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SCHOOL ON SYNCHROTRON RADIATION

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Elements of Solid State Physics

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Overview

- Lecture 1
  - Crystal structures
  - Diffraction in crystals
- Lecture 2
  - General properties of the electronic states in crystals
  - Electronic band structure
- Lecture 3
  - Optical properties
- Lecture 4
  - Lattice vibrations

Solids

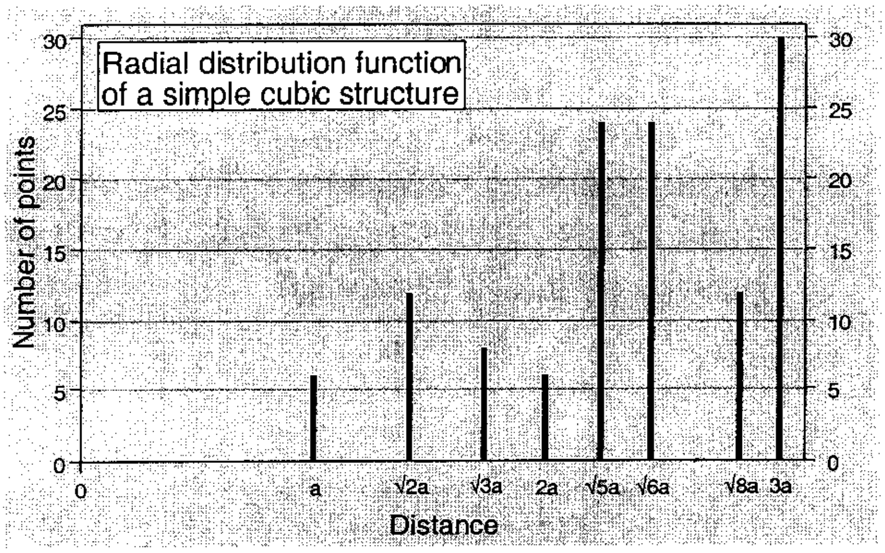
- In a solid, atoms are in fixed positions. The atom arrangament can be:
  - periodic over a large range **(crystals)**
  - locally periodic **(polycrystals)**
  - non periodic **(amorphous solids)**

We can define a "pair correlation function" $g(\vec{r})$ which is the probability of finding an atom in the position $\vec{r}$

Crystals

A one dimensional crystal

$$g(x) \propto \delta(x - na)$$



Crystals

The structure of a crystal is defined by its **space** symmetry and its **point** symmetry.

Space symmetry→periodicity

Point symmetry→operations within a period

The two must be compatible!

Crystals

All the measurable quantities (for example $|\psi(\vec{r})|^2$) associated to the crystal must be invariant under any **space** or **point** symmetry operation

Space Symmetry

Spatial periodicity: define Bravais Lattices as arrangements of points that fulfill:

$$\vec{t}_n = n_1\vec{t}_1 + n_2\vec{t}_2 + n_3\vec{t}_3$$

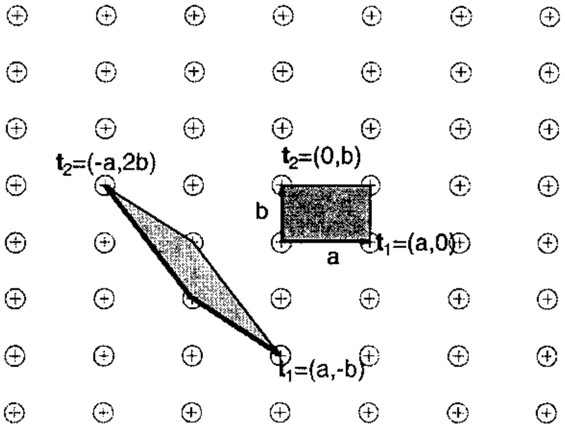
where $\vec{t}_1$, $\vec{t}_2$ and $\vec{t}_3$ are the *primitive translational vectors.* The parallalepiped they form is the *primitive unit cell,* which contains one single lattice point.

Space Symmetry

The choice of primitive vectors (and of primitive unit cell) is not univocal. It is customary to choose the one with the highest symmetry.

All the possible unit cell have the same volume:

$$\Omega = \vec{t}_1 \cdot (\vec{t}_2 \times \vec{t}_3)$$



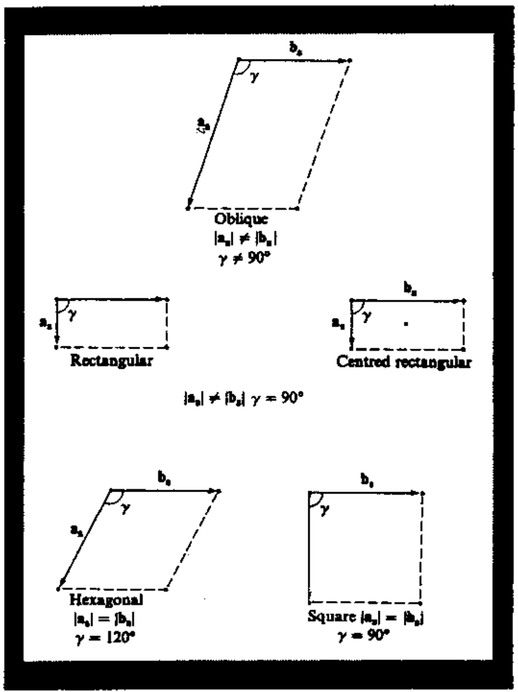
Space Symmetry

Bravais lattices:

Dimensions	# of Bravais lattices
1	1
2	5
3	7

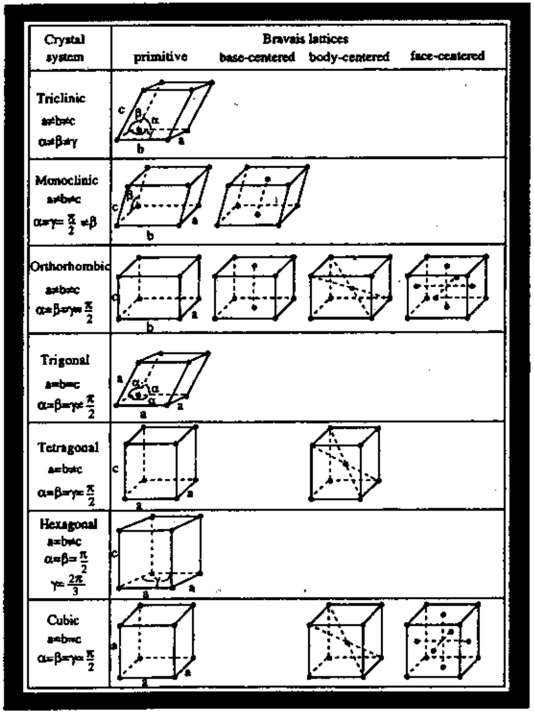
Space Symmetry

The 5 bidimensional Bravais lattices



Space Symmetry

The 14 three dimensional Bravais lattices



Point symmetry

The possible symmetry operations are:

- inversion
- rotations
- screw axes
- glide planes

Point symmetry

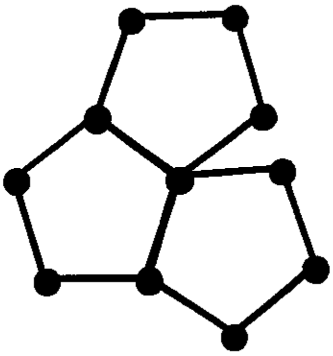
Inversion changes **x** into **-x** so it is described by a matrix:

$$I = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Point symmetry

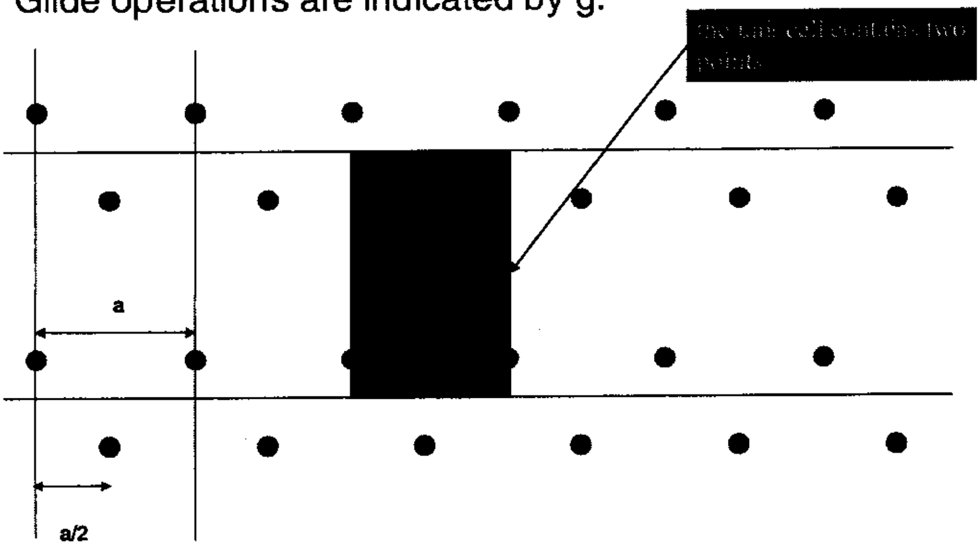
Rotations of an angle $2\pi/n$ are indicated by C_n, where n is a positive integer ≤ 6 and $\neq 5$

