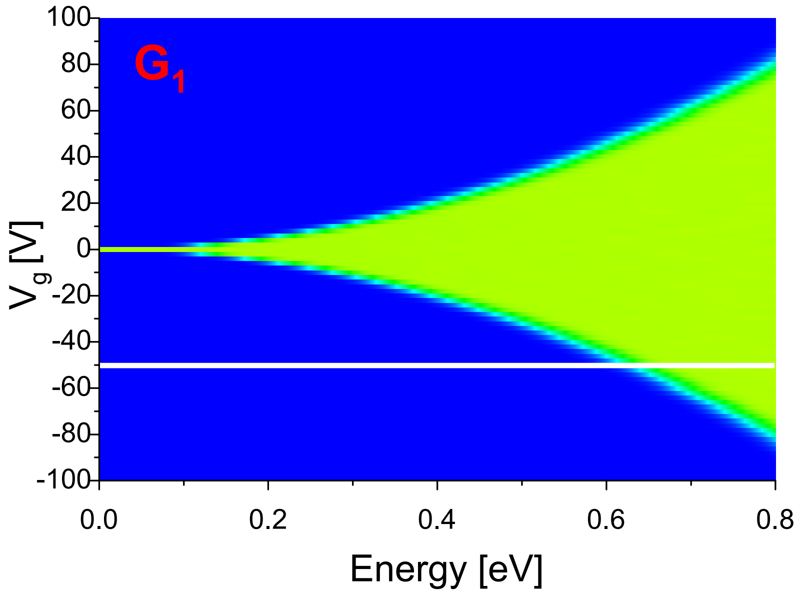


Tight binding results: monolayer graphene

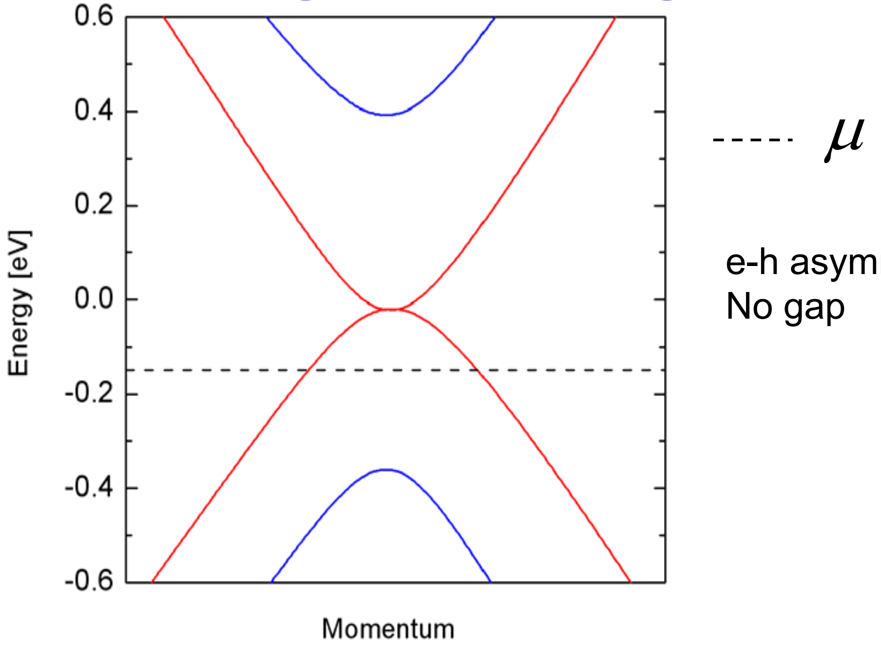




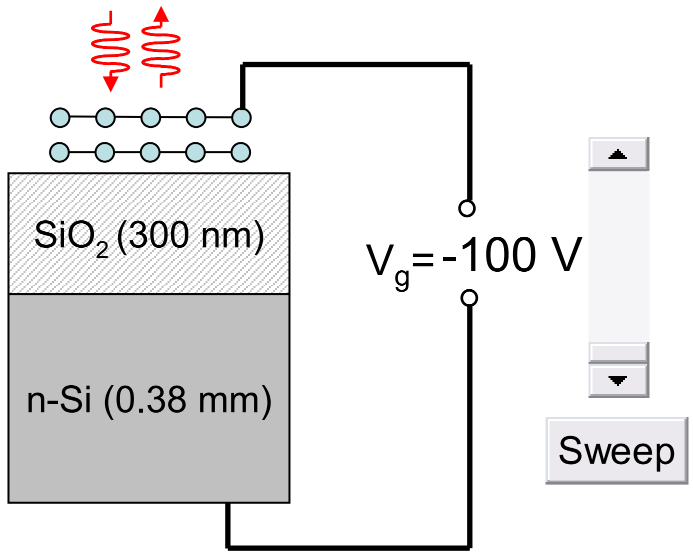


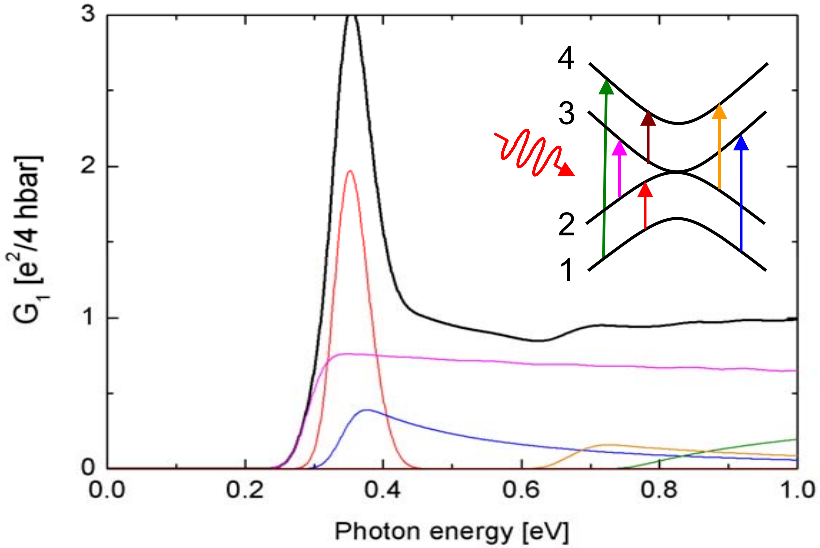


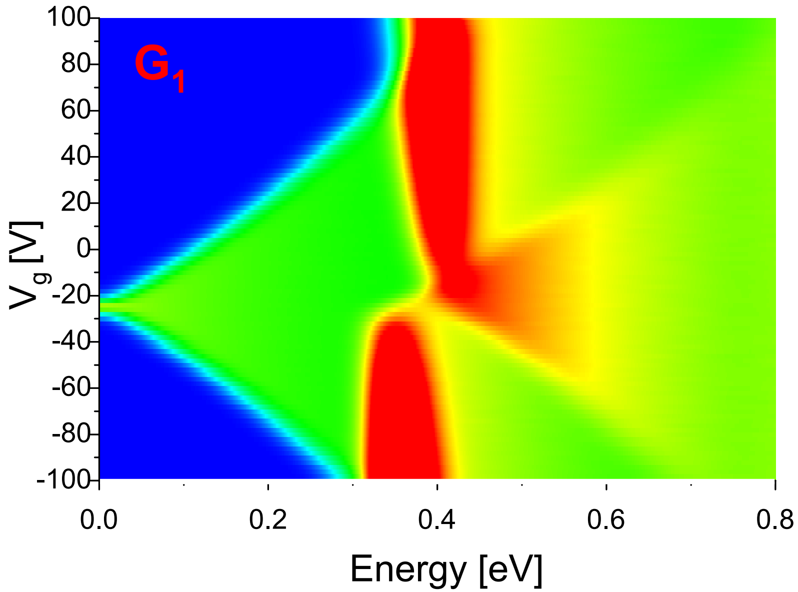
Tight binding results: bilayer graphene



e-h asymmetry
No gap







Deviations from the Drude formula

Standard Drude formula (energy independent scattering) $$\sigma(\omega) = \frac{\omega_p^2}{4\pi}\frac{i}{\omega + i\gamma}$$

Electron-boson scattering: photon creates an electron-hole pair and a boson (e.g. phonon)

$$\sigma(\omega) = \frac{\omega_p^2}{4\pi}\frac{i}{\omega + i\gamma(\omega)} \qquad \gamma(\omega) = \tau^{-1}(\omega) - i\omega\left[\frac{m^*(\omega)}{m_{band}} - 1\right]$$

