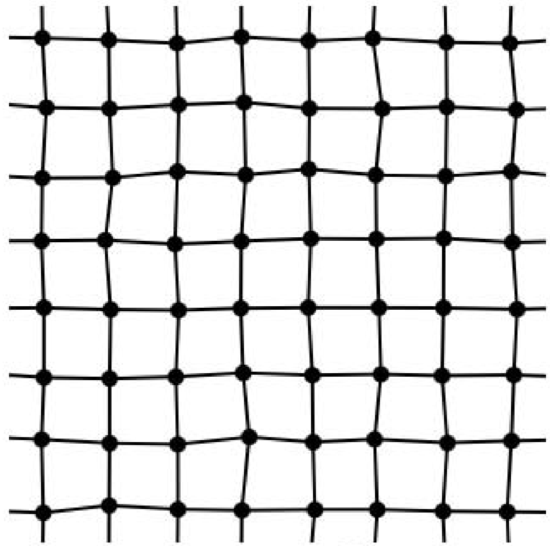
26. Quasiparticles

Jan. 21, 2018

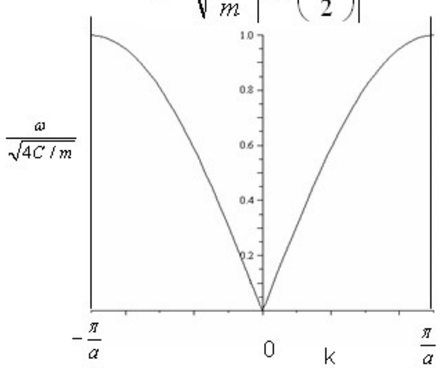
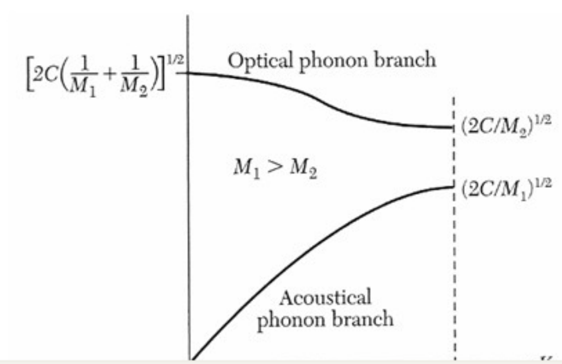
Normal Modes and Phonons

At finite temperatures, the atoms in a crystal vibrate. In the simulation below, the atoms move randomly around their equilibrium positions.



T = 300 K - +

http://lamp.tu-graz.ac.at/~hadley/ss1/phonons/phonontable.html

	Linear Chain $m\frac{d^2u_s}{dt^2} = C(u_{s+1} - 2u_s + u_{s-1})$	**Linear chain 2 masses** $M_1\frac{d^2u_s}{dt^2} = C(v_{s-1} - 2u_s + v_s)$ $M_2\frac{d^2v_s}{dt^2} = C(u_s - 2v_s + u_{s+1})$	**Linear chain 2 spring constants** $M\frac{d^2u_s}{dt^2} = C_1(v_{s-1} - 2u_s + v_s)$ $M\frac{d^2v_s}{dt^2} = C_2(u_s - 2v_s + u_{s+1})$	n
Eigenfunction solutions	$u_s = A_k e^{i(ksa-\omega t)}$	$u_s = ue^{i(ksa-\omega t)}$ $v_s = ve^{i(ksa-\omega t)}$	$u_s = ue^{i(ksa-\omega t)}$ $v_s = ve^{i(ksa-\omega t)}$	
Dispersion relation	$\omega = \sqrt{\frac{4C}{m}}\left\|\sin\left(\frac{ka}{2}\right)\right\|$ 	$\omega^2 = C\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \pm C\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4\sin^2 ka}{M_1M_2}}$ 		

Anharmonic terms

Expand the energy in terms of the normal modes of the linearized problem u_k

$$U = U_0 + \frac{\partial U}{\partial u_k} u_k + \frac{1}{2}\frac{\partial^2 U}{\partial u_j \partial u_k} u_j u_k + \frac{1}{6}\frac{\partial^3 U}{\partial u_i \partial u_j \partial u_k} u_i u_j u_k + \frac{1}{24}\frac{\partial^4 U}{\partial u_h \partial u_i \partial u_j \partial u_k} u_h u_i u_j u_k + \cdots$$

Thermal expansion
Thermal conductivity limited by Umklapp scattering
High temperature limit of specific heat does not approach the Dulong-Petit law

Phonon quasiparticle lifetime

Phonons are the eigenstates of the linearized equations, not the full equations.

Phonons have a finite lifetime that can be calculated by Fermi's golden rule.

$$\Gamma_{i \to f} = \frac{2\pi}{\hbar} \left| \langle f | H_{ph-ph} | i \rangle \right|^2 \delta\left(E_f - E_i\right)$$

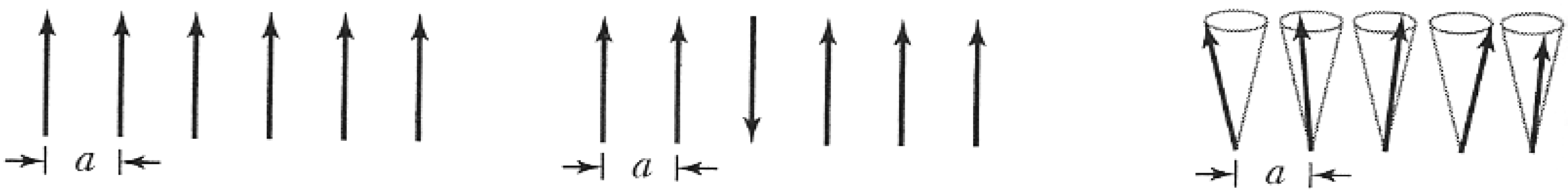
Occupation is determined by a master equation (not the Bose-Einstein function).

$$\begin{bmatrix} \frac{dP_0}{dt} \\ \frac{dP_1}{dt} \\ \vdots \\ \frac{dP_N}{dt} \end{bmatrix} = \begin{bmatrix} -\sum_{i \neq 0} \Gamma_{0 \to i} & \Gamma_{1 \to 0} & \cdots & \Gamma_{N \to 0} \\ \Gamma_{0 \to 1} & -\sum_{i \neq 1} \Gamma_{1 \to i} & \cdots & \Gamma_{N \to 1} \\ \vdots & \vdots & \ddots & \vdots \\ \Gamma_{0 \to N} & \Gamma_{1 \to N} & \cdots & -\sum_{i \neq N} \Gamma_{N \to i} \end{bmatrix} \begin{bmatrix} P_0 \\ P_1 \\ \vdots \\ P_N \end{bmatrix}$$

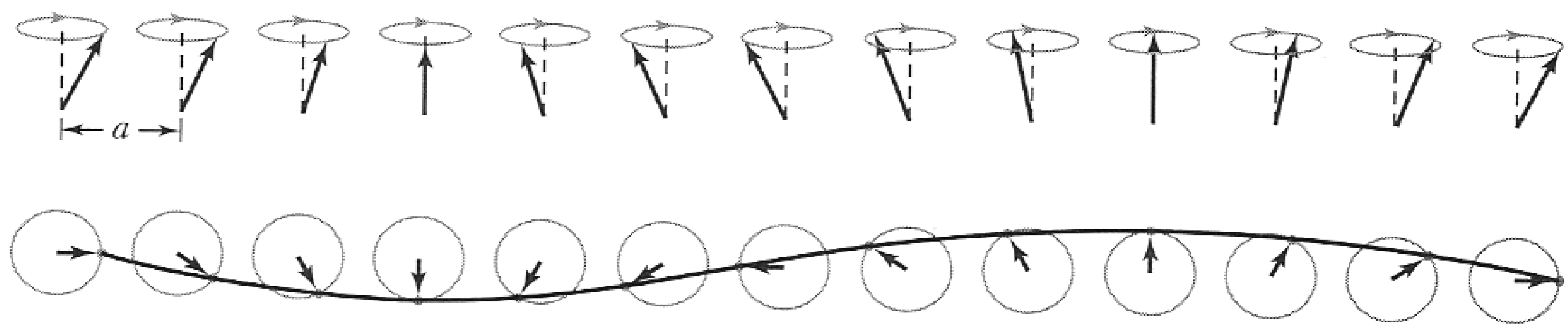
Acoustic attenuation

The amplitude of a monocromatic sound wave decreases as the wave propagates through the crystal as the phonon quasiparticles decay into phonons with other frequencies and directions.

Magnons



Magnons are excitations of the ordered ferromagnetic state



Magnons

Energy of the Heisenberg term involving spin *p*

$$-2J\vec{S}_p \cdot \left(\vec{S}_{p+1} + \vec{S}_{p-1}\right)$$

The magnetic moment of spin *p* is

$$\vec{\mu}_p = -g\mu_B \vec{S}_p$$

$$-\vec{\mu}_p \cdot \left(\frac{-2J}{g\mu_B}\right)\left(\vec{S}_{p+1} + \vec{S}_{p-1}\right)$$

This has the form $-\mu_p \cdot B_p$ where B_p is

$$\vec{B}_p = \left(\frac{-2J}{g\mu_B}\right)\left(\vec{S}_{p+1} + \vec{S}_{p-1}\right)$$

Magnons

$$\vec{\mu}_p = -g\mu_B \vec{S}_p \qquad \vec{B}_p = \left(\frac{-2J}{g\mu_B}\right)\left(\vec{S}_{p+1} + \vec{S}_{p-1}\right)$$

The rate of change of angular momentum is the torque

$$\hbar \frac{d\vec{S}_p}{dt} = \vec{\mu}_p \times \vec{B}_p = 2J\left(\vec{S}_p \times \vec{S}_{p+1} + \vec{S}_p \times \vec{S}_{p-1}\right)$$

If the amplitude of the deviations from perfect alignment along the *z*-axis are small:

$$\hbar \frac{dS_p^x}{dt} = 2J\left|S\right|\left(S_{p+1}^y - 2S_p^y + S_{p-1}^y\right)$$

$$\hbar \frac{dS_p^y}{dt} = 2J\left|S\right|\left(S_{p+1}^x - 2S_p^x + S_{p-1}^x\right)$$

$$\hbar \frac{d\vec{S}_p^z}{dt} = 0$$

Magnons

$$\hbar \frac{dS_p^x}{dt} = 2J\left|S\right|\left(S_{p+1}^y - 2S_p^y + S_{p-1}^y\right)$$

$$\hbar \frac{dS_p^y}{dt} = 2J\left|S\right|\left(S_{p+1}^x - 2S_p^x + S_{p-1}^x\right)$$

$$\hbar \frac{dS_p^z}{dt} = 0$$

These are coupled linear differential equations. The solutions have the form:

$$\begin{pmatrix} S_p^x \\ S_p^y \end{pmatrix} = \begin{pmatrix} u_k^x \\ u_k^y \end{pmatrix} \exp\left[i\left(kpa - \omega t\right)\right]$$

$$-i\hbar\omega u_k^x e^{ikpa} = 2J\left|S\right|\left(-e^{ik(p+1)a} + 2e^{ikpa} - e^{-ik(p-1)a}\right)u_k^y$$

$$-i\hbar\omega u_k^y e^{ikpa} = -2J\left|S\right|\left(-e^{ik(p+1)a} + 2e^{ikpa} - e^{-ik(p-1)a}\right)u_k^x$$

Cancel a factor of e^{ikpa}.