It is impossible to fill space with pentagons



Point symmetry

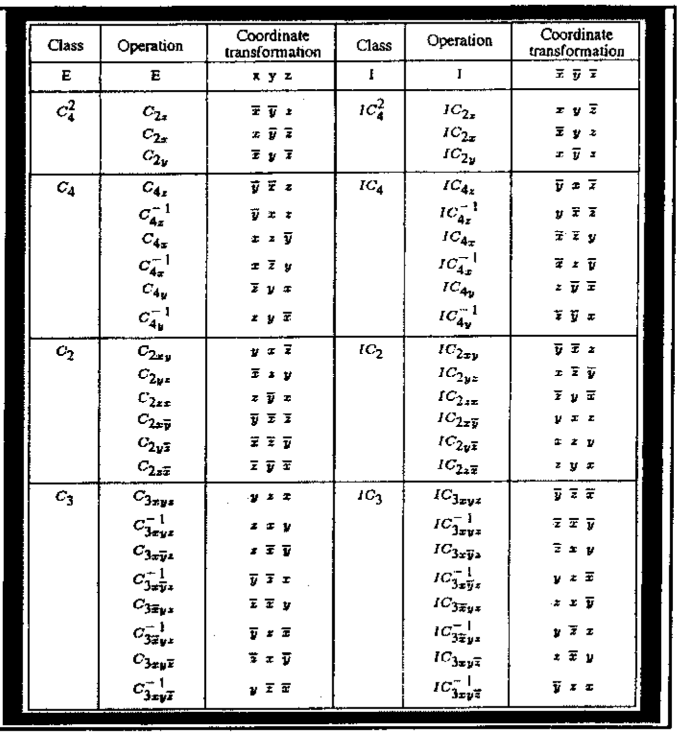
Glide operations are indicated by g:



the unit cell contains two points

Point symmetry

Symmetry operations of the cubic system



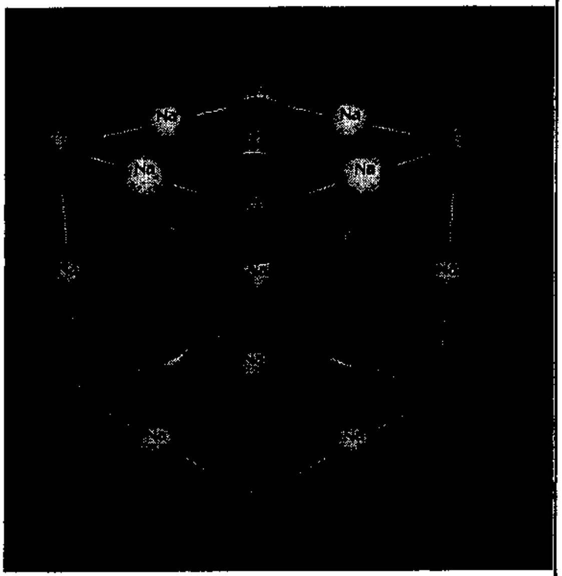
Class	Operation	Coordinate transformation	Class	Operation	Coordinate transformation
E	E	x y z	I	I	$\bar{x}\ \bar{y}\ \bar{z}$
C_4^2	C_{2z}	$\bar{x}\ \bar{y}\ z$	IC_4^2	IC_{2z}	$x\ y\ \bar{z}$
	C_{2x}	$x\ \bar{y}\ \bar{z}$		IC_{2x}	$\bar{x}\ y\ z$
	C_{2y}	$\bar{x}\ y\ \bar{z}$		IC_{2y}	$x\ \bar{y}\ z$
C_4	C_{4z}	$\bar{y}\ x\ z$	IC_4	IC_{4z}	$\bar{y}\ x\ \bar{z}$
	C_{4z}^{-1}	$y\ \bar{x}\ z$		IC_{4z}^{-1}	$y\ \bar{x}\ \bar{z}$
	C_{4x}	$x\ z\ \bar{y}$		IC_{4x}	$\bar{x}\ \bar{z}\ y$
	C_{4x}^{-1}	$x\ \bar{z}\ y$		IC_{4x}^{-1}	$\bar{x}\ z\ \bar{y}$
	C_{4y}	$\bar{z}\ y\ x$		IC_{4y}	$z\ \bar{y}\ \bar{x}$
	C_{4y}^{-1}	$z\ y\ \bar{x}$		IC_{4y}^{-1}	$\bar{z}\ \bar{y}\ x$
C_2	C_{2xy}	$y\ x\ \bar{z}$	IC_2	IC_{2xy}	$\bar{y}\ \bar{x}\ z$
	C_{2yz}	$\bar{x}\ z\ y$		IC_{2yz}	$x\ \bar{z}\ \bar{y}$
	C_{2zx}	$z\ \bar{y}\ x$		IC_{2zx}	$\bar{z}\ y\ \bar{x}$
	$C_{2x\bar{y}}$	$\bar{y}\ \bar{x}\ \bar{z}$		$IC_{2x\bar{y}}$	$y\ x\ z$
	$C_{2y\bar{z}}$	$\bar{x}\ \bar{z}\ \bar{y}$		$IC_{2y\bar{z}}$	$x\ z\ y$
	$C_{2z\bar{x}}$	$\bar{z}\ \bar{y}\ \bar{x}$		$IC_{2z\bar{x}}$	$z\ y\ x$
C_3	C_{3xyz}	$y\ z\ x$	IC_3	IC_{3xyz}	$\bar{y}\ \bar{z}\ \bar{x}$
	C_{3xyz}^{-1}	$z\ x\ y$		IC_{3xyz}^{-1}	$\bar{z}\ \bar{x}\ \bar{y}$
	$C_{3x\bar{y}z}$	$z\ \bar{x}\ \bar{y}$		$IC_{3x\bar{y}z}$	$\bar{z}\ x\ y$
	$C_{3x\bar{y}z}^{-1}$	$\bar{y}\ \bar{z}\ x$		$IC_{3x\bar{y}z}^{-1}$	$y\ z\ \bar{x}$
	$C_{3\bar{x}yz}$	$\bar{z}\ \bar{x}\ y$		$IC_{3\bar{x}yz}$	$z\ x\ \bar{y}$
	$C_{3\bar{x}yz}^{-1}$	$\bar{y}\ z\ \bar{x}$		$IC_{3\bar{x}yz}^{-1}$	$y\ \bar{z}\ x$
	$C_{3xy\bar{z}}$	$\bar{z}\ x\ \bar{y}$		$IC_{3xy\bar{z}}$	$z\ \bar{x}\ y$
	$C_{3xy\bar{z}}^{-1}$	$y\ \bar{z}\ \bar{x}$		$IC_{3xy\bar{z}}^{-1}$	$\bar{y}\ z\ x$

The rocksalt (NaCl) structure is a face centered cubic structure with a basis:

associate to each point in the lattice

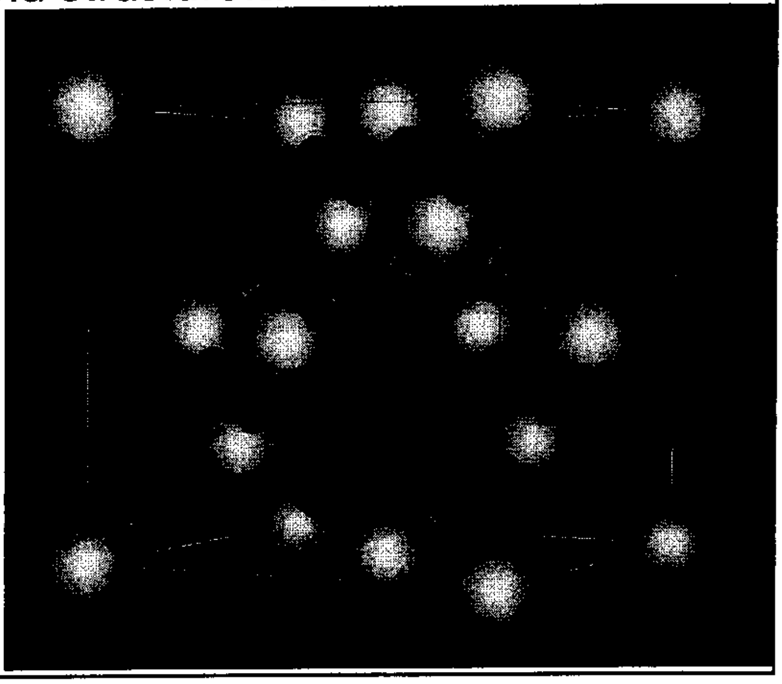
Cl translated by (0,0,0) and

Na translated by (1/2,0,0)



The diamond structure:another fcc with basis

Note: **no** inversion symmetry!



