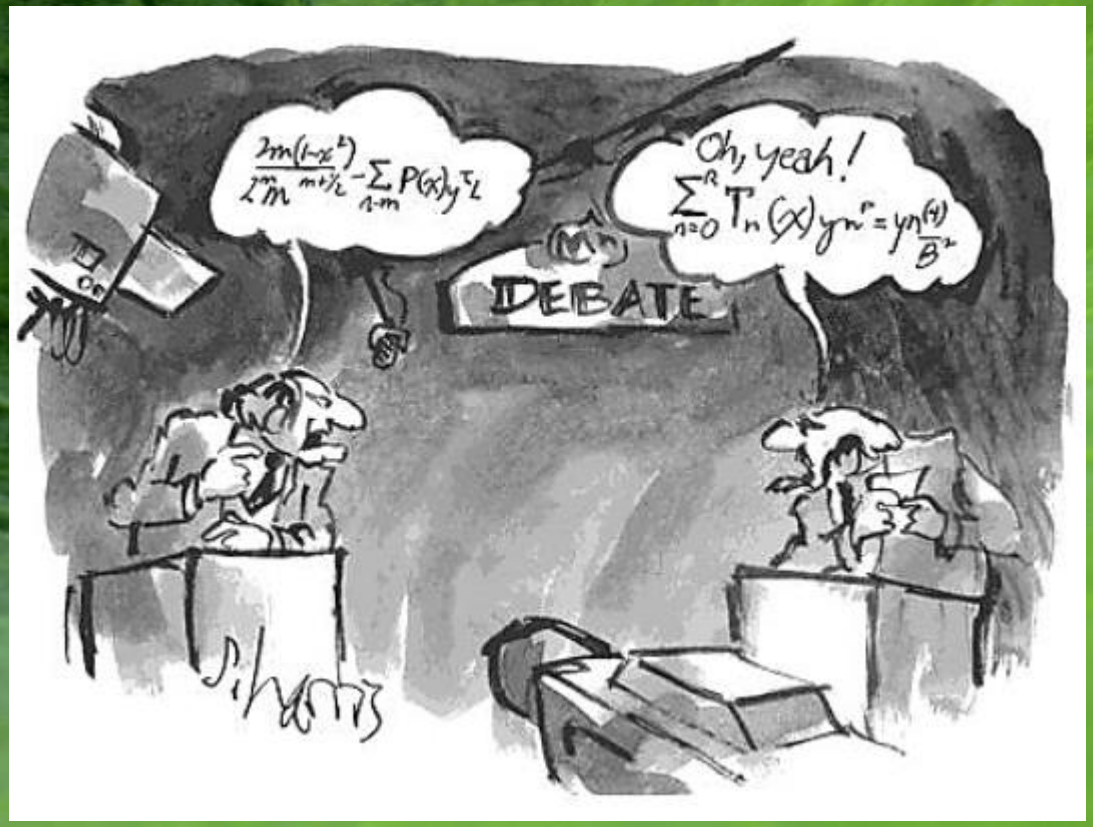
Physics of Condensed Matter I

1100-4INZ`PC



Solid state 2

Faculty of Physics UW

Jacek.Szczytko@fuw.edu.pl

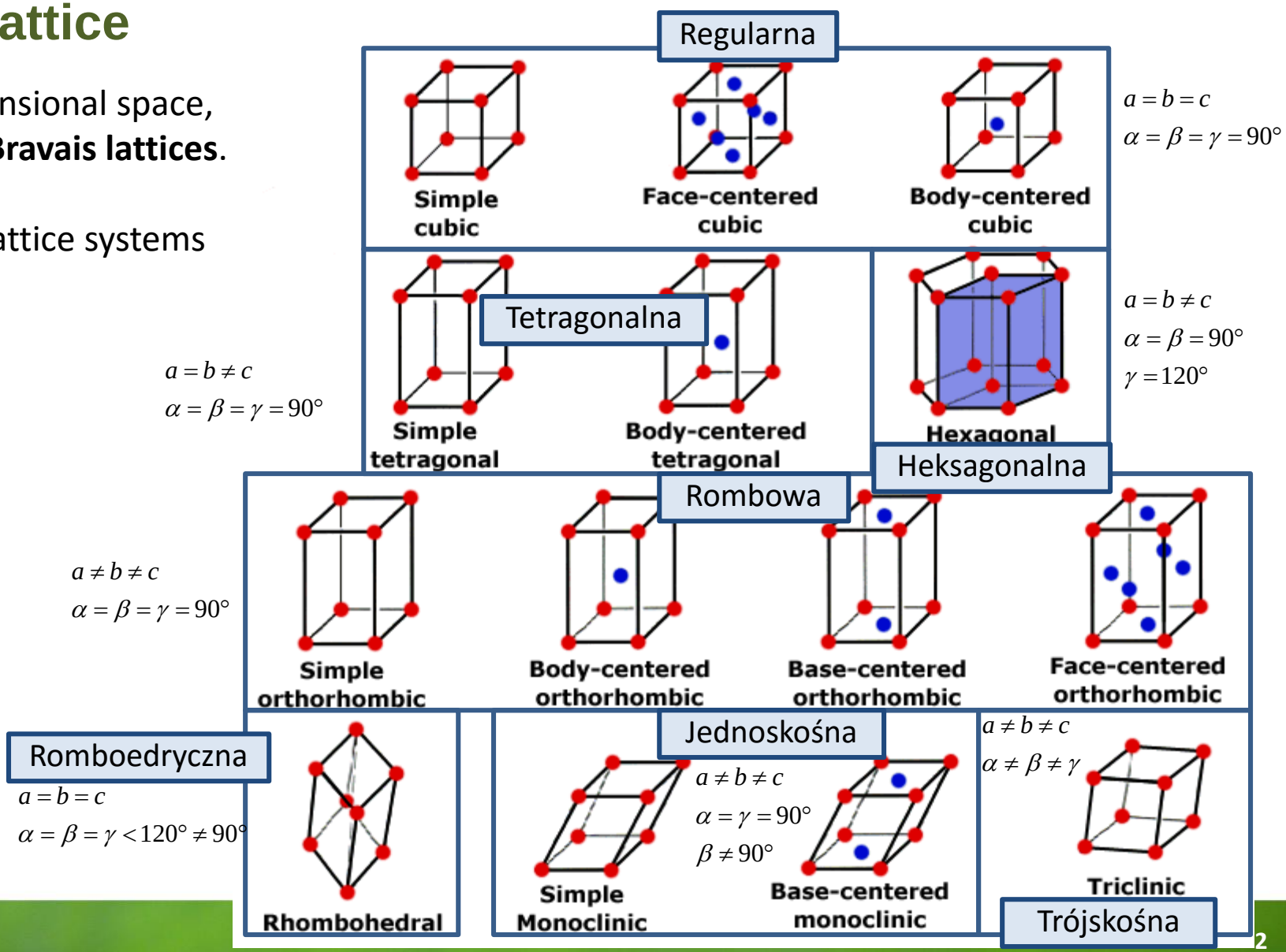
inżynieria nanostruktur

Crystal structure

Bravais lattice

In three-dimensional space, there are 14 **Bravais lattices**.

They form 7 lattice systems



Crystal structure

Planes in the crystal

A family of lattice planes are written (hkl), and denote the family of planes that intercepts the three points:

$$\frac{\vec{a}_1}{h}, \frac{\vec{a}_2}{k}, \frac{\vec{a}_3}{l}$$

If one of the indices is zero, it means that the planes do not intersect that axis (1/0 = infinity)

Also: the family of planes orthogonal to:

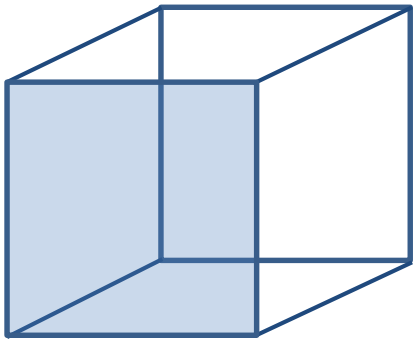
$$h\vec{g}_1 + k\vec{g}_2 + l\vec{g}_3$$

Where $\vec{g}_1$, $\vec{g}_2$, $\vec{g}_3$ are reciprocal lattice vectors