Magnons

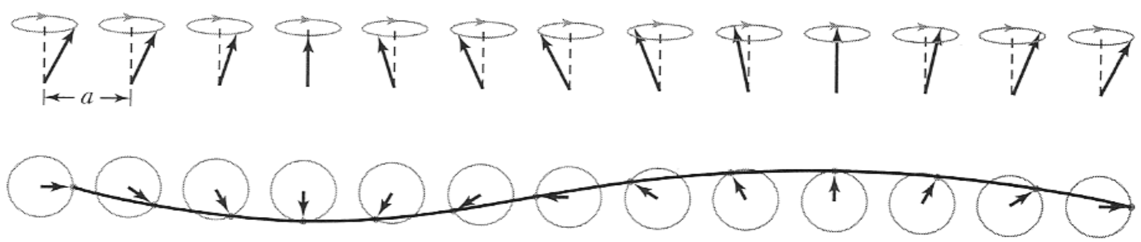
$$-i\hbar\omega u_k^x = 2J|S|\left(-e^{ika}+2-e^{-ika}\right)u_k^y$$
$$-i\hbar\omega u_k^y = -2J|S|\left(-e^{ika}+2-e^{-ika}\right)u_k^x$$

These equations will have solutions when,

$$\begin{vmatrix} i\hbar\omega & 4J|S|\left(1-\cos(ka)\right) \\ -4J|S|\left(1-\cos(ka)\right) & i\hbar\omega \end{vmatrix} = 0$$

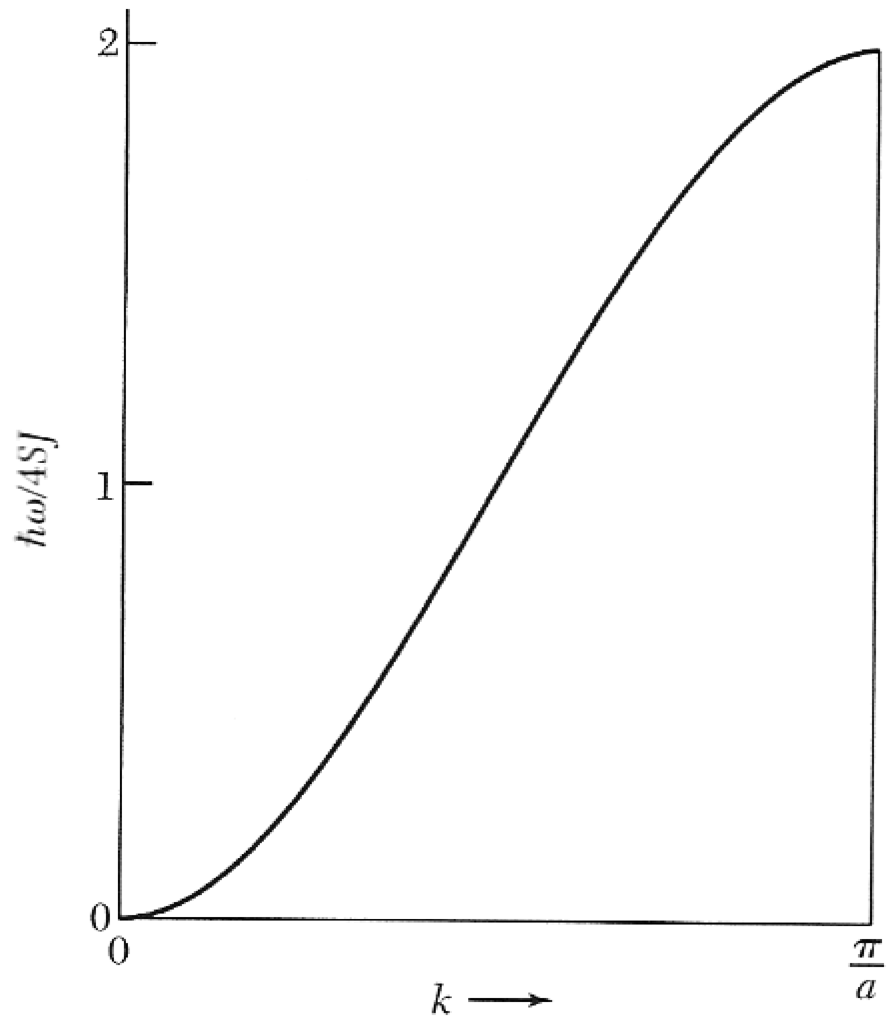
The dispersion relation is:

$$\hbar\omega = 4J|S|\left(1-\cos(ka)\right)$$



Magnon dispersion relation

$$\hbar\omega = 4JS\left(1-\cos(ka)\right)$$



A phonon dispersion relation would be linear at the origin

Magnons

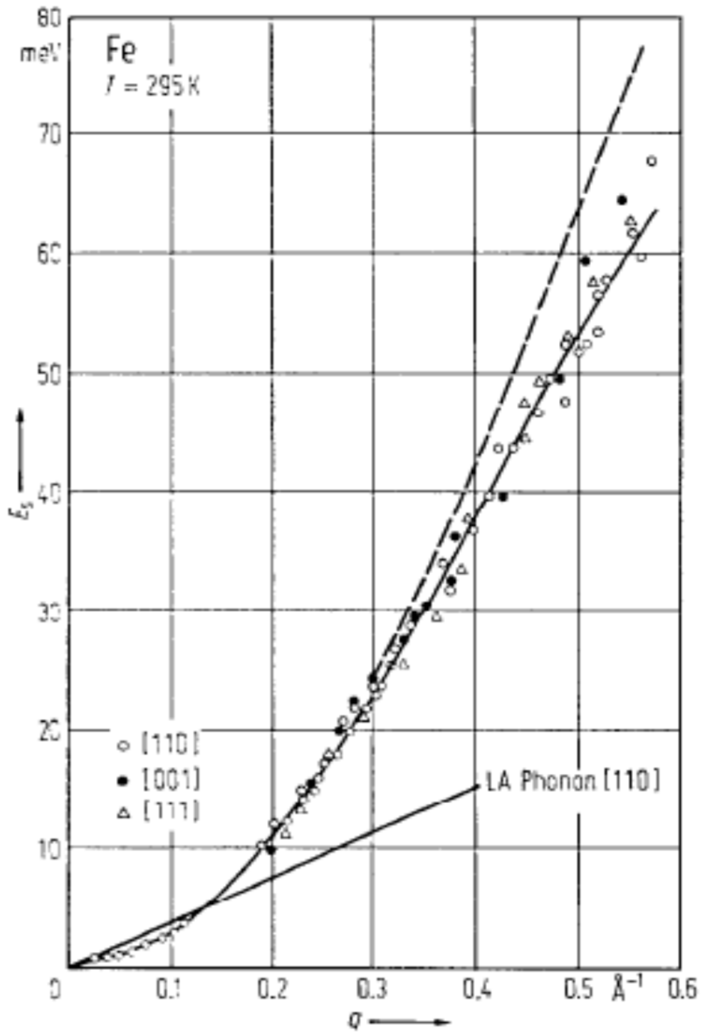


Fig. 1. Constant-E scan TAS-measured spin wave dispersion relation for various directions in a single crystal of Fe at 295 K. The dashed line corresponds to the Heisenberg model with $D = 281$ meV Å^2 and $\beta = 1.0$ Å^2 [68 S 3], see also [73 M 1].

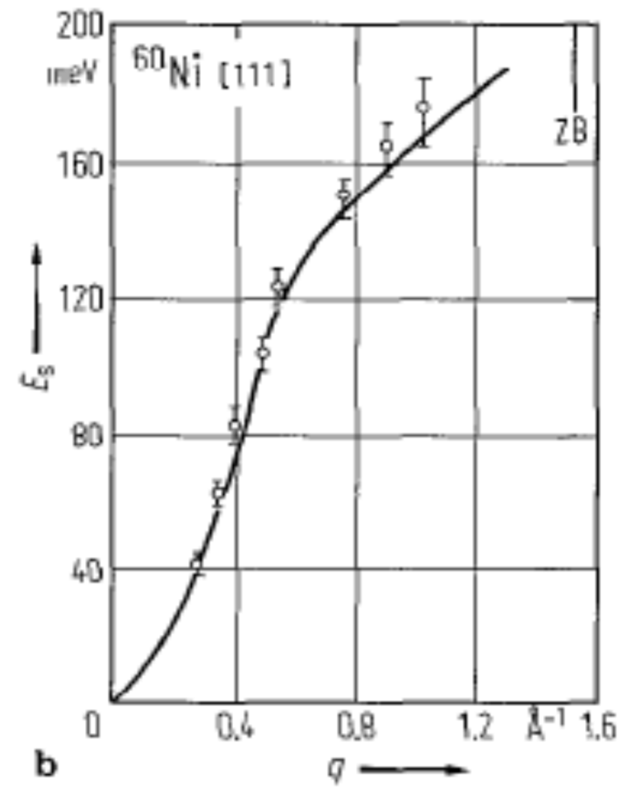
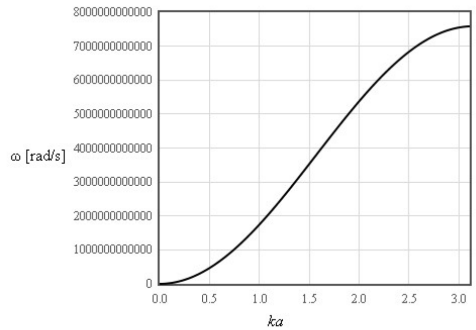
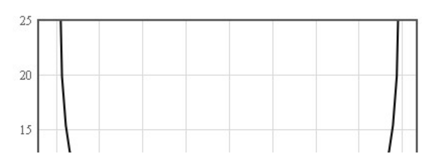


Fig. 6b. Room-temperature spin wave dispersion curve for the [111] direction of ^{60}Ni. ZB shows the position of the zone boundary [85 M 1]. The solid curve is from calculations [85 C 1, 83 C 1].