$\tau^{-1}(\omega)$ ↑ scattering rate

$m^*(\omega)/m_{band}$ ↑ mass renormalization

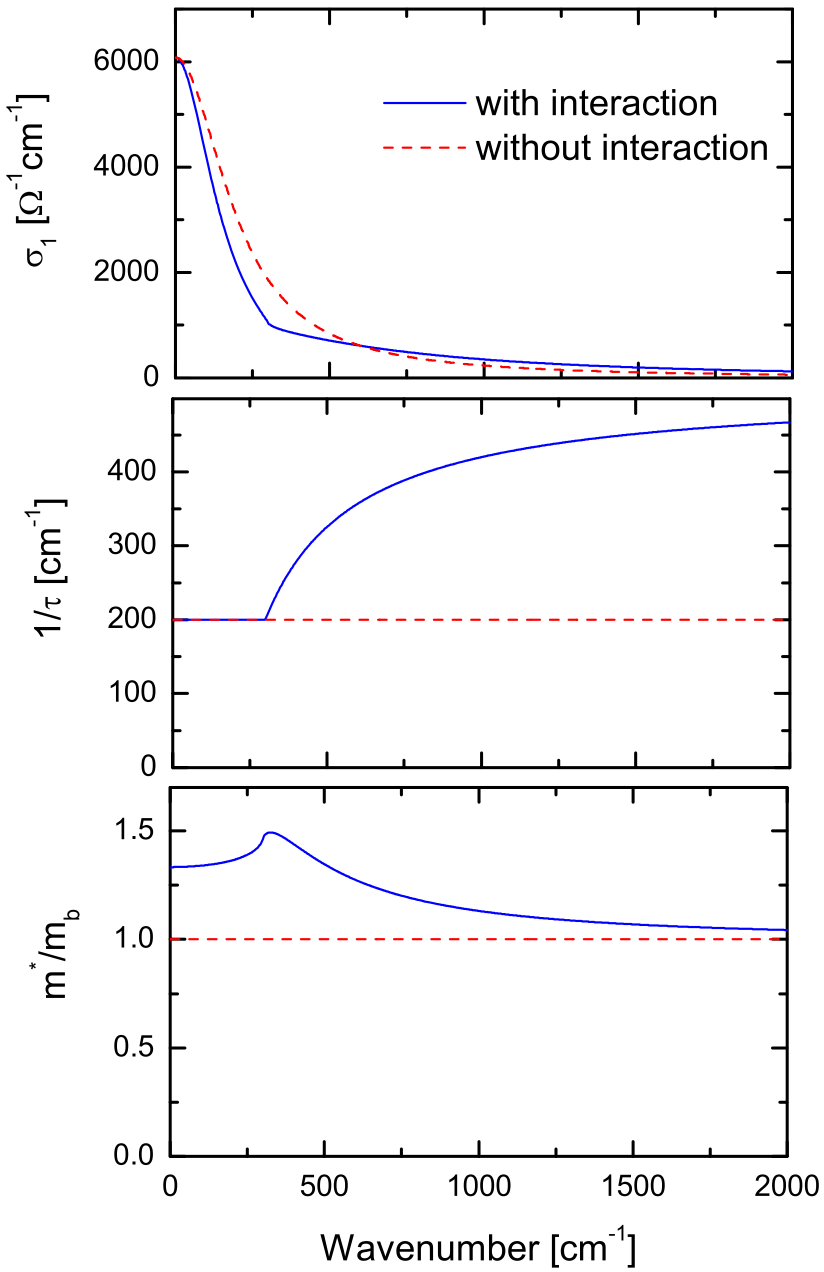
$$\gamma(\omega, T) = \gamma_{imp} + \int_o^\infty d\Omega\, \alpha^2 F(\Omega) K\left(\frac{\omega}{2\pi T}, \frac{\Omega}{2\pi T}\right)$$

$\alpha^2 F(\omega)$ – electron – boson coupling function

$$K(x, y) = \frac{2}{y} - 2i\frac{y-x}{x}\left[\Psi(1 - ix + iy) - \Psi(1 + iy)\right] - 2i\frac{y+x}{x}\left[\Psi(1 - ix - iy) - \Psi(1 - iy)\right],$$

$\Psi(z)$ – digamma function

Deviations from the Drude formula (example)



$$\sigma(\omega) = \frac{\omega_p^2}{4\pi} \frac{i}{\omega + i\gamma(\omega)}$$

$$\gamma(\omega) = \tau^{-1}(\omega) - i\omega\left[\frac{m^*(\omega)}{m_{band}} - 1\right]$$