E.g.: A=2, B=3, C=6, plane (3,2,1)

(hkl) plane
$\{hkl\}$ set of planes
$[hkl]$ diections
$\langle hkl \rangle$ set of directions

(100)



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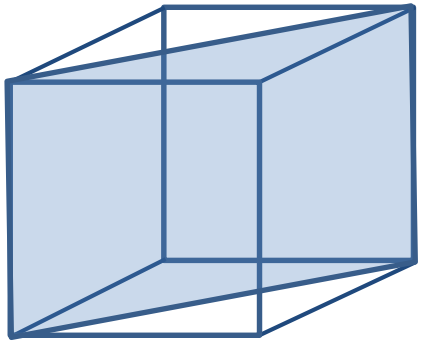

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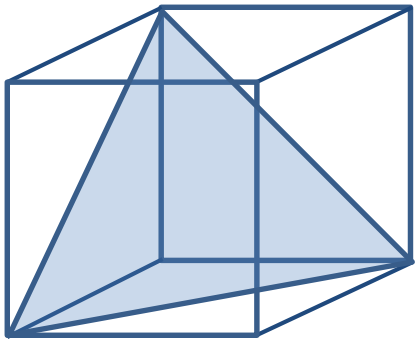
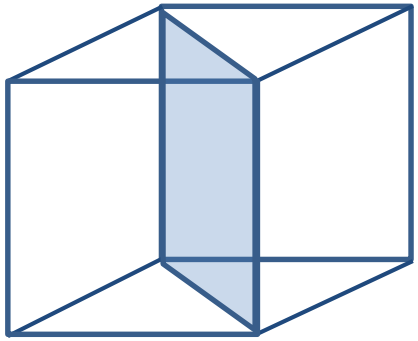


Crystal structure

Planes in the crystal

$(\bar{1}10)$



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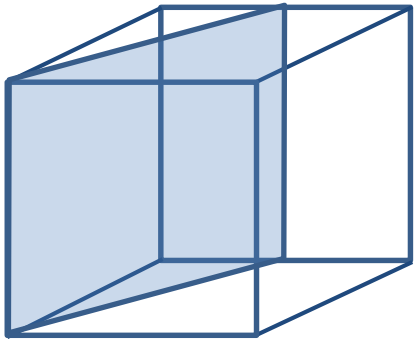

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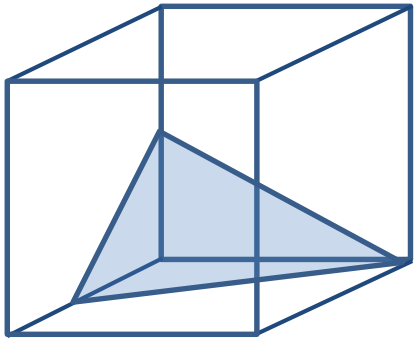

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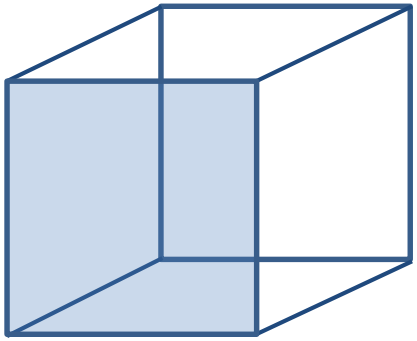

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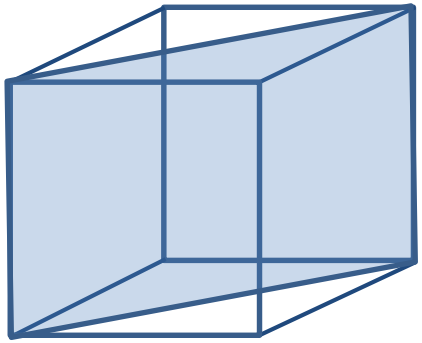