For more crystal structure have a look at:

http://www.theophys.kth.se/symmetrier/intro.html

Reciprocal Lattice

Given a crystal with primitive translation vectors $\vec{t}_1, \vec{t}_2, \vec{t}_3$ it is possible (and useful!) to define a reciprocal lattice whose primitive vectors $\vec{g}_1, \vec{g}_2, \vec{g}_3$ satisfy:

$$\vec{t}_i \cdot \vec{g}_j = 2\pi\delta_{ij}$$

Reciprocal Lattice

From the definition it is easy to show that:

$$\vec{g}_1 = \frac{2\pi}{\Omega}\vec{t}_2 \times \vec{t}_3 \quad ....$$

where

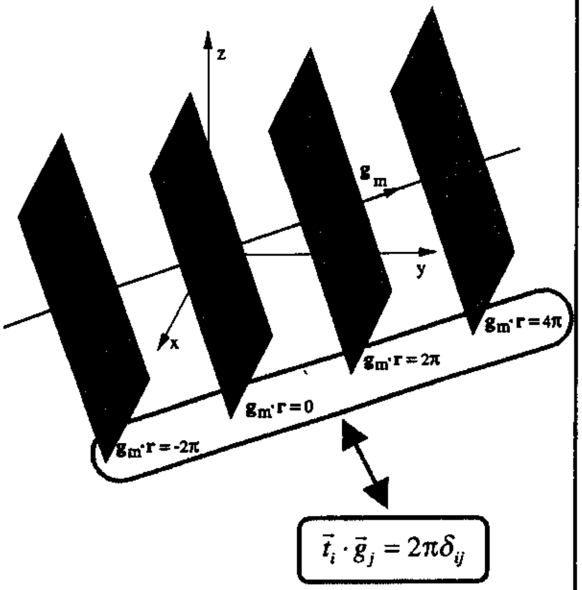
$$\Omega = \vec{t}_1 \cdot \vec{t}_2 \times \vec{t}_3$$

is the volume of the primitive cell in the direct lattice

Reciprocal Lattice

Basic property: every reciprocal lattice vector is normal to a family of parallel and equidistant planes containing all the direct lattice points the distance between two of these planes is:

$$d = \frac{2\pi}{g_m}$$



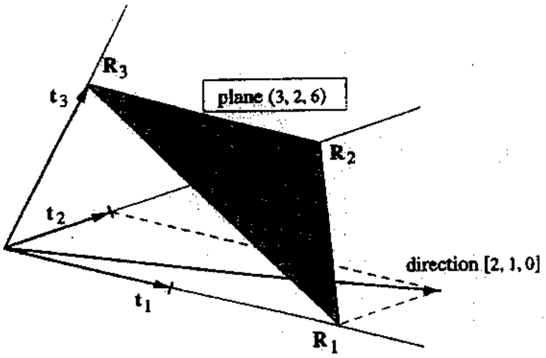
Reciprocal Lattice

A plane in a crystal is usually labelled by Miller indices, which are the reciprocal of the intercepts of the plane with the primitive axis multiplied by the smallest factor to convert them into integer numbers.

the reciprocal lattice vector

$$\vec{g}_m = m_1\vec{g}_1 + m_2\vec{g}_2 + m_3\vec{g}_3$$

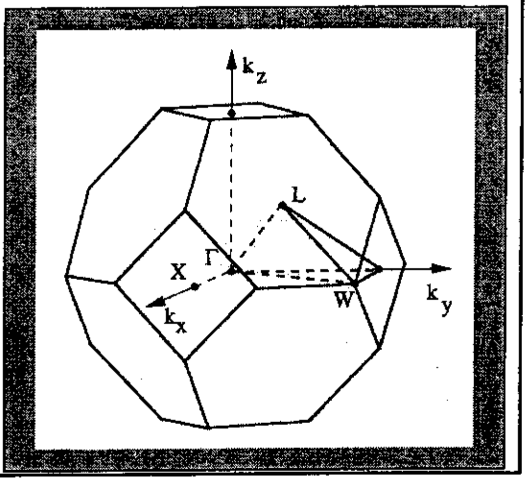
is perpendicular to the planes (m_1,m_2,m_3)



Reciprocal Lattice

The most convenient unit cell in the reciprocal space is called Brillouin zone and is obtained by bisecting with perpendicular nearest neighbours reciprocal lattice vectors, second nearest neighbours (and other orders neighbours, if necessary) and considering the smallest volume enclosed

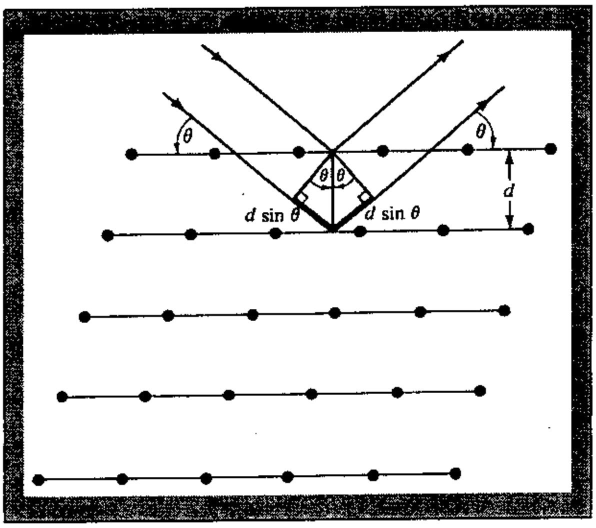
Brillouin zone for the face centered cubic lattice (truncated octaedron). Some high symmetry points are $\Gamma=(0,0,0)$; $X=(2\pi/a)(1,0,0)$; $L=(2\pi/a)(1/2,1/2,1/2)$; $W=(2\pi/a)(1/2,1,0)$



Determination of crystal structures: diffraction

Bragg's law. Radiation of wavelength λ is reflected by the lattice plane. The outgoing waves interfere. Inteference is constructive only if the difference of optical path is a multiple of λ:

$$2d\sin\vartheta = n\lambda$$



Diffraction

Bragg's law implies that the wavelength λ must be of the same order of magnitude as the lattice spacing, typically ≈5 Å

Probe	E(λ)	Scatterers
x-rays	$E=\frac{2\pi\hbar c}{\lambda}$ $E(eV)=\frac{12400}{\lambda(\mathring{A})}$	electrons
electrons	$E=\frac{(2\pi\hbar)^2}{2m}\left(\frac{1}{\lambda}\right)^2$ $E(eV)=\frac{150.4}{(\lambda(\mathring{A}))^2}$	electrons and nuclei
neutrons	$E=\frac{(2\pi\hbar)^2}{2M}\left(\frac{1}{\lambda}\right)^2$ $E(eV)=\frac{8.19\cdot10^{-2}}{(\lambda(\mathring{A}))^2}$	nuclei
atoms (e.g. He)	$E=\frac{(2\pi\hbar)^2}{2MZ}\left(\frac{1}{\lambda}\right)^2$ $E(eV)=\frac{2.05\cdot10^{-2}}{(\lambda(\mathring{A}))^2}$	electrons

Diffraction

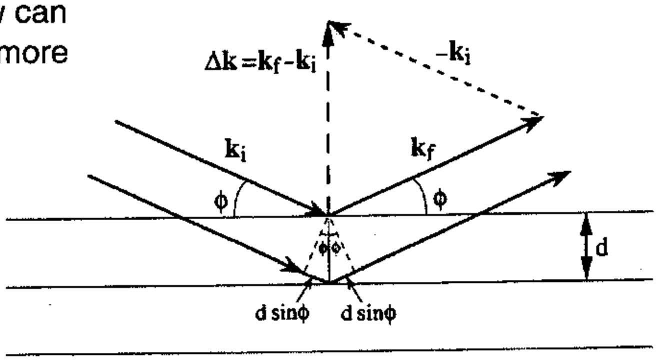
If one considers the wavevector $\vec{k}$ of the plane wave

$$\vec{E}(\vec{r},t)=\vec{E}_0e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

with k=2π/λ, Bragg's law can be expressed in a more general vectorial form:

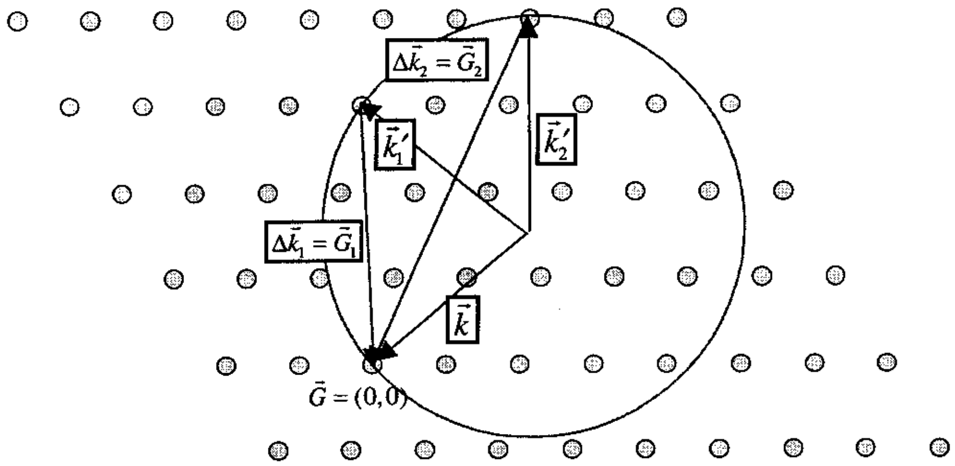
$$\Delta\vec{k}=\vec{G}$$

where $\vec{G}$ is a reciprocal lattice vector



Diffraction

The Ewald construction (reciprocal space!)

