Optical properties of solids

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Intro

- electronics structure of solids.
- electron-photon transitions in solids.
- experimental techniques
- spin-light interactions

Free electron

Free electron's state is described by Schrödinger equation:

$$H\psi = E\psi$$

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})\right)\psi = E\psi, \quad \text{where } U(\mathbf{r}) = 0$$

In case of free electron, the solution of the electron's wavefunction is plane wave, $\psi = \exp(i\mathbf{k}\cdot\mathbf{r})$, and the corresponding electron's energy is:

$$E = \frac{\hbar^2|\mathbf{k}|^2}{2m}.$$

Free electron energy: $E = \dfrac{\hbar^2 |\mathbf{k}|^2}{2m}$

- Relation between wavelength λ and wavevector $\mathbf{k}$ is $\lambda = \dfrac{2\pi}{|\mathbf{k}|}$.
- When compared with the classical relation $E = \frac{p^2}{2m}$, we obtain relation between the linear momentum $\mathbf{p}$ and the wavevector $\mathbf{k}$ (de Broglie relation):

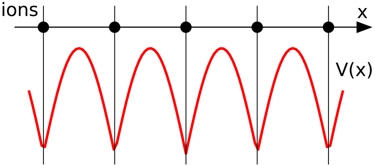
$$\mathbf{p} = \hbar \mathbf{k}.$$

Comparision with photon:

- free electron with energy 1 eV has wavelength 1.23 nm.
- photon with energy 1 eV has wavelength 1240 nm

Electron in periodic potential – Bloch theorem

- Let us assume electron's potential to be periodical: $U_0(\mathbf{r}) = U_0(\mathbf{r} + \mathbf{T})$, where $\mathbf{T}$ is the lattice vector.



- We assume *one-electron approximation*, i.e. interaction with other electrons (exchange, correlation, Coulomb force) are included as the additional effective potential acting on electron, $U_{\mathrm{eff}}(\mathbf{r})$, with the same periodicity as $U_0(\mathbf{r})$: $U(\mathbf{r}) = U_0(\mathbf{r}) + U_{\mathrm{eff}}(\mathbf{r})$.
- Then, the electron's state is described by a wavefunction ψ fulfilling the Schrödinger equation:

$$H\psi = E\psi$$

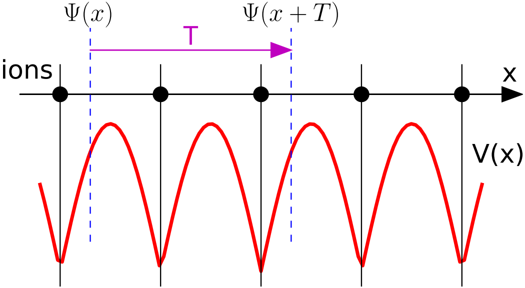
$$\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})\right)\psi = E\psi.$$

Bloch theorem: proof I

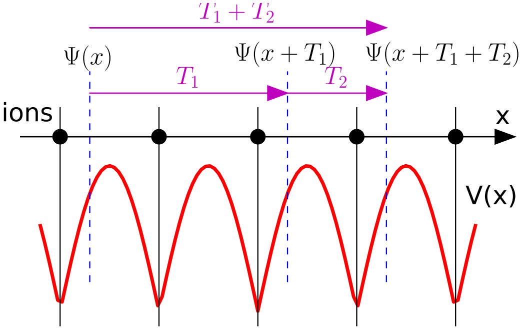
- All observables must have the same periodicity as the lattice. Hence, the electron probability $|\psi|^2$ must fulfill: $|\psi(\mathbf{r})|^2 = |\psi(\mathbf{r}+\mathbf{T})|^2$. Therefore, we can express $\psi(\mathbf{r})$ as:

$$\psi(\mathbf{r}+\mathbf{T}) = e^{i\theta(\mathbf{T})}\psi(\mathbf{r}),$$

where $\theta(\mathbf{T})$ is (at this stage arbitrary) phase, as $|e^{i\theta(\mathbf{T})}|^2 = 1$



Bloch theorem: proof I



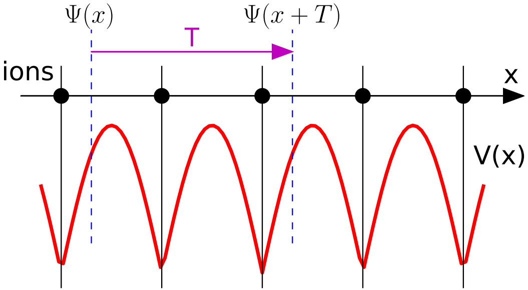
- For two translations $\mathbf{T}_1$ and $\mathbf{T}_2$ we have

$$\psi(\mathbf{r}+\mathbf{T}_1+\mathbf{T}_2) = e^{i\theta(\mathbf{T}_1+\mathbf{T}_2)}\psi(\mathbf{r}) = e^{i\theta(\mathbf{T}_1)}e^{i\theta(\mathbf{T}_2)}\psi(\mathbf{r})$$

Hence, $\theta(\mathbf{T}_1+\mathbf{T}_2) = \theta(\mathbf{T}_1) + \theta(\mathbf{T}_2)$. Hence, the phase $\theta(\mathbf{T})$ has form $\theta(\mathbf{T}) = \mathbf{k}\cdot\mathbf{T}$, as the only this function fulfills the requirement.

Bloch theorem: proof I

- In final, the electron wavefunction of the periodical potential writes: $\psi(\mathbf{r}+\mathbf{T}) = e^{i\mathbf{k}\cdot\mathbf{T}}\psi(\mathbf{r})$. In another words, the translation by a lattice vector $\mathbf{T}$ is equivalent to multiplaying the wavefunction $\psi(\mathbf{r})$ by a phase factor $e^{i\mathbf{k}\cdot\mathbf{T}}$.



Bloch theorem: proof II

- Let us assume, that the solution of $\psi(\mathbf{r})$ is in form:

  $$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}).$$

  Then, we show that $u_{\mathbf{k}}(\mathbf{r})$ has the same periodicity as the lattice.
- In point $\mathbf{r} + \mathbf{T}$ the wavefunction has value:

  $$\psi(\mathbf{r} + \mathbf{T}) = e^{i\mathbf{k}\cdot(\mathbf{r}+\mathbf{T})} u_{\mathbf{k}}(\mathbf{r} + \mathbf{T}),$$

  whereas the previous proof provides:

  $$\psi(\mathbf{r} + \mathbf{T}) = e^{i\mathbf{k}\cdot\mathbf{T}} \psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{T}} e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}).$$

- By comparing both equations, we see:

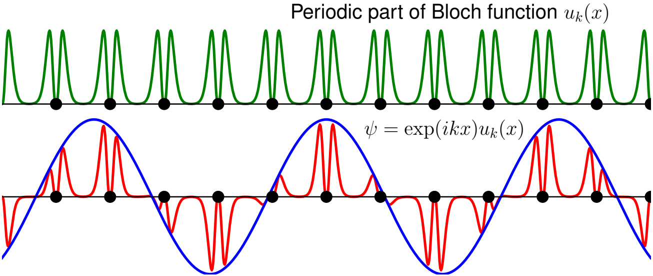
  $$u_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r} + \mathbf{T}),$$

  i.e. $u_{\mathbf{k}}(\mathbf{r})$ has the same periodicity as the lattice.

Wavefunction of the periodic potential is (Bloch theorem):

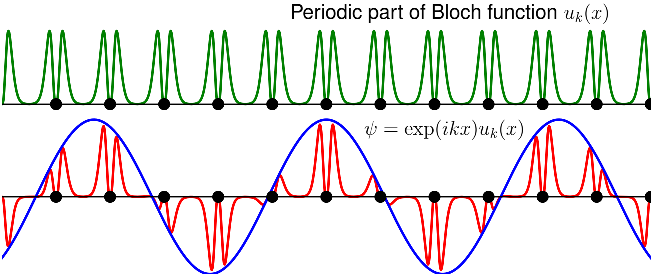
$$\psi_{\mathbf{k}}(\mathbf{r}) = \exp(i\mathbf{k}\cdot\mathbf{r})u_{\mathbf{k}}(\mathbf{r}),$$

- $u_{\mathbf{k}}(\mathbf{r})$ has equal periodicity as the lattice, $u_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r}+\mathbf{T})$.
- $\exp(i\mathbf{k}\cdot\mathbf{r})$ corresponds to free-electron wave (free-electron propagation). It implies that the electron propagates through the crystal like a free (pseudo-free) particle.



$$\psi_{\mathbf{k}}(\mathbf{r}) = \exp(i\mathbf{k}\cdot\mathbf{r})u_{\mathbf{k}}(\mathbf{r}),$$

- Function $u_{\mathbf{k}}(\mathbf{r})$ modulates this free-electron-like wave so that the amplitude oscillates periodically form one cell to the next. It does not affect the basic character of ψ, which is that of a traveling wave. In reality the electron is not free, (it interacts with the lattice, electrons etc), but its propagation has features of a free electron propagation.
- As the electron behaves like a wave with wavevector $\mathbf{k}$, it has a deBroglie wavelength and thus a corresponding momentum $\mathbf{p} = \hbar\mathbf{k}$.



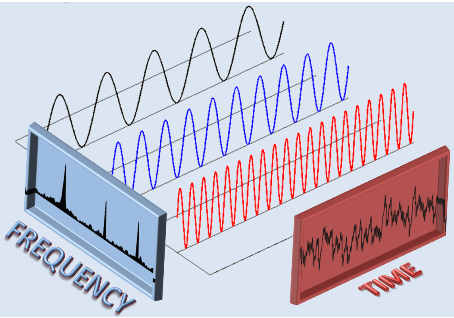
1D Fourier transform

Fourier transform:

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \exp(-ikx) \mathrm{d}x$$

Inverse Fourier transform:

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) \exp(ikx) \mathrm{d}k$$



Build function $f(x)$ as a sum of harmonic functions $\exp(ikx)$ having amplitudes $F(k)$.

1D Fourier transform

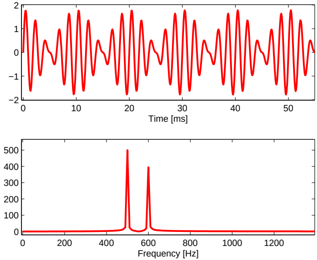
Fourier transform:

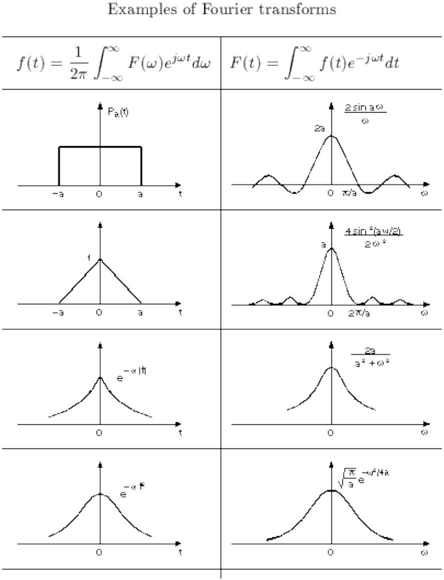
$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \exp(-ikx) \mathrm{d}x$$

Inverse Fourier transform:

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) \exp(ikx) \mathrm{d}k$$

Example: sound in real (time) and reciprocal (frequency) space:





Examples of Fourier transforms

$f(t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}F(\omega)e^{j\omega t}d\omega$	$F(t)=\int_{-\infty}^{\infty}f(t)e^{-j\omega t}dt$

http://www.etc.tuiasi.ro/cin/Downloads/Fourier/Fourier.html

Basic properties of 1D Fourier transformations

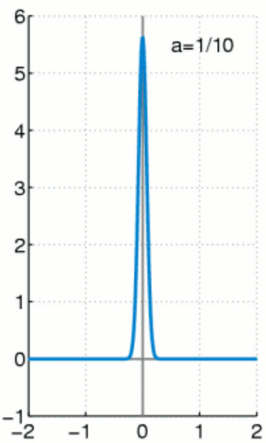
$f(t)$	$F(\omega)$=F.T.$(f(t))$
$f(at)$	$\frac{1}{\lvert a\rvert}F\left(\frac{\omega}{a}\right)$
$f^\star(t)$	$F^\star(-\omega)$ (conjugation)
$f(t-t_0)$	$F(\omega)e^{-it_0\omega}$
$f(t)e^{i\omega_0 t}$	$F(\omega-\omega_0)$
$f(t)\cos(\omega t)$	$\frac{1}{2}\left[F(\omega+\omega_0)+F(\omega-\omega_0)\right]$
$\frac{\mathrm{d}^n f(t)}{\mathrm{d}t^n}$	$(i\omega)^n F(\omega)$
$(-it)^n f(t)$	$\frac{\mathrm{d}^n F(\omega)}{\mathrm{d}\omega^n}$

Dirac δ-function

Definition of δ-function

$$\delta(x) = \begin{cases} +\infty, & x = 0 \\ 0, & x \neq 0 \end{cases}$$

$$\text{so that} \quad \int_{-\infty}^{\infty} \delta(x)\, dx = 1$$



Properties:

$$\int_{-\infty}^{\infty} f(x)\,\delta(x-a)\mathrm{d}x = f(a)$$

$$\delta(ax) = \frac{\delta(x)}{|a|}$$

$$\int_{-\infty}^{\infty} e^{ikx}\mathrm{d}k = 2\pi\delta(x)$$

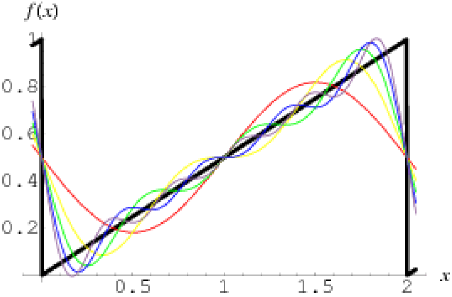
Fourier series

Let us have *periodic* function $f(x)$ with period T, $f(x) = f(x+L)$. Then,

$$f(x) = \sum_{n=-\infty}^{\infty} c_n \exp(in\frac{2\pi x}{L}).$$

where

$$c_n = \frac{1}{L}\int_{-L/2}^{L/2} f(x)\exp(-in\frac{2\pi}{L}x)\mathrm{d}x$$



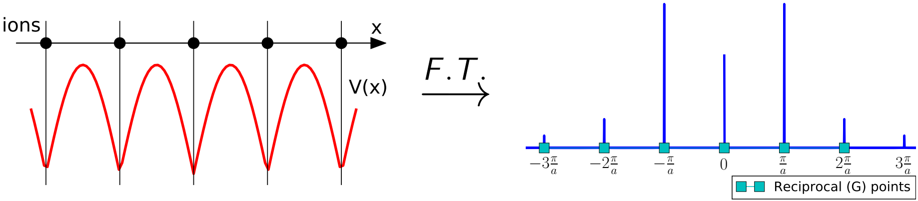
Fourier series and Fourier transformation

Periodic function $f(x) = \sum_{n=-\infty}^{\infty} c_n \exp(in\frac{2\pi x}{L})$.

Fourier transform of periodic function $f(x)$ is:

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \exp(-ikx) \mathrm{d}x = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} c_n \int_{-\infty}^{\infty} \exp\left[ix(-n\frac{2\pi}{L} + k)\right]$$

$$= \sum_{n=-\infty}^{\infty} \sqrt{2\pi} c_n \delta(k - n\frac{2\pi}{L}).$$



Periodic function becomes a train of δ-functions with equidistant spacing.

Reciprocal space (k-space)

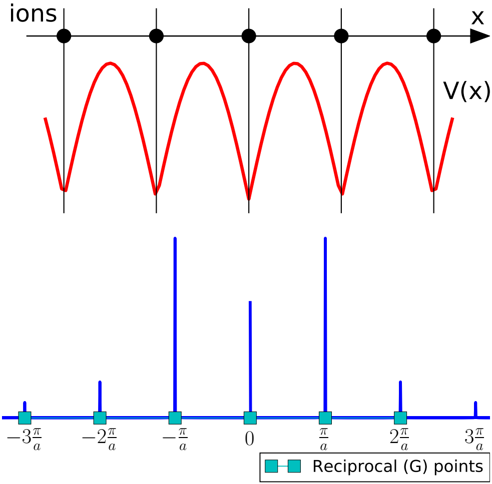
- In the real space, the quantities are expressed as function of positions, e.g. $V(\mathbf{r})$, $\psi_{\mathbf{k}}(\mathbf{r})$.
- In the reciprocal space, the quantities are expressed as function of wave-vector $\mathbf{k}$ or momentum $\mathbf{p} = \hbar\mathbf{k}$.
- Conversion between real and reciprocal space is Fourier transform, e.g. $V(\mathbf{k}) = \mathrm{F.T.}(V(\mathbf{r}))$, and $V(\mathbf{r}) = \mathrm{inv.F.T.}(V(\mathbf{k}))$.

Reciprocal space (k-space): potential $V(x)$

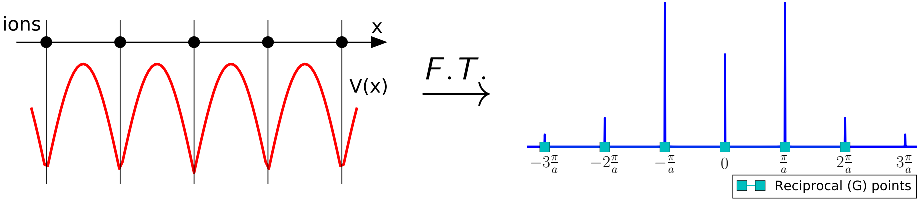
Potential $V(\mathbf{x})$ of the crystal is periodical. Hence, in the reciprocal space, $V(\mathbf{k})$ consists of train (lattice) of δ-functions.

$V(r)$
real space

$V(k)$
reciprocal
space



Reciprocal space (k-space): potential $V(x)$



- the position of δ-functions are called reciprocal points or G-points, forming reciprocal lattice
- the distance between G-points is given only by periodicity of the function

⇒ any periodic function with equal periodicity is described by δ functions at identical G-points

⇒ any periodic property of crystal (potential, electron density) is expressed at identical G-points

- the shape of the function is given by amplitudes of the δ-functions

Reciprocal space of 2D periodic function $f(\mathbf{r})$

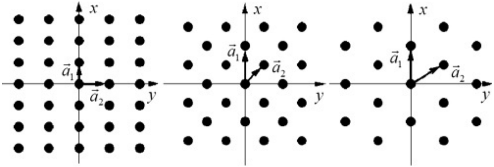
- 2-dimensional (2D) periodic function $f(\mathbf{r}) = f(\mathbf{r} + \mathbf{R_u})$, $\mathbf{u} \in \mathbb{Z}$, where translation vectors $\mathbf{R} = u_1\mathbf{a}_1 + u_2\mathbf{a}_2$ form *Bravais lattice*

→ $\mathbf{a}_1$, $\mathbf{a}_2$ called primitive vectors

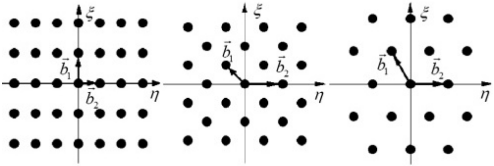
- Fourier transform of $f(\mathbf{r})$ consists of 2D lattice of δ-functions

→ each reciprocal point denotes position of δ-function

Bravais (real) lattice:



Reciprocal lattice:

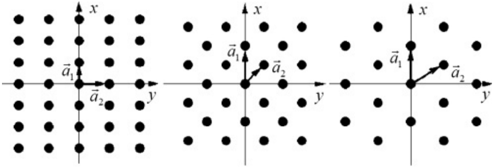


Lin-Wei et al, JOSAA 25, 203 (2008)

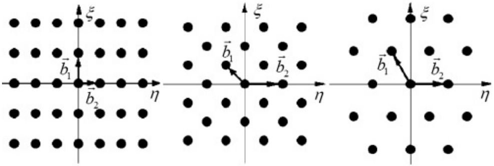
Reciprocal space of 2D periodic function $f(\mathbf{r})$

- position of reciprocal points $\mathbf{G_m}$ are determined by relation $\mathbf{G_m} \cdot \mathbf{R_u} = 2\pi n$, $n \in \mathbb{Z}$, originating from condition $\exp(i\mathbf{G_m} \cdot \mathbf{R_u}) = 1$
- primitive vector of reciprocal lattice are $\mathbf{b}_1$, $\mathbf{b}_2$, providing $\mathbf{G_m} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2$
- similar for 3D reciprocal lattice

Bravais (real) lattice:



Reciprocal lattice:



Lin-Wei et al, JOSAA 25, 203 (2008)

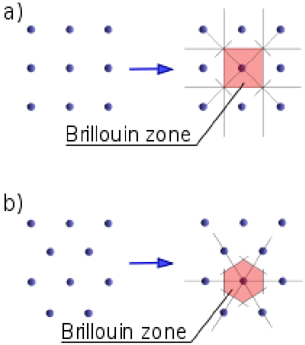
(First) Brillouin zone

Definitions:

Def1: First Brillouin zone is a smallest possible cell in reciprocal space, which by translation can form whole reciprocal space.