Student project

Make a table of magnon properties like the table of phonon properties

Magnons

	1-D ferromagnetic magnons	1-D antiferromagnetic magnons	3-D low temperature limit	
Equations of motion in mean field theory				
Eigenfunction solutions	$\begin{pmatrix}S_p^x\\S_p^y\end{pmatrix}=\begin{pmatrix}u_k^x\\u_k^y\end{pmatrix}\exp\left[i\left(kpa-\omega t\right)\right]$			
Dispersion relation	$\hbar\omega = 4JS\left(1-\cos(ka)\right)$  Calculate ω(k)			
				$D(E)$

Fe bcc
Ni fcc
Co hcp

1 student / column

Longitudinal plasma waves

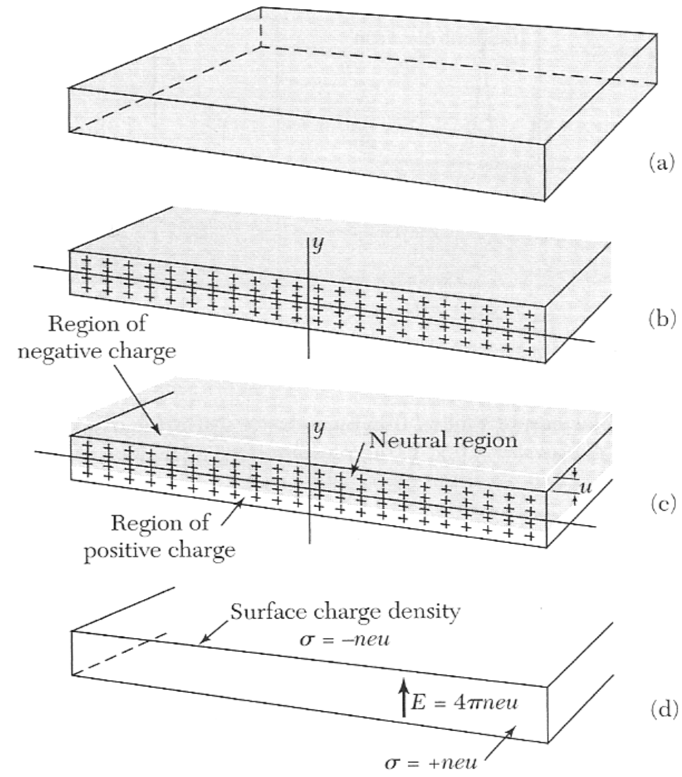
$$nm\frac{d^2y}{dt^2} = -neE$$

$$E = \frac{ney}{\varepsilon_0}$$

$$nm\frac{d^2y}{dt^2} = -\frac{n^2e^2y}{\varepsilon_0}$$

$$\frac{d^2y}{dt^2} + \omega_p^2 y = 0$$

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



Kittel

There is no magnetic component of the wave.

Plasma waves can be quantized like any other wave

Transverse optical plasma waves

The dispersion relation for light

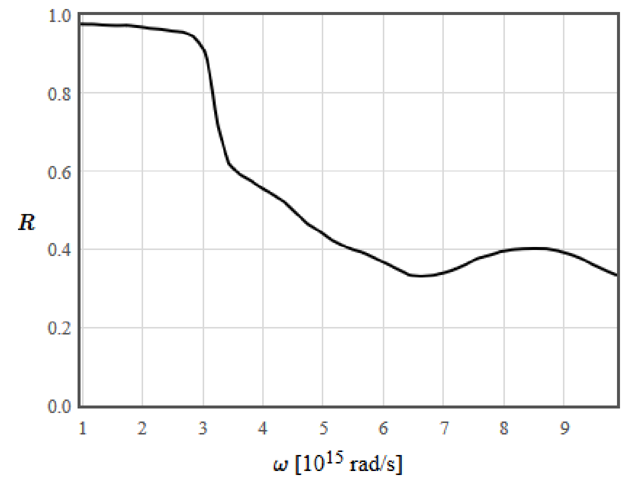
$$\varepsilon\varepsilon_0\mu_0\omega^2 = \frac{\varepsilon\omega^2}{c^2} = k^2$$

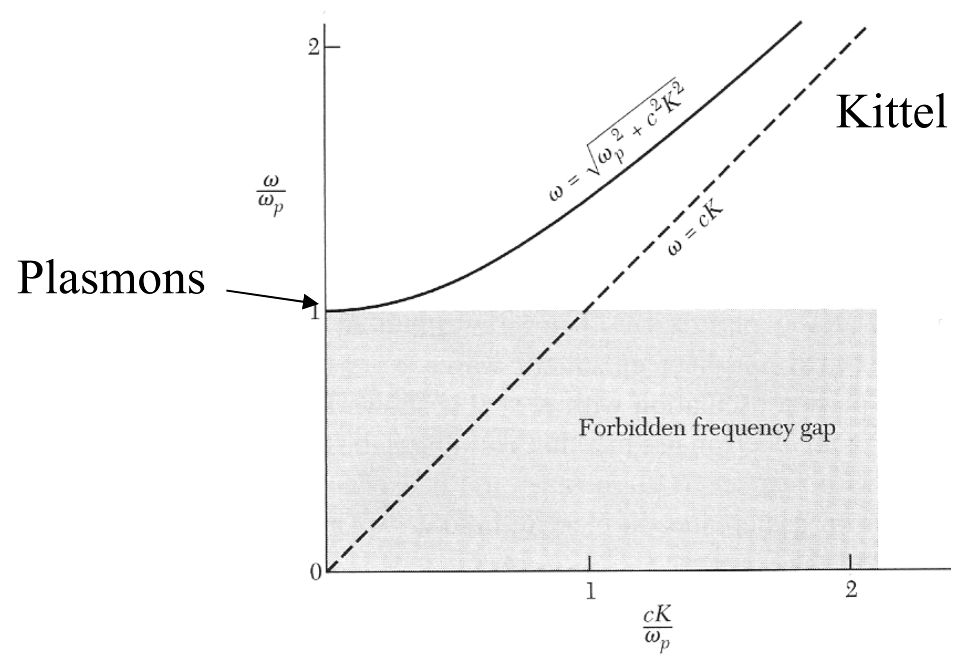
For a free electron gas

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

$$\left(1 - \frac{\omega_p^2}{\omega^2}\right)\omega^2 = c^2k^2$$

$$\omega^2 = \omega_p^2 + c^2k^2$$





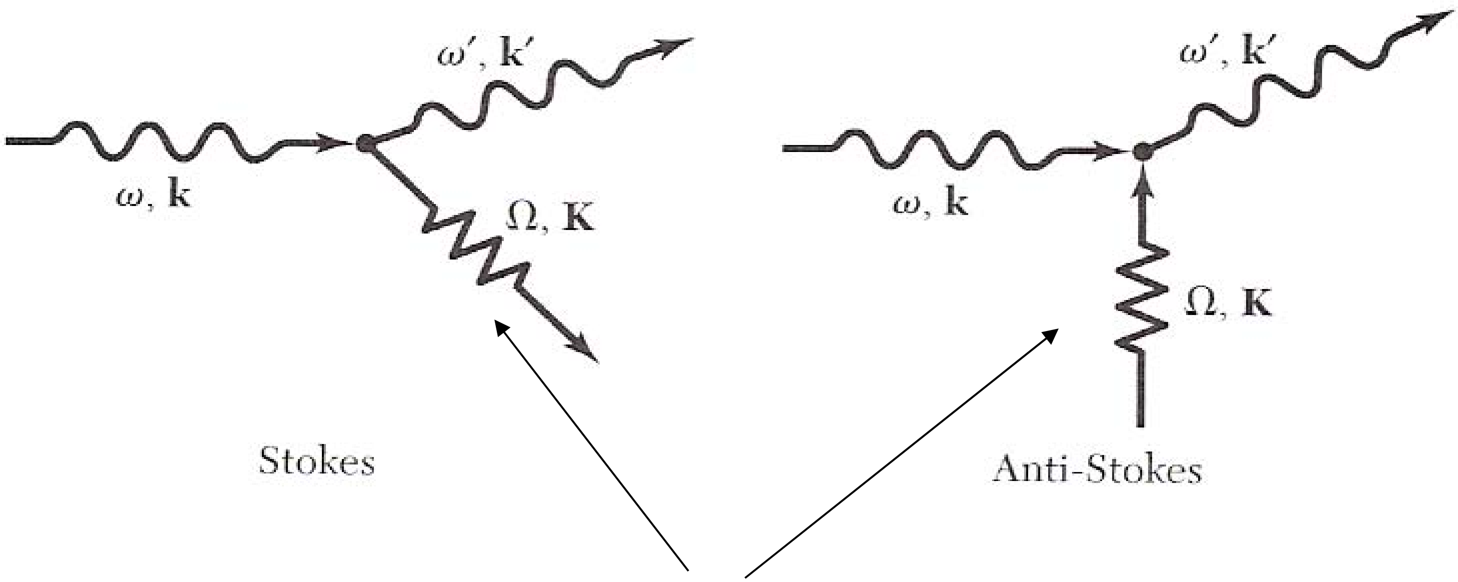
Raman Spectroscopy

C. V. Raman

Inelastic light scattering

$$\omega = \omega' \pm \Omega$$

$$\vec{k} = \vec{k}' \pm \vec{K} \pm \vec{G}$$



Phonons, magnons, plasmons, polaritons, ...

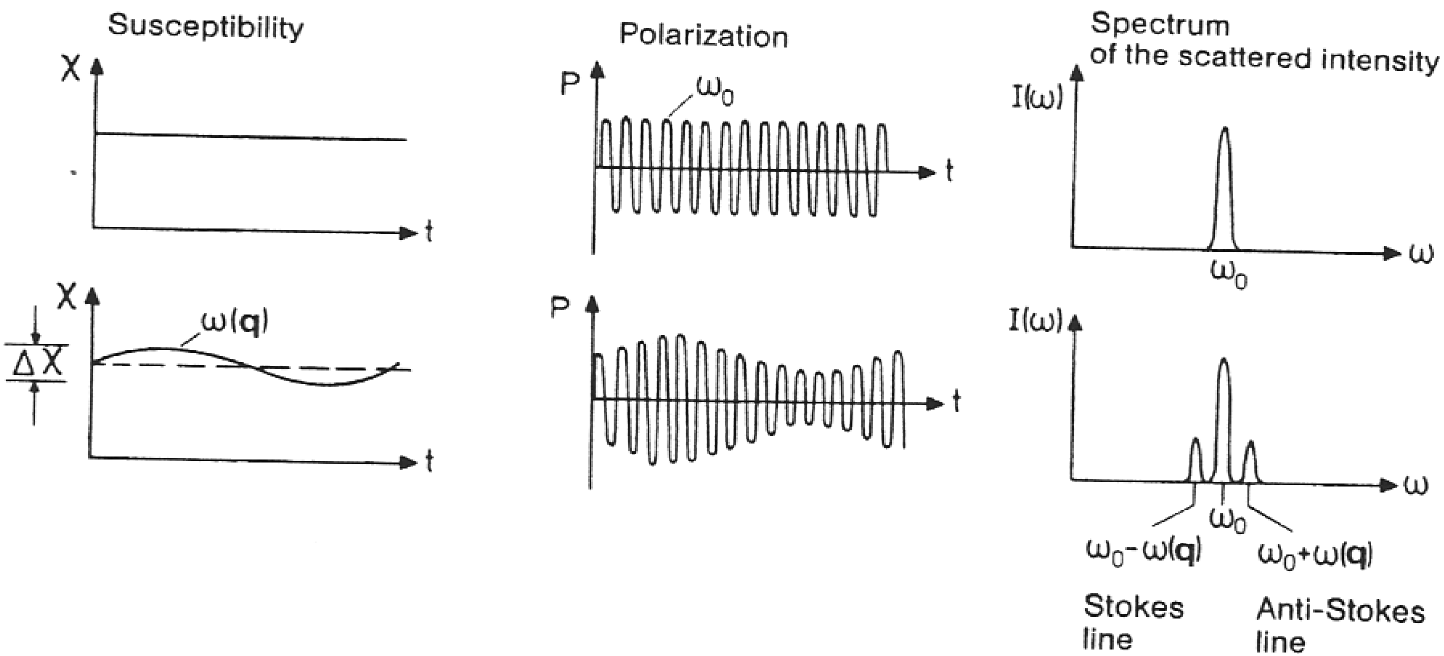
$$\vec{K} \approx 0$$

Raman Spectroscopy

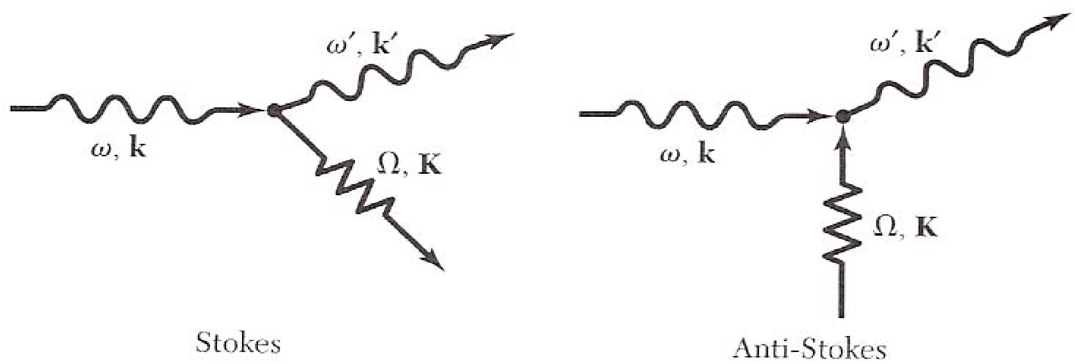
$$\chi = \chi_0 + \frac{\partial \chi}{\partial X} X \cos(\Omega t)$$