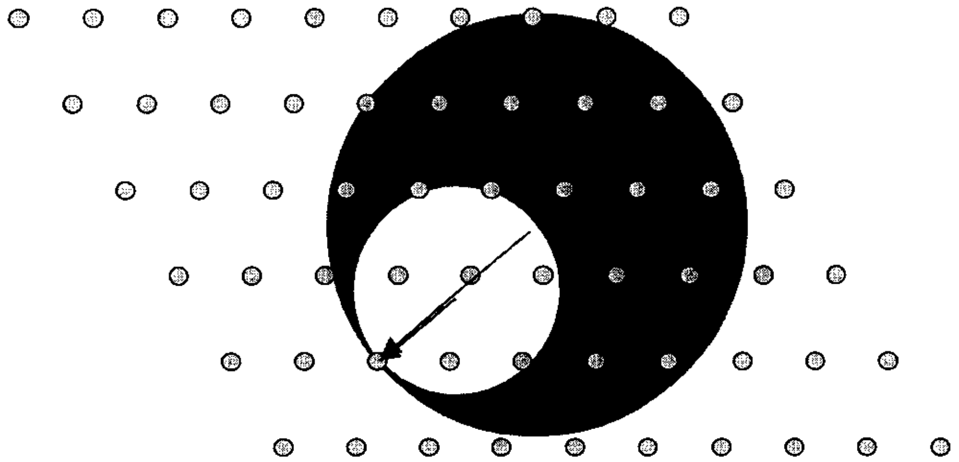


Diffraction

If the Ewald sphere does not intersect any reciprocal space point there are no diffracted beams. It is necessary to change **k** in modulus (i.e change the wavelength of the incoming beam) and/or direction (i.e. rotate the crystal) to get diffraction.

Diffraction

As an example, one can use a continuous range of wavelengths to get more diffracted beams (Laue method)



Diffraction

A Laue pattern: Si(100)

Diffraction

Bragg's law shows that the angular distribution of diffracted beams is related to hte space symmetry of the lattice.

The intensities of the beams are related to the point symmetry

$$F(\vec{G}) = N\sum_{\vec{d}} e^{-i\vec{G}\cdot\vec{d}} f_a(\vec{G})$$

structure factor

sum over all atoms in the unit cell

$$f_a(\vec{G}) = \int e^{-i\Delta\vec{k}\cdot\vec{r}} n_a(\vec{r})\,d\vec{r}$$

atomic form factor

electrondensity of atom a

Tutorial programs:

http://www.ruph.cornell.edu/sss/sss.html

Lecture two: electronic levels

- Schrödinger equation for a crystal
- Bloch's theorem
- Band structure

Schrödinger equation

The total non-relativistic Hamiltonian for a crystal is:

$$H_{tot} = \sum_i \frac{\vec{p}_i^{\,2}}{2m} + \sum_I \frac{\vec{P}_I^{\,2}}{2M_I} + \sum_i \sum_I \frac{-Z_I e^2}{\left|\vec{r}_i - \vec{R}_I\right|} + \frac{1}{2}\sum_{i \neq j} \frac{e^2}{\left|\vec{r}_i - \vec{r}_j\right|} + \frac{1}{2}\sum_{I \neq J} \frac{Z_I Z_J e^2}{\left|\vec{R}_I - \vec{R}_J\right|}$$

kinetic energy of the electrons

kinetic energy of the nuclei

electrons-nuclei attractive potential

repulsion between electrons

repulsion between nuclei

Schrödinger equation

Nuclei are much heavier than electrons. If we want to study the electrons, we can neglegt the motion of nuclei *(Born-Oppenheimer approximation)*:

$$H_{el} = \sum_i \frac{\vec{p}_i^{\,2}}{2m} + \sum_i \sum_I \frac{-Z_I e^2}{|\vec{r}_i - \vec{R}_I|} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} + const$$

Schrödinger equation

Further approximation: *the independent electron approximation*. The wave function is written as a Slater determinant

$$\psi(\tau_1 \tau_2 \ldots \tau_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(\tau_1) & \psi_1(\tau_2) & \ldots & \psi_1(\tau_N) \\ \psi_2(\tau_1) & \psi_2(\tau_2) & \ldots & \psi_2(\tau_N) \\ \ldots & \ldots & \ldots & \ldots \\ \psi_N(\tau_1) & & & \psi_N(\tau_N) \end{vmatrix}$$

Schrödinger equation

Introducing Slater's determinant into Schrödinger equation we get:

$$-\frac{\hbar^2}{2m}\nabla^2\psi_i(\vec{r})-\sum_I\frac{-Z_Ie^2}{\left|\vec{r}_i-\vec{R}_I\right|}\psi_i(\vec{r})+\left[\sum_j e^2\int\frac{\psi_j^*(\vec{r}')\psi_j(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}'\right]\psi_i(\vec{r})+$$

$$-\left[\sum_j e^2\int\frac{\psi_j^*(\vec{r}')\psi_j(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}'\right]\psi_j(\vec{r})=E_i\psi_i(\vec{r})$$

"exchange" interaction

This is stil a difficult problem!

Schrödinger equation

We assume it is possible to define a mean crystal field so that:

$$\left(-\frac{\hbar^2}{2m}\nabla^2+U_{crystal}(\vec{r})\right)\psi(\vec{r})=E\psi(\vec{r})$$

is Schrödinger equation for each electron

Schrödinger equation

The problem of finding an appropriate form for $U_{crystal}$ is difficult but we know it must be invariant under symmetry operations! In particular it has to have translational periodicity and can be expressed as a Fourier series:

$$U_{crystal}(\vec{r}) = \sum_{\vec{g}_m} U(\vec{g}_m) e^{i\vec{g}_m \cdot \vec{r}}$$

where the $\vec{g}_m$ are reciprocal lattice vectors

Schrödinger equation

Consider the matrix element:

$$\left\langle e^{i\vec{k}'\cdot\vec{r}} \middle| U_{crystal}(\vec{r}) \middle| e^{i\vec{k}\cdot\vec{r}} \right\rangle = \sum_{\vec{g}_m} U(\vec{g}_m) \int e^{i(\vec{g}_m - \vec{k}' + \vec{k})\cdot\vec{r}} d\vec{r}$$

The integrals vanish unless

$$\vec{g}_m - \vec{k}' + \vec{k} = 0$$

i.e. the wavevectors must differ by a reciprocal lattice vector and wavevectors within the first Brillouoin zone are good quantum numbers which can be used to classify the eigenstates

Schrödinger equation

The wavefunctions can be written as:

$$\psi(\vec{k},\vec{r}) = \sum_{\vec{g}_n} a_n(\vec{k}) e^{i(\vec{g}_m+\vec{k})\cdot\vec{r}} = e^{i\vec{k}\cdot\vec{r}} \underbrace{\boxed{\sum_{\vec{g}_n} a_n(\vec{k}) e^{i\vec{g}_m\cdot\vec{r}}}}_{\boxed{\text{periodic function}}}$$

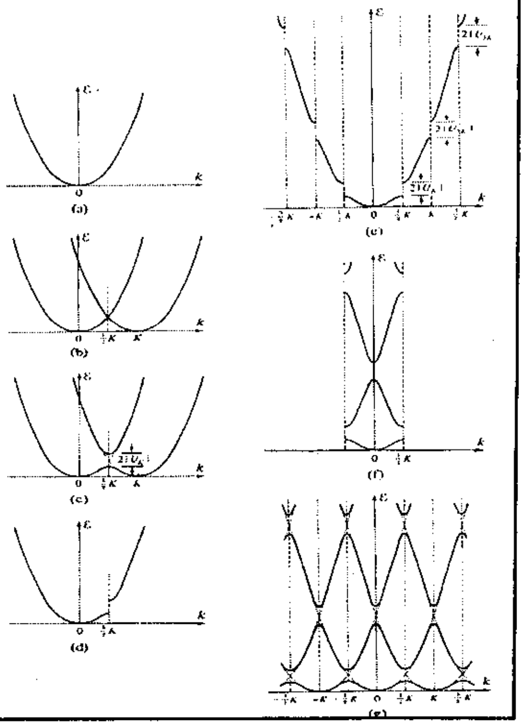
Bloch's theorem

The wavefunctions of the crystal Hamiltonian can be written as the product of a plane wave of wavevector $\vec{k}$ within the first Brillouin zone, times an appropriate periodic function

$$\boxed{\psi(\vec{k},\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u(\vec{k},\vec{r})}$$