Def2: Any point of the reciprocal space $\mathbf{k}$ can be reached from the first Brillouin zone $\mathbf{k}_{\text{inside\_1st\_Brillouin\_zone}}$ added to a translation vector of the reciprocal lattice $\mathbf{G}_{mn}$:

$$\mathbf{k} = \mathbf{k}_{\text{inside\_1st\_Brillouin\_zone}} + \mathbf{G}_{mn}.$$

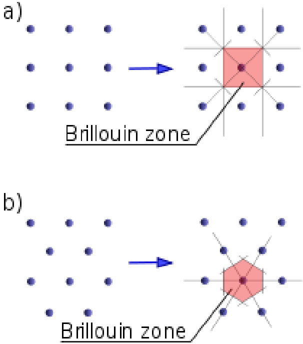


Properties of Brillouin zone:

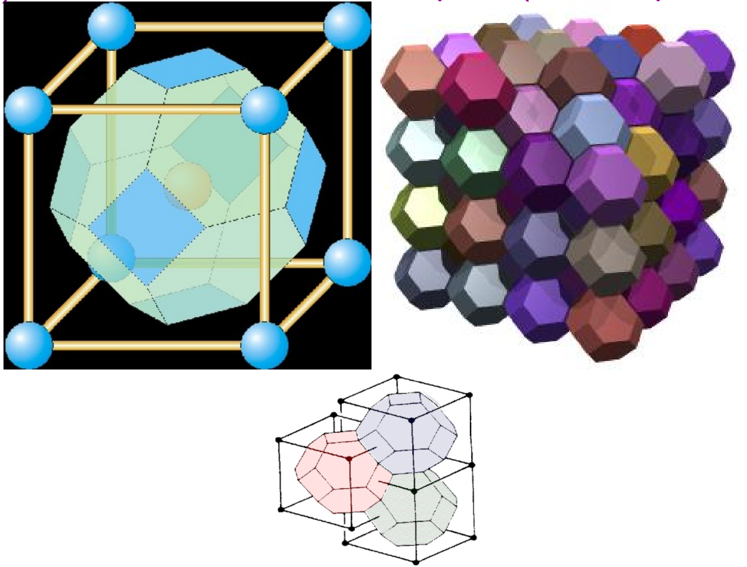
- Volume of the (first) Brillouin zone $V_{\mathbf{k}}$ is inversely proportional to volume of unit cell of the real (direct) lattice $V_{\mathbf{r}}$:

$$V_{\mathbf{k}} = \frac{(2\pi)^N}{V_{\mathbf{r}}}$$

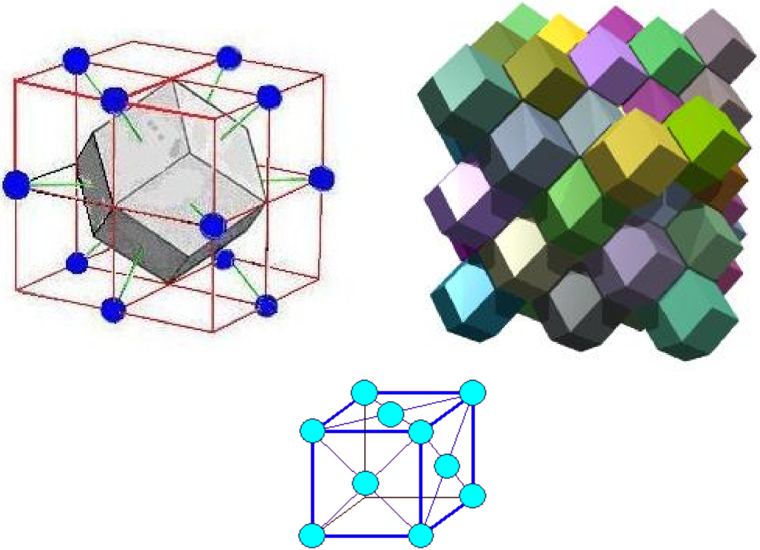
N - dimension of lattice (2D or 3D)



(First) Brillouin zone of fcc real space (bcc reciprocal)



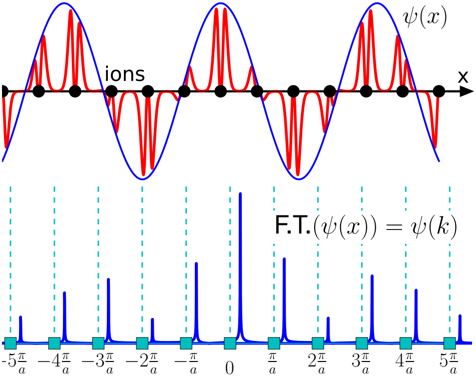
(First) Brillouin zone of bcc real space (fcc reciprocal)



Bloch's $\psi(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r})$ in the reciprocal space

- $u_{\mathbf{k}}(\mathbf{r})$ periodical part of Bloch's function
- $\exp(i\mathbf{k}\cdot\mathbf{r})$ plane wave.

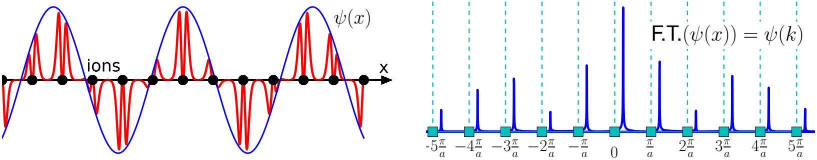
As $\psi(\mathbf{r})$ is not periodic in $\mathbf{r}$, $\psi(\mathbf{k})$ is expressed by train of δ-functions shifted by $\mathbf{k}$ from the reciprocal points as F.T.$(f(x)\exp(ik_0x))$=$F(k-k_0)$.



$\psi(r)$
real space

$\psi(k)$
reciprocal
space

Bloch's $\psi(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r})$ in the reciprocal space



- as $\psi(\mathbf{k})$ is described by a train of δ-functions in the reciprocal space, it is enough to use **k** from the 1st Brillouin zone

⇒ reduction to the first Brillouin zone

- wavevector **k** is a quantum number of the wavefunction:

⇒ **k** in crystal must be described by integer and hence must be *quantized number*

→ Pauli principle: No two electrons in an atom/crystal can have identical all quantum numbers.

⇒ Inside whole crystal, there can be only two electrons at each **k** state (spin-up and spin-down)

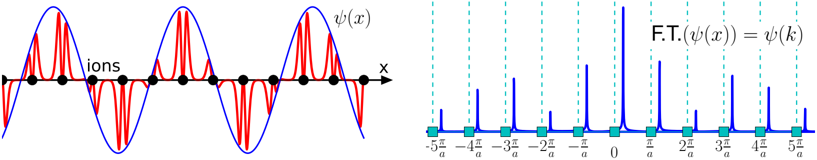
- So, how many **k**-states is in the crystal?

Note: conservation of momentum $\mathbf{p} = \hbar\mathbf{k}$ in a crystal

Energy conservation E: due to time-invariant space.

Momentum conservation $\mathbf{p}$: due to translation-invariant space.

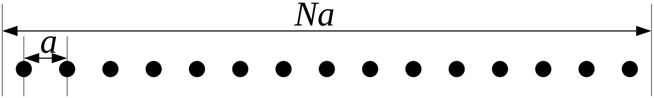
Angular momentum conservation $\mathbf{L}$: due to rotation-invariant space.



- in crystal, there is no invariance of space in both translation and rotation.

⇒ momentum $\mathbf{p} = \hbar\mathbf{k}$ of the electron in crystal is not uniquely defined, and it can behave as having any value $\mathbf{p} = \hbar(\mathbf{k} + \mathbf{G_m})$, $\mathbf{G_m}$ being any reciprocal vector in the lattice.

How many **k**-states is in the crystal?

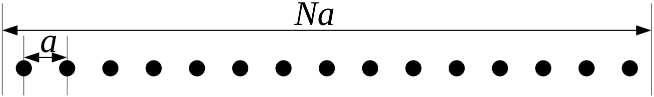


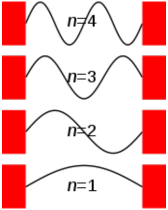
We need to know, how many **k**-states are available inside whole (macroscopic) crystal having N unit cells. Hence, boundary conditions of $\psi(\mathbf{r})$ on crystal's interface must be described.

Number of k states in the Brillouin zone:

There is exactly as many allowed **k**-vector states in the Brillouin zone as there is number of the unit cells in the crystal.

Boundary conditions of $\psi(\mathbf{r})$ on interface of the crystal:





1st opt: Describe standing waves inside the 1D box, having boundary conditions $\psi(x<0)=\psi(x>Na)=0$, where a is inter-atomic distance and N is a number of atoms in x-direction. However, difficult to handle analytically.

2nd opt: Cyclic (Born – von Kármán) boundary conditions $\psi(x)=\psi(x+Na)$. Not a real (physical) boundary conditions, but accounts correct number of allowed k-states.

Cyclic boundary conditions:

Let us demonstrate cyclic boundary conditions in x-direction:

$$\psi(x) = \psi(x + Na)$$

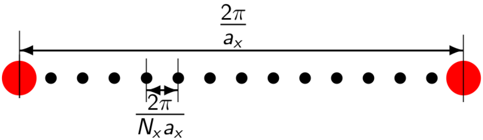
For Bloch electron in x-direction:

$$\psi(x) = e^{ikx} u_k(x)$$
$$\psi(x + Na) = e^{ikNa} e^{ikx} u_k(x) = e^{ikNa} \psi(x)$$

And hence: $e^{ikNa} = 1$, providing $kNa = 2\pi m$, $m \in \mathbb{Z}$. Hence, allowed values of k are:

$$k_m = \frac{2\pi}{a} \frac{m}{N}$$

Cyclic boundary conditions:



Due to the boundary conditions, not all values of k-vector are allowed. Only allowed values of k are ($m \in \mathbb{Z}$):

$$k_m = \frac{2\pi}{a}\frac{m}{N} = G\frac{m}{N},$$

i.e. the reciprocal translation vector $G = 2\pi/a$ is divided to N parts.

To generalize to 3D and general unit cell (general Brillouin zone):

Number of k states in the Brillouin zone:

There is exactly as many allowed **k**-vector states in the Brillouin zone as there is number of the unit cells in the crystal.

Free electron in 2D cubic crystal

Let us assume an electron inside 2D periodic lattice. However, we assume wavefunction $\psi = e^{i\mathbf{k}\cdot\mathbf{r}}$ (which is solution for $U(\mathbf{r}) = 0$), with energy $E = \frac{\hbar^2 k^2}{2m}$ (free electron approximation).

- Assume crystal has N unit cells in 2D crystal, and Z electrons per unit cell. Hence, whole crystal contains NZ electrons.
- Pauli principle states that on each quantum state (i.e. for each value of k-vector), the $\mathbf{k}$-stae can contain only two electrons (with spin-up and spin-down).
- The electrons are filled to the electronic structure starting from smaller energies, i.e. in our case from smaller $\mathbf{k}$-vectors.

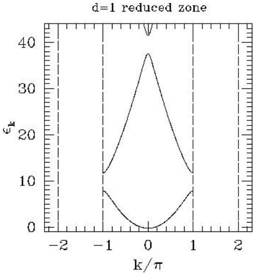
Reduction to the Brillouin zone

In case of electron with **k**-vector outside Brillouin zone, the **k**-vector can be shifted back to the first Brillouin zone,

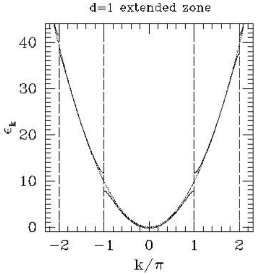
$$\mathbf{k} = \mathbf{k}_{\mathrm{inside\_1st\_Brillouin\_zone}} + \mathbf{G}_{mn}$$

In free electron model, electron energy is $E = \frac{\hbar^2 k^2}{2m}$.
Hence shift of **k** to the Brillouin zone provides electron bands (with principal quantum number $n > 0$).

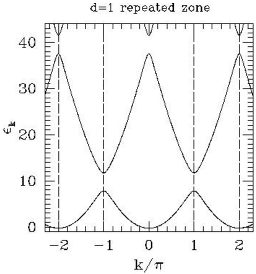
reduced zone



extended zone



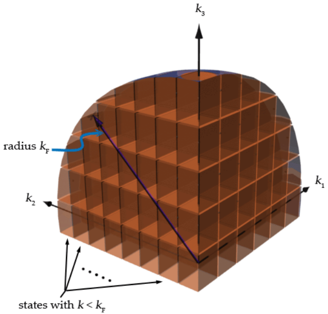
repeated zone



- 2D volume of the Brillouin zone $V_k = 4\pi^2/V_r$ contains 2N electrons' **k**-states (times 2 because of two spins).
- The electron energy depends solely on $|\mathbf{k}|$, the area of constant energy is a sphere in the reciprocal space.

- When all available electrons fill the **k**-spaces, a circle is formed up to the highest occupied energy (*Fermi level*), with **k**-vector k_F.
- This 2D circle occupies reciprocal space $V_k = \pi k_F^2$, providing $\pi k_F^2/(NZ) = (4\pi^2/V_r)/(2N)$. Hence, the Fermi level of this circle has radius:

$$k_F = \sqrt{\frac{2\pi}{V_r} Z} \equiv \sqrt{\frac{2\pi}{V} NZ}.$$



This figure should be 2D!

$$E_F = \frac{\hbar^2 k_F^2}{2m}$$

Free electron in 2D cubic crystal

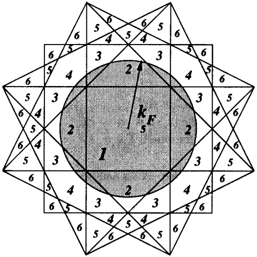
$Z = 4$

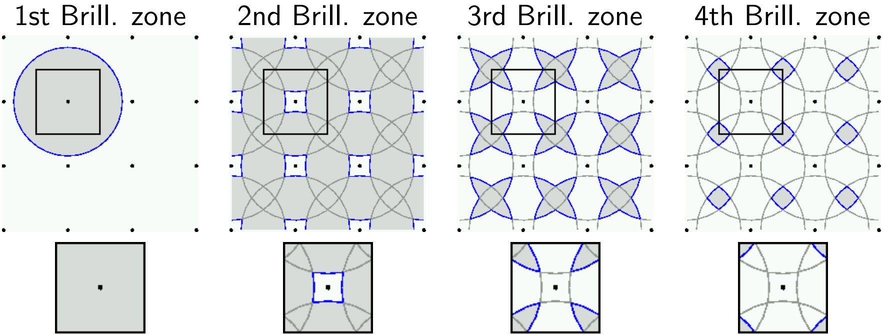
What states are occupied and what are filled?

square length: $k_a = 2\pi/a = 6.28/a$

$k_F = \sqrt{2\pi Z/(a^2)} = 5.01/a$

$k_F/(k_a/2) = 1.60 > \sqrt{2}$




1st Brill. zone

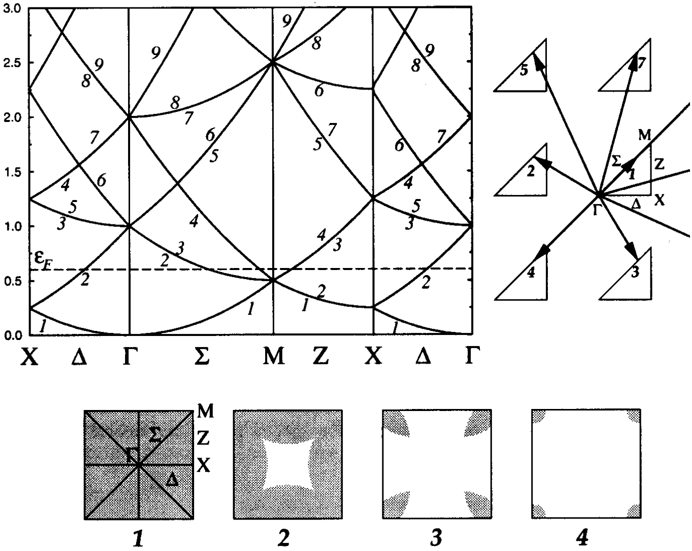
2nd Brill. zone

3rd Brill. zone

4th Brill. zone

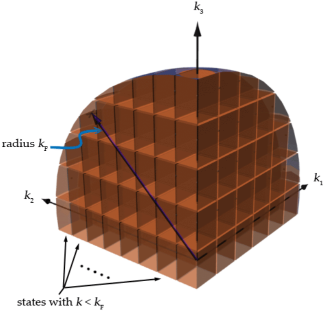
http://phycomp.technion.ac.il/~nika/fermi_surfaces.html

Band structure of 2D electrons in cubic crystal



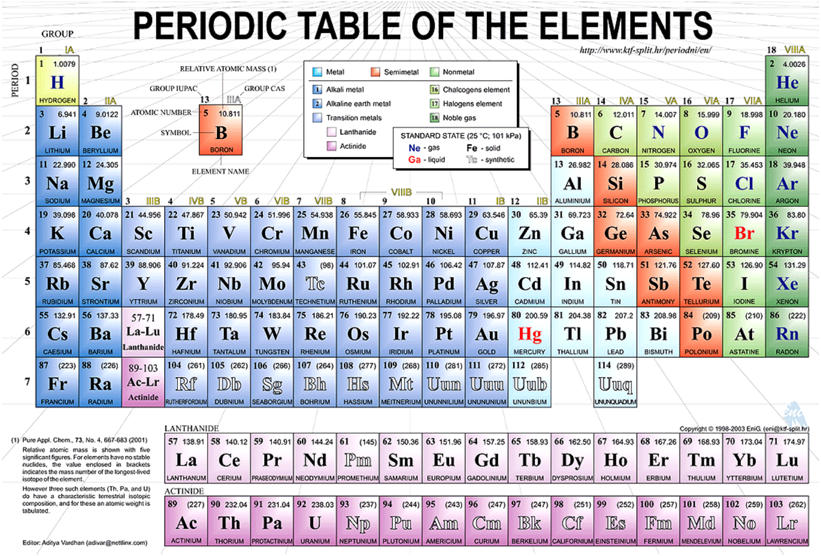
Free electron in 3D

- In the volume of the Brillouin zone $V_k = 8\pi^3/V_r$ there is 2N electrons' k-states.
- The electron energy depends solely on $|\mathbf{k}|$, the area of constant energy is a sphere in the reciprocal space.
- When all NZ available electrons fill the $\mathbf{k}$-spaces, they form a sphere called Fermi sphere (terminated by *Fermi surface*), with maximal k-vector k_F.
- This sphere occupies reciprocal space $V_k = \frac{4}{3}\pi k_F^3$, providing $\frac{4}{3}\pi k_F^3/(NZ) = (8\pi^3/V_r)/(2N)$. Hence, the Fermi sphere has radius:



$$k_F = \sqrt[3]{\frac{3\pi^2}{V_r}Z} \equiv \sqrt[3]{\frac{3\pi^2}{V}NZ}.$$

$$E_F = \frac{\hbar^2 k_F^2}{2m}$$



PERIODIC TABLE OF THE ELEMENTS

http://www.ktf-split.hr/periodni/en/

🟦 Metal	🟥 Semimetal
🟩 Nonmetal	
1 Alkali metal	16 Chalcogens element
2 Alkaline earth metal	17 Halogens element
Transition metals	18 Noble gas
Lanthanide	
Actinide	

STANDARD STATE (25 °C; 101 kPa)
Ne - gas
Fe - solid
Ga - liquid
Tc - synthetic

PERIOD	1 IA	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8	9	10	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1	1 1.0079 H HYDROGEN																	2 4.0026 He HELIUM
2	3 6.941 Li LITHIUM	4 9.0122 Be BERYLLIUM											5 10.811 B BORON	6 12.011 C CARBON	7 14.007 N NITROGEN	8 15.999 O OXYGEN	9 18.998 F FLUORINE	10 20.180 Ne NEON
3	11 22.990 Na SODIUM	12 24.305 Mg MAGNESIUM											13 26.982 Al ALUMINIUM	14 28.086 Si SILICON	15 30.974 P PHOSPHORUS	16 32.065 S SULPHUR	17 35.453 Cl CHLORINE	18 39.948 Ar ARGON
4	19 39.098 K POTASSIUM	20 40.078 Ca CALCIUM	21 44.956 Sc SCANDIUM	22 47.867 Ti TITANIUM	23 50.942 V VANADIUM	24 51.996 Cr CHROMIUM	25 54.938 Mn MANGANESE	26 55.845 Fe IRON	27 58.933 Co COBALT	28 58.693 Ni NICKEL	29 63.546 Cu COPPER	30 65.39 Zn ZINC	31 69.723 Ga GALLIUM	32 72.64 Ge GERMANIUM	33 74.922 As ARSENIC	34 78.96 Se SELENIUM	35 79.904 Br BROMINE	36 83.80 Kr KRYPTON
5	37 85.468 Rb RUBIDIUM	38 87.62 Sr STRONTIUM	39 88.906 Y YTTRIUM	40 91.224 Zr ZIRCONIUM	41 92.906 Nb NIOBIUM	42 95.94 Mo MOLYBDENUM	43 (98) Tc TECHNETIUM	44 101.07 Ru RUTHENIUM	45 102.91 Rh RHODIUM	46 106.42 Pd PALLADIUM	47 107.87 Ag SILVER	48 112.41 Cd CADMIUM	49 114.82 In INDIUM	50 118.71 Sn TIN	51 121.76 Sb ANTIMONY	52 127.60 Te TELLURIUM	53 126.90 I IODINE	54 131.29 Xe XENON
6	55 132.91 Cs CAESIUM	56 137.33 Ba BARIUM	57-71 La-Lu Lanthanide	72 178.49 Hf HAFNIUM	73 180.95 Ta TANTALUM	74 183.84 W TUNGSTEN	75 186.21 Re RHENIUM	76 190.23 Os OSMIUM	77 192.22 Ir IRIDIUM	78 195.08 Pt PLATINUM	79 196.97 Au GOLD	80 200.59 Hg MERCURY	81 204.38 Tl THALLIUM	82 207.2 Pb LEAD	83 208.98 Bi BISMUTH	84 (209) Po POLONIUM	85 (210) At ASTATINE	86 (222) Rn RADON
7	87 (223) Fr FRANCIUM	88 (226) Ra RADIUM	89-103 Ac-Lr Actinide	104 (261) Rf RUTHERFORDIUM	105 (262) Db DUBNIUM	106 (266) Sg SEABORGIUM	107 (264) Bh BOHRIUM	108 (277) Hs HASSIUM	109 (268) Mt MEITNERIUM	110 (281) Uun UNUNNILIUM	111 (272) Uuu UNUNUNIUM	112 (285) Uub UNUNBIUM		114 (289) Uuq UNUNQUADIUM				

LANTHANIDE

57 138.91 La LANTHANUM	58 140.12 Ce CERIUM	59 140.91 Pr PRASEODYMIUM	60 144.24 Nd NEODYMIUM	61 (145) Pm PROMETHIUM	62 150.36 Sm SAMARIUM	63 151.96 Eu EUROPIUM	64 157.25 Gd GADOLINIUM	65 158.93 Tb TERBIUM	66 162.50 Dy DYSPROSIUM	67 164.93 Ho HOLMIUM	68 167.26 Er ERBIUM	69 168.93 Tm THULIUM	70 173.04 Yb YTTERBIUM	71 174.97 Lu LUTETIUM

ACTINIDE

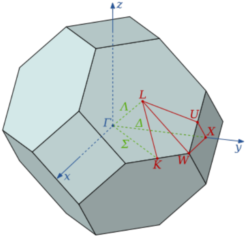
89 (227) Ac ACTINIUM	90 232.04 Th THORIUM	91 231.04 Pa PROTACTINIUM	92 238.03 U URANIUM	93 (237) Np NEPTUNIUM	94 (244) Pu PLUTONIUM	95 (243) Am AMERICIUM	96 (247) Cm CURIUM	97 (247) Bk BERKELIUM	98 (251) Cf CALIFORNIUM	99 (252) Es EINSTEINIUM	100 (257) Fm FERMIUM	101 (258) Md MENDELEVIUM	102 (259) No NOBELIUM	103 (262) Lr LAWRENCIUM

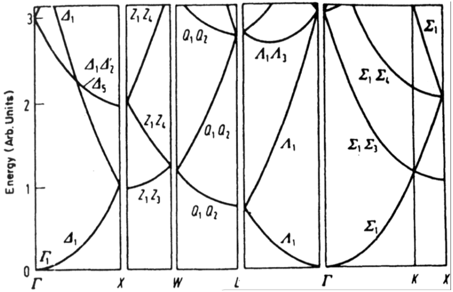
(1) Pure Appl. Chem., **73**, No. 4, 667-683 (2001)
Relative atomic mass is shown with five significant figures. For elements have no stable nuclides, the value enclosed in brackets indicates the mass number of the longest-lived isotope of the element.

However three such elements (Th, Pa, and U) do have a characteristic terrestrial isotopic composition, and for these an atomic weight is tabulated.