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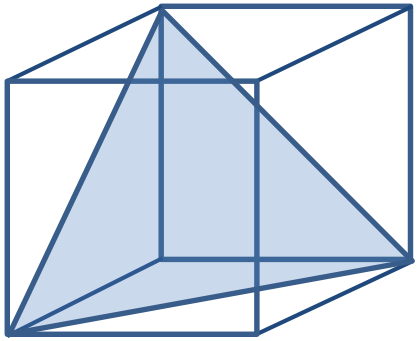
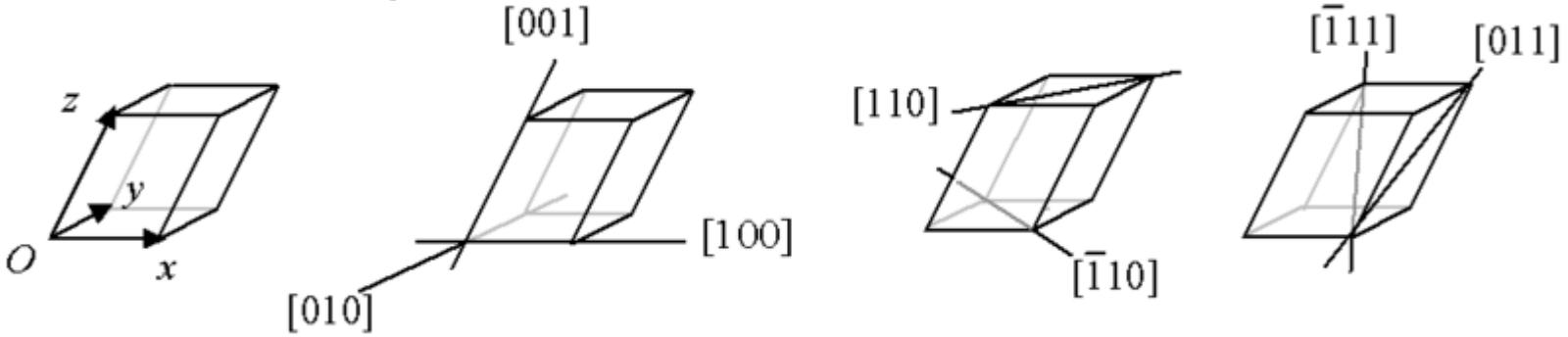
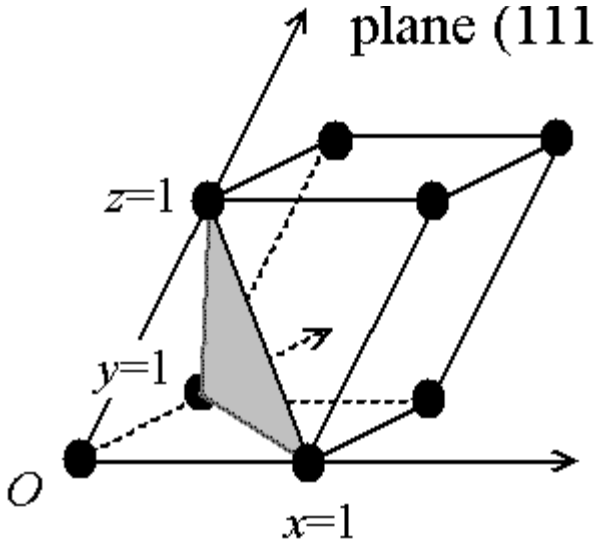
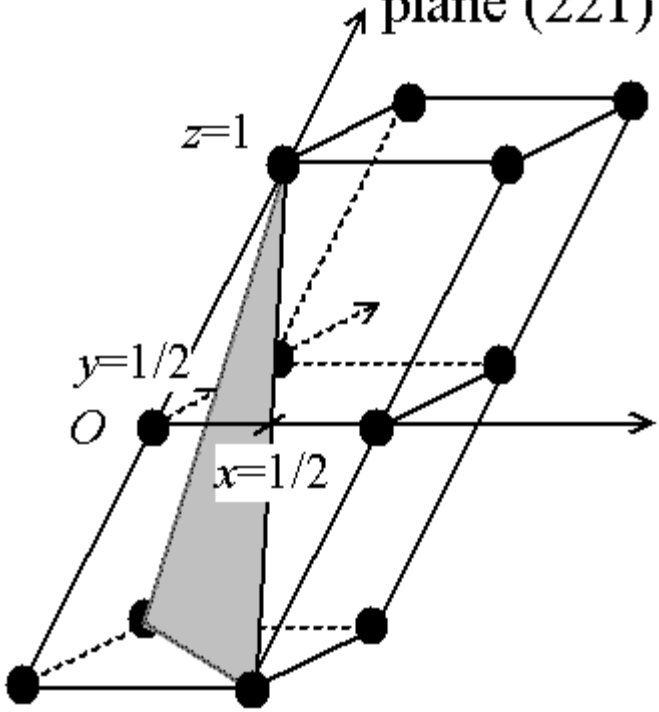