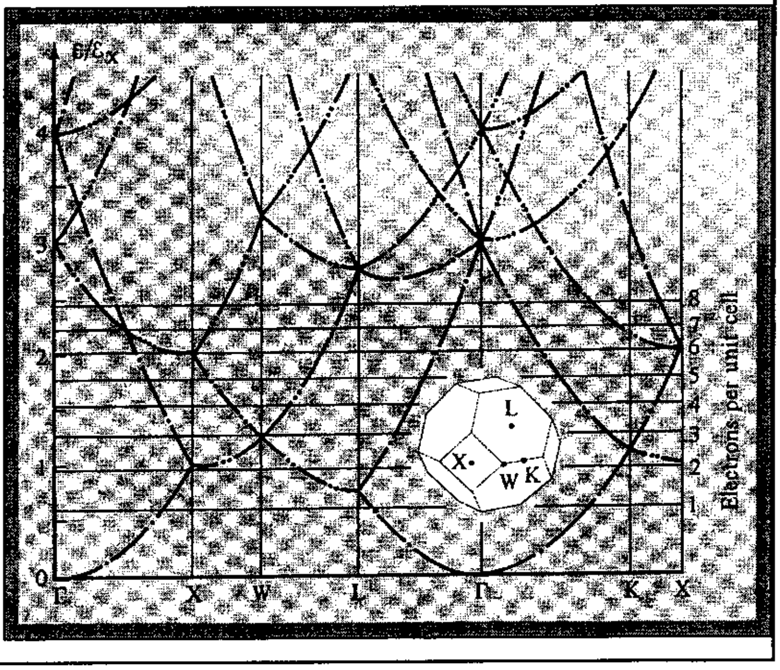
Energy bands

In a weak periodic potential, the energy bands have little deviation fron the parabolic free electron behavior. The most important piece of news is the opening of energy gaps.



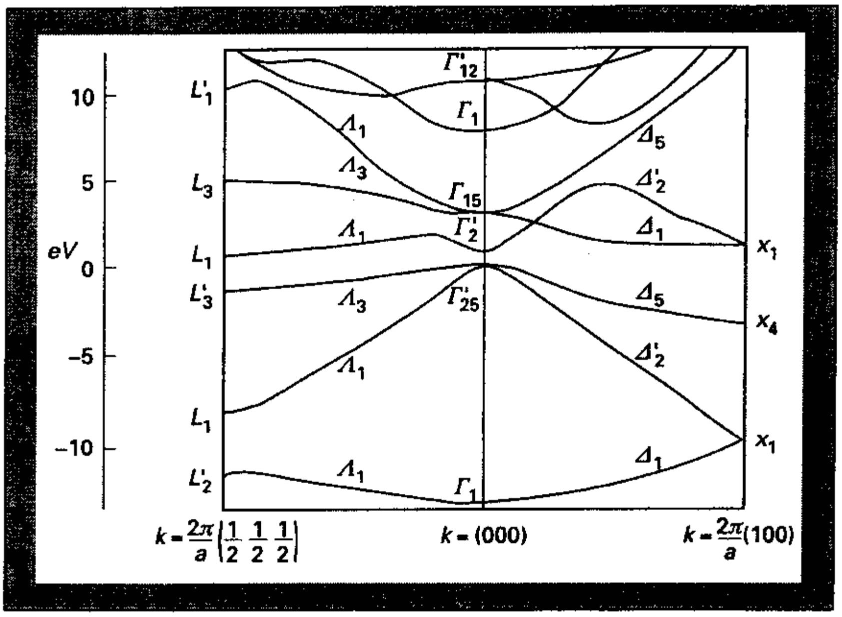
Energy bands

Free electron bands in an fcc crystal.



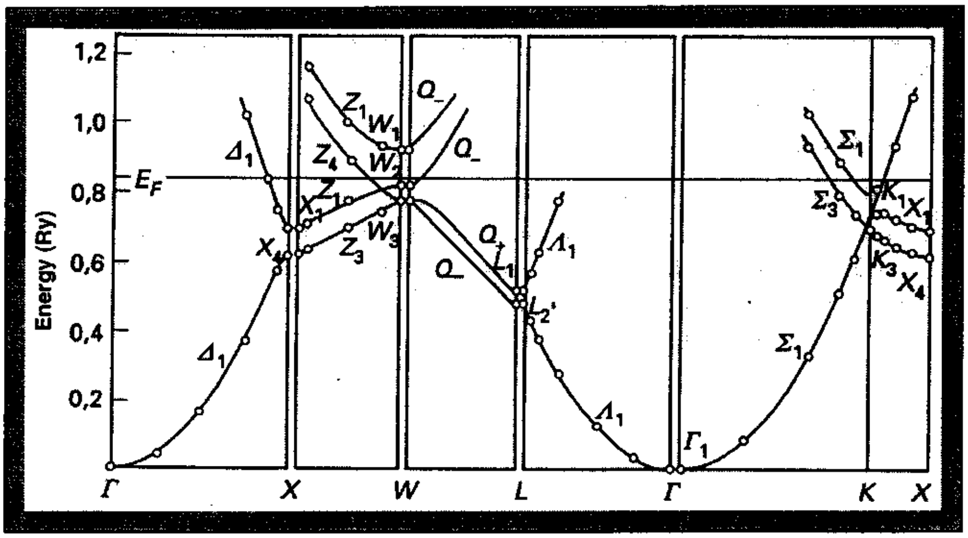
Energy bands

A semiconductor: Germanium



Energy bands

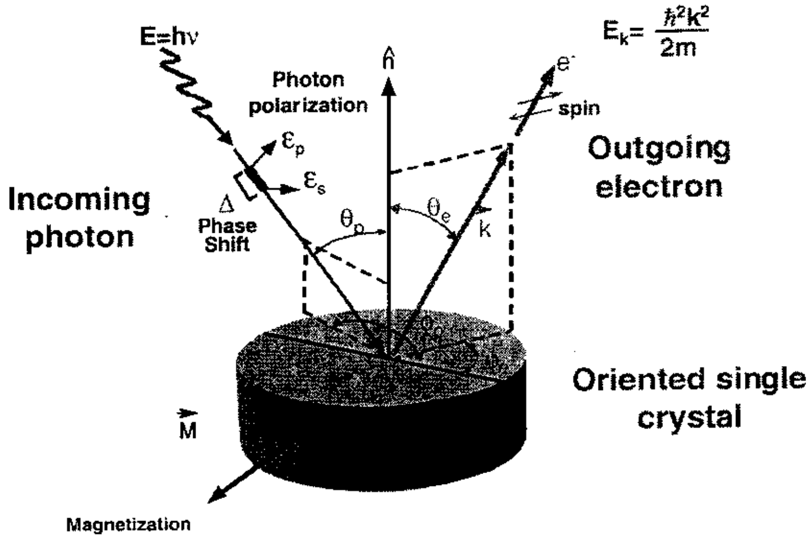
A metal: Aluminum



Energy bands

Experimental determination of
band structure

The photoemission experiment



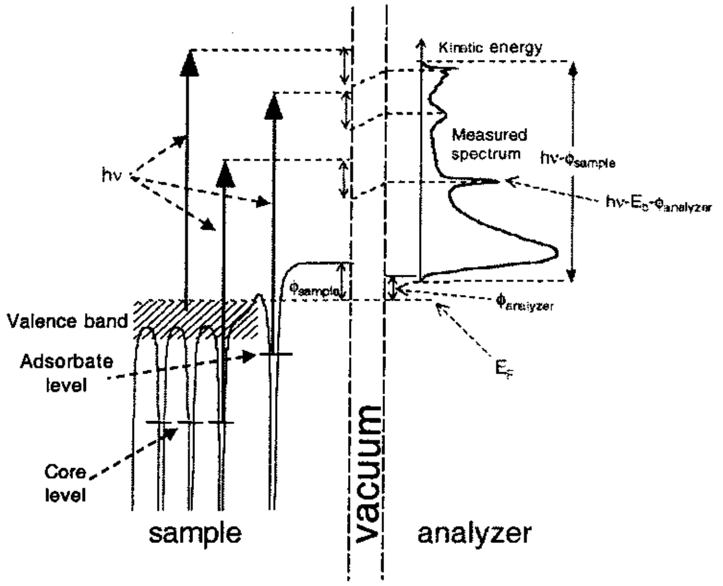
Incoming photon

Outgoing electron

Oriented single crystal

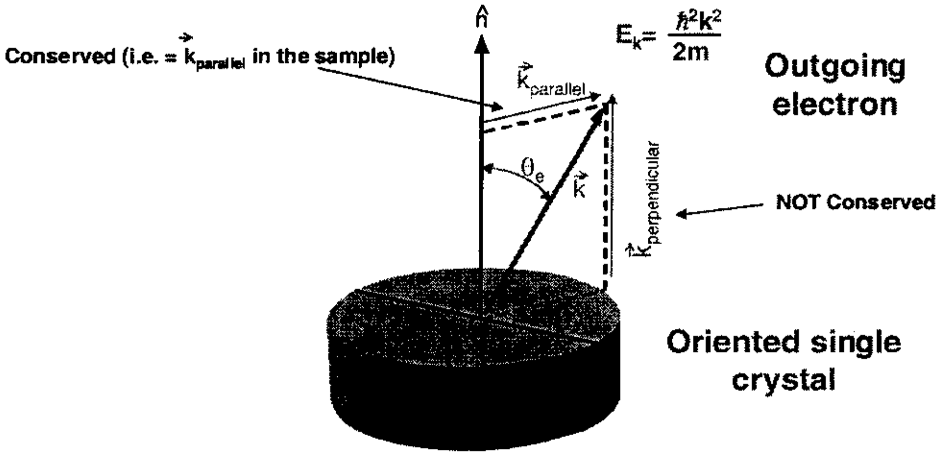
The electron must overcome the sample work function Φ_{sample} in order to reach the vacuum; afterwards its energy is changed by the difference in work function between the analyzer and the sample. So:

$$E_k^{meas} = h\nu - E_b - \phi_{analyzer}$$

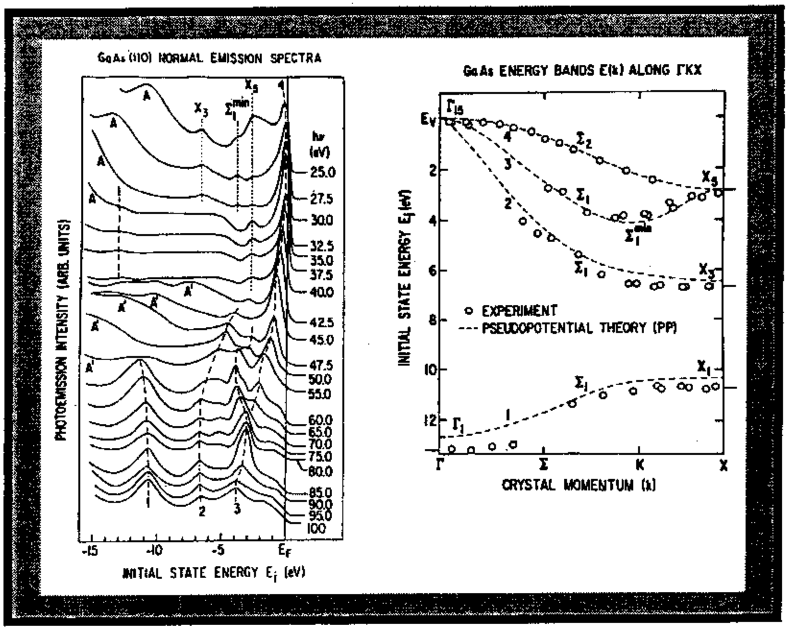


Momentum conservation

The surface breaks the traslational symmetry along $\hat{n}$



Band mapping: GaAs



Optical properties

- Macroscopic theory
- Drude-Lorentz theory
- Interband transitions
- Examples
  - Metals
  - Semiconductors

Macroscopic theory

Maxwell equations
(no charge, no current)

$$\vec{\nabla}\cdot\vec{D}=0$$

$$\vec{\nabla}\cdot\vec{B}=0$$

$$\vec{\nabla}\times\vec{E}=-\frac{1}{c}\frac{\partial\vec{B}}{\partial t}$$

$$\vec{\nabla}\times\vec{H}=-\frac{1}{c}\frac{\partial\vec{D}}{\partial t}+\frac{4\pi}{c}\vec{J}$$

Properties of the medium

$$\vec{D}=\vec{E}+4\pi\vec{P}$$

$$\vec{B}=\vec{H}+4\pi\vec{M}$$

Macroscopic theory

Linear approximation

$$\begin{matrix}\vec{P}=\alpha\vec{E}\\ \vec{J}=\sigma\vec{E}\end{matrix}\quad\longrightarrow\quad\begin{matrix}\vec{D}=\varepsilon\vec{E}\\ \varepsilon=1+4\pi\alpha\end{matrix}$$

σ is the conductivity → absorption
α is the polarizability → dispersion

Macroscopic theory

For a periodic electric field $\vec{E} = \vec{E}_0 e^{-i\omega t}$

it is convenient to introduce a complex dielectric function $\boxed{\tilde{\varepsilon} = \varepsilon_1 + i\varepsilon_2 = \varepsilon + i\frac{4\pi\sigma}{\omega}}$

to treat absorption and dispersion simultaneously. This is similar to the concept of complex impedance for the analysis of a.c. circuts

Macroscopic theory

by inserting the complex dielectric function into Maxwell equations we find:

$$\nabla^2 \vec{E} - \frac{\tilde{\varepsilon}}{c^2}\frac{\partial^2 \vec{E}}{\partial t^2} = 0$$

waves travellig at v=c/$\sqrt{\varepsilon_1}$

solutions of the form

$$\vec{E} = \vec{E}_0 e^{i(\vec{q}\cdot\vec{r}-\omega t)} + c.c. \longrightarrow \omega^2 = \frac{c^2}{\tilde{\varepsilon}} q^2$$

Macroscopic theory

The introduction of the compex dielectric function allows us to introduce other complex functions (complex refraction index, complex reflectivity...) and extend the relations found in simple optics keeping into account absorption and dispersion simultaneously.

complex refraction index:

$$\tilde{n} = n + i\kappa$$

$$\tilde{n}^2 = \tilde{\varepsilon}$$

$$n^2 - \kappa^2 = \varepsilon_1$$

$$2n\kappa = \varepsilon_2$$

Macroscopic theory

Kramers-Kronig dispersion relations

The dielectric constant describes the response of the system to an e.m. field.

It is possible to apply the causality principle (i.e. the response must follow the stimulus) and derive relations between the real and imaginary part:

$$\varepsilon_1(\omega_0) = 1 + \frac{2}{\pi} P \int_0^{\infty} \frac{\omega \varepsilon_2(\omega)}{\omega^2 - \omega_0^2} d\omega$$

$$\varepsilon_2(\omega_0) = -\frac{2}{\pi} P \int_0^{\infty} \frac{\varepsilon_1(\omega) - 1}{\omega^2 - \omega_0^2} d\omega$$

Macroscopic theory

Lorentz-Drude model

A medium composed of charged particles whose density is N behaving like harmonic oscillators

$$\tilde{\varepsilon} = 1 + \frac{4\pi N e^2}{m} \frac{1}{(\omega_0^2 - \omega^2) - i\gamma\omega}$$

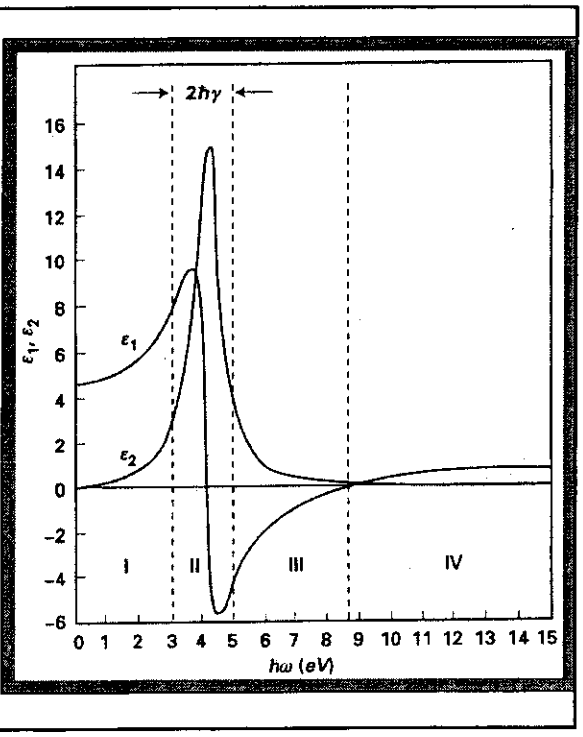
ω_0 resonance

γ damping

Macroscopic theory

Lorentz-Drude model

A medium composed of N charged particles behaving like harmonic oscillators



Macroscopic theory

Metals

Lorentz-Drude model with ω_0=0.