Editor: Aditya Vardhan (adivar@netlinx.com)

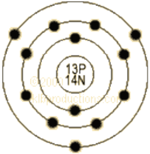
Free electron in fcc:

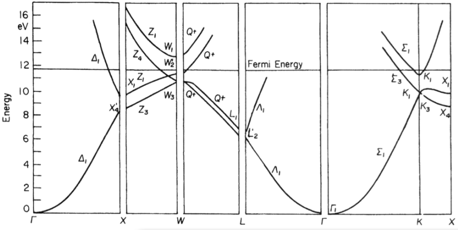




Aluminium (fcc):

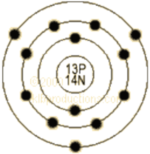
- $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$
- three unbounded electrons

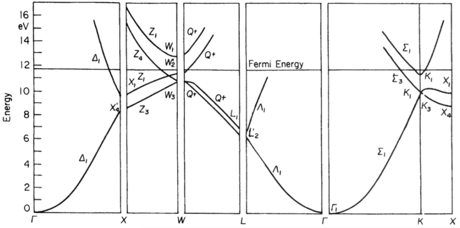




Aluminium (fcc):

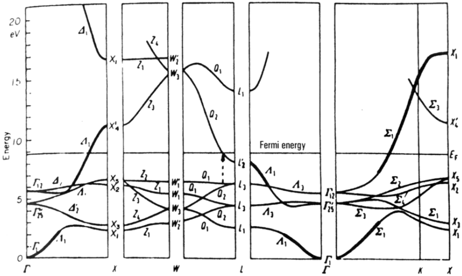
- $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$
- three unbounded electrons





Cuprum (fcc):

- $[Ar]\ 3d^{10}\ 4s^1$
- eleven unbounded electrons



Density of states (DOS):

Density of states (DOS): number of electron's states per energy interval:

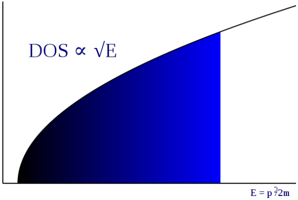
$$g = \frac{\mathrm{d}(NZ)}{\mathrm{d}E}.$$

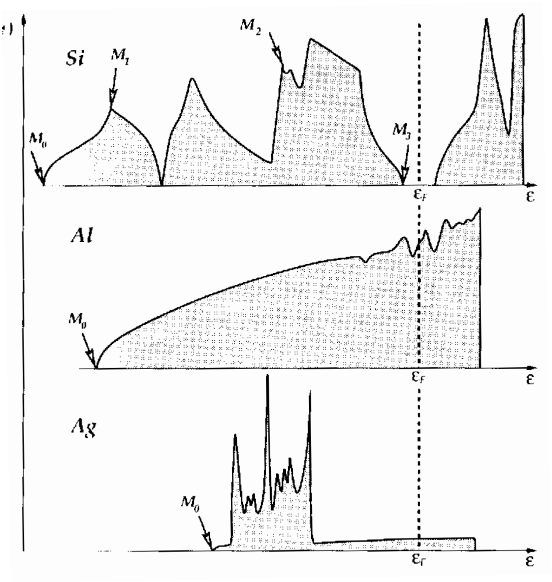
For free elecctron, $E_F = \frac{\hbar^2 k_F^2}{2m}$, where $k_F = \sqrt[3]{\frac{3\pi^2}{V} NZ}$.
Hence:

$$NZ = \frac{V}{3\pi^2} \left(\frac{2mE}{\hbar^2} \right)^{3/2}$$

Therefore, Density of states $g(E)$ of free electron is:

$$g(E) = \frac{\mathrm{d}(NZ)}{\mathrm{d}E} = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{E}$$





Si: complicated DOS, contains gap at Fermi level.

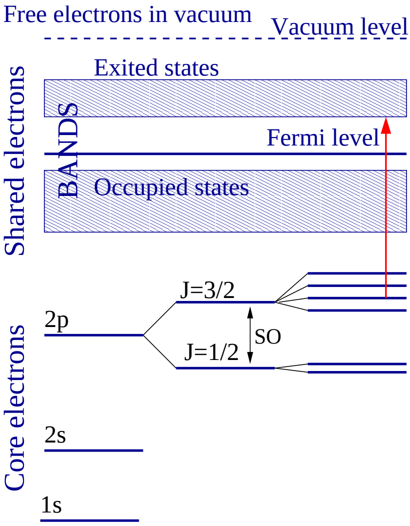
Al: nearly free electrons DOS $\sim \sqrt{E}$.

Ag: *d* electrons are burried and the only electrons on the Fermi level are *s*-electrons.

Complete energy levels in solids:

Core states:

- Electrons in the spherical potential of the nucleus (bounded, not shared, electrons).
- Approximately, they correspond to electrons in filled electronic shells.
- They provide sharp energies.
- Quantum numbers **without** spin-orbit coupling: n, l, $m \equiv l_z$, s, s_z
- Quantum numbers **with** spin-orbit coupling: n, l, s, j, j_z



Complete energy levels in solids:

Occupied states:

Electrons shared through the crystal. They approximately correspond to valence electrons of the atoms. They form energy bands.

Fermi level:

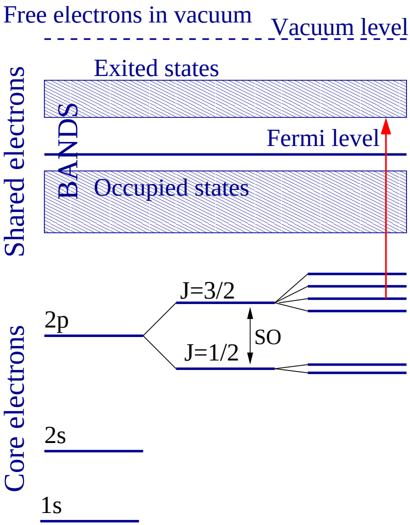
Energy level separating occupied and unoccupied states.

Excited states:

Empty energy levels above Fermi level. Electrons can be excited to those states and then they relax back.

Vacuum level:

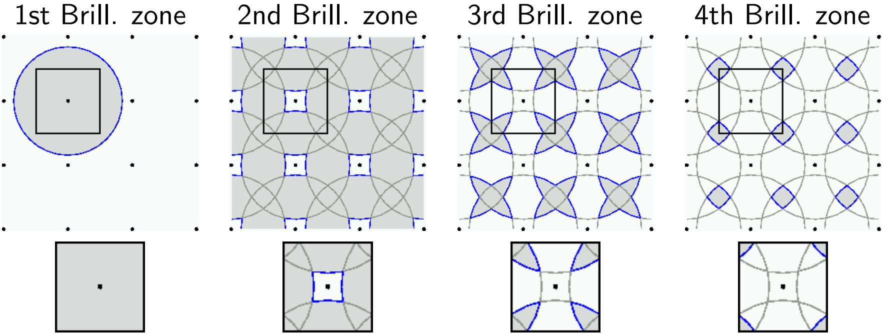
Overcoming this barrier, electrons do not feel periodical potential of the crystal and become free.



Fermi surface

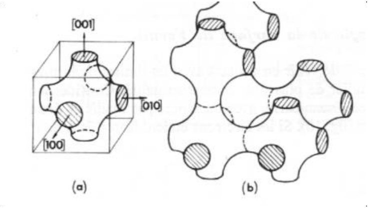
As electrons fill the reciprocal space up to E_F, they create a boundary in the reciprocal space between filled and empty k-spaces. This boundary is called Fermi surface.

Fermi surface in 2D, cubic (blue line):



Fermi surface in 3D

cubic:

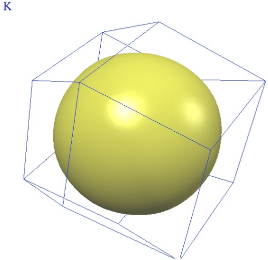


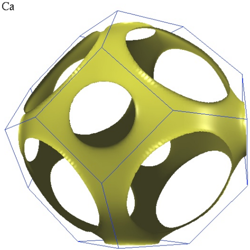
Real atoms:

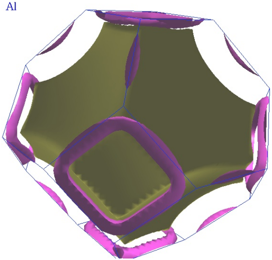
K(bcc) [Ar] $4s^1$

Ca(fcc) [Ar] $4s^2$

Al (fcc) [Ne] $3s^2$ $3p^1$

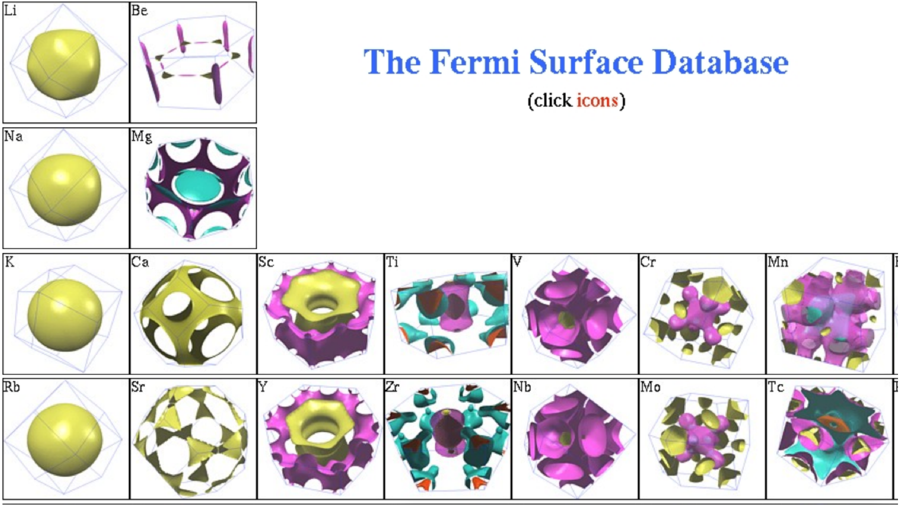






`http://www.phys.ufl.edu/fermisurface/`

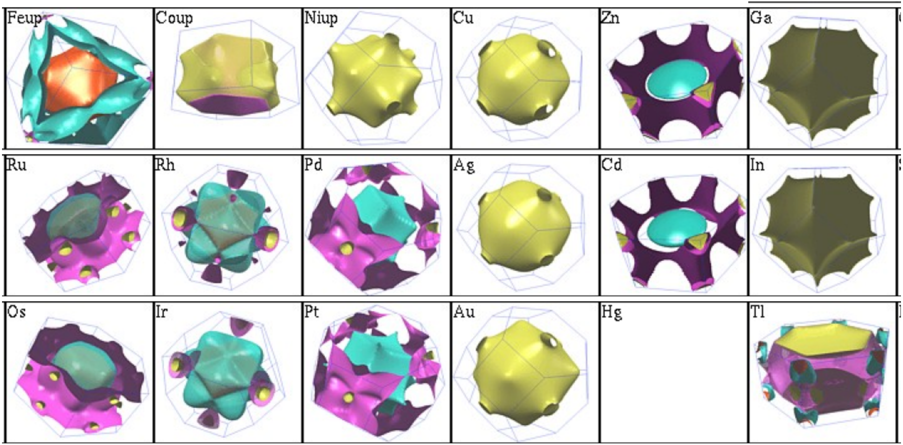
Example of some elements' Fermi surfaces.



The Fermi Surface Database

(click icons)

Example of some elements' Fermi surfaces.



Comments on Fermi surface

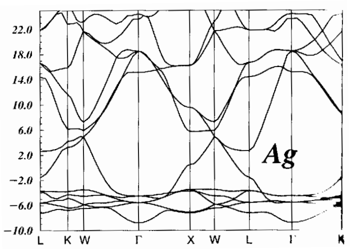
- Fermi surface is formed by free (unbounded or easily excited) electrons. Such electrons are provides e.g. electrical or thermal conductivity.
- Hence, the metal can be defined as 'material having Fermi surface'.
- Semiconductors and insulators do not have Fermi surfaces, because they do not have free electrons on Fermi level. In this case, one Brillouin zone is completely full and next Brillouin zone is completely empty.

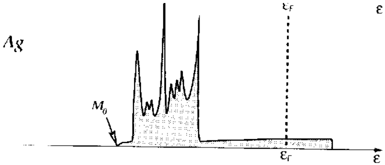
Basic classification of materials (according to DOS):

metal

no gap at Fermi level

Fermi surface

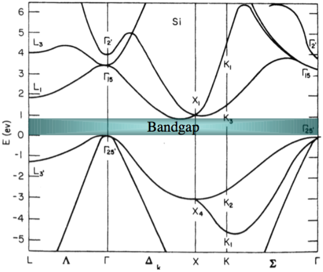


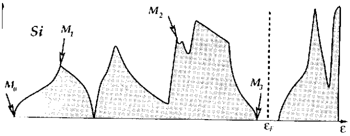


semiconductor/isolator

gap at Fermi level

no Fermi surface (filled BZ)

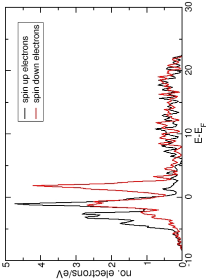




Basic classification of materials (according to DOS):

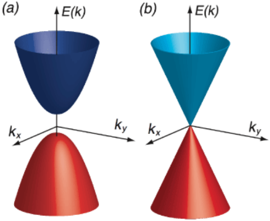
ferromagnet

different DOS for up and down electrons
Fe(bcc): [Ar]$4s^2 3d^6$



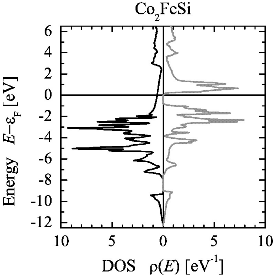
Dirac cone

Fermi surface is a dot.
(graphene, Nobel price 2010)



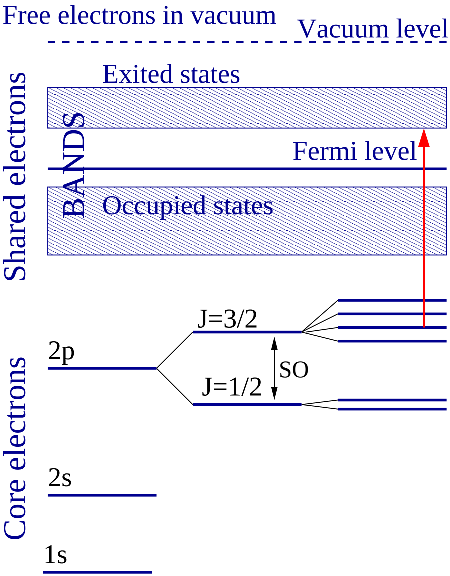
half-metal

gap only for spin down (or only for spin up)



Sketch of the electronic structure in solids:

Core electrons: localized electrons on each atoms.
Shared electrons: form occupied band structure.
Excited electrons: excited to excited states of the crystal, still interacting wit (bonded to) the crystal.
Ionized electrons: excited above vacuum level and hence they are free (no interaction with the crystal).



Photon spectroscopies (absorption) I:

The optical properties are based on probability of photon absorption:

1. material's absorption of photons i.e. imaginary part of permittivity $\Im(\varepsilon)$ [determined usually by electric-dipole approximations].
2. real part of permittivity $\Re(\varepsilon)$ by Kramers-Kronig relations Then, the optical properties are then described by complex numbers, e.g. complex permittivity ε or complex refraction index N or complex conductivity σ, $\varepsilon = N^2 = 1 + i\sigma/\omega$

Photon spectroscopies (absorption) II:

Different photon energy ranges excites and probes different part of the electronic structure of the matter.

dc conductivity, THz=far-infrared: energy about $kT \approx 30\,\text{meV}$. Excites vicinity of the Fermi surface (charge, spin and heat transfer and their combinations).

extended visible light (mid-infrared – far-UV): $\sim 30\,\text{meV}$ - $100\,\text{eV}$. Both starting and final states are in the band structure (both not simply identified) (reflectometry, ellipsometry, MOKE).

X-ray: $\sim 120\,\text{eV}$ – $120\,\text{keV}$. Excites deep core levels of the atoms. XAS (X-ray absorption spectroscopy). Starting levels are from core levels and hence they are easy to identify.

Time dependent perturbation theory I

(according Solid State Physics, M. S. Dresselhaus, `http://web.mit.edu/course/6/6.732/www/6.732-pt2.pdf`)

Unperturbated Hamiltonian with eigenstates

$$H_0 \left|n\right\rangle = E_n \left|n\right\rangle$$

is perturbated by time-dependent perturbation $H'(t)$

$$H = H_0 + H'(t)$$

and we search for solutiuon of Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \left|\psi\right\rangle = (H_0 + H'(t)) \left|\psi\right\rangle$$

The solution is searched as a sum of H_0 eigenstates weighted by time-dependent expansion coefficients $a_n(t)$

$$\left|\psi(t)\right\rangle = \sum_n a_n(t) \left|n\right\rangle \exp(-iE_n t/\hbar)$$

Time dependent perturbation theory II

$$|\psi(t)\rangle = \sum_n a_n(t)\,|n\rangle \exp(-iE_n t/\hbar)$$

By substituting $|\psi(t)\rangle$ to Schr. Eq., multiplying from left by $\langle k|$ and using ortonormality $\langle k|n\rangle = \delta_{nk}$

$$\dot{a}_k(t) = \frac{1}{i\hbar}\sum_n a_n(t)\,\langle k|H'(t)|n\rangle \exp(i\omega_{kn}t)$$

which is exact solution up-to now and where $\hbar\omega_{kn} = E_k - E_n$. Assuming (i) $H'(t)$ is small (ii) at $t = 0$, quantum state is only $|l\rangle$, i.e. $a_l(0) = 1$, $a_{n\neq l}(0) = 0$.

$$\dot{a}_k(t) = \frac{1}{i\hbar}\,\langle k|H'(t)|l\rangle \exp(i\omega_{kl}t)$$

which can be integrated to obtain $a_k(t) = \int_0^t \mathrm{d}t'\dot{a}_k(t')$.

Time dependent perturbation theory III

Assuming, that hamiltonian perturbation is harmonic, $H'(t) = H'(0)\exp(\pm i\omega t)$:

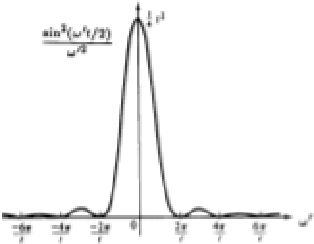
$$\begin{aligned} a_k(t) &= \frac{1}{i\hbar}\langle k|H'(0)|l\rangle \int_0^t \mathrm{d}t' \exp(i(\omega_{kl} \pm \omega)t') \\ &= \frac{1}{i\hbar}\langle k|H'(0)|l\rangle \frac{\exp(i(\omega_{kl} \pm \omega)t) - 1}{i(\omega_{kl} - \omega)} \end{aligned}$$

with amplitude of $a_k(t)$ being (using identity $|\exp(ix) - 1|^2 = 4\sin^2(x/2)$)

$$|a_k(t)|^2 = \frac{|\langle k|H'(0)|l\rangle|^2}{\hbar^2} \frac{4\sin^2((\omega_{kl} \pm \omega)t/2)}{(\omega_{kl} \pm \omega)^2}$$

Time dependent perturbation theory IV

$$|a_k(t)|^2 = \frac{|\langle k|H'(0)|l\rangle|^2}{\hbar^2} \frac{4\sin^2((\omega_{kl} \pm \omega)t/2)}{(\omega_{kl} \pm \omega)^2}$$



- $|a_k(\omega)|^2$ has peak at $\omega = \omega_{kl}$, i.e. at resonance
- the peak width is about $2\pi/t$
  - however, Heisenberg uncertainity principle states

$$\Delta E \Delta t \sim 2\pi\hbar, \qquad \text{i.e.} \qquad \Delta\omega_{kl} \sim \frac{2\pi}{t}$$

  - Hence, the time of transition probability is so small, that the uncertainity in energy (frequency) covers about full width of the peak.

Fermi golden rule I

We introduce probability of transition from state $|l\rangle$ to state $|k\rangle$ per time W_k. Second, as in solid state, there is large number of similar **k**-states in the solids, we sum-up also transition probabilities, where the transition happens at or nearby **k**-state. Hence, we sum transition probability over all possible **k**-states accesible due to uncertainity principle. Number of states in the vicinity of energy ω_{kl} is given by (joint) density of states $\mathrm{d}N = \rho(E_{kl})\,\mathrm{d}E = \rho(E_{kl})\hbar\mathrm{d}\omega_{kl}$.

$$W_k = \frac{1}{t}\int \mathrm{d}N|a_k(t)|^2 = \frac{\hbar}{t}\int \mathrm{d}\omega_{kl}|a_k(t)|^2\rho(\hbar\omega_{kl})$$

integrated over energies (frequencies).

The only quickly changing function is the peak, sinc(x), and hence

$$W_k = \frac{4\hbar}{\hbar^2 t}\,\langle k|H'|l\rangle\,\rho(E_{kl})\int \mathrm{d}\omega_{kl}\frac{\sin^2((\omega_{kl}\pm\omega)t/2)}{(\omega_{kl}\pm\omega)^2}$$

Fermi golden rule II

Using

$$\int_{-\infty}^{\infty} \frac{sin^2 x}{x^2} \mathrm{d}x = \pi$$
$$x = (\omega_{kl} \pm \omega) t/2$$

we finally get (Fermi golden rule = transition probability per time per volume)

$$W_{l \to k} \equiv W_k = \frac{2\pi}{\hbar} | \langle k | H'(0) | l \rangle |^2 \rho(E_{kl})$$

Perturbation Hamiltonian for oscillating electromagnetic field I

- $\mathbf{A}$: vector potential, $\mathbf{B} = \nabla \times \mathbf{A}$, $\mathbf{E} = -\nabla\phi - \frac{\partial}{\partial t}\mathbf{A}$
- ϕ can be zero for electromagnetic wave (charge is zero and gauge transformation can be selected in such a way)
- Then, electromagnetic field can be written as $\mathbf{A}(t) = \mathbf{A}(0)\exp(-i\omega t)$, $\mathbf{E} = i\omega\mathbf{A}$
- Then, perturbated Hamiltonian is (introducing non-zero vector potential $\mathbf{A}$ by substitution $\mathbf{p} \to \mathbf{p} - e\mathbf{A}$)

$$H = H_0 + H' = \frac{1}{2m}(\mathbf{p} - e\mathbf{A})^2 + e\phi - \boldsymbol{\mu}\cdot\mathbf{B} + U(\mathbf{r})$$

Perturbation Hamiltonian for oscillating electromagnetic field II

$$H = H_0 + H' = \frac{1}{2m}(\mathbf{p} - e\mathbf{A})^2 + e\phi - \boldsymbol{\mu}\cdot\mathbf{B} + U(\mathbf{r})$$

Two perturbations appeares:

- $H' = -\frac{e}{m}\mathbf{p}\cdot\mathbf{A}$: el-mag field 'moves' electron charge. It provides so called electric dipolar transitions. Dominant term for interband and intraband optical transitions, i.e. photon absorption process for dc, optical and X-ray frequency range.
- $H' = -\boldsymbol{\mu}\cdot\mathbf{B} = \frac{e\hbar}{2m}\boldsymbol{\sigma}\cdot\mathbf{B}$: el-mag field 'moves' electron spin. It providing so called magnetic dipole transitions. It governs effects changing spin direction e.g. creation of magnon, FMR excitation, absorption in NMR, where electric dipole transitions are not allowed.