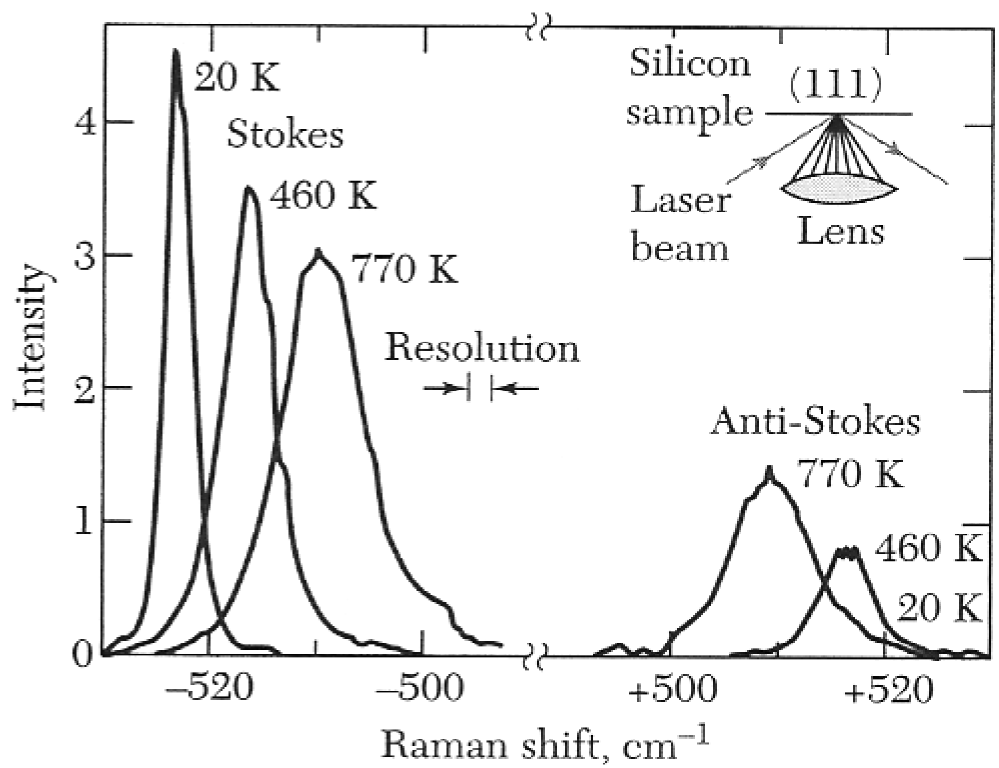
$$\vec{P} = \varepsilon_0 \chi \vec{E} \cos(\omega t) + \varepsilon_0 \frac{\partial \chi}{\partial X} X \cos(\Omega t) \vec{E} \cos(\omega t)$$

There are components of the polarization that oscillate at $\omega \pm \Omega.$



Raman Spectroscopy





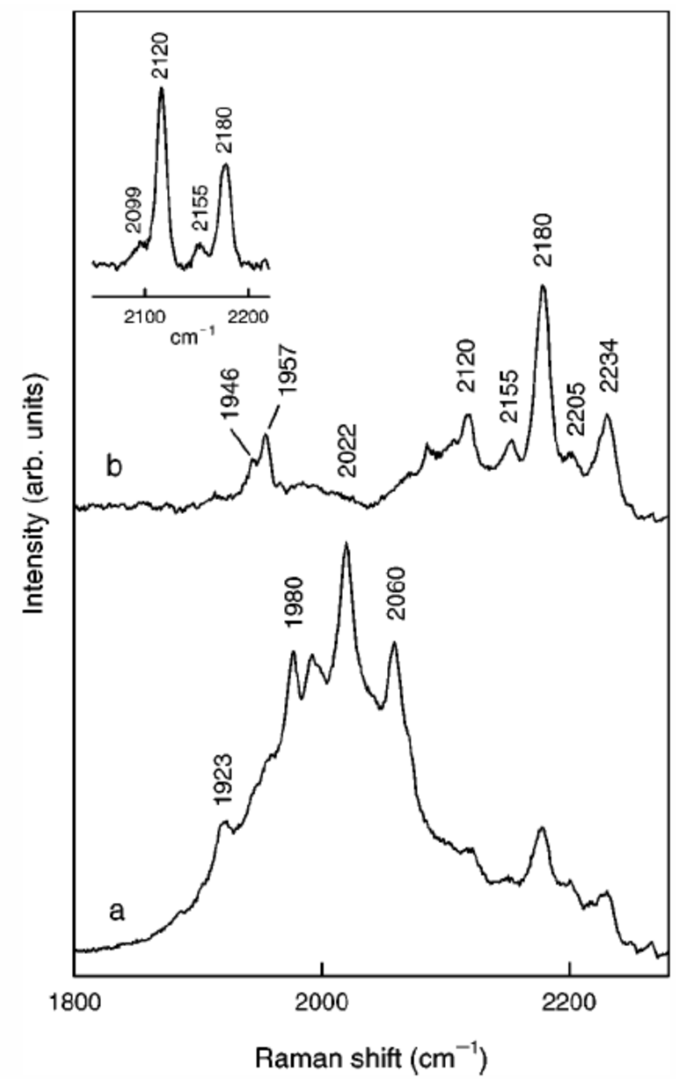
PHYSICAL REVIEW B, VOLUME 64, 035204

Vacancy-hydrogen defects in silicon studied by Raman spectroscopy

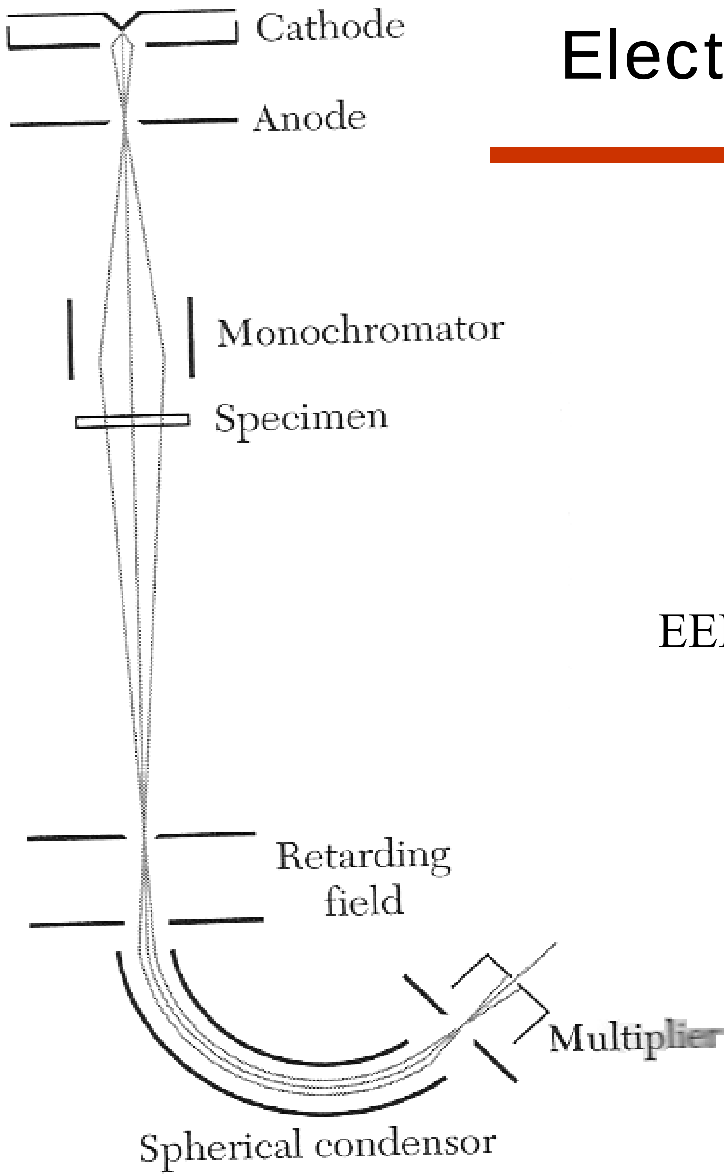
E. V. Lavrov* and J. Weber

Raman spectroscopy

FIG. 1. Raman spectra measured at room temperature on the H_2-implanted sample: (a) as-implanted sample, (b) after annealing at 400 °C for 2 min. Spectra are offset vertically for clarity.