Crystal structure

Planes in the crystal





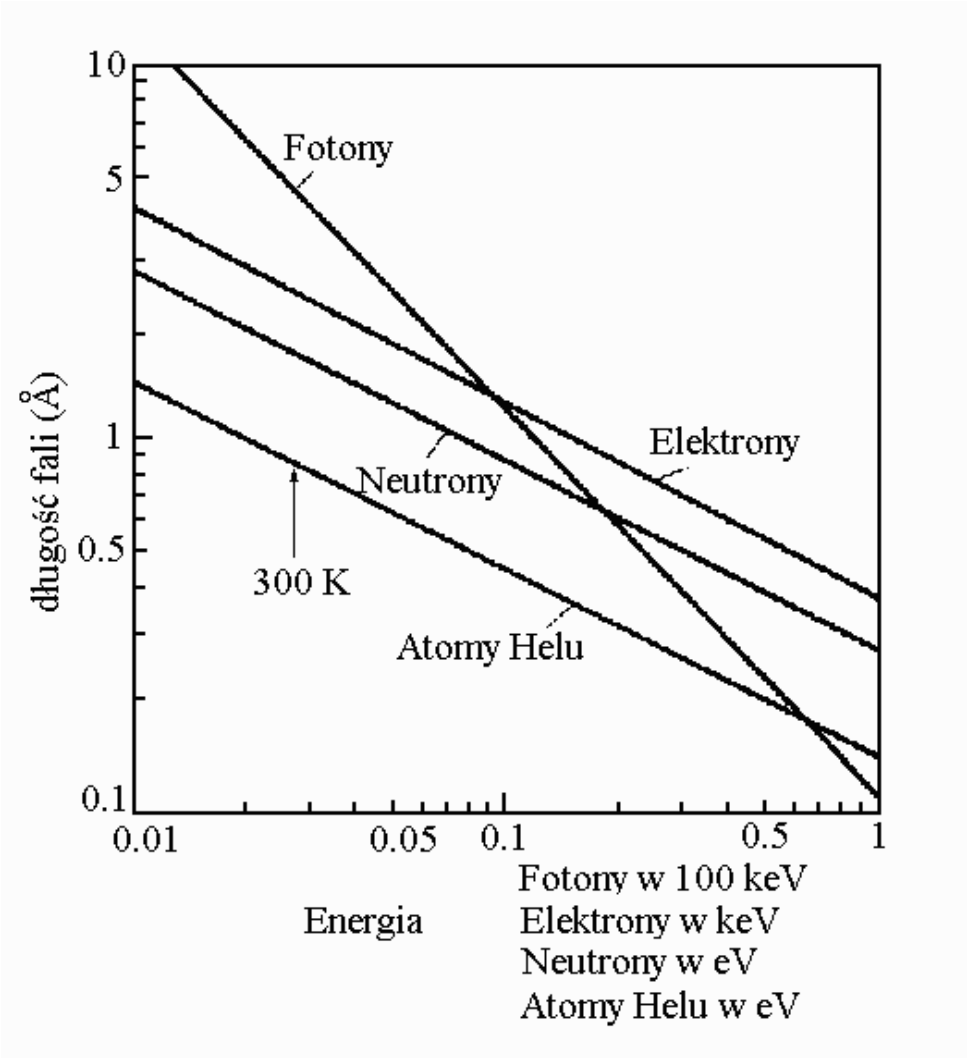


http://pl.wikipedia.org/wiki/Wskaźniki_Millera

Crystalography

Planes in the crystal

The crystalline structure is studied by means of the diffraction of photons, neutrons, electrons or other light particles



Crystalography

Crystals

1912 - Max von Laue noted that the wavelength of X-rays are comparable to the distances between atoms in the crystal. This suggestion was quickly confirmed by Walter Friedrich and Paul Knipping

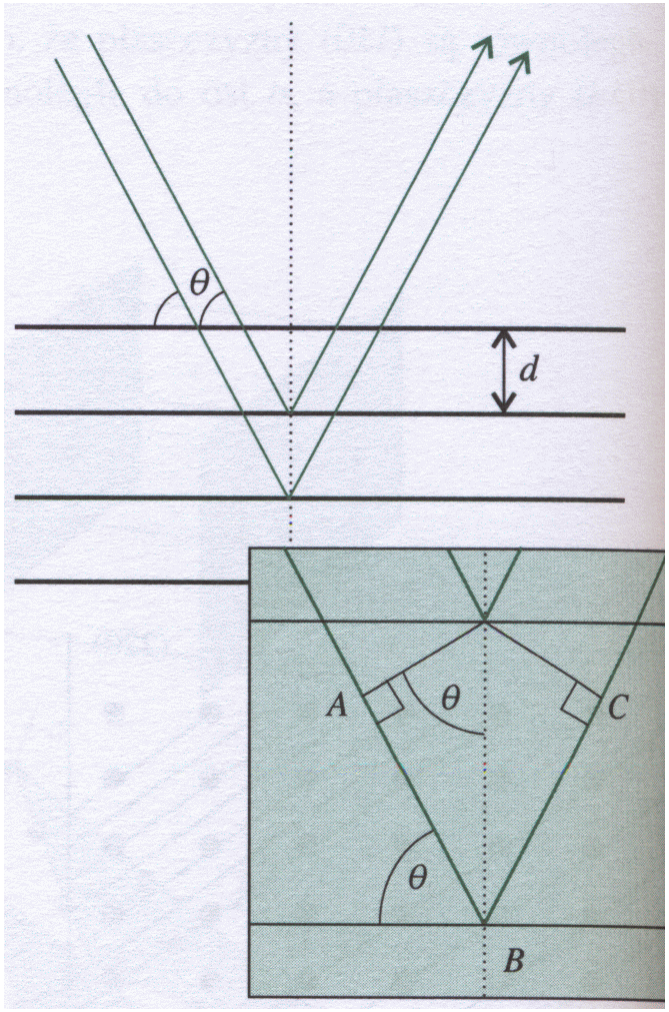
Max von Laue
1879 - 1960

Model of the crystal: set of discrete parallel planes separated by a constant parameter d

$$2dsin\theta = n\lambda$$

William Lawrence Bragg (son) and William Henry Bragg (father), 1913

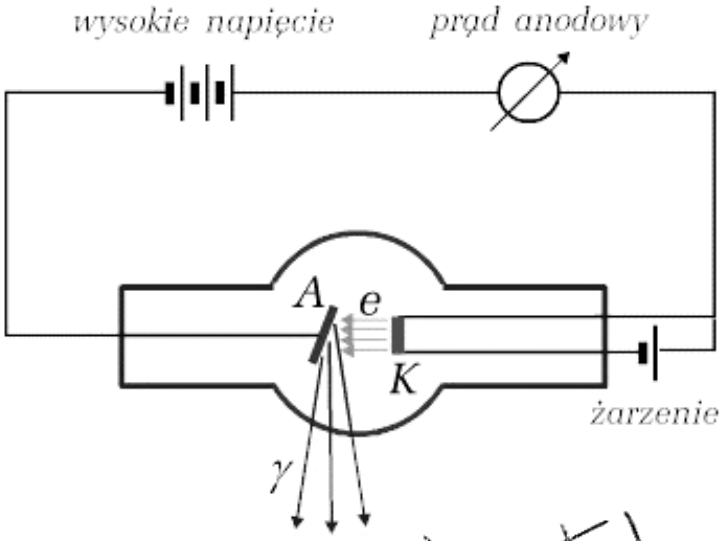
e.g . λ=1,54 Å, d = 4 Å, crystals with cubic symmetry, the first reflex $\theta = 11°$