Electric-dipole transitions:

- The largest contribution to the photon absorption is given by so-called electric-dipole transitions valid for $\lambda \gg a$.
- Hence, whole vast energy range can be described by so-called Kubo formula, determining conductivity (absorption) for a given photon energy .

As **k**-vector is conserved during optical transitions from conductive to valence band, the joint density of states is

$$\rho_{cv}(\hbar\omega) = \frac{2}{8\pi^3} \int_{BZ} \mathrm{d}^3\mathbf{k}\,\delta(E_c(\mathbf{k}) - E_v(\mathbf{k}) - \hbar\omega)$$

Substituting this to Fermi golden rule, and assuring the transition goes from occupied to unoccupied state, we obtain Kubo formula expressing light absorption in matter.

Kubo formula

Conductivity (propertional to probability of photon absorption)

$$\Im(\varepsilon_{xx}) \sim \Re(\sigma_{xx}) \sim$$

$$\sum_{i,f} [f(E_i) - f(E_f)] \times [|\langle i|p_+|f\rangle|^2 + |\langle i|p_-|f\rangle|^2] \times \delta(E_f - E_i - \hbar\omega)$$

where

- $\langle i|$, $|f\rangle$: initial and final states, respectively.
- $p_\pm = p_x \pm i p_y$, $p_x = i\hbar\partial/\partial x$, momentum operator
- terms in the Kubo formula means:
    - summation over all initial and final states, $\langle i|$ and $|f\rangle$
    - $f(E_f)$, $f(E_i)$: electron occupancy of initial and final states.
    - $|\langle i|p_\pm|f\rangle|^2$: probability of the photon to be absorbed between $\langle i|$ and $|f\rangle$ states for circularly left/right polarized light (non-zero only when electric-dipole selection rules are fulfilled).
    - $\delta(E_f - E_i - \hbar\omega)$ assures energy conservation.

Selection rules of electric-dipole transitions:

Electric dipole transition is allowed when following conditions are fulfilled:

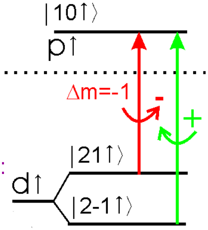
Energy: $E_f - E_i = \hbar\omega$ (absorbed photon energy is difference between energies of the final and initial electron states)

Momentum: $\hbar\omega/c \approx 0$ (photon has negligible momentum compared to one of the electron. I.e. the momentum of the electron is kept between initial and final state (vertical transitions)).

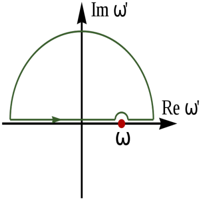
Electron spin : $\Delta s = 0$ (probability photon's spin=1 is transferred to electron's spin is tiny ⇒ electron's spin is preserved for electric dipole transitions)

Orbital momentum: $\Delta l = \pm 1$ (photon has angular momentum $1\hbar$). Therefore only $s \leftrightarrow p$, $p \leftrightarrow d$ etc. transitions are allowed.

Orbital momentum along z-axis (magnetic number): $\Delta m = \pm 1$ (determines if photon is circularly right or left polarized).



Kramers-Kroning relations I



0) Kramers-Kroning relations relates real and imaginary of the complex function, e.g. of the optical spectra of the permittivity.
Purely based on mathematical relation between real and imaginary part of 'polite' functions (Cauchy integral).
1) mathematics: Cauchy residual theorem states (for any function without poles in integration area):

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

2) for function $\chi(\omega')/(\omega' - \omega)$, we create pole in point $\omega' = \omega$. Hence Cauchy integral becomes (assuming the integral over 'arc' is zero, i.e. function χ is enough small at infinity):

$$\oint \frac{\chi(\omega')}{\omega' - \omega}\, d\omega' = \mathcal{P}\int_{-\infty}^{\infty} \frac{\chi(\omega')}{\omega' - \omega}\, d\omega' - i\pi\chi(\omega) = 0.$$

I.e. function in point $\chi(\omega)$ equals to the integral over whole ω'!

Kramers-Kroning relations II

Rearranging:

$$\chi(\omega) = \frac{1}{i\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{\chi(\omega')}{\omega' - \omega}\, d\omega'.$$

3) Amplitude of $\chi(t)$ is real. Further, $\chi(\omega)$=F.T.($\chi(t)$). Hence $\chi(\omega) = \chi^*(-\omega)$. Hence, relation between $\Re(\chi)$ and $\Im(\chi)$ is

$$\Re(\chi(\omega)) = \frac{2}{\pi}\mathcal{P}\int_{0}^{\infty} \frac{\omega'\Im(\chi(\omega'))}{\omega'^2 - \omega^2}\, d\omega'$$

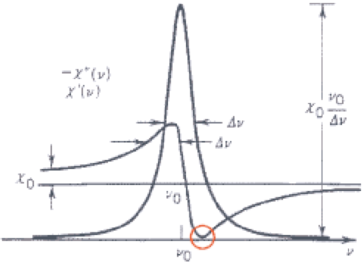
$$\Im(\chi(\omega)) = -\frac{2\omega}{\pi}\mathcal{P}\int_{0}^{\infty} \frac{\Re(\chi(\omega'))}{\omega'^2 - \omega^2}\, d\omega'$$

Which are famous Kramers-Kronig relations.

Kramers-Kroning relations III

- Absorption line (i.e. $\Im(\varepsilon)$) is described by Lorenzian function. Kramers-Kronig then determines its real part.
- notice finite shift in $\Re(\varepsilon)$ even for $\omega \ll \omega_0$. It corresponds to e.g. situation when light propagating in glass is not not absored, however, its propagation speed is smaller to c due to absorption at higher frequencies.

Example: Lorenzian function



Kramers-Kroning relations IV

Comment on Kramers-Kronig relations:

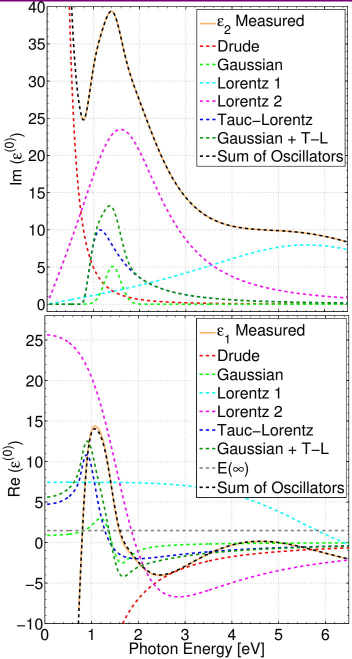
- In Kubo formula, $\Re(\varepsilon)$ can be equally obtained by introducing finite linewidth Γ, i.e. by replacing δ-function by finete-width Lorenzian function:

$$\delta(E_f - E_i - \hbar\omega) \rightarrow \frac{1}{E_f - E_i - \hbar\omega + i\Gamma}$$

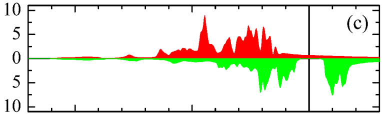
Contributions to optical permittivity

Optical permittivity ε: $\varepsilon = \Re(\varepsilon) + i\Im(\varepsilon)$

- $\Im(\varepsilon)$ means light absorption.
- $\Re(\varepsilon)$ and $\Im(\varepsilon)$ are related by Kramers-Kronig (KK) relations.
- the light absorption consist of several contributions; their sum provides resulting light absorption
  1. vaccum permittivity: $\varepsilon_\infty = 1$
  2. Drude term (free electron).
  3. Lorentz term (resonance line).
  4. Tauc-Lorentz (semiconductor gap).
  5. many others



Example:
Heusler compound
$Co_2FeAl_{0.5}Si_{0.5}$
Balke et al



Lorentz oscillator (Lorentz contribution)

photon absorption due to bound states

$$\varepsilon_{\mathrm{Lorentz}} = \frac{A^2}{\omega_0^2 - \omega^2 - i\Gamma\omega}$$

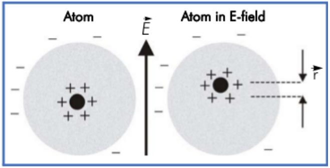


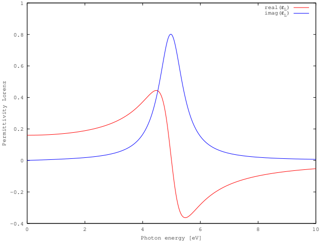
Fig. 4 Polarization of the electronic cloud due to external E-field.

ω: Photon energy

ω_0: Energy distance between the energy levels (i.e. resonance energy)

A: Amplitude (probability of the absorption)

Γ: Width of the line (sharpness of the absorption) (i.e. full width at half maxima: FWHM)



Can be determined also from damped oscillator model:

$$m\frac{\mathrm{d}^2 y}{\mathrm{d}t^2} + m\Gamma\frac{\mathrm{d}y}{\mathrm{d}t} + m\omega_0^2 y = E\cos(\omega t)$$

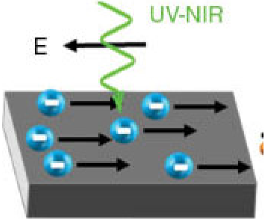
where material's polarization is $P = \varepsilon_0 \varepsilon E = yNq$.

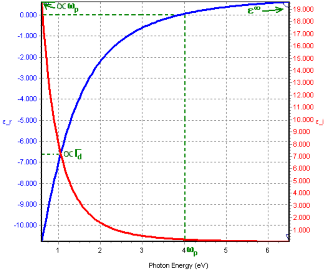
Free electron contribution: Drude contribution

$$\varepsilon_{\text{Drude}} = \frac{A^2}{-\omega^2 - i\Gamma\omega}$$

- photon absorption due to free electrons (i.e. due to conductivity)
- Drude is like Lorenz, for $\omega_0 = 0$
- amplitude A also called plasma frequency ω_p; at this frequency $\Re(\varepsilon_{\text{Drude}}) = 0$ for $\varepsilon_\infty = 1$
- when Drude is expressed in permittivity, $\lim_{\omega\to 0} \Im(\varepsilon_{\text{Drude}}) = \infty$
- driving equation

$$m\frac{\mathrm{d}^2 y}{\mathrm{d}t^2} + m\Gamma\frac{\mathrm{d}y}{\mathrm{d}t} = E\cos(\omega t)$$



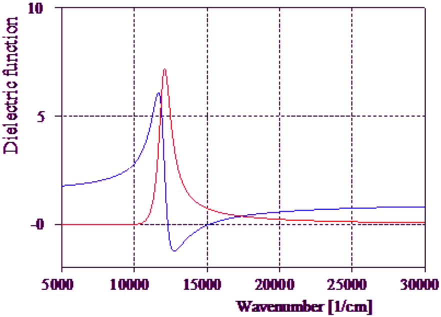


Tauc-Lorentz contribution

Tauc-Lorentz contribution describes optical properties of (amorphous) semiconducor at photon energies near the gap:

$$\varepsilon_{\mathrm{TL}} = A\left(\frac{\omega-\omega_{\mathrm{gap}}}{\omega}\right)^2 H(\omega-\omega_{\mathrm{gap}})\Im\left(\frac{1}{\omega_0^2-\omega^2-i\omega\Gamma}\right)$$

i.e. Tauc-Lorentz is expressed by multiplication of Lorentz function, parabolic function, and Heaviside step function



**With more careful calculations, one can win;
with less, one cannot.
How much less chance of victory has one who makes no calculations at all!**

Sun Tzu: The Art of War

Spin-orbit coupling: Dirac equation

Spin-orbit coupling term couples spin of the electron $\boldsymbol{\sigma} = 2\mathbf{S}/\hbar$ with movement of the electron $m\mathbf{v} = \mathbf{p} - e\mathbf{A}$ in presence of electrical field $\mathbf{E}$.

$$H_{SOC} = -\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma} \cdot [\mathbf{E} \times (\mathbf{p} - e\mathbf{A})]$$

The maximal coupling is obtained when all three componets are perpendicular each other.
The spin-orbit term can be determined from solution of electron state in relativistic case. The equation describing relativistic electron is called Dirac equation, relativistic analogue of Schrodinger equation.

Dirac equation: introduction I

- Relativity describes nature at high speeds, $v \approx c$.
- Relativity unites time and space, described by Lorentz transformation

$$x' = \frac{x - vt}{\sqrt{1 - \frac{v^2}{c^2}}} \qquad t' = \frac{t - \frac{vx}{c^2}}{\sqrt{1 - \frac{v^2}{c^2}}}$$

$\Rightarrow$ relativistic quantum theory must do the same. Schrodinger equation does not fulfils this, as it it has first derivative in time and second in space.

Dirac equation: introduction II

Relativistic theory expresses total energy of the particle as:

$$W^2 = p^2 c^2 + m_0^2 c^4 \tag{1}$$

Quantum operator substitution: $\mathbf{p} \to \hat{\mathbf{p}} = -i\hbar\nabla$,
$W \to \hat{W} = i\hbar\partial/\partial t$. It follows in Klein-Gordon equation

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m_0^2 c^2}{\hbar^2}\right)\psi(\mathbf{r}, t) = 0 \tag{2}$$

This Eq. reduces to Eq. (1) for plane wave (free particle) $\psi(\mathbf{r}, t) = \exp[i(\mathbf{r} \cdot \mathbf{p} - Wt)/\hbar]$. This condition limits following solutions to particles with spin $1/2$, as space-time wavefunction is symmetric, and hence spin-part must be antisymmetric.

Dirac equation: derivation I

1. let as ASSUME, the Dirac equation will have first derivative in time. Then, it must be also in first derivative in space.
2. wave function is superposition of N base wavefunctions $\psi(\mathbf{r},t)=\sum\psi_n(\mathbf{r},t)$
3. must fulfil Klein-Gordon equation, Eq. (2)

General expression of condition 1:

$$\frac{1}{c}\frac{\partial\psi_i(\mathbf{r},t)}{\partial t}=-\sum_{w=x,y,z}\sum_{n=1}^{N}\alpha_{i,n}^{w}\frac{\partial\psi_n}{\partial w}-\frac{imc}{\hbar}\sum_{n=1}^{N}\beta_{i,n}\psi_n(\mathbf{r},t) \qquad (3)$$

Dirac equation: derivation II

When expressed in matrix form (ψ is column vector, $\alpha^k_{i,n}$ is $3 \times N \times N$ matrix, $\beta_{i,n}$ is $N \times N$ matrix)

$$\frac{1}{c}\frac{\partial \psi(\mathbf{r},t)}{\partial t} = -\tilde{\boldsymbol{\alpha}} \cdot \nabla \psi(\mathbf{r},t) - \frac{imc}{\hbar}\tilde{\beta}\psi(\mathbf{r},t) \tag{4}$$

Substituting quantum operators $\hat{\mathbf{p}} \rightarrow -i\hbar\nabla$, we get Dirac equation

$$i\hbar\frac{\partial \psi(\mathbf{r},t)}{\partial t} = \hat{H}\psi(\mathbf{r},t) = (c\tilde{\boldsymbol{\alpha}} \cdot \hat{\mathbf{p}} + \tilde{\beta}mc^2)\psi(\mathbf{r},t) \tag{5}$$

where matrices $\tilde{\alpha}$, $\tilde{\beta}$ are unknown.

Dirac equation: non-relativistic limit

When Dirac equation is solved up to order $1/c^2$, we get

$$\begin{aligned}\hat{H} =& \frac{1}{2m}\left(\frac{\hbar}{i}\nabla - e\mathbf{A}(\mathbf{r})\right)^2 + V(\mathbf{r}) + mc^2 \qquad \text{Unrelativistic Hamiltonian}\\ & - \frac{e\hbar}{2m}\boldsymbol{\sigma}\cdot\mathbf{B} \qquad \text{Zeeman term}\\ & - \frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot[\mathbf{E}\times(\mathbf{p}-e\mathbf{A})] \qquad \text{Spin} - \text{orbit coupling}\\ & - \frac{1}{8m^3c^2}(\mathbf{p}-e\mathbf{A})^4 \qquad \text{Mass of electron increases with speed}\\ & + \frac{\hbar^2 e}{8m^2c^2}\nabla^2 V(\mathbf{r}) \qquad \text{Darwin term}\end{aligned}$$

Darwin term: electron is not a point particle, but spread in volume of size of Compton length $\approx \hbar/mc$.

Spin-orbit coupling: discussion I

Spin-orbit coupling term can be sepaarted into two components:

$$-\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot[\mathbf{E}\times(\mathbf{p}-e\mathbf{A})] = -\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot[\mathbf{E}\times\mathbf{p}] + \frac{e^2\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot[\mathbf{E}\times\mathbf{A}]$$
$$= H_{SOC} + H_{AME}$$

AME=Angular magneto-electric

- The electric field $\mathbf{E} = -\frac{1}{e}\nabla V - \frac{\partial}{\partial t}\mathbf{A}$
- canonical momentum $\mathbf{p} = -i\hbar\nabla$ (conjugate variable of position; $\frac{\partial H}{\partial x_i} = -\dot{p}_i$, $\frac{\partial H}{\partial p_i} = \dot{x}_i$)
- kinetical momentum $m\mathbf{v} = \mathbf{p} - e\mathbf{A}$ (defines kinetic energy and represents velocity)

H_{SOC} in spherical potential, static case

$$H_{SOC} = -\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot[\mathbf{E}\times\mathbf{p}]$$

Spherical potential $V(\mathbf{r}) = V(|\mathbf{r}|) = V(r)$; static case $\frac{\partial}{\partial t}\mathbf{A} = 0$:

$$e\mathbf{E} = -\nabla V(|\mathbf{r}|) = \frac{dV(r)}{dr}\frac{\mathbf{r}}{|\mathbf{r}|}$$

providing:

$$H_{SOC} = \frac{\hbar}{4m^2c^2}\frac{1}{r}\frac{dV}{dr}\boldsymbol{\sigma}\cdot(\mathbf{r}\times\mathbf{p}) = \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV}{dr}\mathbf{S}\cdot\mathbf{L} = \xi\mathbf{S}\cdot\mathbf{L}$$

where spin angular momentum $\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$ and orbital angular momentum $\mathbf{L} = \mathbf{r}\times\mathbf{p}$

Understanding spin-orbit coupling: spherical potential

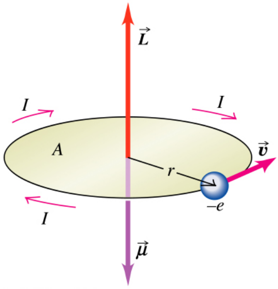
- spin of the electron creates electron's magnetic moment (in SI)

$$\boldsymbol{\mu}_S = -\frac{e}{m}\mathbf{S} = -\frac{e}{m}\frac{h}{2}\boldsymbol{\sigma} = -\mu_b\boldsymbol{\sigma} = -\frac{2\mu_B}{\hbar}\mathbf{S}$$

  where $\mu_B = \frac{e\hbar}{2m}$ is Bohr magneton.
- orbital moment (around atomic core) creates magnetic moment too

$$\boldsymbol{\mu}_L = -\frac{e}{2m}\mathbf{L} = -\frac{\mu_B}{\hbar}\mathbf{L} = -\mu_B l$$

  (or can be understood as creating magnetic field H_{eff} due to current created by electron orbital)
- the mutual static energy of spin and orbital is then $E_{SO,approx} = -\boldsymbol{\mu}_S \cdot \mathbf{B}_{eff}$ or just electrostatic interaction between both magnetic dipoles.



Understanding spin-orbit coupling: Lorentz transformation

Electromagnetic field appears different as observing frame is moved. For example, if a charge is moving in the laboratory frame (unprimed), we observe both electric and magnetic fields. In the frame of the moving charge (primed), only electric field is observed and the current and magnetic field are absent. Lorentz transformation of el.-mag. fields between both frames is:

$$\mathbf{E}'_{\parallel} = \mathbf{E}_{\parallel} \qquad \mathbf{B}'_{\parallel} = \mathbf{B}_{\parallel}$$

$$\mathbf{E}'_{\perp} = \frac{(\mathbf{E} + \mathbf{v} \times \mathbf{B})_{\perp}}{\sqrt{1 - \frac{v^2}{c^2}}} \qquad \mathbf{B}'_{\perp} = \frac{(\mathbf{B} - \mathbf{v}/c^2 \times \mathbf{E})_{\perp}}{\sqrt{1 - \frac{v^2}{c^2}}}$$

where $\perp$ and $\parallel$ are relative to the direction of the velocity $\mathbf{v}$. I.e. for small speeds, $\mathbf{E}' = \mathbf{E} + \mathbf{v} \times \mathbf{B}$ and $\mathbf{B}' = \mathbf{B} - \frac{\mathbf{v}}{c^2} \times \mathbf{E}$

Understanding spin-orbit coupling: Lorentz transformation

For electron flying by speed $\mathbf{v}$ through static electric field $\mathbf{E}$, in its frame the electron feels magnetic field $\mathbf{B}' = -\frac{-\mathbf{v}}{c^2} \times \mathbf{E}$, which torques/acts on its spin. The Hamiltonian is given by Zeeman interaction

$$H_{SO,E\to B} = -\boldsymbol{\mu}_S \cdot \mathbf{B}' \tag{6}$$

$$= -\left(-\frac{e\hbar}{2m}\boldsymbol{\sigma}\right) \cdot \left(-\frac{1}{c^2}(-\mathbf{v}) \times \mathbf{E}\right) \tag{7}$$

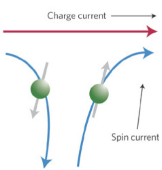
$$= -\frac{e\hbar}{2m^2c^2}\boldsymbol{\sigma} \cdot (\mathbf{E} \times \mathbf{p}) \tag{8}$$

which is twice larger compared to H_{SOC} derived from Dirac equation. Missing half is due to Thomas precession (in case of electron orbiting nucleus, it is the precession of the electron rest frame as it orbits around the nucleus).

Lorentz transformation: extrinsic spin Hall effect

In laboratory frame, spin-Hall effect provides scattering of electrons on charged impurity along to electron spin.

In electron frame, it can be understood as charge current from impurities, providing magnetic field, according which the electron spin aligns.



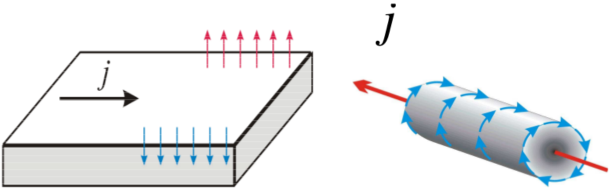


Figure 1. The Spin Hall Effect. An electrical current induces spin accumulation at the lateral boundaries of the sample. In a cylindrical wire the spins wind around the surface, like the lines of the magnetic field produced by the current. However the value of the spin polarization is much greater than the (usually negligible) equilibrium spin polarization in this magnetic field.