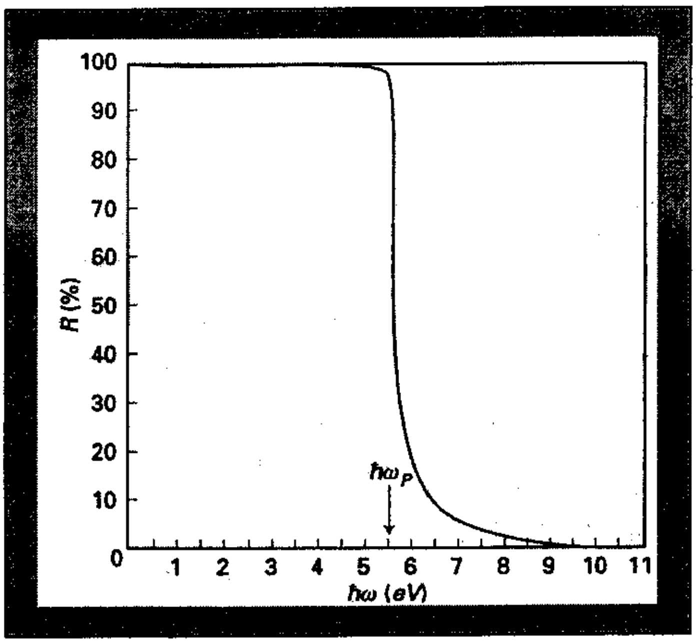
$$\tilde{\varepsilon} = 1 + \frac{\omega_p^2}{\omega^2 - \gamma^2} + i\frac{\gamma\omega_p^2}{\omega^3 + \gamma^3\omega}$$

plasma frequency $\longrightarrow \omega_p^2 = \frac{4\pi e^2 N}{m}$

Macroscopic theory

Metals

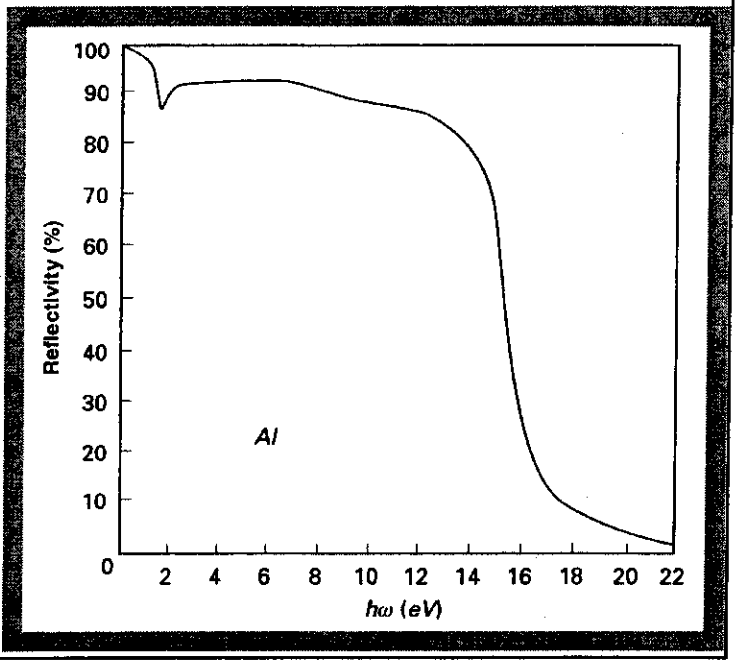
Reflectivity



Macroscopic theory

Metals

Reflectivity of a real metal: Aluminum



Quantum Theory

The hamiltonian for a system with an external em field,described by a vector potential $\vec{A}$ and a scalar potential ϕ is:

$$H=\frac{1}{2m}\left(\vec{p}+e\frac{\vec{A}(\vec{r},t)}{c}\right)^2-e\phi(\vec{r},t)+V(\vec{r})$$

With the transverse gauge (no charges, no currents)

$$\left.\begin{array}{l}\boxed{\vec{\nabla}\cdot\vec{A}=0}\\ \phi(\vec{r},t)=0\end{array}\right\}\rightarrow\nabla^2\vec{A}+\frac{1}{c^2}\frac{\partial^2\vec{A}}{\partial t^2}=0$$

So the Hamiltonian becomes:

$$H=\frac{1}{2m}p^2+\frac{e}{2mc}\left(\underbrace{\boxed{\vec{p}\cdot\vec{A}}}_{=0}+\vec{A}\cdot\vec{p}\right)-\underbrace{\boxed{\frac{e}{2mc^2}A^2}}_{\approx 0}+V(\vec{r})$$

Quantum Theory

We can write: $H = H_0 + H_1$

where $H_1 = \frac{ie\hbar}{mc}\vec{A}\cdot\vec{\nabla}$ is the perturbation.

The incoming radiation can be described as a superposition of plane waves of the form:

$$\vec{A}(\vec{r},t) = \vec{A}_\omega e^{i(\vec{q}\cdot\vec{r}-\omega t)}$$

We put all this into the time dependent perturbation theory to get:

$$c_{f,i} = -\frac{2\pi e}{mc}\vec{A}_\omega\cdot\langle f|e^{i\vec{q}\cdot\vec{r}}\vec{\nabla}|i\rangle\delta\left(\omega-\frac{E_f-E_i}{\hbar}\right)$$

For optical transitions the wavelength $\lambda=2\pi/|q|$ is always much longer than the size of the atoms. So we can approximate the exponential with 1

$$\boxed{c_{f,i} = -\frac{2\pi e}{mc}\vec{A}_\omega\cdot\langle f|\vec{\nabla}|i\rangle\delta\left(\omega-\frac{E_f-E_i}{\hbar}\right) = -\frac{2\pi ie}{mc\hbar}\vec{A}_\omega\cdot\langle f|\vec{p}|i\rangle\delta\left(\omega-\frac{E_f-E_i}{\hbar}\right)}$$

this formula represents the so-called **dipole approximation**

Quantum Theory

In a solid one has to consider all possible energy conserving transitions:

$$\varepsilon_2 = \frac{4\pi^2e^2}{m^2\omega^2}\sum_{v,c}\int_{BZ}\frac{2d\vec{k}}{(2\pi)^3}c_{i,f}(\vec{k})\delta\left(E_c(\vec{k})-E(\vec{k})_v-\hbar\omega\right)$$

Quantum Theory

It is often possible to neglect the variation of the matrix element with momentum so for a pair of bands ε_2 is proportional to:

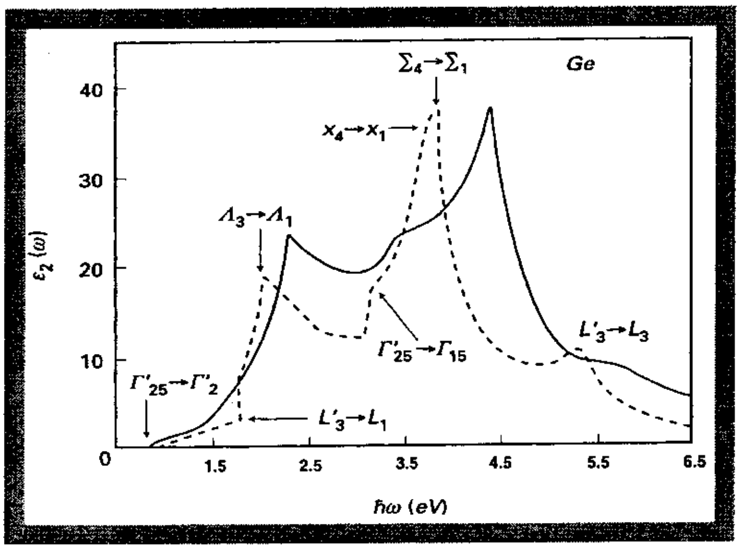
$$J_{c,v}(\hbar\omega)=\int_{BZ}\frac{2d\vec{k}}{(2\pi)^3}\delta\left(E_c(\vec{k})-E(\vec{k})_v-\hbar\omega\right)$$

the joint density of states, which can be written as:

$$\boxed{J_{c,v}(\hbar\omega)=\int_{E_c(\vec{k})-E(\vec{k})_v=\hbar\omega}\frac{2dS}{|\nabla_k(E_c(\vec{k})-E(\vec{k})_v)|}}$$

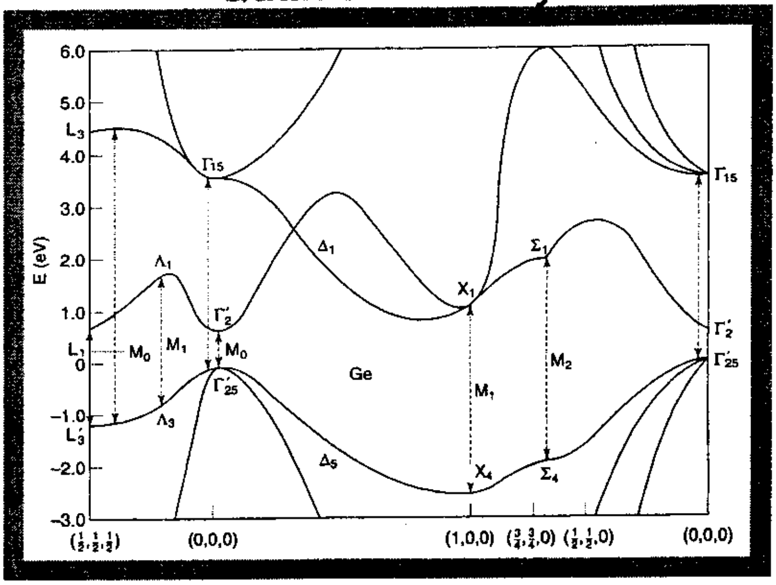
high contribution from parallel bands

Quantum Theory



Comparison between theoretical (--) and experimental (—) determination of the optical properties of Germanium