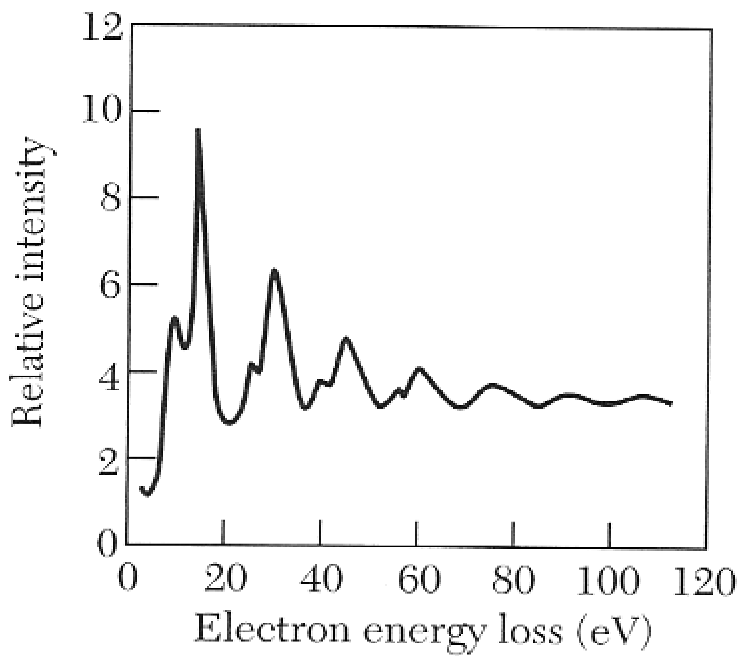
Electron energy loss spectroscopy

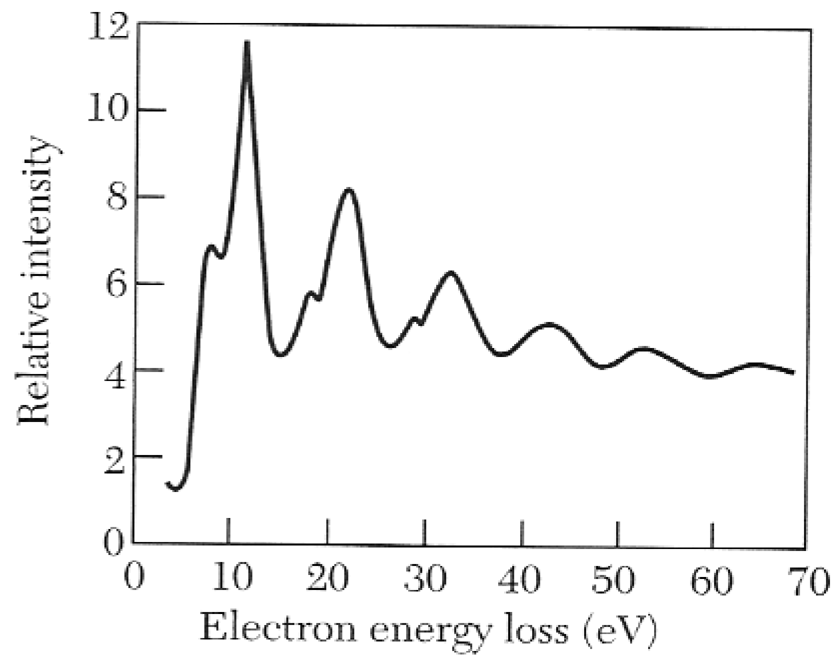


$$\Delta E = n\hbar\omega_p$$

EELS is often used to measure phonons

Electron energy loss spectroscopy





Aluminum

Plasmons 15.3 eV

Surface plasmons 10.3 eV

Magnesium

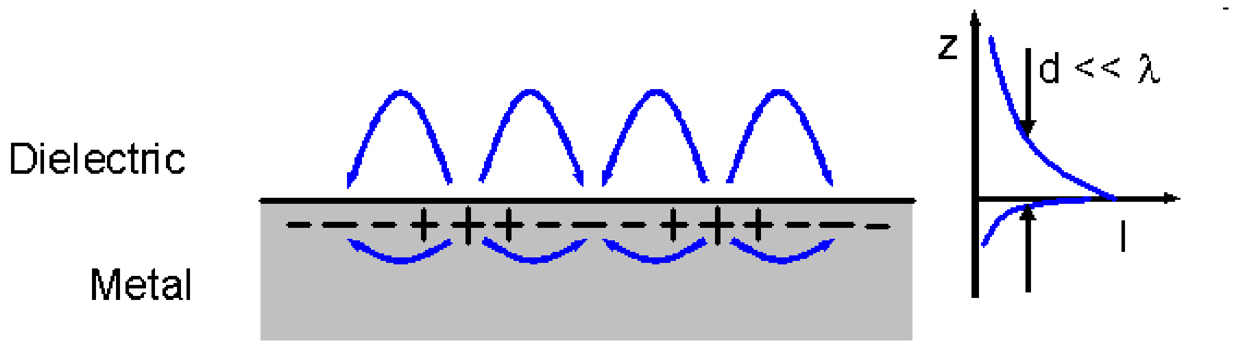
Plasmons 10.6 eV

Surface plasmons 7.1 eV

Surface Plasmons

Waves in the electron density at the boundary of two materials.

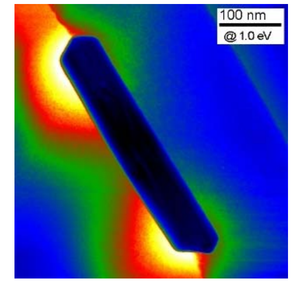
Surface plasmons have a lower frequency that bulk plasmons. This confines them to the interface.



Surface Plasmons

High-resolution surface plasmon imaging of gold nanoparticles by energy-filtered transmission electron microscopy

PHYSICAL REVIEW B 79, 041401 R 2009



Surface plasmons on nanoparticles are efficient at scattering light.

Green and blue require different sized particles.

Nature Photonics

LETTERS

Organic plasmon-emitting diode

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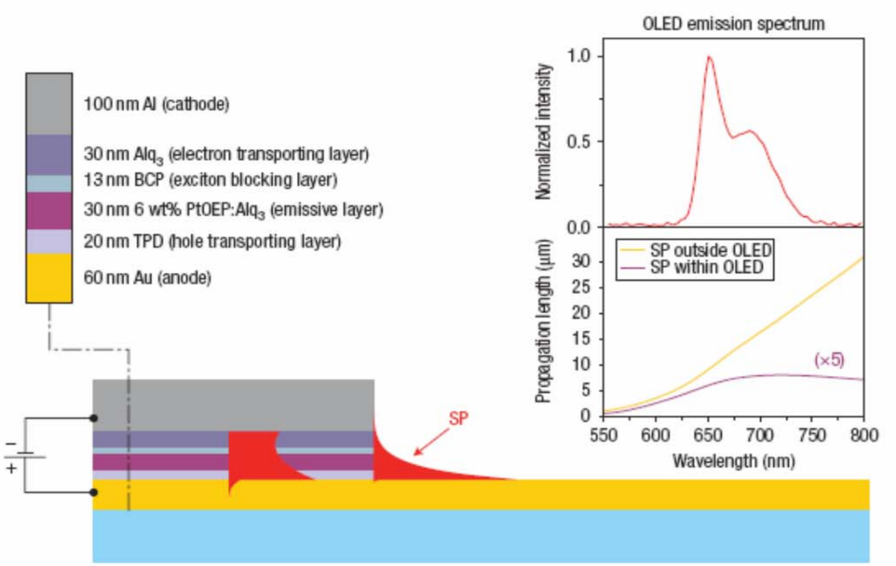
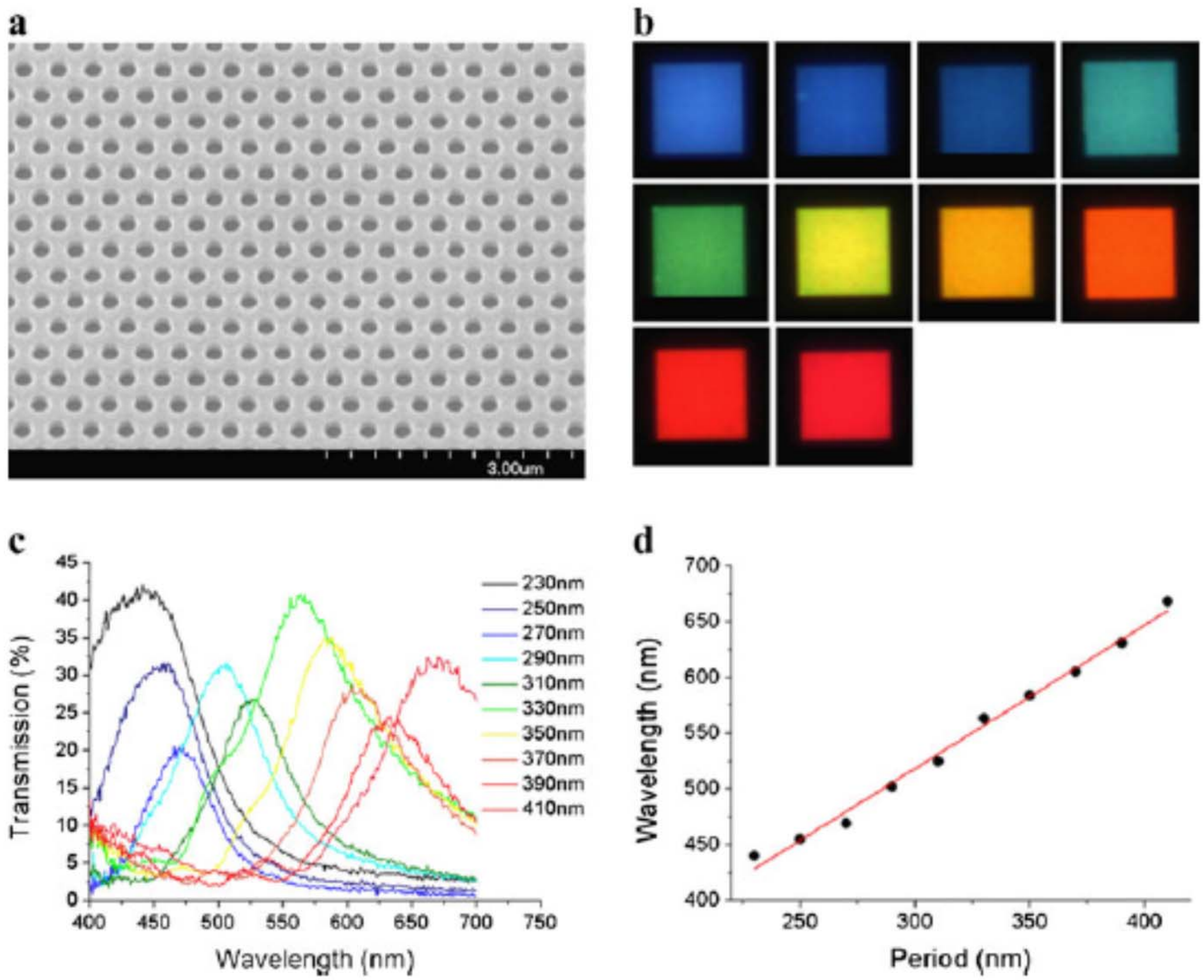
Surface plasmons are hybrid modes of longitudinal electron oscillations and light fields at the interface of a metal and a dielectric[1,2]. Driven by advances in nanofabrication, imaging and numerical methods[3,4], a wide range of plasmonic elements such as waveguides[5,6], Bragg mirrors[7], beamsplitters[8], optical modulators[9] and surface plasmon detectors[10] have recently been reported. For introducing dynamic functionality to plasmonics, the rapidly growing field of organic optoelectronics[11] holds strong promise due to its ease of fabrication and integration opportunities. Here, we introduce an electrically switchable



Surface plasmons are used for biosensors.