Examples of spin-orbit effects

$$H_{SOC} = -\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma} \cdot [\mathbf{E} \times (\mathbf{p} - e\mathbf{A})]$$

Various SOC effects are obtained by different origins of **A** and $\mathbf{E} = \frac{1}{e}\nabla V - \frac{\partial}{\partial t}\mathbf{A}$.
Examples:

- SOC in spherical potential (already discussed)
- optical spin pumping: excitation of electrons with selective spins in GaAs
- **E** has contribution originating from interface of two materials: → Rasha effect
- **A** has contribution of incident light: coupling between angular momentum of light and electron spin (optomagnetic field)

Example: splitting of atomic levels by SOC

Splitting of atomic levels due to spin-orbit coupling (without magnetic field). The energy levels corresponds to different values of the total angular momentum **J**

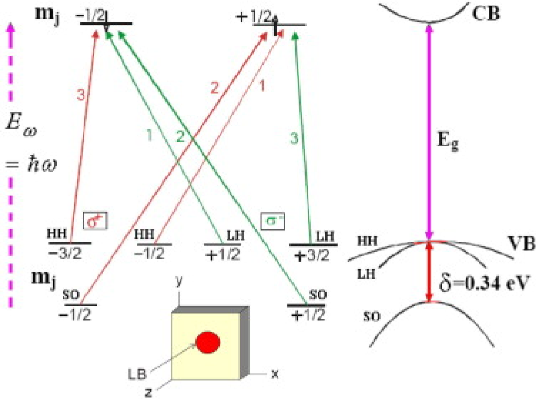
$$\begin{aligned}\mathbf{J} &= \mathbf{L} + \mathbf{S} \\ \mathbf{J}\cdot\mathbf{J} &= (\mathbf{L}+\mathbf{S})\cdot(\mathbf{L}+\mathbf{S}) = \mathbf{L}\cdot\mathbf{L} + \mathbf{S}\cdot\mathbf{S} + 2\langle\mathbf{L}\cdot\mathbf{S}\rangle \\ j(j+1) &= l(l+1) + s(s+1) + 2\langle\mathbf{L}\cdot\mathbf{S}\rangle \\ \langle\mathbf{L}\cdot\mathbf{S}\rangle &= \frac{1}{2}\left[j(j+1) - l(l+1) - s(s+1)\right]\end{aligned}$$

For p states, $l = 1$, $s = 1/2$ and $j = 3/2$ (4 electrons) or $1/2$ (2 electrons). So, due to spin-orbit coupling (without magnetic field), the energy level of electron splits into two levels.
Thus, the spin-orbit interaction does not lift all the degeneracy for atomic states. To lift this additional degeneracy it is necessary to apply a magnetic field.

Optical spin orientation

Electron excitation by circularly polarized beam in GaAs excites electrons with selective spins.

- for $\hbar\omega$ between E_g and $E_g + \Delta_{SO}$, only the light and heavy hole subband are excited. Then for zinc-bland structure (e.g. GaAs), the spin-polarization is $P_n = -1/2$.
- Light polarization can also be used to detect spin polarization in semiconductors.

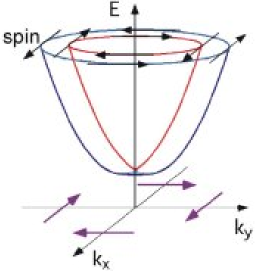


Rashba effect I

Rashba Hamiltonian: electric field **E** is created on interface, **E** $\parallel \hat{z}$:

$$H_{\mathrm{Rashba}} = \alpha(\boldsymbol{\sigma} \times \mathbf{p}) \cdot \hat{\mathbf{z}}$$

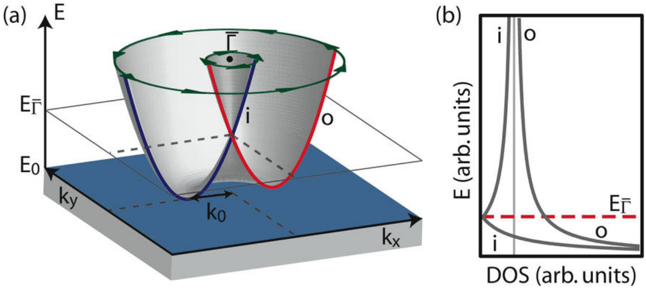
α: Rasba coupling
p: electron's momentum
σ: spin direction (Pauli matrix vector)



The Rashba effect is a momentum dependent splitting of spin bands in two-dimensional condensed matter systems (heterostructures and surface states). It originates from concurrent appearance of

- spin-orbit coupling
- asymmetry of the potential in the direction $\hat{z}$ perpendicular to the two-dimensional plane, creating electric field $\mathbf{E} = E_z\hat{z} = -\frac{1}{e}\nabla V$

Rashba effect II



`http://www.sps.ch/fr/articles/progresses/`

- For $\mathbf{p} = p_x$ and $H_{\text{Rashba}} = \alpha(\boldsymbol{\sigma} \times \mathbf{p}) \cdot \hat{z} \Rightarrow H_{\text{Rashba}} = -\alpha p_x \sigma_y$
- splitting of energy states according to **p** and $\boldsymbol{\sigma}$ directions.
- max. splitting when z, **p** and $\boldsymbol{\sigma}$ are perpendicular each other.
- when crystal lacks inversion symmetry, internal electric field **E** is created.

Optomagnetic field I

according to: Paillard, Proc. of SPIE 9931, 99312E-1 (2016)

$$H_{AME} = -\frac{e^2\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot[\mathbf{E}\times\mathbf{A}]$$

Assume electric field as plane wave

$$\mathbf{E}_{\mathrm{ext}} = -\frac{\partial\mathbf{A}}{\partial t} = \Re\left(\mathbf{E}_0\exp[i(\mathbf{k}\cdot\mathbf{r}-\omega t)]\right)$$

providing vector potential as $\mathbf{A} = \Re(-\frac{i}{\omega}\mathbf{E}_0\exp[i(\mathbf{k}\cdot\mathbf{r}-\omega t)])$

- Electric field acting on electron has two contributions, $\mathbf{E} = \mathbf{E}_{\mathrm{int}} + \mathbf{E}_{\mathrm{ext}}$, $\mathbf{E}_{\mathrm{int}} = -1/e\nabla V$ provided by crystal and $\mathbf{E}_{\mathrm{ext}}$ provided by incoming el.-mag. field.
- term $[\mathbf{E}_{\mathrm{int}}\times\mathbf{A}]$ vanishes as $\mathbf{E}_{\mathrm{int}}$ varies much quicker compared to $\mathbf{A}$ (due to $a \ll \lambda$).

Optomagnetic field II

$$H_{AME} = -\frac{e^2\hbar}{8m^2c^2\omega}\boldsymbol{\sigma} \cdot \Re[i\mathbf{E}_0 \times \mathbf{E}_0^*] = -\boldsymbol{\mu}_B \cdot \mathbf{B}_{OM}$$

$$\mathbf{B}_{OM} = -\frac{\mu_B}{\varepsilon_0 c^3\omega\hbar} I \boldsymbol{\sigma}_{\text{helicity}}$$

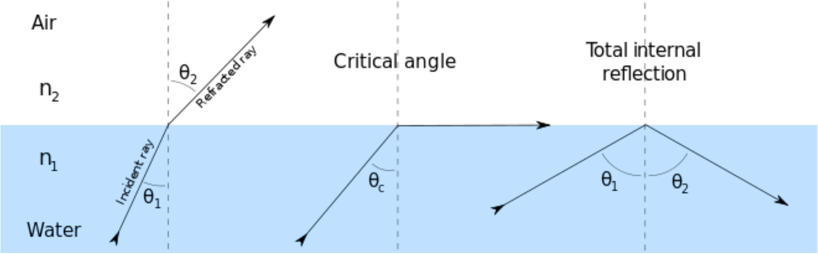
- $\boldsymbol{\mu} = -\mu_b\boldsymbol{\sigma}$: electron magnetic moment, $\mu_b = e\hbar/(2m)$ Bohr magneton
- $\boldsymbol{\sigma}_{\text{helicity}} = \Re[i\mathbf{u} \times \mathbf{u}]$: helicity of beam, where $\mathbf{u}$ is beam polarization, $\mathbf{u} = \mathbf{E}_0/E_0$
- $I = \frac{c\varepsilon_0}{2}E_0^2$: beam intensity
- direction of $\mathbf{B}_{OM}$ is determined by helicity of the incident beam $\boldsymbol{\sigma}_{\text{helicity}}$

Note: although $\mathbf{B}_{OM}$ contributes to magnetization torque by induced light, it is not probably the dominanting term.

Techniques using evanescent light wave

Attenuated total reflection & Surface plasmon polariton

Reflection and total reflection



Snell law:

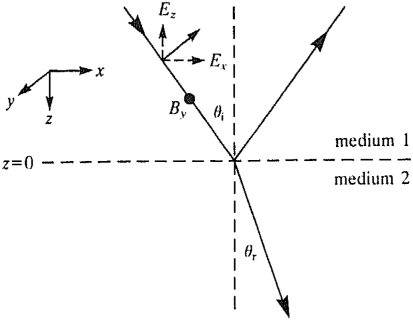
$$\sqrt{\varepsilon_1}\sin\varphi_1 = \sqrt{\varepsilon_2}\sin\varphi_2$$

Critical angle:

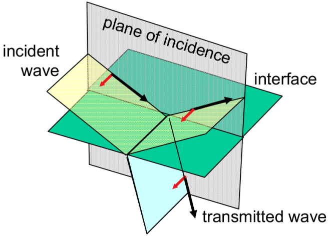
$$\sin\varphi_c = \sqrt{\frac{\varepsilon_2}{\varepsilon_1}}$$

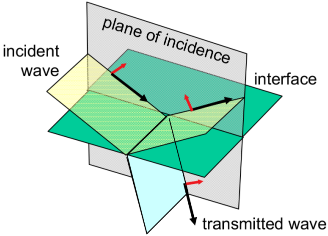
Light reflection on the interface

1. Maxwell equations
2. solution as plane wave
   $E = E_0 \exp(i(\mathbf{k} \cdot \mathbf{r} - \omega t))$
3. boundary conditions at the interface:
   $\mathbf{E}, \mathbf{H}$ fields: continuous transverse $(x,\ y)$ components
   $\mathbf{D}, \mathbf{B}$ fields: continuous normal (z) components
4. for total reflection, solution of transverse wave is in form so called evanescent wave, non-propagating in z-direction
   $E = E \exp(-k_z z)$



Light reflection on the interface





s-polarized light:

$$r_\perp = \frac{n_i \cos(\theta_i) - n_t \cos(\theta_t)}{n_i \cos(\theta_i) + n_t \cos(\theta_t)}$$

$$t_\perp = \frac{2n_i \cos(\theta_i)}{n_i \cos(\theta_i) + n_t \cos(\theta_t)}$$

p-polarized light:

$$r_\parallel = \frac{n_i \cos(\theta_t) - n_t \cos(\theta_i)}{n_i \cos(\theta_t) + n_t \cos(\theta_i)}$$

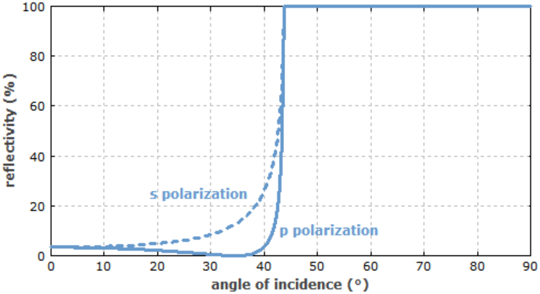
$$t_\parallel = \frac{2n_i \cos(\theta_i)}{n_i \cos(\theta_t) + n_t \cos(\theta_i)}$$

And, for <u>both</u> polarizations: $n_i \sin(\theta_i) = n_t \sin(\theta_t)$

`http://www.ece.rice.edu/~daniel/262/pdf/lecture14.pdf`

Light reflection on the interface

Reflection on glass/air



Total reflection

Critical angle:

$$\sin \varphi_c = \sqrt{\frac{\varepsilon_2}{\varepsilon_1}} = \frac{n_2}{n_1}$$

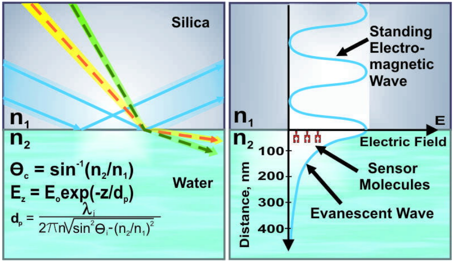
Evanescent wave:

$$E = E_t \exp(-z/\delta - i\omega t)$$

Penetration depth:

$$\delta = \frac{1}{k_0\sqrt{(n_1 \sin \varphi_1)^2 - (n_2^2)}}$$

Example: glass(n_1)/water(n_2) inteerface; $n_1 > n_2$



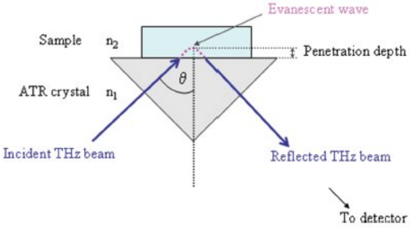
http://www.tirftechnologies.com/principles.php

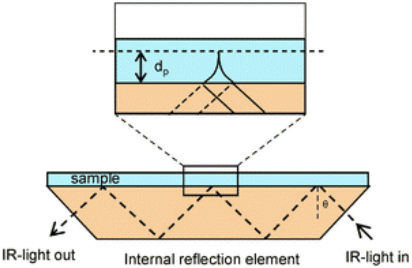
Attenuated total reflectance (ATR)

- probes sample by evanescent wave

⇒ sensitive to surface of the sample

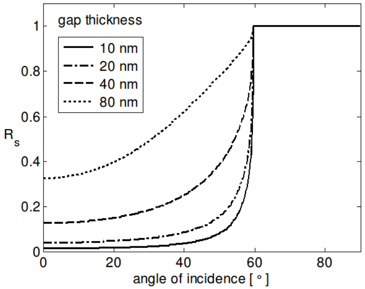
- sample modifies evanescent wave → partial absorption or transmission of light in sample → total reflection is decreased (attenuated).



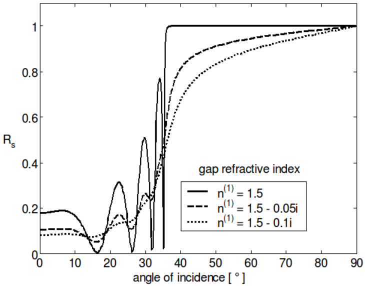


Attenuated total reflectance (ATR): gap effect

Gap thickness (refractivity of gap=1):



Absorption in gap (gap thickness 960 nm):



Surface plasmon (electrical excitation providing two adjacent evanescent waves in the vicinity of the interface)

Electric field in the vicinity of the interface:

$$E = E_O \exp[i(k_x x + k_z z - \omega t)]$$

where

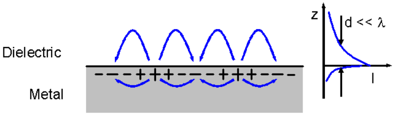
$$k^2 = k_x^2 + k_z^2 = \epsilon\,(\omega/c)^2 = \epsilon k_0^2 \qquad (9)$$

At the interface of two materials ϵ_1 and ϵ_2:
(a) k_x continuous over the interface;

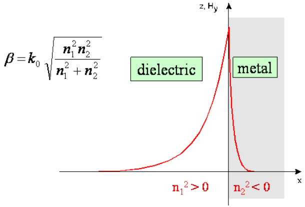
$$k_{x1} = k_{x2} \qquad (10)$$

(b) D_z and E_x continuous over the interface

$$k_{z1}/\epsilon_1 = k_{z2}/\epsilon_2 \qquad (11)$$



Surface Plasmon Resonance



Note! There is only a single p-polarized (TM) surface plasmon !

`http://www.physics.uwo.ca/~smittler/`

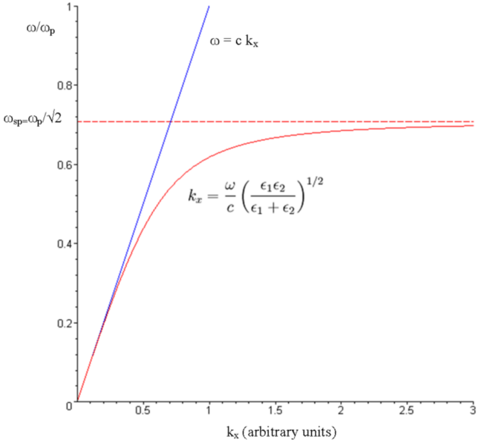
Surface plasmon II: dispersion relation

- From Eqs.(9–11) follows dispersion relation for surface plasmon:

$$k_x = k_0 \sqrt{\left(\frac{\epsilon_1 \epsilon_2}{\epsilon_1 + \epsilon_2}\right)}, \qquad (12)$$

where $k_0 = \omega / c$.

- Surface plasmon appears only for p-polarized (TM) wave, as this mode has normal (z) component of $D = \epsilon \epsilon_0 E$ field.

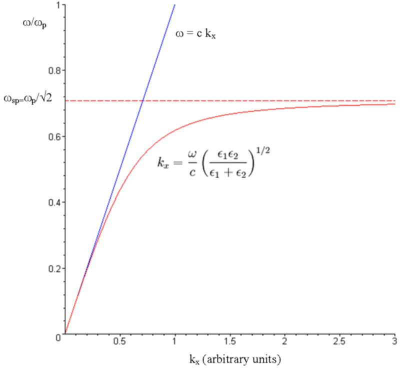


Surface plasmon III: example

Example: assuming $\epsilon_1 = 1$ (air) and $\epsilon_2 = 1 - \frac{\omega_p^2}{\omega^2}$ (metal as free electron model of an electron gas = Drude, neglecting absorption). Then

$$k_x = \frac{\omega}{c}\sqrt{\left(\frac{\omega^2 - \omega_p^2}{2\omega^2 - \omega_p^2}\right)} \qquad (13)$$

Hybridization between photon ($\omega = ck_0$) and plasmon $\omega_{SP} = \omega_p/\sqrt{2}$.



Surface plasmon resonance (SPR) I

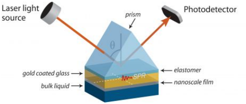
- Resonance between incident wave photon and surface plasmon. Resonance means that both (pseudo)-particles have equal ω and $k_x = k_{x,inc} = \Re(k_{x,sp})$.
- Description of incident wave from material ϵ_1 under angle φ:

$$k_{x,inc} = \frac{\omega}{c}\sqrt{\epsilon_1}\sin\varphi \tag{14}$$

- Description of surface plasmon:

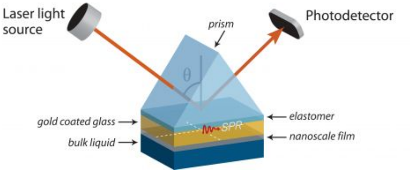
$$k_{x,sp} = \left(\frac{\omega}{c}\right)\sqrt{\left(\frac{\epsilon_1\epsilon_2}{\epsilon_1+\epsilon_2}\right)}, \tag{15}$$

Condition for existence of the resonance: $\Re(\epsilon_2) < -\epsilon_1$ (i.e. $\Re(\epsilon_2)$ must be negative; fulfilled by coinage metals, Au, Ag, Cu). Here, ϵ_1 is assumed to be non-absorbing material (i.e. $\Im(\epsilon_1) = 0$).



Surface plasmon resonance (SPR) II

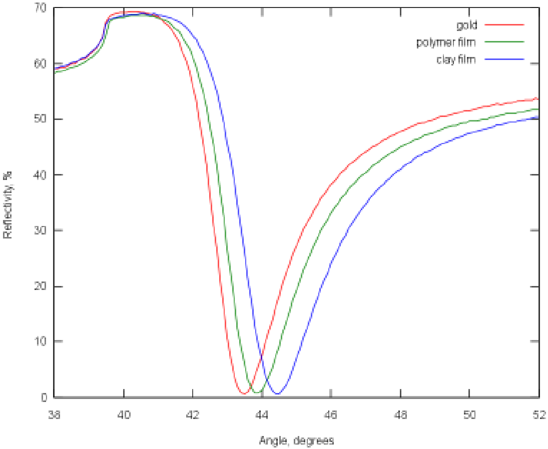
Surface plasmons are very sensitive to slight perturbations within the skin depth ⇒ surface plasmons are often used to probe tiny changes of refraction index near the interface (extreme sensitive detector of small changes of the refraction index).
⇒ Readout of many bio-sensors based on this detection technique.



http://www.bionavis.com/technology/spr/

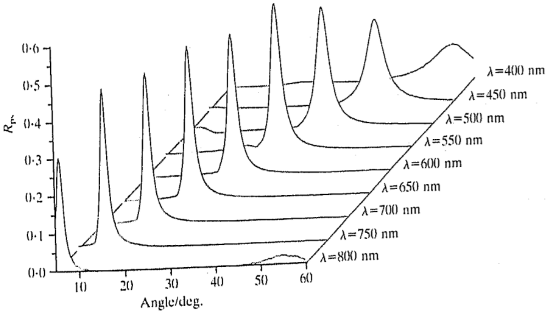
SPR: detection I

- presence of resonance increases absorption and reduces reflectivity.
- position of reflection minima very sensitive to refractivity index in position of the evanescent wave.

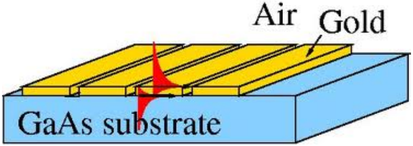


SPR: detection II

- presence of resonance increases absorption and reduces reflectivity.
- position of reflection minima very sensitive to refractivity index in position of the evanescent wave.



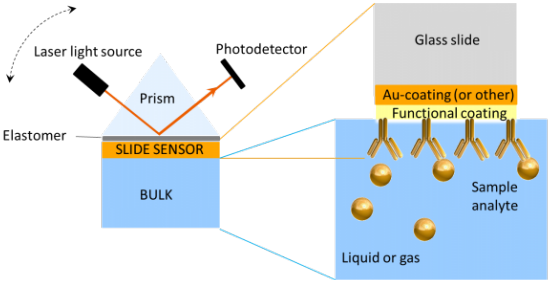
SPR: how to couple surface plasmon and photon?



- couple light by high-refraction index prism
- lateral modulation of the interface (roughness or structuring)

$$\omega/c \sin\varphi + 2\pi/b = \omega/c\sqrt{\frac{\varepsilon_2}{\varepsilon_2+1}} \tag{16}$$

SPR: bio sensors



`http://www.bionavis.com/technology/spr/`

Spin-orbit interaction of light

K.Y. Bliokh, Nature Photon. 9, 796 (2015)
Similar to spin-orbit coupling of electron, there is spin-orbit coupling also for photon (for light beam).

- Spin-orbit interaction of electron: connect spin wavefunction and space wavefunction
- Spin orbit coupling of photon: connects beam trajectory and its polarization state (also know as optical spin-Hall effect).