Quantum Theory



Optical transitions in Ge with high joint density of states

Lattice vibrations

Consider an expansion of the total ground state energy:

$$E_0(\{s_n\}) = E_0(0) + \frac{1}{2}\sum_{n,n'}\left(\frac{\partial^2 E_0}{\partial s_n \partial s_{n'}}\right) s_n s_{n'} + O(s^3)$$

where the *s*'s are displacements of the nuclei with respect to their equilibrium positions

Lattice vibrations

Consider an axpansion of the total ground state energy:

$$m_i \ddot{s}_{ij} = \sum_{i'j'} D_{ij,i'j'} \vec{s}_{i'j'}$$

where the *s*'s are displacements of the nuclei with respect to their equilibrium positions and the j's represent equivalent lattice points

Lattice vibrations

vibrations must be consistent with bloch's theorem and therefore

$$\vec{s}_{ij}(\vec{k}) = \vec{s}_{ij}^{\,0} e^{i(\vec{k}\cdot\vec{\tau}_j - \omega t)}$$

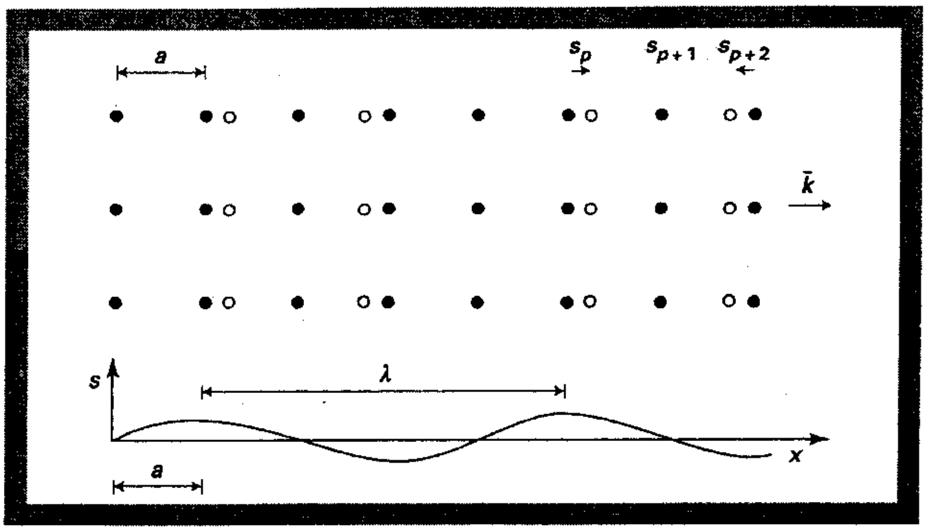
which gives

$$-\omega^2 m_i \vec{s}_{ij}^{\,0} = \sum_{i'j'} D_{ij,i'j'} \vec{s}_{i'j'}^{\,0}(\vec{k})$$

Lattice vibrations

Unidimensional monoatomic case. First neighbour interaction

$$m\ddot{s}_p = C(s_{p+1} - s_p + s_{p-1} - s_p) = C(s_{p+1} + s_{p-1} - 2s_p)$$

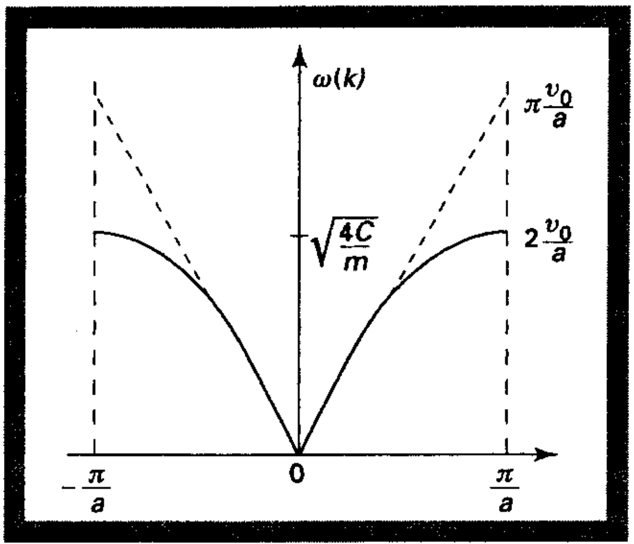


Lattice vibrations

Unidimensional monoatomic case. First neighbour interaction

$$-\omega^2 m s_p = C(e^{ika} + e^{ika} - 2)s_p$$

$$\omega = \sqrt{\frac{4C}{m}}\left|\sin\frac{ka}{2}\right|$$

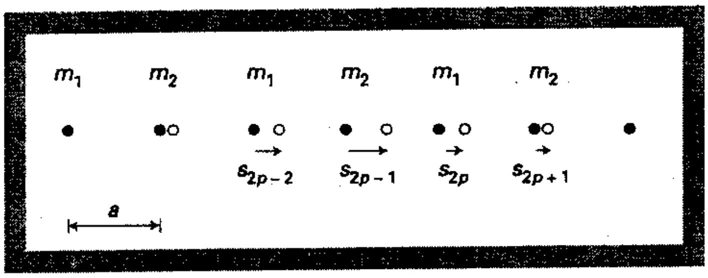


Lattice vibrations

Unidimensional biatomic case. First neighbour interaction

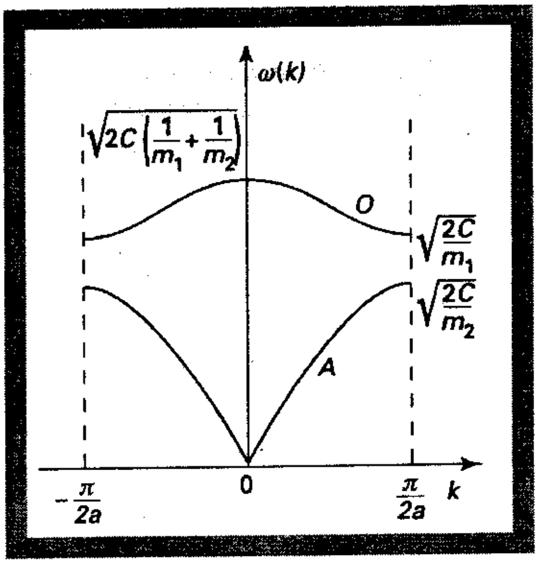
$$m_1\ddot{s}_{2p} = C(s_{2p+1} - s_{2p} + s_{2p-1} - s_{2p})$$

$$m_2\ddot{s}_{2p+1} = C(s_{2p+2} - s_{2p+1} + s_{2p} - s_{2p+1})$$

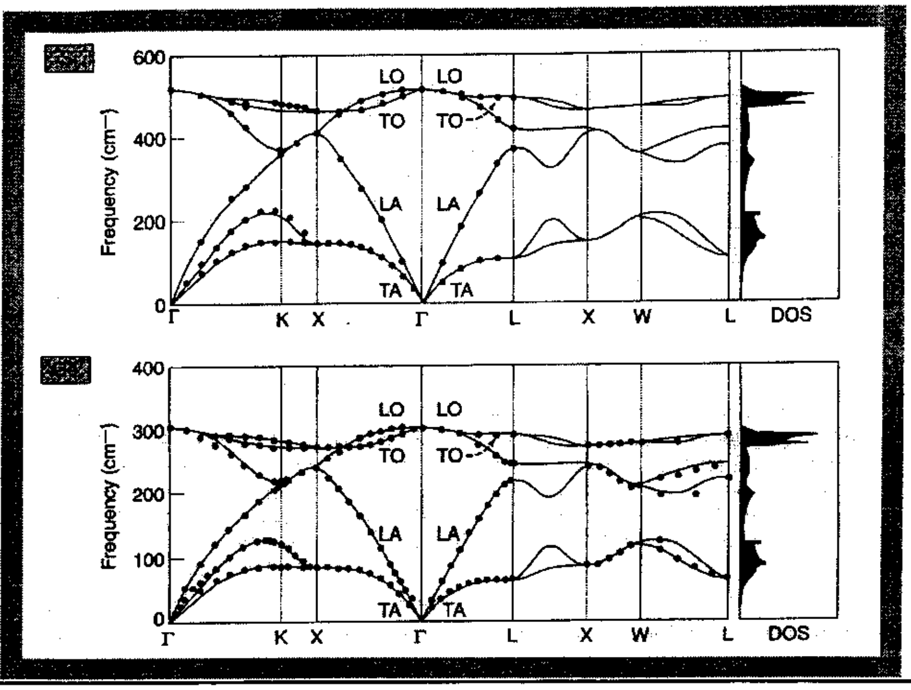


Lattice vibrations

Unidimensional biatomic case. First neighbour interaction



Lattice vibrations



Lattice vibrations

Experimental determination by synchrotron radiation