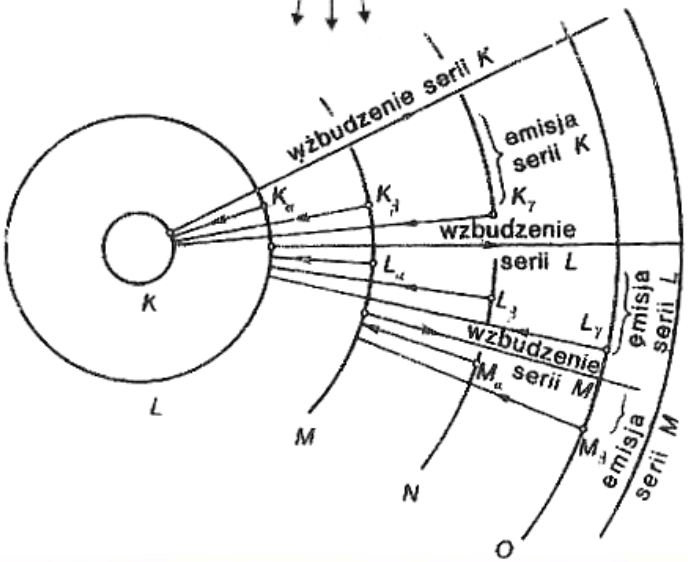


P. Atkins

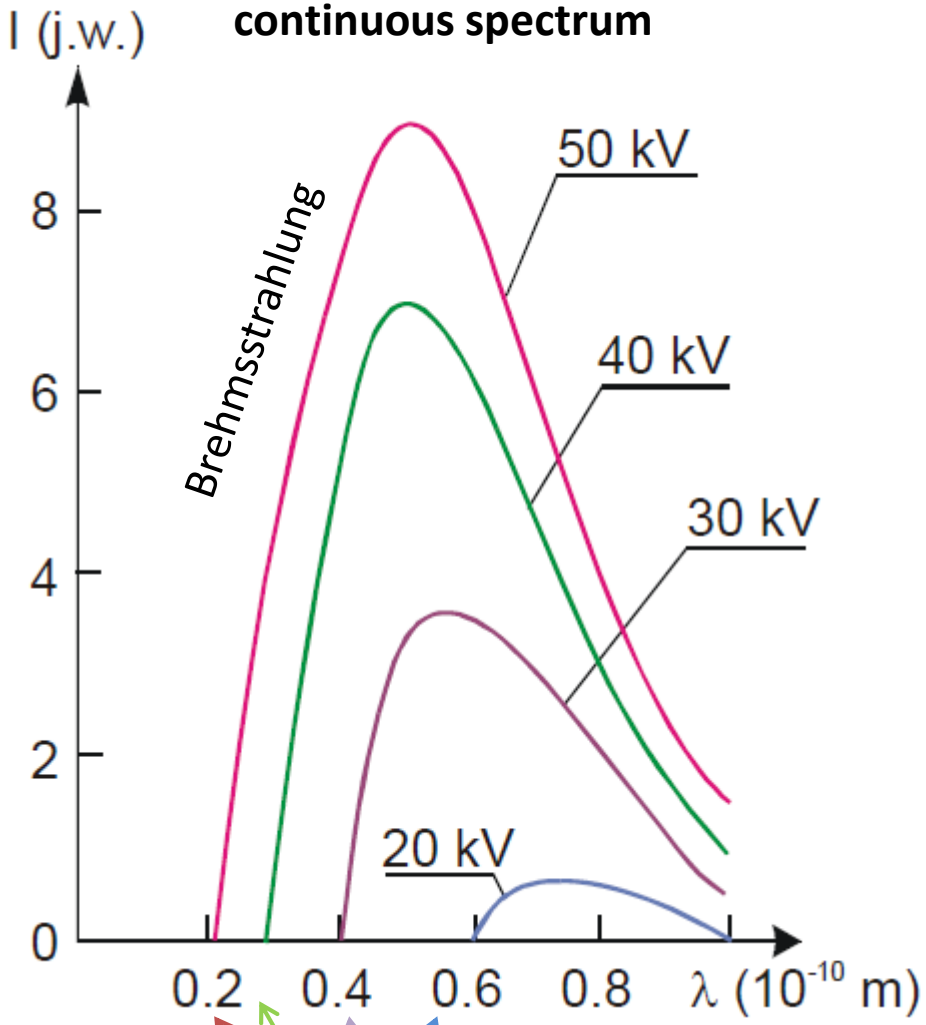
Brehmsstrahlung – *promieniowanie hamowania*