Einstein oscillator

$$\alpha^2 F(\omega) = A\delta(\omega - \omega_0)$$

$$T = 0$$

$$\omega_0 = 300 \text{ cm}^{-1}$$

$$\omega_p = 8500 \text{ cm}^{-1}$$

$$\gamma_{imp} = 200 \text{ cm}^{-1}$$

Extended Drude analysis

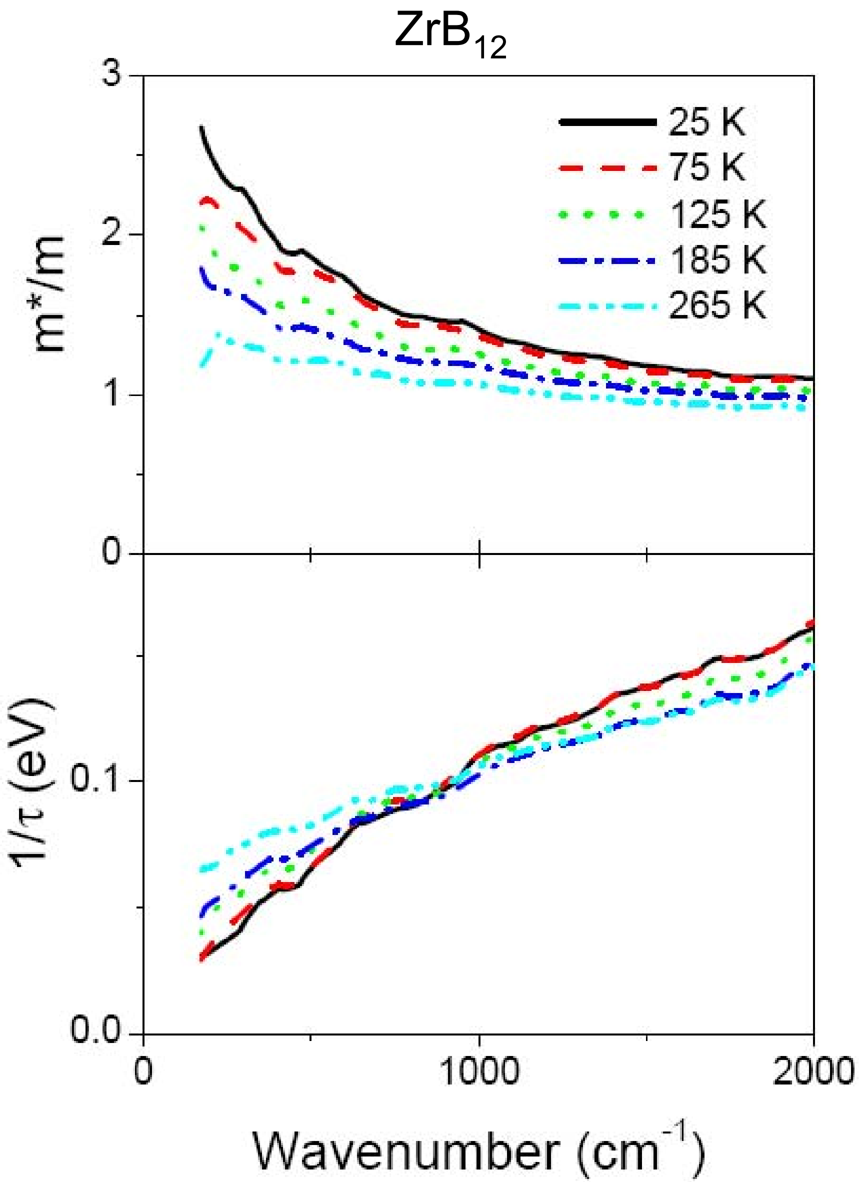
$$\sigma(\omega) = \frac{\omega_p^2}{4\pi} \frac{i}{\omega + i\gamma(\omega)}$$

$$\tau^{-1}(\omega) = \frac{\omega_p^2}{4\pi} \mathrm{Re}\left[\frac{1}{\sigma(\omega)}\right]$$

$$1 + \frac{m^*(\omega)}{m_b} = \frac{\omega_p^2}{4\pi\omega} \mathrm{Im}\left[-\frac{1}{\sigma(\omega)}\right]$$

Can be used to extract the coupling function $\alpha^2 F(\omega)$

There should be only one Drude component !



J. Teyssier et al. Phys. Rev. B **75**, 134503 (2007)