Plasmon filter

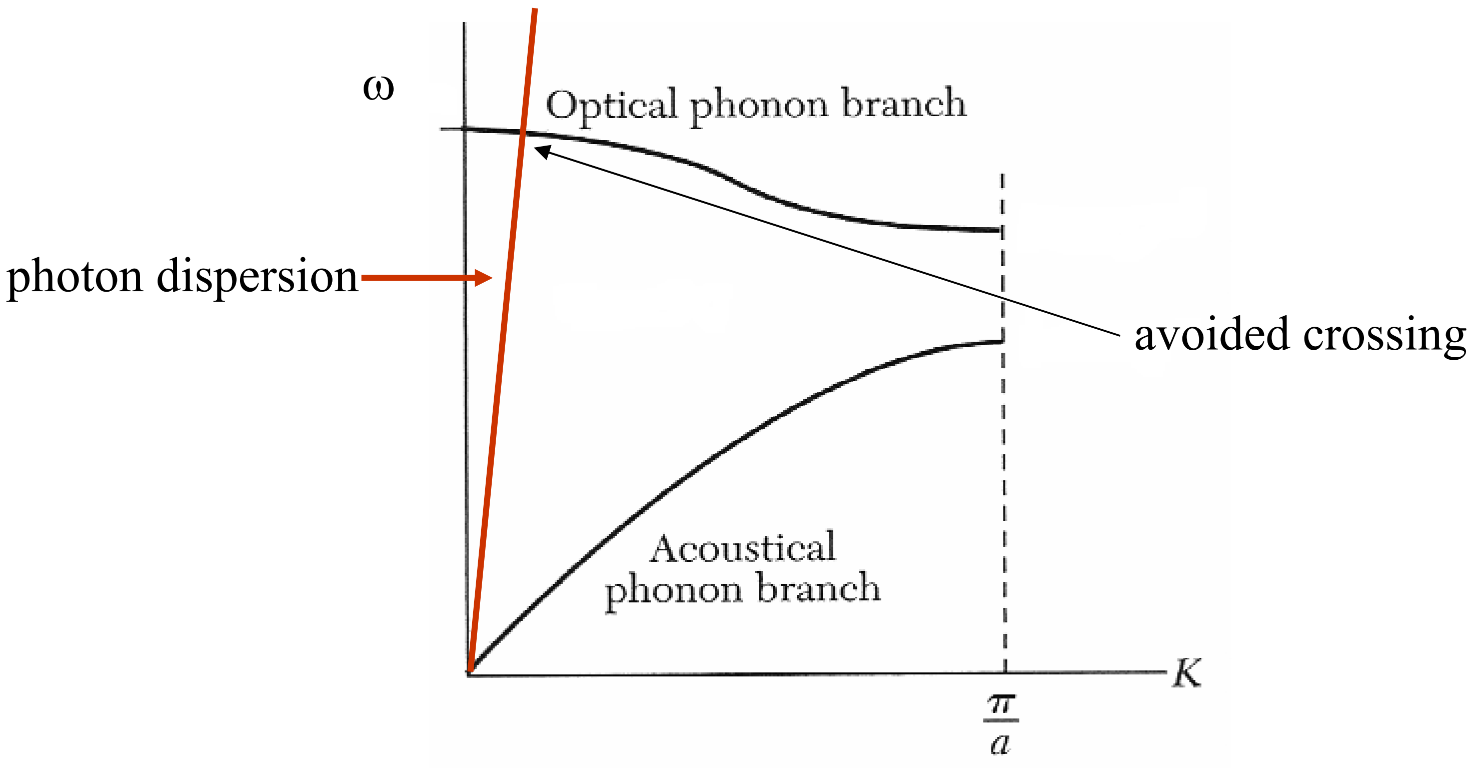


Plasmon modes on the other side of the metal films are excited.

http://web.pdx.edu/~larosaa/Applied_Optics_464-564/Lecture_Notes_Posted/2010_Lecture-7_SURFACE%20PLASMON%20POLARITONS%20AT%20%20METALINSULATOR%20INTERFACES/Lecture_on_the_Web_SURFACE-PLASMONS-POLARITONS.pdf

Polaritons

Transverse optical phonons will couple to photons with the same ω and *k*.



Light Bragg reflects off the sound wave; sound Bragg reflects off the light wave.

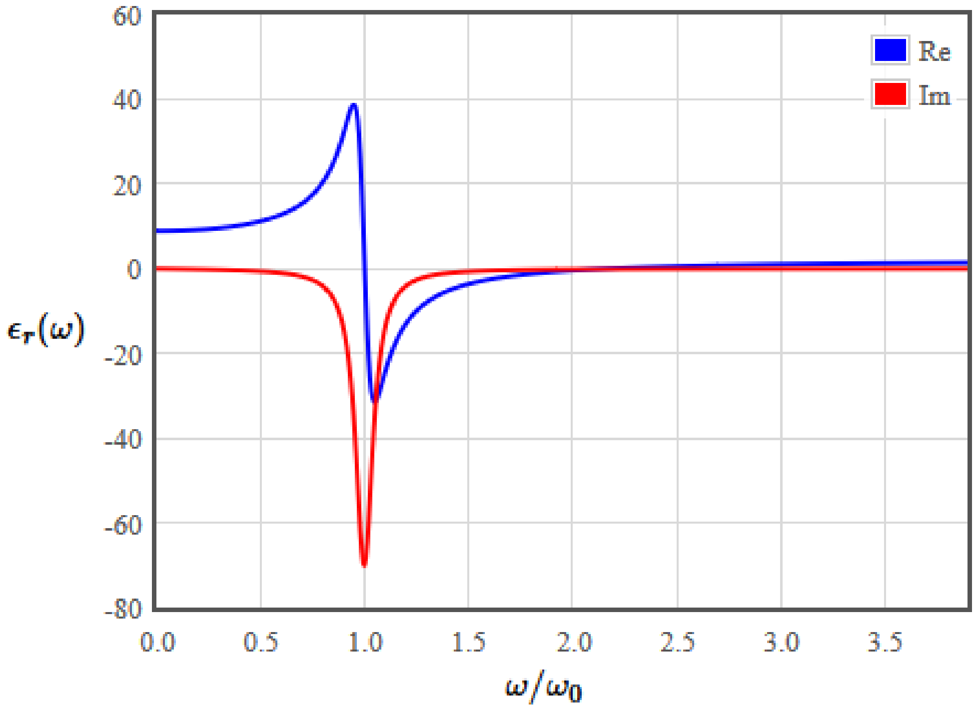
Polaritons

The dispersion relation for light

$$\varepsilon\varepsilon_0\mu_0\omega^2 = \frac{\varepsilon\omega^2}{c^2} = k^2$$

For an insulator

$$\epsilon_r(\omega) = \epsilon(\infty) + \frac{\omega_0^2(\epsilon(0)-\epsilon(\infty))}{\omega_0^2-\omega^2+i\gamma\omega}$$



The description of polaritons is already built into the dielectric function.

Polaritons

Ignore the loss term $i\gamma\omega$

$$\varepsilon(\omega) = \varepsilon(\infty) + \frac{\omega_0^2\left(\varepsilon(0) - \varepsilon(\infty)\right)}{\omega_0^2 - \omega^2}$$

Use a common denominator

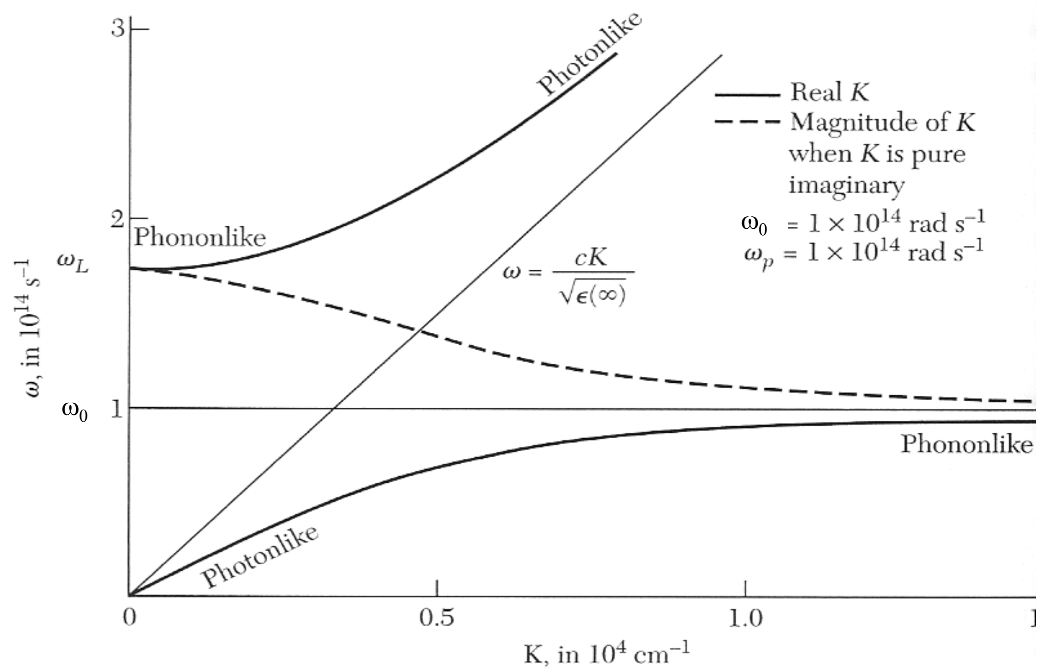
$$\varepsilon(\omega) = \frac{\varepsilon(\infty)\left(\omega_0^2 - \omega^2\right) + \omega_0^2\left(\varepsilon(0) - \varepsilon(\infty)\right)}{\omega_0^2 - \omega^2}$$

Define ω_L $\quad \omega_0^2\varepsilon(0) = \varepsilon(\infty)\omega_L^2$

$$\varepsilon(\omega) = \varepsilon(\infty)\frac{\omega_L^2 - \omega^2}{\omega_0^2 - \omega^2}$$

Polaritons

$$\varepsilon(\infty)\frac{\omega_L^2-\omega^2}{\omega_0^2-\omega^2}\frac{\omega^2}{c^2}=k^2$$

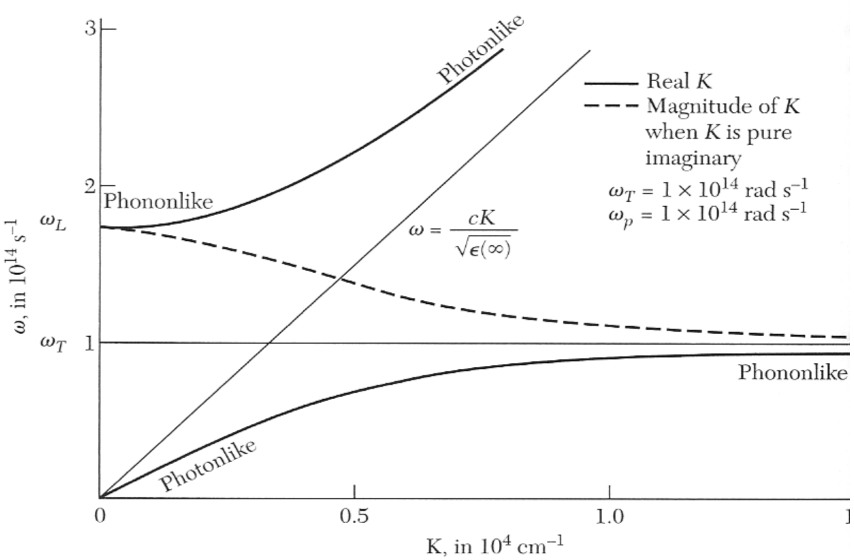


There are two solutions for every *k*, one for the upper branch and one for the lower branch.

Polaritons are the normal modes near the avoided crossing.

A gap exists in frequency.