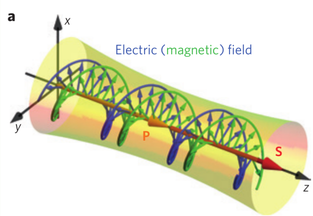
Angular momenta of light I

Spin angular momentum S:

degree of circular polarization (helicity)

$\sigma = (-1, 1)$

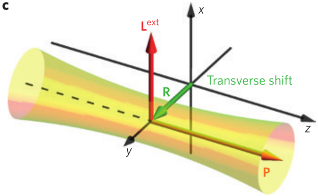
$$\mathbf{S} = \sigma \frac{\mathbf{k}}{k} = \sigma \frac{\mathbf{p}}{p}$$



Extrinsic orbital angular momentum $\mathbf{L}^{ext}$:

determined by the trajectory of the beam **R**

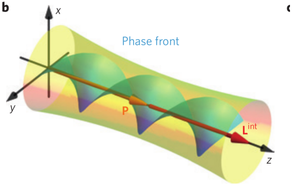
$\mathbf{L}^{ext} = \mathbf{R} \times \mathbf{p}$

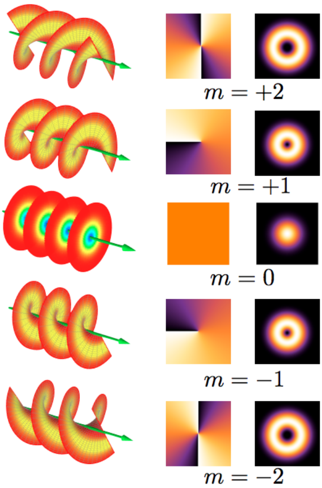


Angular momenta of light II

Intrinsic angular momentum L^{int}:
helical phase front: phase of the beam depends on position inside beam, approximately $E(r, z, \phi) \approx E_0(r, z)\exp[il\phi]$, where r, z, ϕ are coordinates in cylindrical coordinates.

$$L^{int} = l\frac{\mathbf{k}}{k}, \qquad l \in \mathbb{Z}$$





Optical spin Hall effect I

Interactions between those three angular momenta of light represents spin-orbit coupling of light.

Example: optical spin Hall effect:

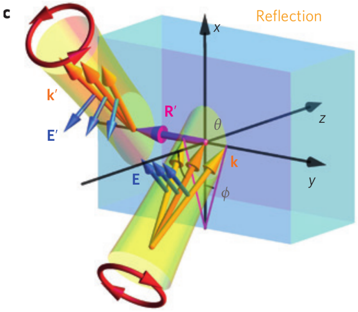
The light beam on reflection displaces (shifts) according to the beam helicity σ. Consequence of total angular momentum conservation:

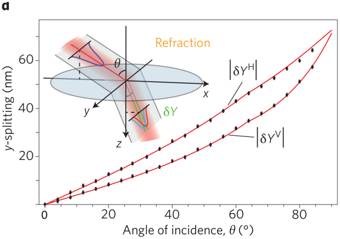
$$\mathbf{J} = \mathbf{S} + \mathbf{L}^{ext} = \mathbf{S} + \mathbf{R} \times \mathbf{p}$$

adjusting coordinates that incident beam has $\mathbf{R} = 0$ and hence $\mathbf{L}^{ext} = 0$

$$\mathbf{S} - \mathbf{S}' \approx \mathbf{R}' \times \mathbf{p}'$$

K.Y. Bliokh, Nature Photon. 9, 796 (2015)





Optical spin Hall effect II

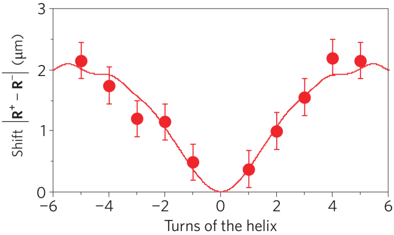
$$\mathbf{J} = \mathbf{S} + \mathbf{L}^{ext} = \mathbf{const.}$$

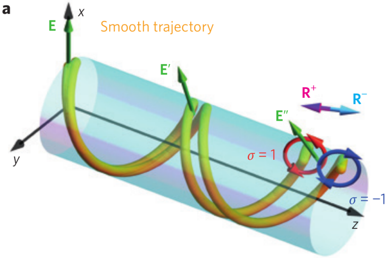
displacement of beam due to light helicity inside the glass cylinder with gradient of refraction index.

$$\dot{\mathbf{p}} = \nabla n(\mathbf{R}) \qquad \dot{\mathbf{R}} = \frac{\mathbf{p}}{p} - \frac{\sigma}{k_0}\frac{\mathbf{p}\times\dot{\mathbf{p}}}{p^3}$$

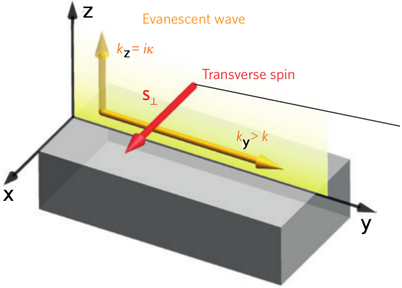
(overdot denotes derivation according to the trajectory)

Bliokh Nature Photon. 2, 748 (2008)





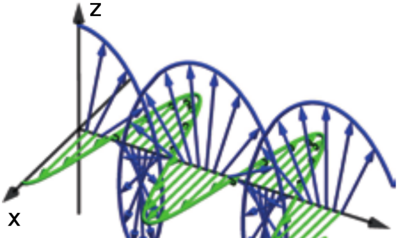
Spin trasnfer by evanescent wave



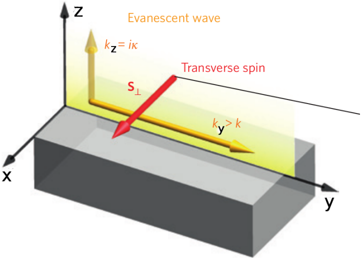
Electrical field of the evanescent wave (propagation along y, recall $\mathbf{E} \cdot \mathbf{k} = 0$):

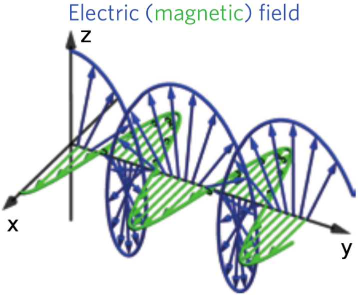
$$\mathbf{k} = \begin{bmatrix} 0 \\ k_y \\ iK \end{bmatrix} \qquad \mathbf{E} = \begin{bmatrix} 0 \\ i(-K/k_y)E_z \\ E_z \end{bmatrix}$$

Electric (magnetic) field

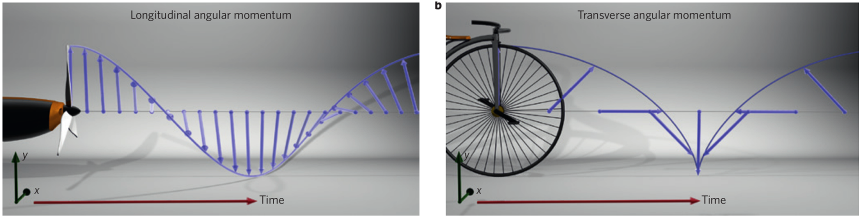


Profile of electric field



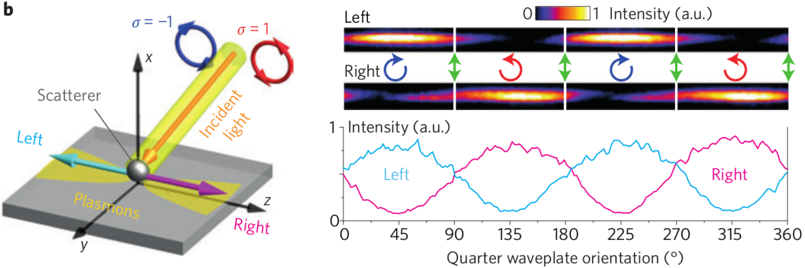


Profiles of electric field in paraxial beam and evanescent beam, providing longitudinal and transverse spin angular momentum.



Selection of evanescent wave propagation

As spin of the evanescent wave is given by propagation of spinwave, the polarization (helicity) of incoming beam determines propagation direction of the evanescent wave.



"Remarkably, the universal character of spin-direction locking in evanescent waves can be associated with the quantum spin-Hall effect of photons, which makes it an optical counterpart of the quantum spin-Hall effect of electrons in topological insulators"

Polariton I

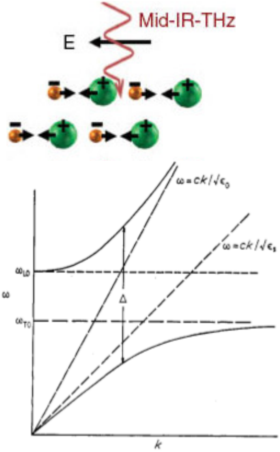
Polariton: coupling between photon and excitation of the matter. Here we discuss coupling with optical phonon.

$$m\frac{\mathrm{d}^2 u}{\mathrm{d}t} + \omega_{TO}^2 m = eE\cos(\omega t)$$

- u: amplitude of optical phonon
- E: driving electrical field at ω

$$u = \frac{P}{Ne} = \frac{eE/m}{\omega_{TO}^2 - \omega^2}$$

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{\Omega_p^2}{\omega_{TO}^2 - \omega^2}$$

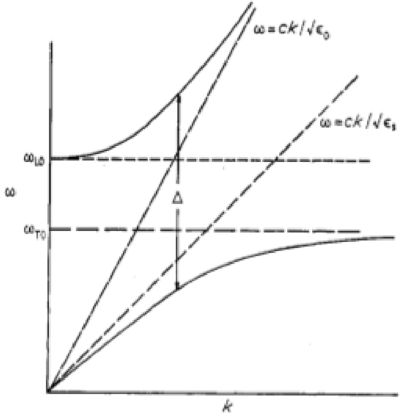


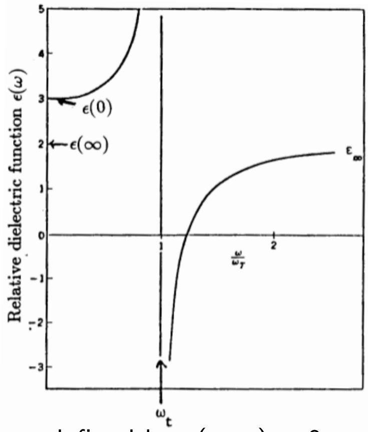
Mills, Rep. Prog. Phys. 37, 817 (1974)

Polariton II

Polariton dispersion:

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{\Omega_p^2}{\omega_{TO}^2 - \omega^2}$$



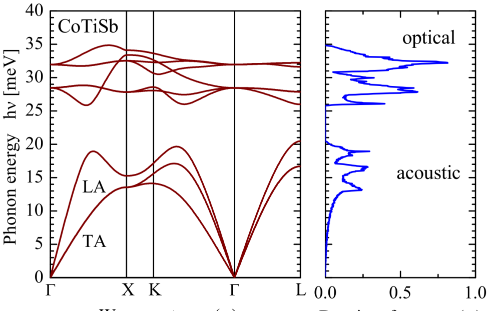


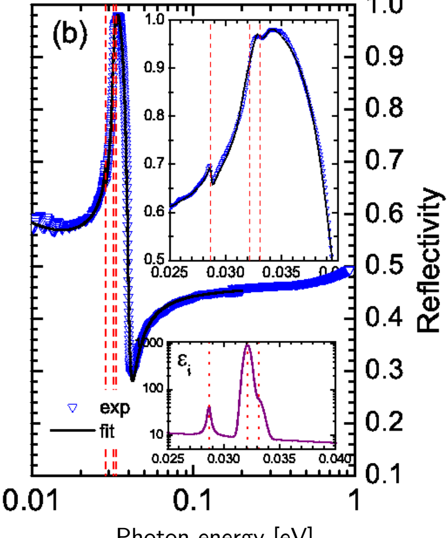
Note: longitudinal mode frequency ω_{LO} defined by $\varepsilon(\omega_{LO}) = 0$

Polariton example: CoTiSb

Infrared (IR) reflectivity:

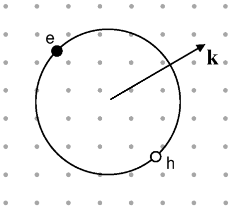
- One dominant and one satellite peaks → originating from atomic vibrations (phonons).
- Described by weak Drude and three sharp Lorenzians.
- Phonon energies at Γ-point agrees perfectly well with exp. (≈30 meV).

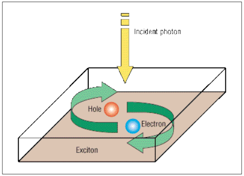


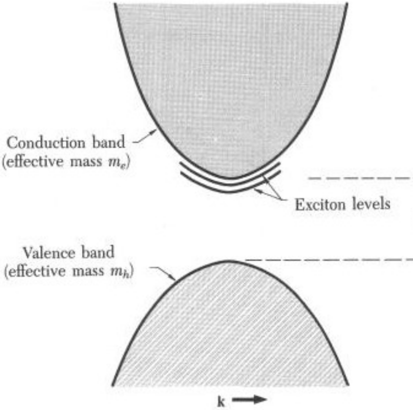


Excitons

- Excition is electron-hole pair binded by Coulomb's electrostatic attraction.
- This is very similar to a hydrogen atom, like an electron orbiting around a proton. However, the binding energy is much lower, due to small effective masses of the excited electron and hole. $E_{\text{exciton}} \sim 1/n^2$, $n \in \mathbb{N}$

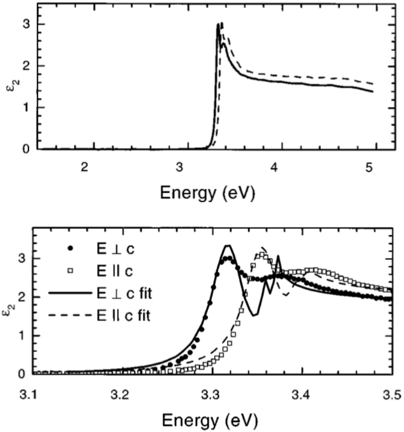




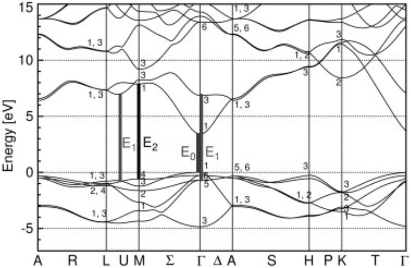


Excitons in ZnO

- ZnO: large gap direct semiconductor (3.3 eV @ RT)
- Strong excitonic binding energy ≈60 meV
- excitons add sharp absorptions to optical spectra



Jellison PRB 58, 3586 (1998)



Schmidt-Grund, Thin Solid Films 455, 500 (2004)

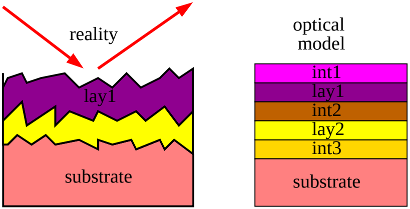
Optics of multilayers I

Total optical response of multilayer described by reflection matrix:

$$R = \begin{bmatrix} r_{ss} & r_{sp} \\ r_{ps} & r_{pp} \end{bmatrix}$$

Reflection matrix is the only quantity accessible for sample investigations by optical means. Roughness of the interfaces is included by:

1. usually described by effective sub-layers.
2. their optical properties described by e.g. effective-medium-approximation (EMA).



Optics of multilayers II

Total optical response of multilayer described by reflection matrix:

$$R = \begin{bmatrix} r_{ss} & r_{ps} \\ r_{sp} & r_{pp} \end{bmatrix}$$

Different quantities can be investigated on reflection:

- reflectivity (unpolarized light): $I = 1/2(|r_{ss}|^2 + |r_{pp}|^2)$
- reflectivity of *s*-polarized light: $I_s = |r_{ss}|^2$
- magneto-optical Kerr *s*-effect: $\Phi_s = \theta_s + i\epsilon_s = \frac{r_{sp}}{r_{ss}}$
- ellipsometry: $\rho = \tan\Psi \exp(-i\Delta) = \frac{r_{pp}}{r_{ss}}$
- magnetic linear dichroism for *s*-wave (**M** in-plane): $MLD = |r_{ss}(M \parallel s)|^2 - |r_{ss}(M \parallel p)|^2$

Light in multilayer system

1) Solution of Maxwell equations in homogeneous (but generally anisotropic) material:

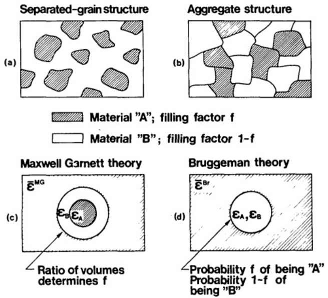
$$\mathbf{k}^2\mathbf{E} - \mathbf{k}(\mathbf{k}\cdot\mathbf{E}) = \frac{\omega^2}{c^2}\mathbf{E}\cdot\mathbf{E}$$

general solution are four waves, two propagating in two directions ('up', 'down'), each having different polarization.
2) on surfaces, boundary conditions are applied (transversal components of E and H fields are continuous over the interface)

Optical properties of mixtures

spherical inclusions of materials 1 and 2:

$$\frac{\varepsilon_{eff} - \varepsilon_h}{\varepsilon_{eff} + 2\varepsilon_h} = f\,\frac{\varepsilon_1 - \varepsilon_h}{\varepsilon_1 + 2\varepsilon_h} + (1-f)\,\frac{\varepsilon_2 - \varepsilon_h}{\varepsilon_2 + 2\varepsilon_h}$$



ε_{eff} : effective medium permittivity

ε_h : host medium permittivity

$1 - f$: volume fraction of the first, second material

ε_1, ε_2 : permittivities of the first, second material

Maxwell-Garnett : $\varepsilon_h = \varepsilon_1$ (host medium is one of the constituent media)

Lorentz-Lorenz : $\varepsilon_h = 1$ (host medium is air)

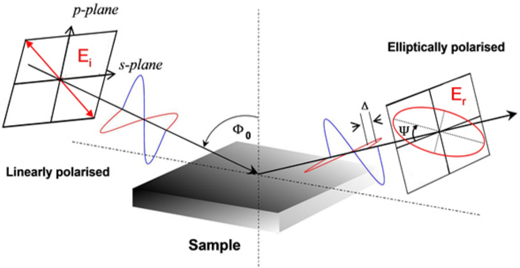
Bruggeman : (also known as EMA=Effective medium approximation)
$\varepsilon_h = \varepsilon_{eff}$: host medium is effective mediuam itself

Ellipsometry I

Ellipsometry measures complex ratio of diagonal reflection coefficients:

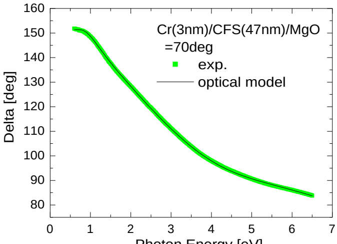
$$\rho = \tan\Psi \exp(-i\Delta) = \frac{r_{pp}}{r_{ss}}$$

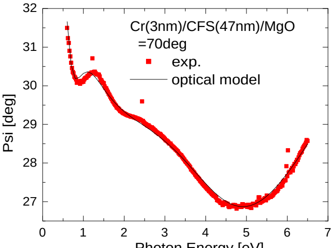
- Ψ, Δ: so-called ellipsometric angles Ψ, Δ
- Ψ expresses ratio of reflected s- and p-waves
- Δ expresses phase difference of reflected s- and p- waves.



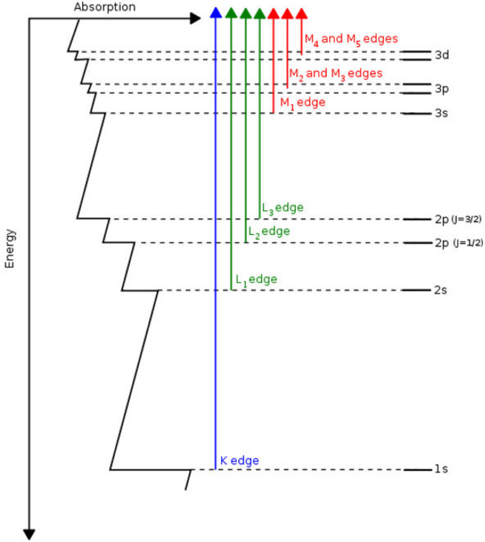
Ellipsometry II

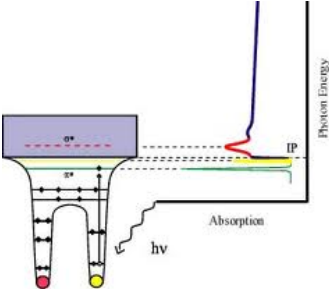
- experimental setup provides spectra of Ψ, Δ
- those spectra are fitted into optical model, where various parameters can be free parameters in the fit (but not all at the same fit):
    - optical constants of a given layer (can be further described by a various functions)
    - layer thicknesses
    - interface roughnesses
- Example of fit to spectra of Ψ, Δ





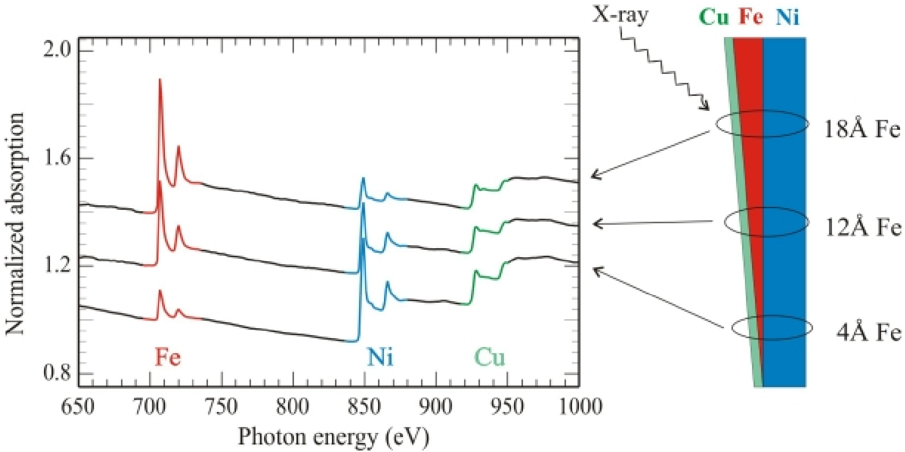
X-ray absorption spectroscopy (XAS):





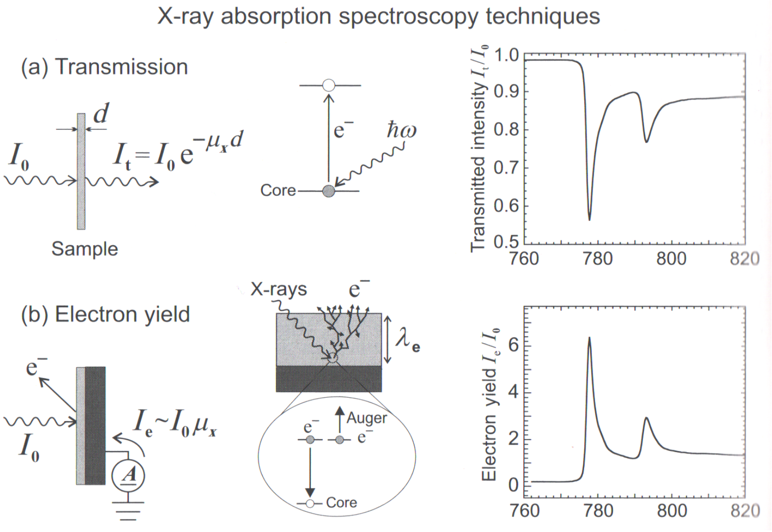
http://news.softpedia.com

X-rays can pick materials apart: layer-by-layer



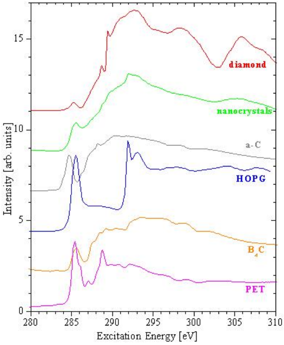
https://www-ssrl.slac.stanford.edu/stohr/xmcd.htm

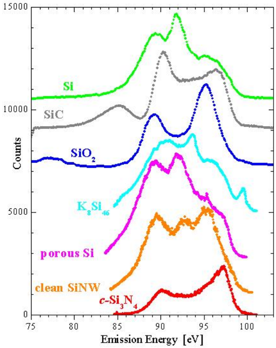
Experimental setup of XAS


X-ray absorption spectroscopy techniques

X-ray absorption spectroscopy (XAS):

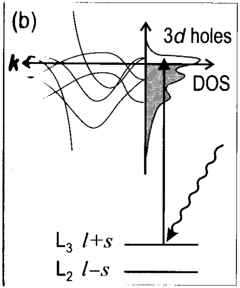
XAS is extremely sensitive to the chemical state each element, as each element have its own characteristic binding energies. XAS measurements can distinguish the form in which the element crystallizes (for example one can distinguish diamond and graphite, which both entirely consist of C), and can also distinguish between different sites of the same element.