Crystals





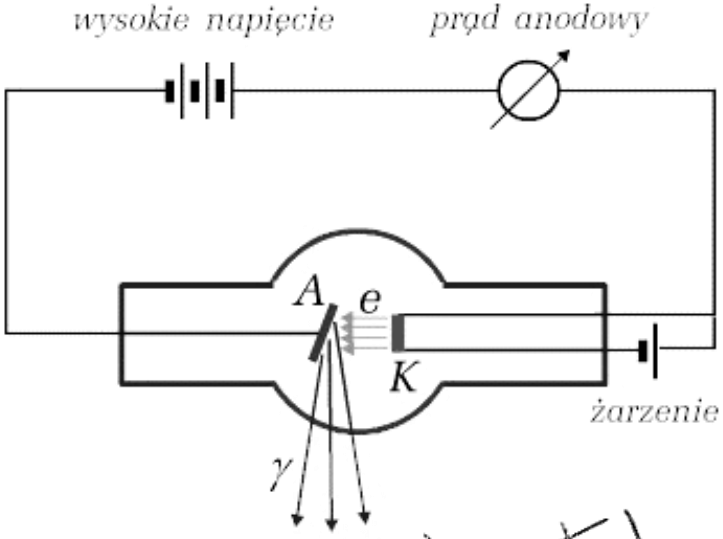
continuous spectrum

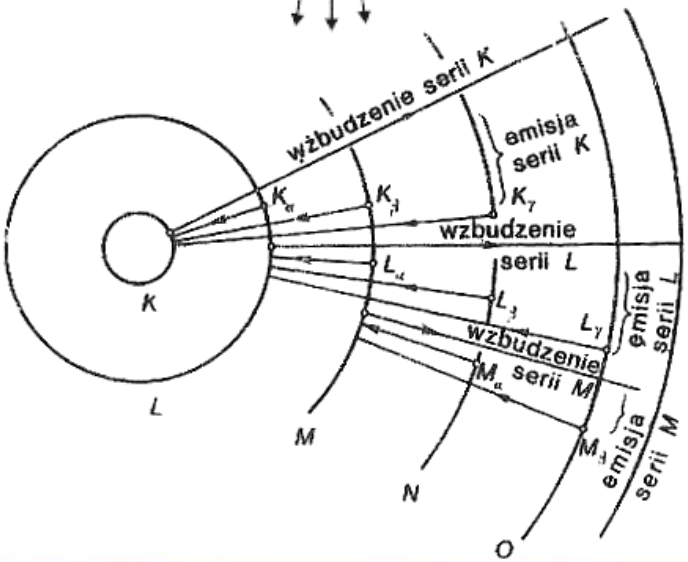


$$h\nu_{max} = h\frac{c}{\lambda_{min}} = eV$$

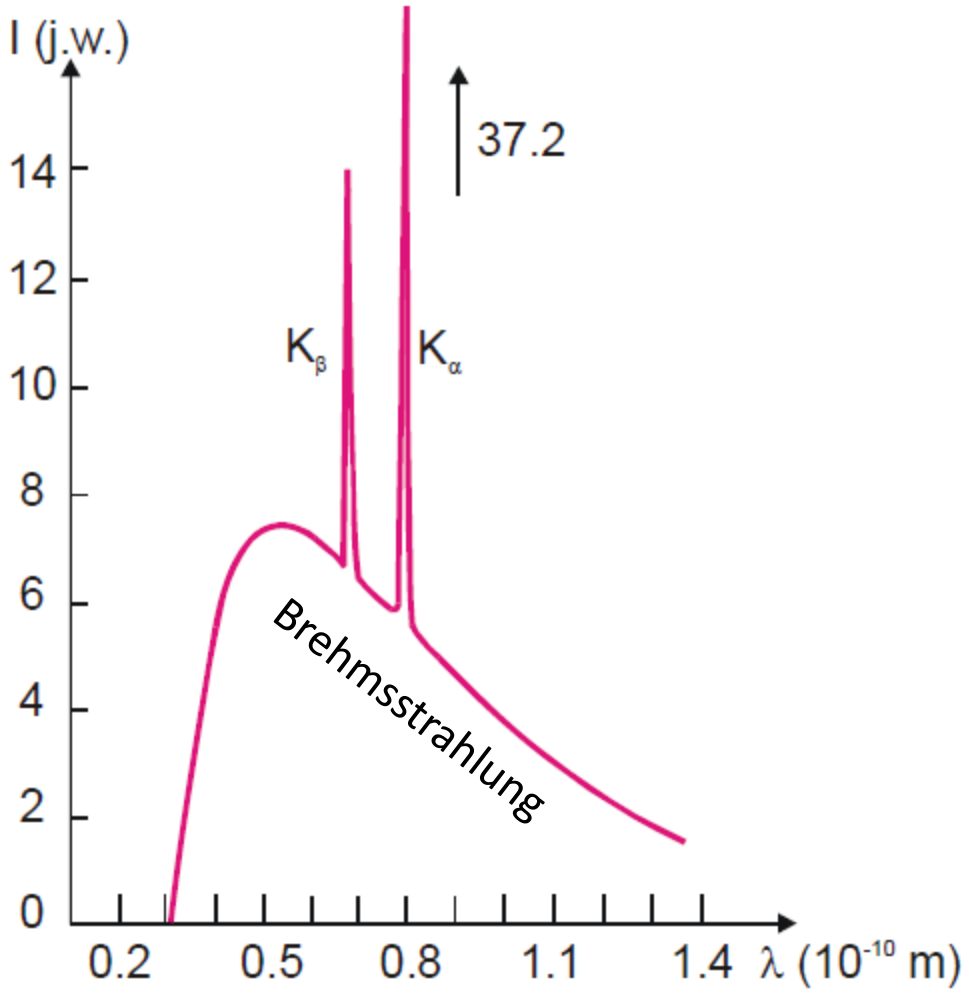
Crystalography

Crystals





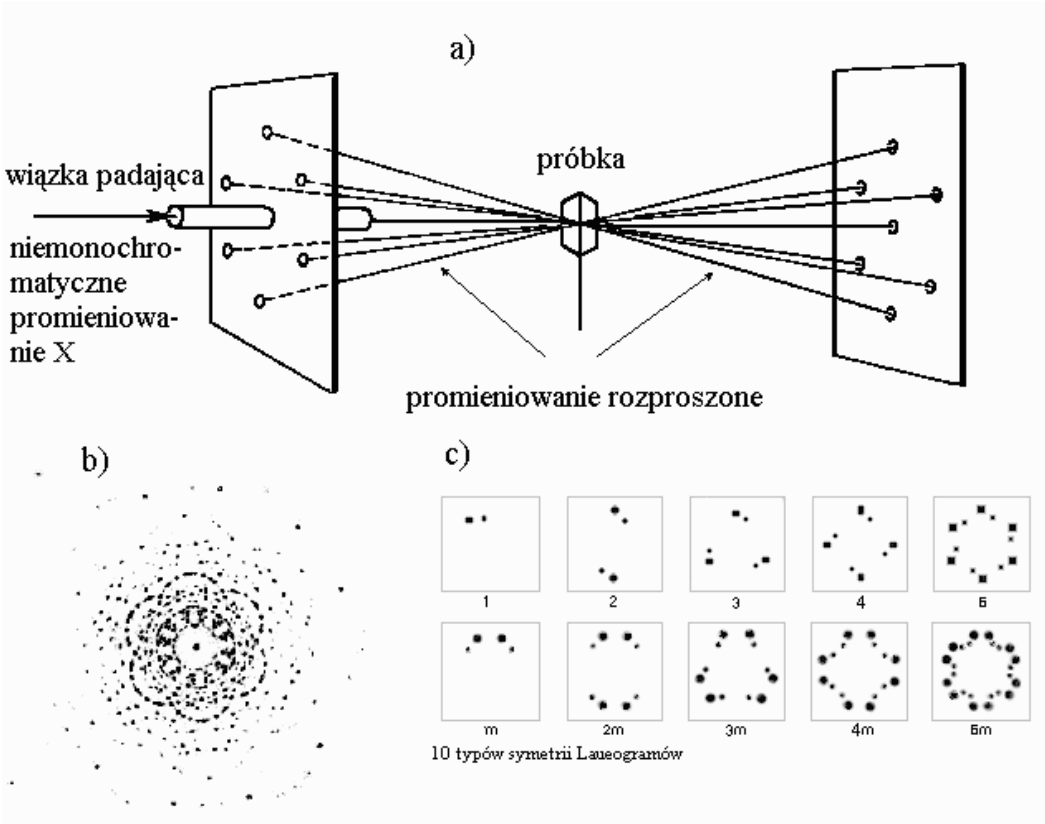
characteristic spectrum



Crystalography

Laue method

- The crystal is illuminated with white light.
- As a result of scattering the waves of different wavelengths are distributed in different directions. We get different points for different colors (wavelengths).