Polaritons allow us to study the properties of phonons using optical measurements



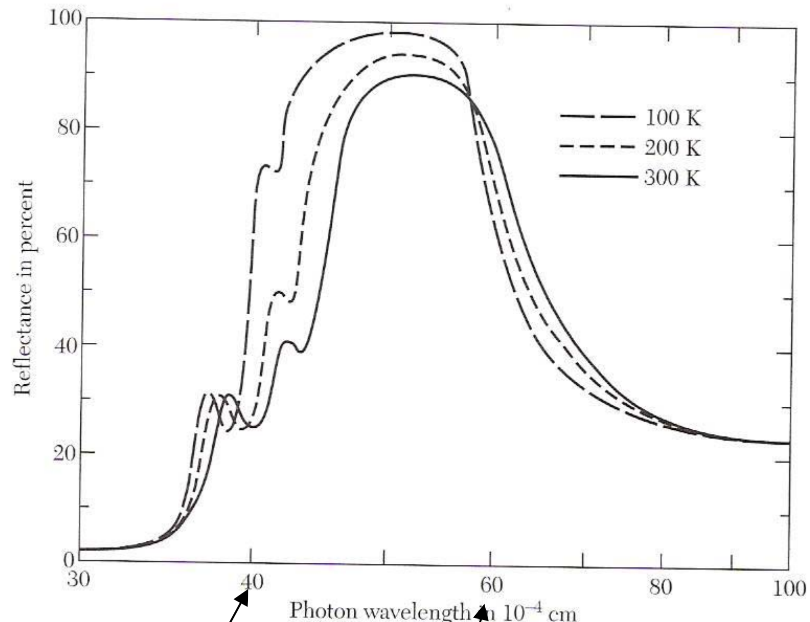


Figure 15 Reflectance of a crystal of NaCl at several temperatures, versus wavelength. The nominal values of ω_L and ω_T at room temperature correspond to wavelengths of 38 and 61 × 10^{-4} cm, respectively. (After A. Mitsuishi et al.)

ω = 4.7E13

ω = 3.1E13

Kittel

By looking at the reflectance in different crystal directions, you can determine the frequencies of the transverse optical phonons.

Polaritons and optical properties

TU Graz

Print version

Advanced Solid State Physics

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
Superconductivity
Exam questions
Appendices
Lectures
Books
Course notes
TUG students
Making presentations

Optical properties of insulators and semiconductors

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

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

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

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

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

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

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

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

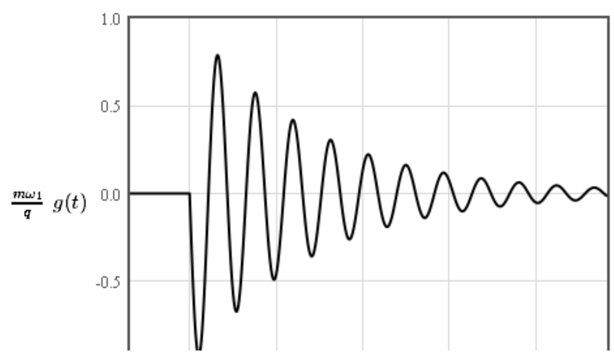
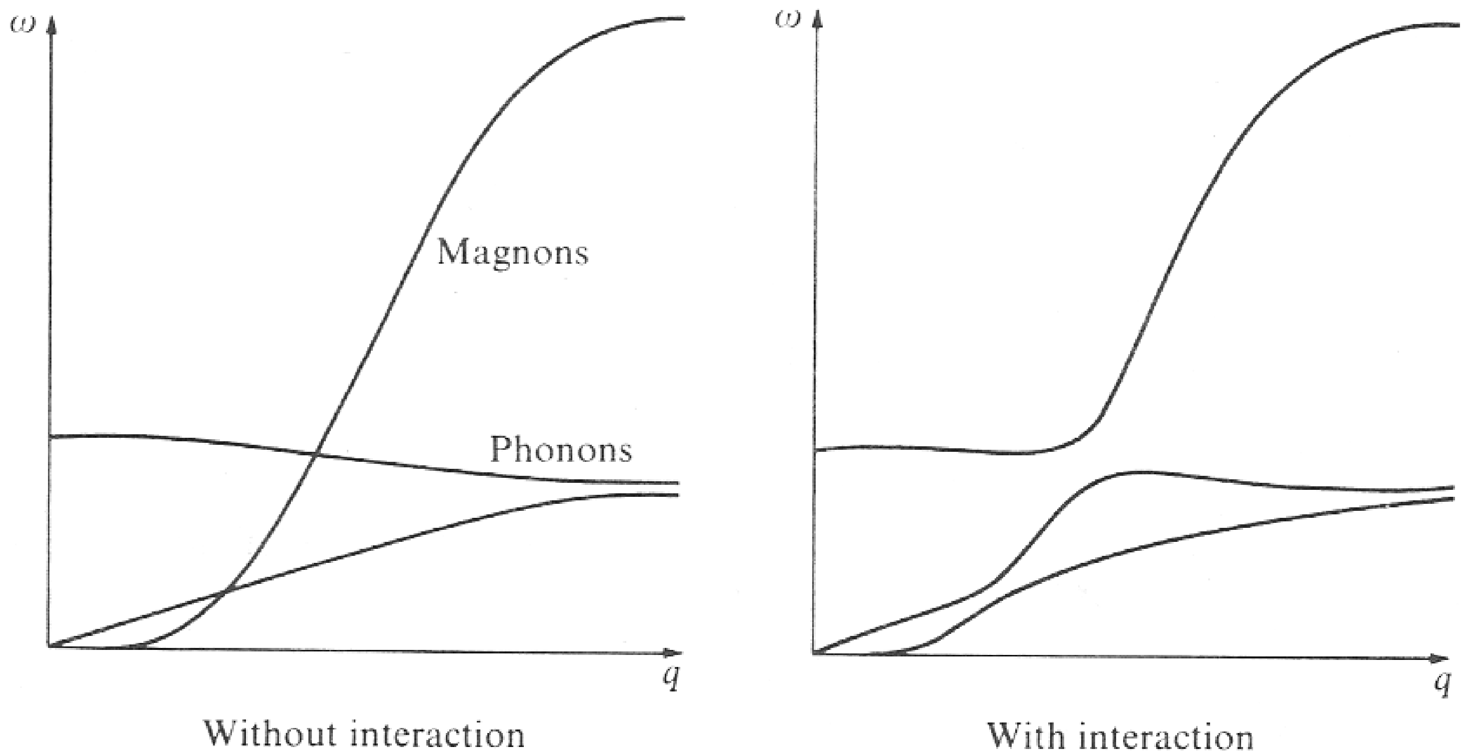


Fig. 5.7 Schematic magnon and phonon dispersion curves. The magnon curve has been compressed by a factor of order 10 for illustrative purposes.



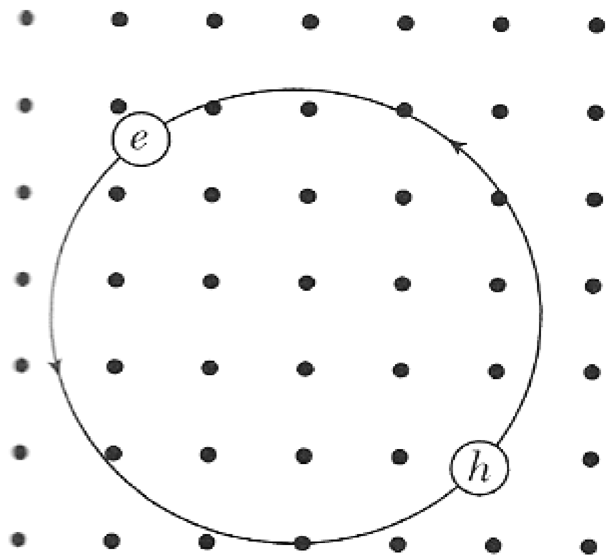
From: *Solid State Theory*, Harrison

Excitons

Bound state of an electron and a hole in a semiconductor or insulator

Mott Wannier excitons

(like positronium)



Mott-Wannier Excitons

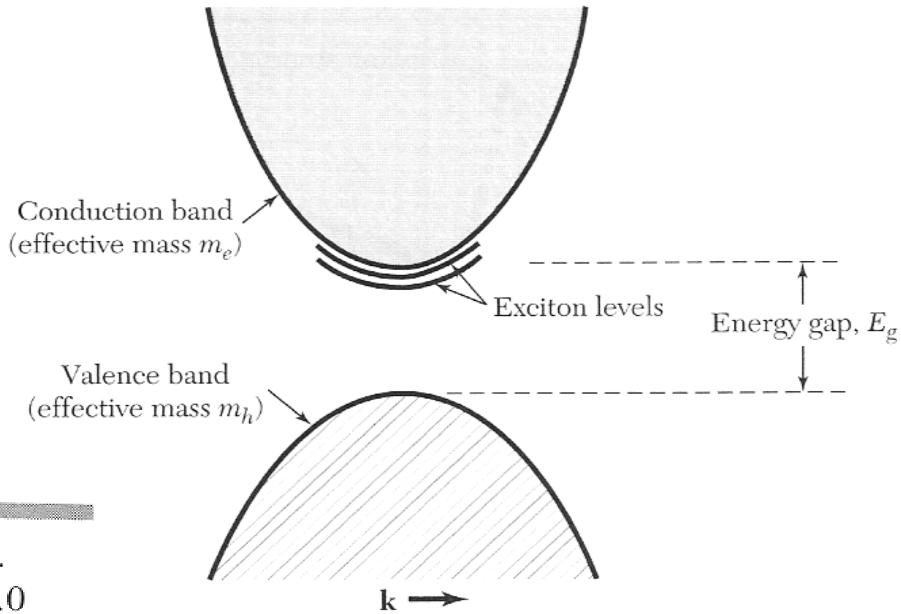
Bound state of an electron and a hole in a semiconductor or insulator (like positronium)

Hydrogenic model

$$E_{n,K} = E_g - \frac{\mu^* e^4}{32\pi^2\hbar^2\varepsilon^2\varepsilon_0^2 n^2} + \frac{\hbar^2 K^2}{2\left(m_h^* + m_e^*\right)}$$