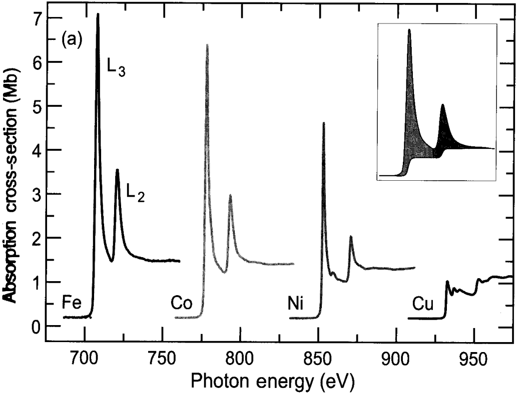


`http://beamteam.usask.ca/`

XAS on Fe:



Stöhr, Siegmann, Magnetism: From fundamentals to nanoscale dynamics



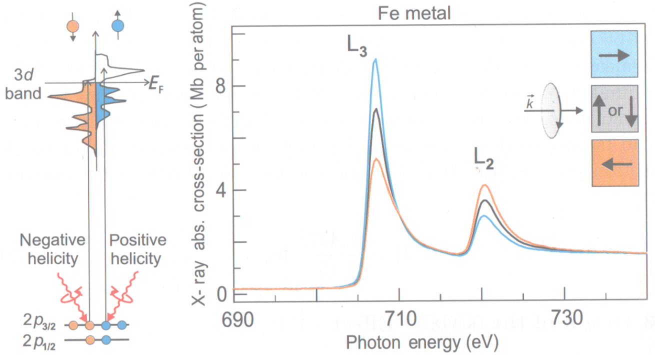
Starting L2, L3 edge (i.e. 2p$^{1/2}$, 2p$^{3/2}$, respectively):

$$I_{XAS,\ p\rightarrow d} \sim N_h$$

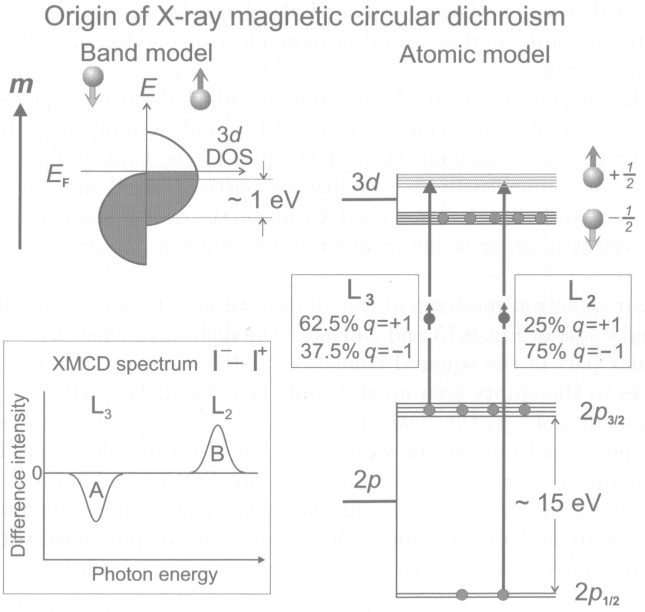
N_h: number of free d-states. $p \rightarrow s$ has small contribution.

XMCD: X-ray Magnetic circular dichroism:

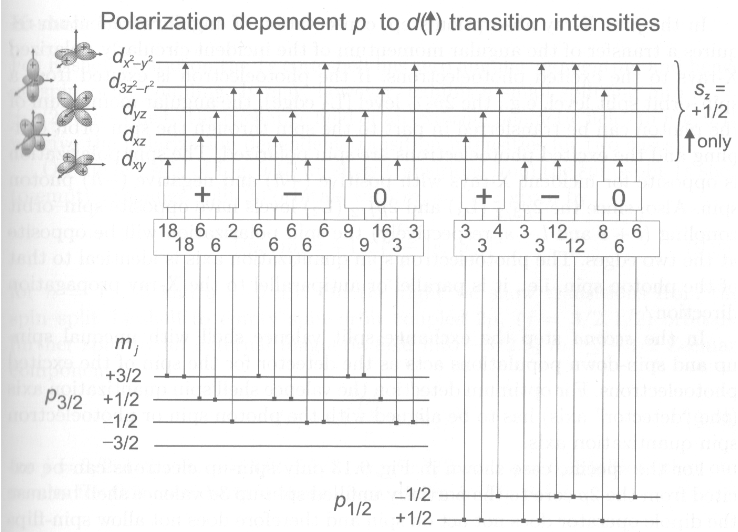
Circular Dichroism: different absorption for circularly left and right light polarization.



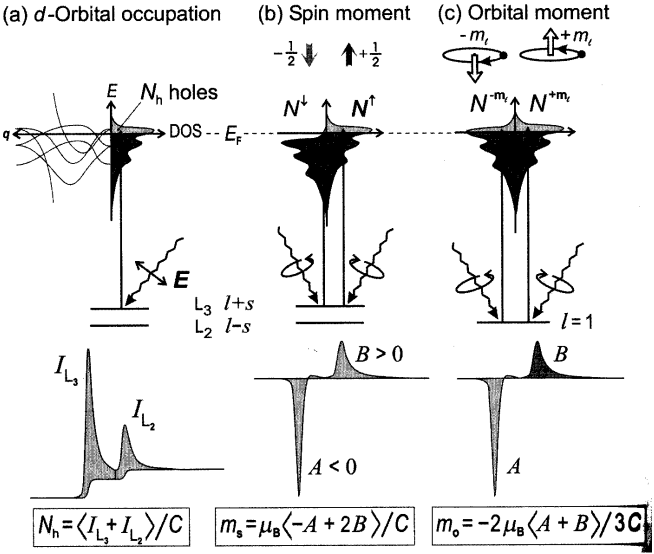
Different absorbed intensity for opposite magnetization orientations.


Origin of X-ray magnetic circular dichroism
Band model
Atomic model
m
E
3d
DOS
E_F
~ 1 eV
3d
+1/2
−1/2
L_3
62.5% q=+1
37.5% q=−1
L_2
25% q=+1
75% q=−1
XMCD spectrum I⁻ − I⁺
Difference intensity
0
L_3
L_2
A
B
Photon energy
2p_3/2
2p
~ 15 eV
2p_1/2

XMCD: Detailes p $\rightarrow$ d transition



XMCD: sum rules:



Advantages of X-ray spectroscopies:

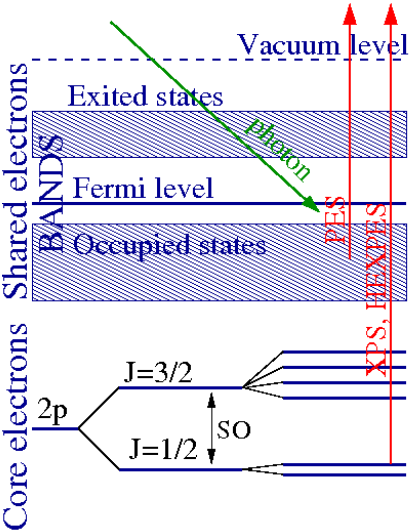
- element selective.
- quantitative determination of material characterization (e.g. magnetic moment, orbital moment).
- can be both interface or bulk sensitive.
- can provide excellent lateral resolution ($\sim$ 15 nm).
- can provide excellent time resolution ($\sim$ 100 fs).

Disadvantages:

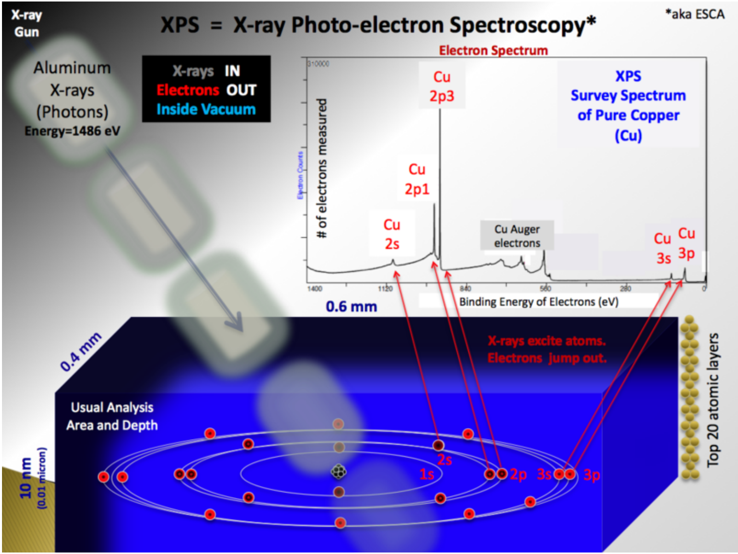
- due to width of the initial (core) line, the energy resolution is limited to $\sim$1 eV.
- synchrotron needed.

Photoemission spectroscopy (PES)

- Photon in, electron out.
- Based on the photoelectric effect (electrons kick out by incoming photon).
- Also called Photoelectron spectroscopy.
- Probes density of states below Fermi level.

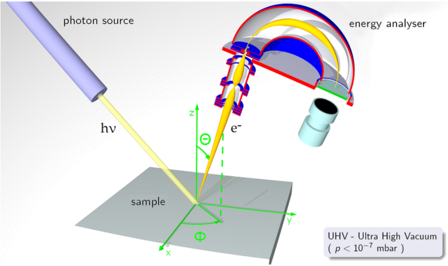


Photoemission spectroscopy (PES or XPS)



Photoemission spectroscopy (PES)

- photon in (known energy), electron out (energy measured)
- elemental composition of the surface (top 1–10 nm usually).
- detect all elements except H and He.
- chemical or electronic state of each element in the surface.
- mapping of elemental composition across the surface.

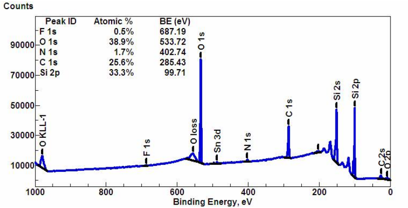


Photoemission spectroscopy principle

$$E_{\mathrm{photon}} = E_{\mathrm{ionized\ electron}} + E_{\mathrm{binding}}$$

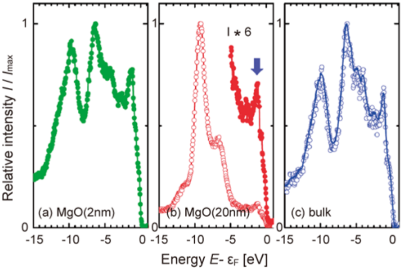
⇒ when ionizing core-levels, outgoing dependence electron yield on detected electron kinetic energy E_{electron} provides sharp peaks.
⇒ when exciting valence band, valence band occupancy can be found.

probing core levels



Peak ID	Atomic %	BE (eV)
F 1s	0.5%	687.19
O 1s	38.9%	533.72
N 1s	1.7%	402.74
C 1s	25.6%	285.43
Si 2p	33.3%	99.71

probing valence bands by HAXPES



Photoemission spectroscopy (PES)

- Ultraviolet photoemission spectroscopy (UPS)
  - vacuum UV radiation (photon energy of $E = 10\text{–}45\ \text{eV}$) to examine valence levels.
  - when varied detection angles, one can map out energy in the reciprocal space.
- X-ray photoemission spectroscopy (XPS)
  - soft x-rays ($E = 200\text{–}2000\ \text{eV}$) to examine down to core-levels.
  also known as Electron Spectroscopy for Chemical Analysis (ESCA).
- Hard X-ray photoemission spectroscopy (HAXPES, HX-PES):
  - using hard X-ray to excite down to deep core levels.
  - bulk sensitive

Angle resolved photoemission spectroscopy (ARPES):

Both energy and direction of the ionized electrons are measured.

Momentum conservation:

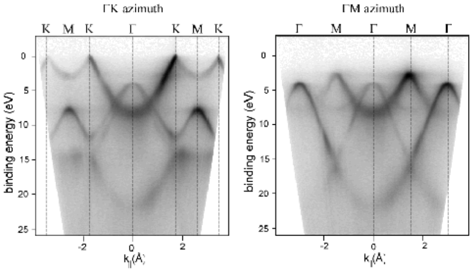
$$\mathbf{p}_{\text{ionized electron}} = \mathbf{p}_{\text{photon}} + \mathbf{p}_{\text{bound electron}} + \hbar \mathbf{K}$$

as $\mathbf{p}_{\text{photon}} \approx 0$, hence $\mathbf{p}_{\text{ionized electron}} = \mathbf{p}_{\text{bound electron}} + \hbar \mathbf{K}$.

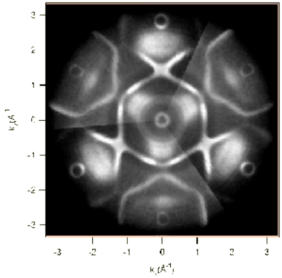
- hence, the ionized electron has the same momentum as the original bound electron (plus $\hbar \mathbf{K}$ due to lattice periodicity).
- hence, by measuring the excitation angle with respect to crystallographic direction, one can determine the dispersion relation $E(\mathbf{k})$ of the electrons inside the matter.

Angle resolved photoemission spectroscopy (ARPES)

Electronic structure of graphite



Fermi surface of $Cu_3Au(111)$

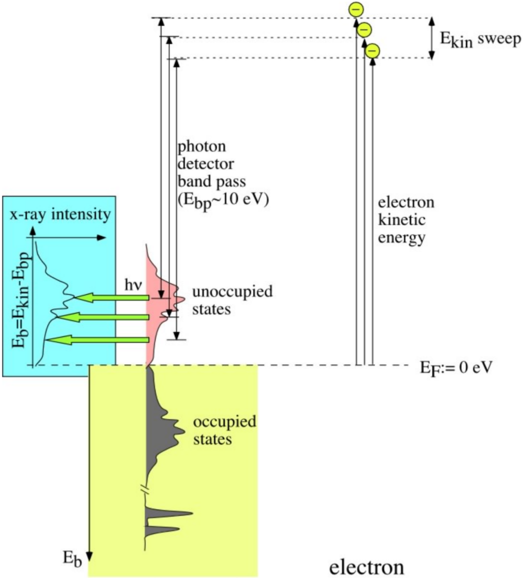


`http://www.tp2.uni-erlangen.de`

Inverse photoelectron spectroscopy (IPES)

Electron in, photon out.

- low incidence electron energy E_{kin} ($\sim 20\,\text{eV}$).
$\rightarrow$ those electrons couple to unoccupied states E_{kin} above Fermi level
$\rightarrow$ when electrons decays to lower states, radiates photon.
- when photons pass narrow-band filter (i.e. only one energy passes), unoccupied DOS measured.

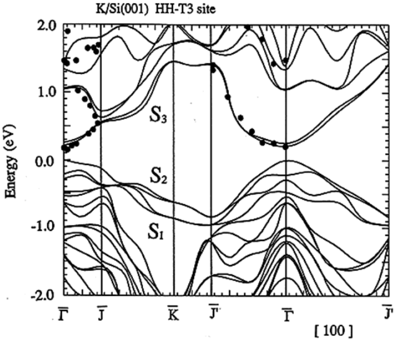


http://rsl.eng.usf.edu

Inverse photoelectron spectroscopy (IPES): properties

- as small electron energy, only surface is tested.
- can provide k-resolution, as ARPES.
- can provide spin-resolution.

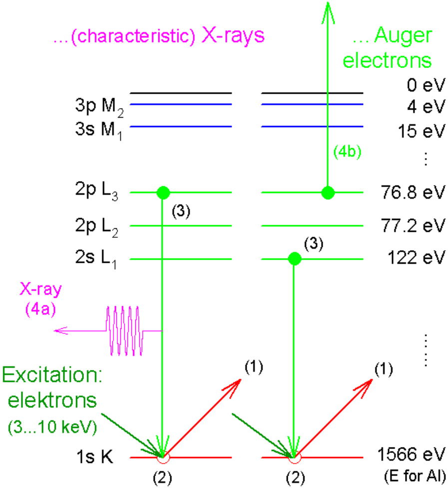
Example of IPES on Si(100) surface



http://e1.physik.uni-dortmund.de

Auger electron spectroscopy (AES) and characteristic X-ray

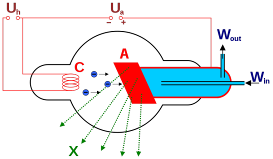
- electron in (~ 3 –10 keV).
- inner shell of an atom is ionized.
- the vacancy is filled by an electron from an outer shell.
- the released energy is emitted as (characteristic) X-ray or is transferred by electromagnetic interaction to a 3rd electron. If it gets sufficient energy it can leave the atom as Auger electron.
- energy of both radiations is determined by the energy levels of the atom and makes analysis of the composition possible.

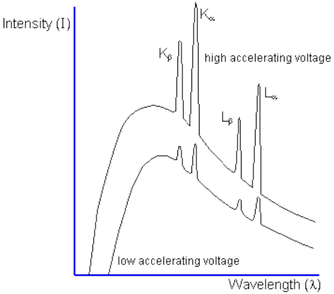


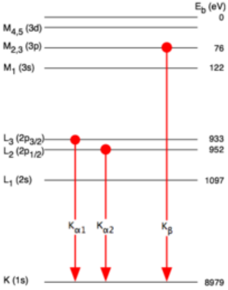
http://www.ifw-dresden.de/institutes/ikm/organisation/dep-31/methods/auger-electron-spectroscopy-aes

Characteristic X-ray radiation

Characteristic X-ray radiation is used to generate X-ray radiation in X-ray tubes. (most common X-ray source used e.g. in medical X-rays or X-ray diffractometers).







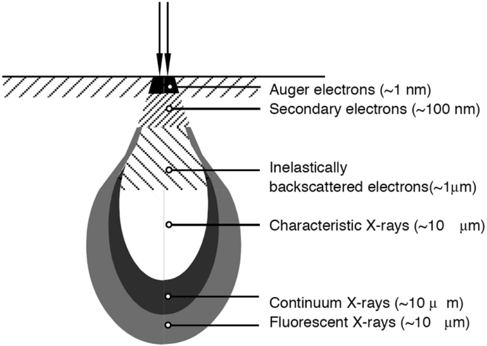
Radiation consists of characteristic single-energy radiation (denoted K_{α},

Auger electron spectroscopy:

- Only H and He do not emit Auger electrons (The Auger process).
- measured Auger electron spectra.

⇒ element and chemical states identification.

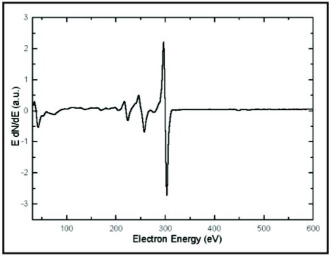
- element detect limit about $\leq 1\%$.
- depth information 0.5–5 nm (surface technique).
- in combination with electron microscopy, local analysis (points, areas, lines) are possible.
- Disadvantage: high energy and current density of the primary electron beam, producing many defects.



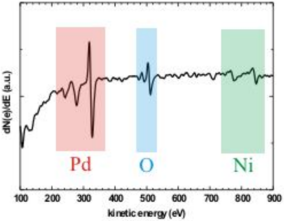
http://www.ifw-dresden.de/institutes/ikm/organisation/dep-31/methods/auger-electron-spectroscopy-aes

Examples of Auger spectra

Rh(111)

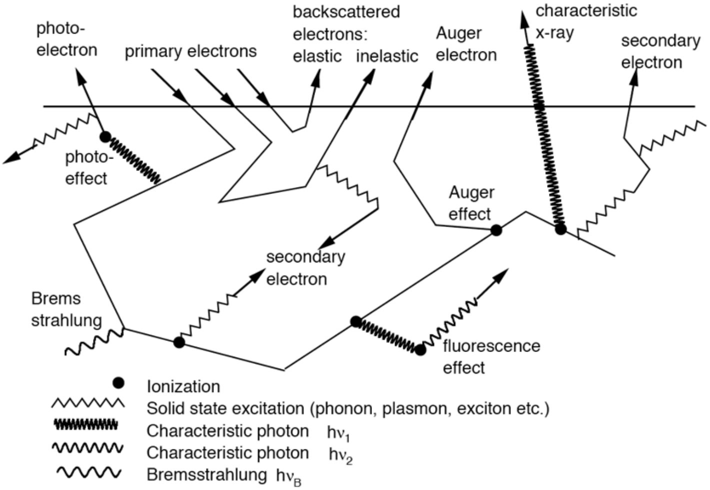


monolayer of NiO on Pd

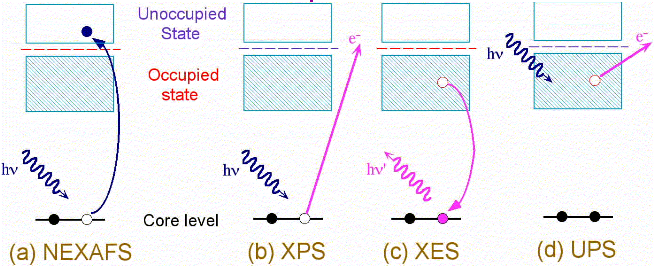


http://surface-science.uni-graz.at/main_frame/techniques/aes.htm

Processes related with electron-in



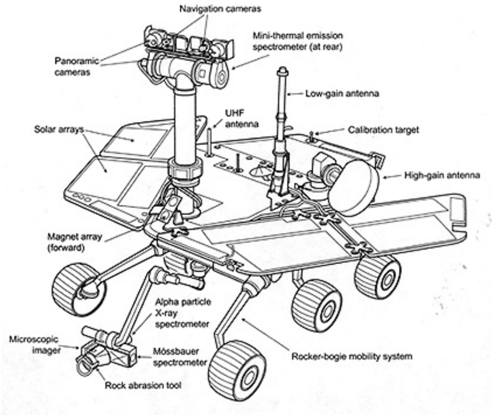
Processes related with photon-in



XAS	X-ray absorption spectroscopy
XMCD	X-ray magnetic circular dichroism
NEXAFS	near edge absorption fine structure
PES, XPS	photoemission spectroscopy, photoelectron spectroscopy
UPS	ultraviolet absorption spectroscopy
XES, XFS	X-ray emission spectroscopy, X-ray fluorescence spectroscopy
HAXPES	hard X-ray absorption photoemission spectroscopy

http://www.theochem.kth.se/research/xspectra/index.html

NASA's Mars Exploration Rover Spirit



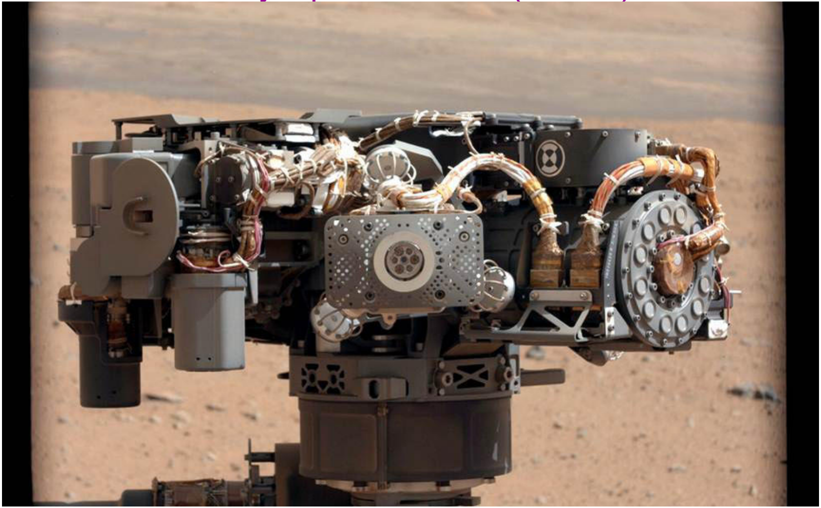
Mars Exploration Rover

Rock named Clovis:

The Rovers are both designed to search for water using a variety of instruments, including a mini-Thermal Emission Spectrometer, a Mossbauer Spectrometer, and Alpha Particle X-ray Spectrometer.