- the pattern of the spots has a symmetry of the crystal along the direction of the incident wave

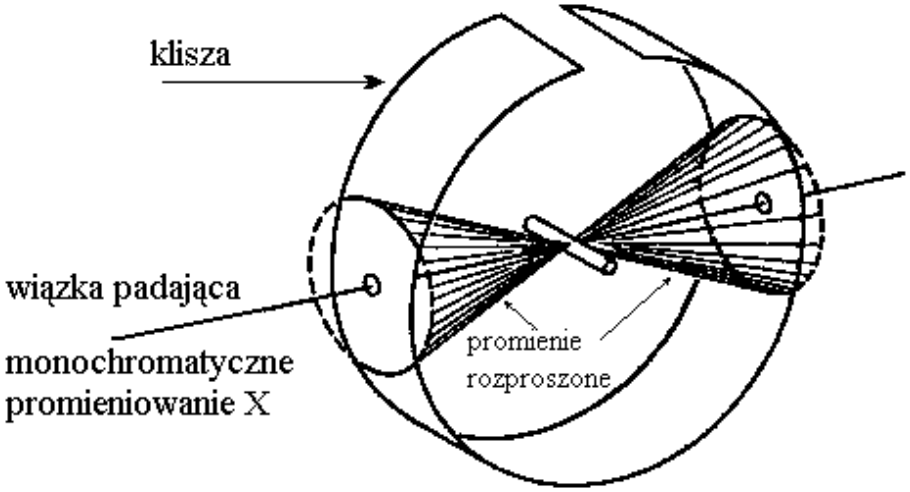


Crystalography

Debaye-Scherer method

Peter Joseph Debye
1884 – 1966

Paul Scherrer
1890 - 1969

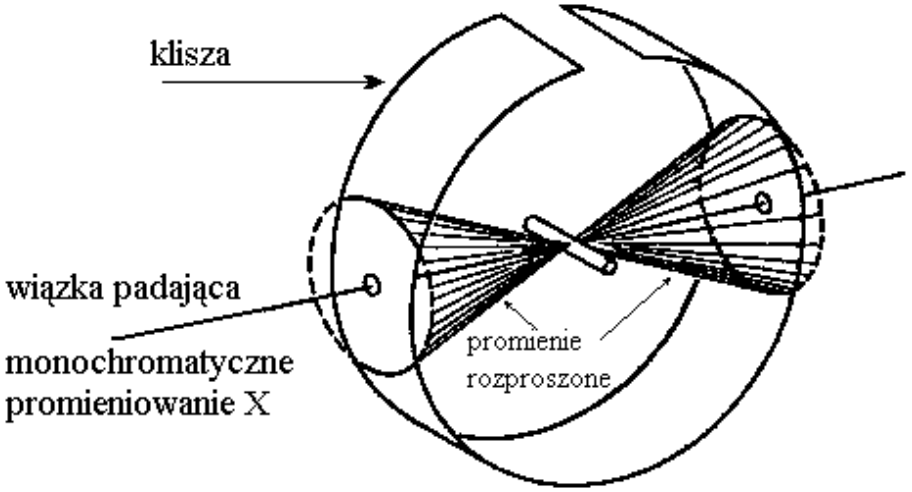


Typowy debajogram

Crystalography

Debaye-Scherer method

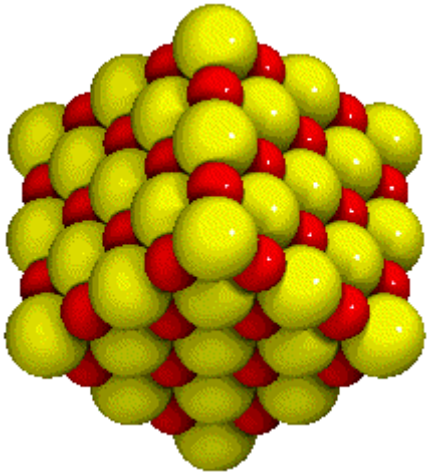
The powder of the crystals with chaotic orientation in space is measured. It is illuminated by the monochromatic wave. X-rays scattered by the differently oriented crystals creates arcs corresponding to the planes on which the X-ray wave was scattered.