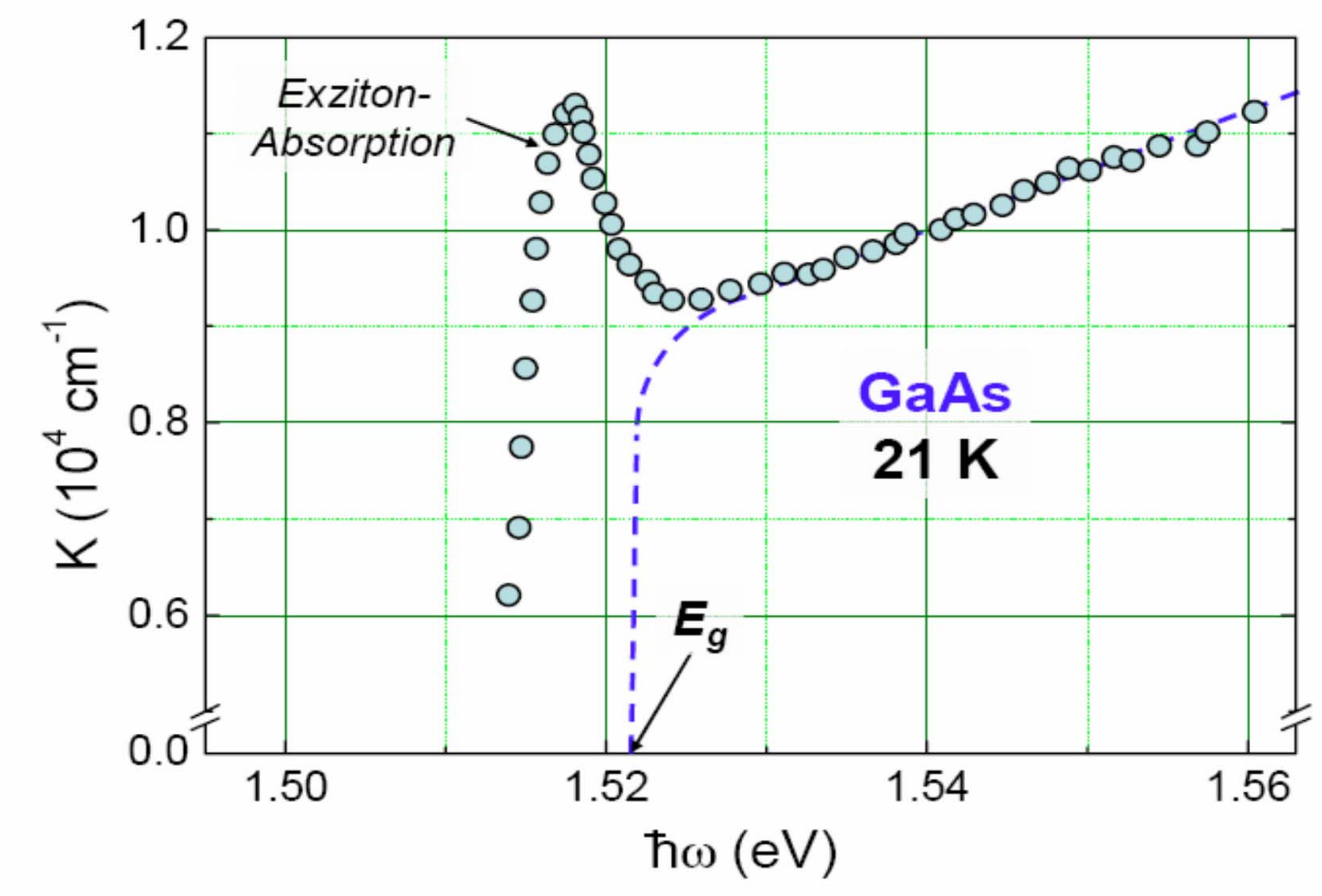
Table 1 Binding energy of excitons, in meV

Si	14.7	BaO	56.
Ge	4.15	InP	4.0
GaAs	4.2	InSb	(0.4)
GaP	3.5	KI	480.
CdS	29.	KCl	400.
CdSe	15.	KBr	400.



Kittel

Excitons



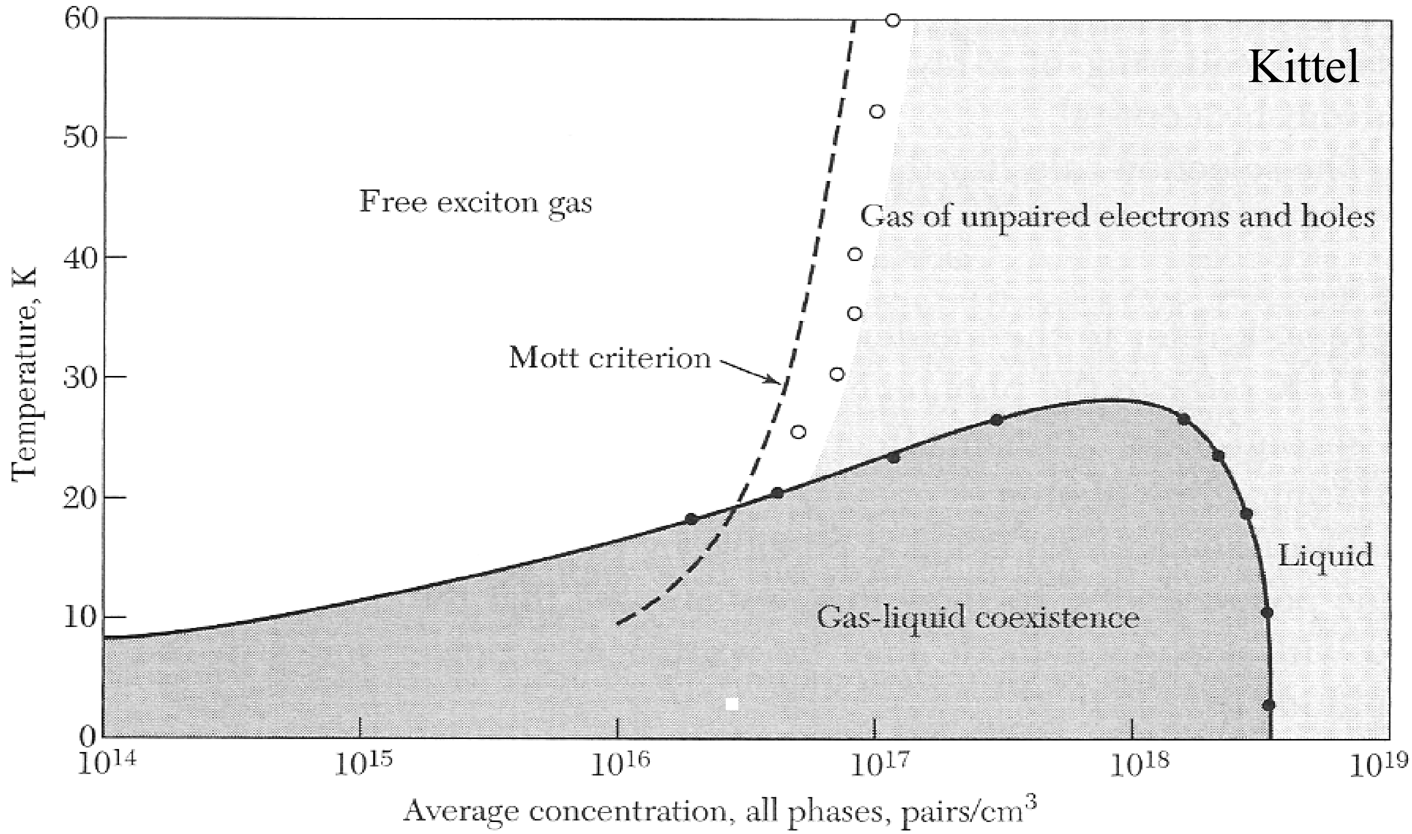
Gross & Marx

Excitons

Biexcitons H_2?

Metallic plasma droplets

Observe with an infrared camera



Phase diagram for photoexcited electrons and holes in unstressed silicon.

See: C. D. Jeffries, Electron-Hole Condensation in Semiconductors, Science 189 p. 955 (1975).

Frenkel Excitons

A Frenkel exciton is localized on an atom or molecule in a crystal.

The band gap of solid krypton is 11.7 eV. Lowest atomic transition in the solid is 10.17 eV.

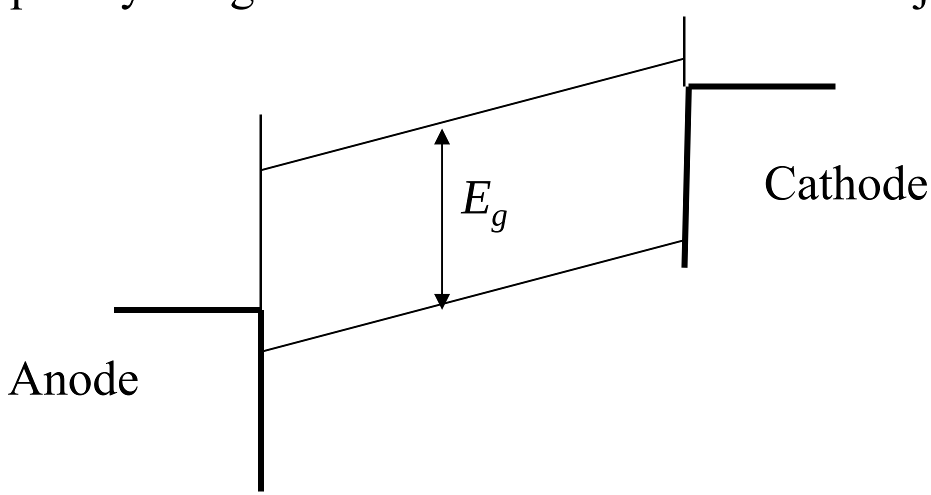
Excitons transport energy but not charge. Frenkel excitons are occur in organic solar cells, organic light emitting diodes, and photosynthesis.

OLEDs

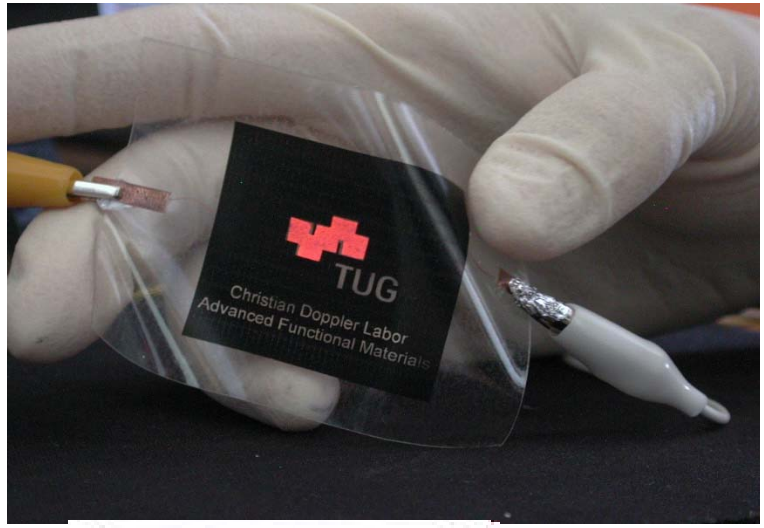
Aluminum cathode
Electron transport layer
Emission layer
Hole transport layer
ITO anode
Glass

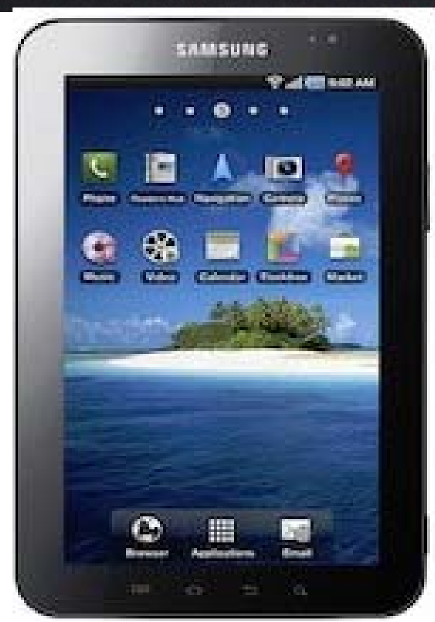
Cathode is typically a low work function material Al, Ca - injects electrons

Anode is typically a high work function material ITO - injects holes



OLEDs





Galaxy Tab