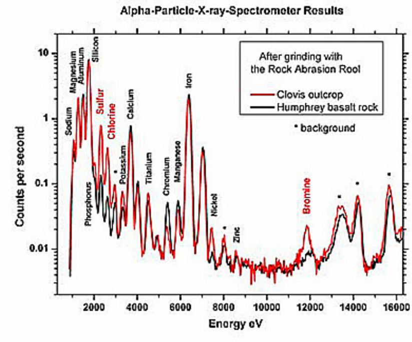
http://rst.gsfc.nasa.gov/Sect19/Sect19_13a.html

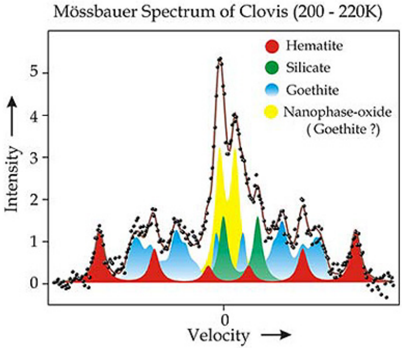
Alpha Particle X-Ray Spectrometer (APXS) on Rover



"... will expose the material to alpha particles and X-rays emitted during the radioactive decay of the element curium." "When X-rays and alpha particles interact with atoms in the surface material, they knock electrons out of their orbits, producing

NASA's Mars Exploration Rover Spirit



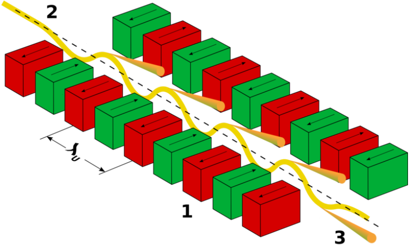


"On Earth, Goethite - a very common mineral associate with Limonite - is found as an alteration product or as a direct precipitate in the so-called "bog iron" deposits, which result from a reducing, water-rich swampy environment. That form of Goethite is usually produced with the aid of bacteria but can also form inorganically. The mode of origin of the Clovis Goethite is still "up for grabs" but the presence of this mineral suggests a significant role for water in Mars' past."

X-ray beam generation in synchrotrons

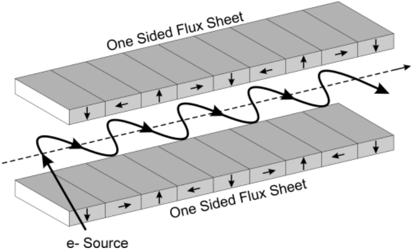
Undulator:

small electron oscillation amplitude, narrow energy band emission, smaller light intensity.



Wiggler:

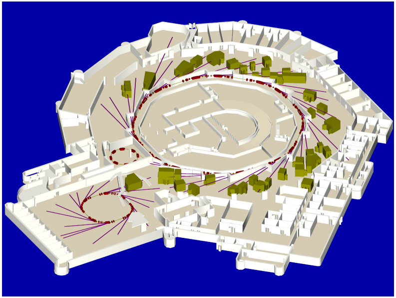
large electron oscillation amplitude, wide energy band emission, higher light intensity



- Electron trajectory determines light polarization.
- Photon energy can be from IR to hard X-ray. Mostly used is X-ray.
- Quick X-ray pulses (up to 100 fs) are possible.

Synchrotron radiation source:

National Synchrotron Light source, USA



Grenoble

Magneto-optical Kerr effect:

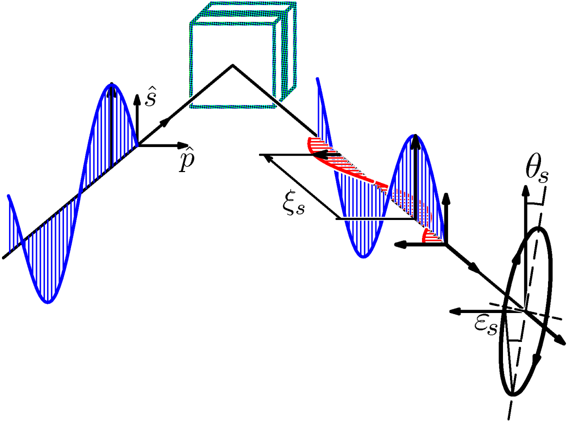
- Change of optical properties (polarization state, reflectivity) by presence/change of magnetization of the sample.

One can separate usage of magneto-optical (MO) effects to:

- MO as a metrology tool to study magnetism:
    - MO magnetometry (study of magnetization reversal).
    - MO microscopy (study of domain wall and its propagation).
    - Magnetization dynamic studies (precession etc.)
    - MO as a tool for ultrafast magnetization processes.
- MO spectroscopy to study optical properties of the MO effect:
    - Magnetism is understand as a perturbation, reducing symmetry of the solids and hence introducing new optical features.
    - Study of spin-orbit interaction.
    - Interaction between light and magnetism – a very fundamental interaction.

MO effect I: Magneto-optical Kerr effect (MOKE):

- For example: incident s-polarized wave.
- Magnetized sample
  $\Rightarrow$ hence: also p-polarized wave appears on the reflection.



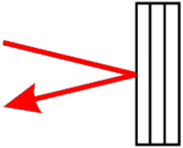
MOKE linear in **M**

Kerr and Faraday magneto-optical effect:

Due to historical reasons, there are different names for MO effects measured in reflection and transmission.

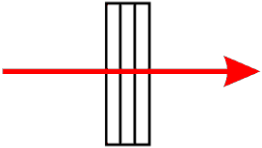
Kerr effect:

- measured in reflection.
- discovered 1876.



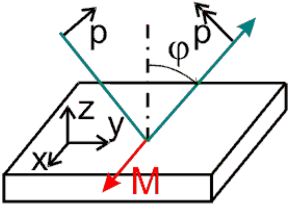
Faraday effect:

- measured in transmission.
- discovered 1845.



MO effect II: transversal MOKE:

- Incident p-polarized wave.
- Magnetization in-plane and perpendicular to the incident plane (so-called transversal magnetization direction).
- Change of the reflected p-polarized intensity due to magnetization in the sample (in this particular case, on change in polarization of the reflected light appears).



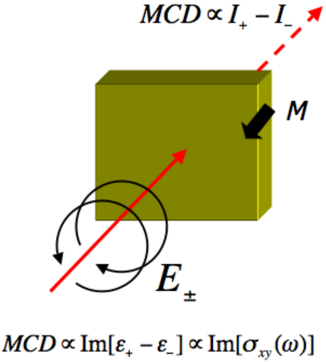
MO effect III: Magnetic dichroism and birefringence:

Dichroism: different damping of both light's eigen-modes.

Birefringence: different propagation speed of both light's eigen-modes.

Magnetic circular dichroism (MCD):

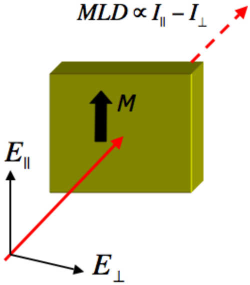
- Different absorption for circularly left and right polarized light.
- MCD linear in **M**.
- MOKE and MCD has the same microscopic origin, they just manifest in different ways.



MO effect IV: Voigt effect:

- Discovered 1899.
- Different absorption or phase shift for linear polarization parallel and perpendicular with the magnetization.
- Quadratic in **M** ($\sim M^2$).
- Also called Cotton-Mouton effect or linear magnetic dichroism/birefringence (LMD/LMB)
- The same microscopic origin as quadratic MOKE (QMOKE) (more precisely, Voigt effect is simplest case of QMOKE).

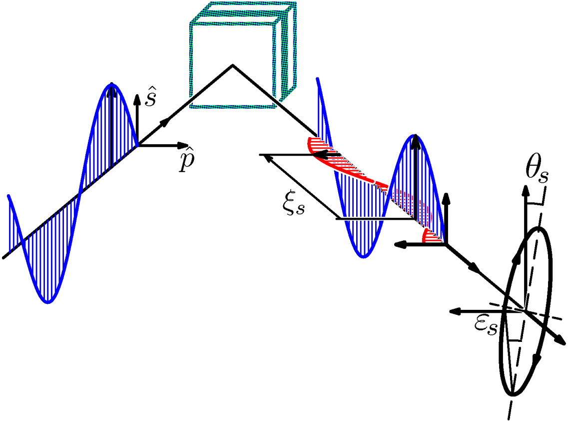
$MLD \propto I_{\parallel} - I_{\perp}$



$MLD \propto \mathrm{Im}[\varepsilon_{\parallel} - \varepsilon_{\perp}] \propto \mathrm{Re}[\sigma_{\parallel} - \sigma_{\perp}]$

Classification of the MO effects:

- Even / odd effect in magnetization.
- Measured in transmission / reflection.
- Detected change of intensity / polarization.
- Probing light is linearly / circularly polarized.

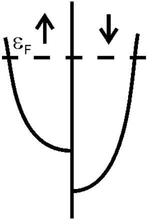


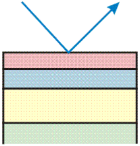
Family of magneto-optical effects:

Linear pol.	Detected: Polariz.	Detected: Intensity
Linear in M	MOKE, (Kerr and Faraday effect) [Hall effect]	Transversal-MOKE
Quadratic in M	QMOKE, Voigt effect, Linear Magnetic Birefringence (LMB)	Linear Magnetic Dichroism (LMD) [AMR]
Circular pol.	Detected: Polariz.	Detected: Intensity
Linear in M	Mag. Circular Birefringence (MCB)	Magnetic Circular Dichroism (MCD)
Quadratic in M	?	quadratic-MCD (?)

[...] denotes nomenclature in research of conductivity.

Origin of MO effect (microscopical):





Electronic structure of the FM material

[microscopic description]

$$\Downarrow$$

Permittivity tensor of each layer

[phenomenological description]

$$\varepsilon = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{bmatrix}$$

$$\Downarrow$$

Reflectivity matrix of whole sample

[maximal accessible optical information]

$$R = \begin{bmatrix} r_{ss} & r_{sp} \\ r_{ps} & r_{pp} \end{bmatrix}$$

$$\Downarrow$$

Measured Kerr effect: $\Phi_s = \frac{r_{ps}}{r_{ss}}$

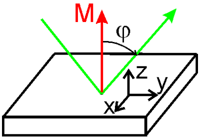
$$\Downarrow$$

Signal measured by MO setup

MOKE configurations and permittivity tensor:

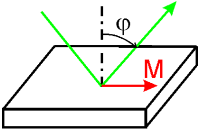
Polar MOKE

$M \perp$ sample surface



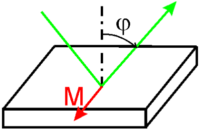
Longitudinal MOKE

$M \parallel$ plane of incidence



Transversal MOKE

$M \perp$ plane of incidence



Polarization induced by magnetization: $\Delta \mathbf{P}_M = \varepsilon_1 (\mathbf{M} \times \mathbf{E})$

$$\begin{bmatrix} \varepsilon_0 & -\varepsilon_1 m_z & 0 \\ \varepsilon_1 m_z & \varepsilon_0 & 0 \\ 0 & 0 & \varepsilon_0 \end{bmatrix} \qquad \begin{bmatrix} \varepsilon_0 & 0 & \varepsilon_1 m_y \\ 0 & \varepsilon_0 & 0 \\ -\varepsilon_1 m_y & 0 & \varepsilon_0 \end{bmatrix} \qquad \begin{bmatrix} \varepsilon_0 & 0 & 0 \\ 0 & \varepsilon_0 & -\varepsilon_1 m_x \\ 0 & \varepsilon_1 m_x & \varepsilon_0 \end{bmatrix}$$

$$\Phi_{s/p}(m_z) \qquad \Phi_{s/p}(m_y) \qquad \Delta r_{pp}(m_x)$$

MO effects and permittivity tensors

[Note: tensors on this slide are only illustrative.]

⇒ Linear MOKE: PMOKE, LMOKE, TMOKE, MCD, MCB, [Hall]

$$\begin{bmatrix} \varepsilon_0 & -\varepsilon_1 m_z & \varepsilon_1 m_y \\ \varepsilon_1 m_z & \varepsilon_0 & -\varepsilon_1 m_x \\ -\varepsilon_1 m_y & \varepsilon_1 m_x & \varepsilon_0 \end{bmatrix} \qquad \text{MO signal} \sim \varepsilon_1(m_i)$$

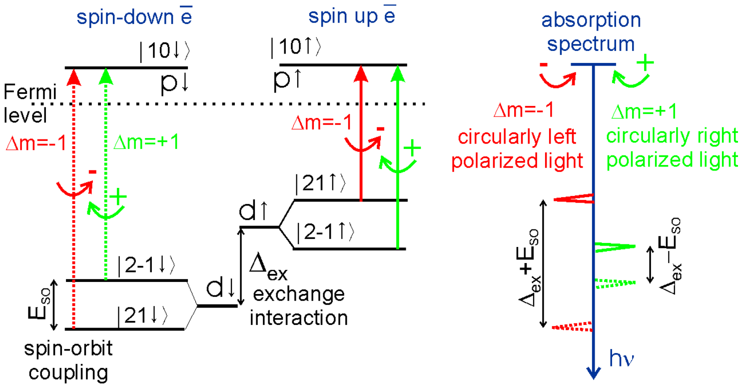
⇒ Quadratic MOKE:

$$\begin{bmatrix} \varepsilon_0 & \varepsilon_1(m_i m_j) & 0 \\ \varepsilon_1(m_i m_j) & \varepsilon_0 & 0 \\ 0 & 0 & \varepsilon_0 \end{bmatrix} \qquad \text{MO signal} \sim \varepsilon_1(m_i m_j)$$

⇒ Voigt effect: MLD, MLD, [AMR]

$$\begin{bmatrix} \varepsilon_{xx}(m_i m_j) & 0 & 0 \\ 0 & \varepsilon_{yy}(m_i m_j) & 0 \\ 0 & 0 & \varepsilon_{zz}(m_i m_j) \end{bmatrix} \qquad \text{MO signal} \sim \sqrt{\varepsilon_{zz}(m_i m_j) - \varepsilon_{yy}(m_i m_j)}$$

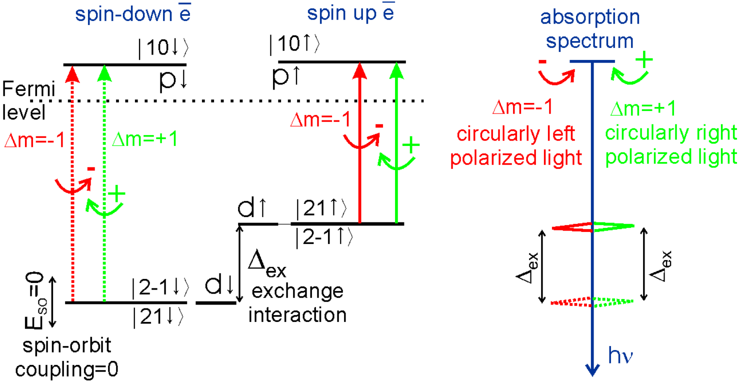
Magneto-optical spectroscopy microscopic picture



Simplified electronic structure for one point of the *k*-space.

No spin-orbit coupling assumed:

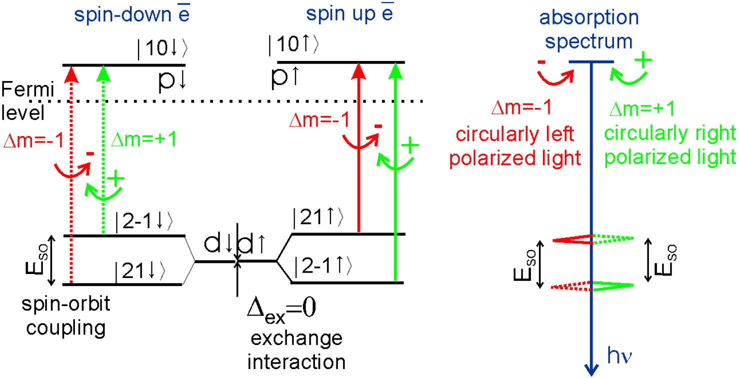
⇒ no MOKE effect



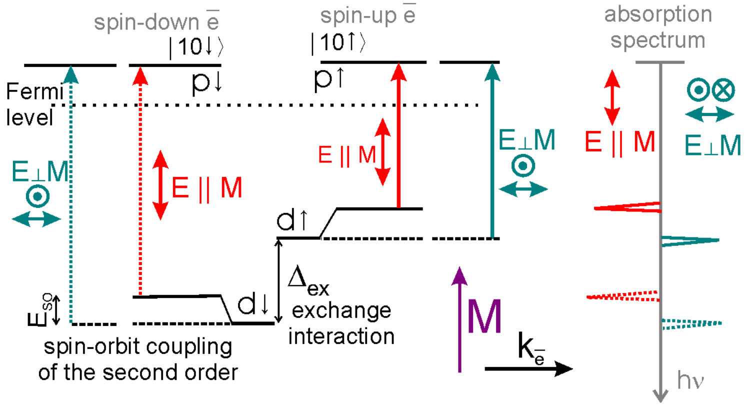
No exchange assumed:

$\Rightarrow$ no MOKE effect

$\Rightarrow$ both SO coupling and exchange must be present to have MOKE.

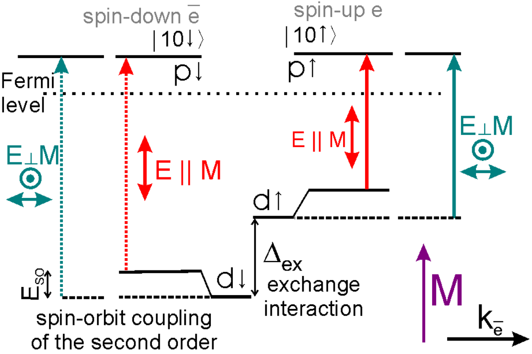


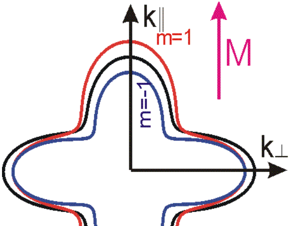
Quadratic Magneto-optical Kerr effect (QMOKE):



QMOKE arises from different absorptions for **E** ⊥ **M** and **E**||**M**.

Quadratic Magneto-optical Kerr effect (QMOKE):





Condutivity (and hence absorption of the photon)

Kubo formula: conductivity determination.

$$\Re[\sigma_{xx}] \sim \sum_{i,f} [f(E_i) - f(E_f)] \times [|\langle i|p_+|f\rangle|^2 + |\langle i|p_-|f\rangle|^2] \times \delta(E_f - E_i - \hbar\omega)$$

$$\Im[\sigma_{xy}] \sim \sum_{i,f} [f(E_i) - f(E_f)] \times [|\langle i|p_+|f\rangle|^2 - |\langle i|p_-|f\rangle|^2] \times \delta(E_f - E_i - \hbar\omega)$$

where

- $\langle i|$, $|f\rangle$: initial and final states, respectively.
- $p_\pm = p_x \pm ip_y$, $p_x = i\hbar\partial/\partial x$, momentum operator
- terms in the Kubo formula means:
  - summation over all initial and final states, $\langle i|$ and $|f\rangle$.
  - $f(E_f)$, $f(E_i)$: electron occupancy of initial and final states.
  - $|\langle i|p_\pm|f\rangle|^2$: probability of the photon to be absorbed between $\langle i|$ and $|f\rangle$ states for circularly left/right polarized light (non-zero only when electric-dipole selection rules are fulfilled).
  - $\delta(E_f - E_i - \hbar\omega)$ assures energy conservation.

MOKE advantages and disadvantages:

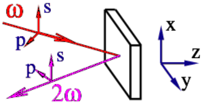
- spatial resolution limited by wavelength limit (∼300nm for visible light) → but sub-wavelength resolution demonstrated.
- investigation on distance, light can be transported nearby sample by a fibre.
- no need of vacuum or special sample preparation.
- depth resolution about 30nm.
- measurements do not influence sample magnetization.
- high time resolution.
- depth selectivity.
- vectorial resolution (possible to determine all magnetization components).
- robust, cheap technique.

BUT:

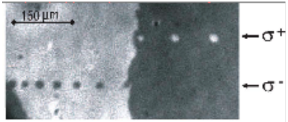
- spatial resolution limited by wavelength limit.
- easy to overcome Kerr signal by spurious noise (S/N ratio problem).
- not direct information about the electronic structure or magnetic moments etc.

Extensions of MOKE:

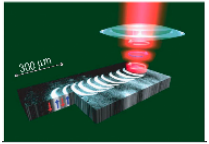
- XMCD, XMLD for high photon energy.
- Non-linear magneto-optics
  ⇒ MO second harmonic generation.



- Inverse Faraday effect (ultrafast optical switching).



(Stanciu et al, PRL 99, 047601 (2007))



- Observation of spin accumulation in GaAs (spin Hall effect).