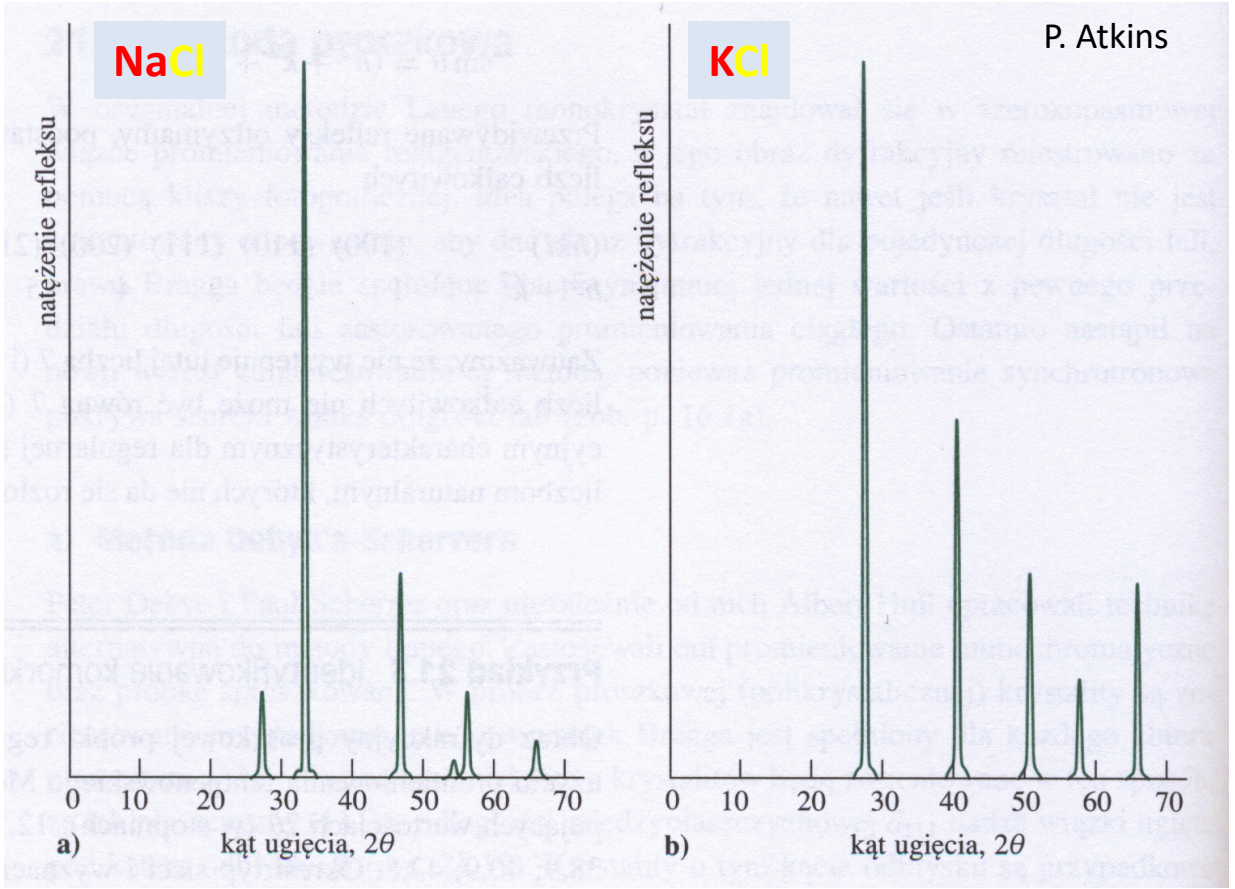


Typowy debajogram

Crystalography

Atomic form factor (*czynnik atomowy*)

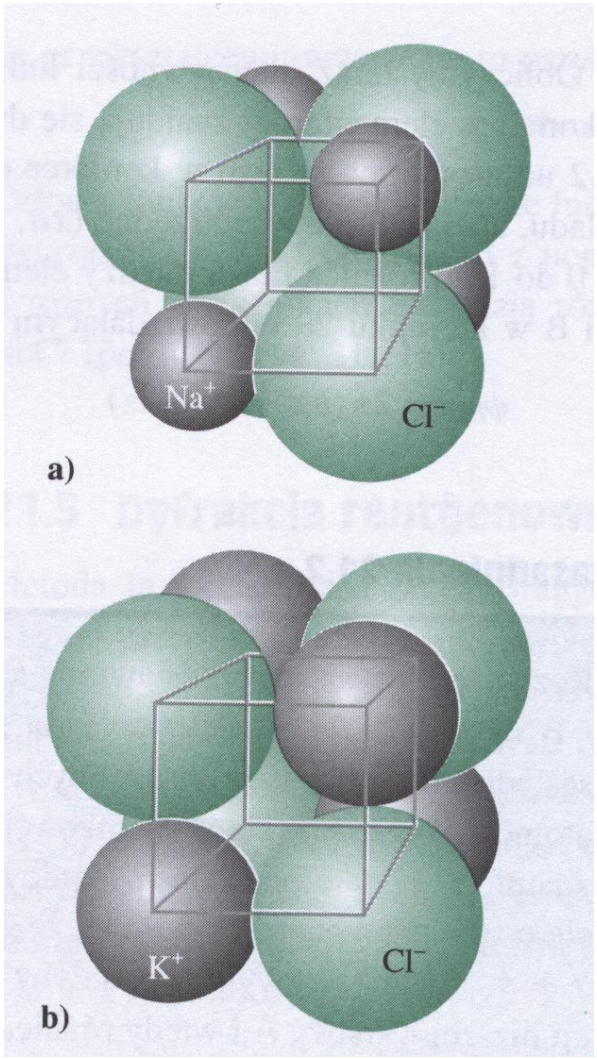


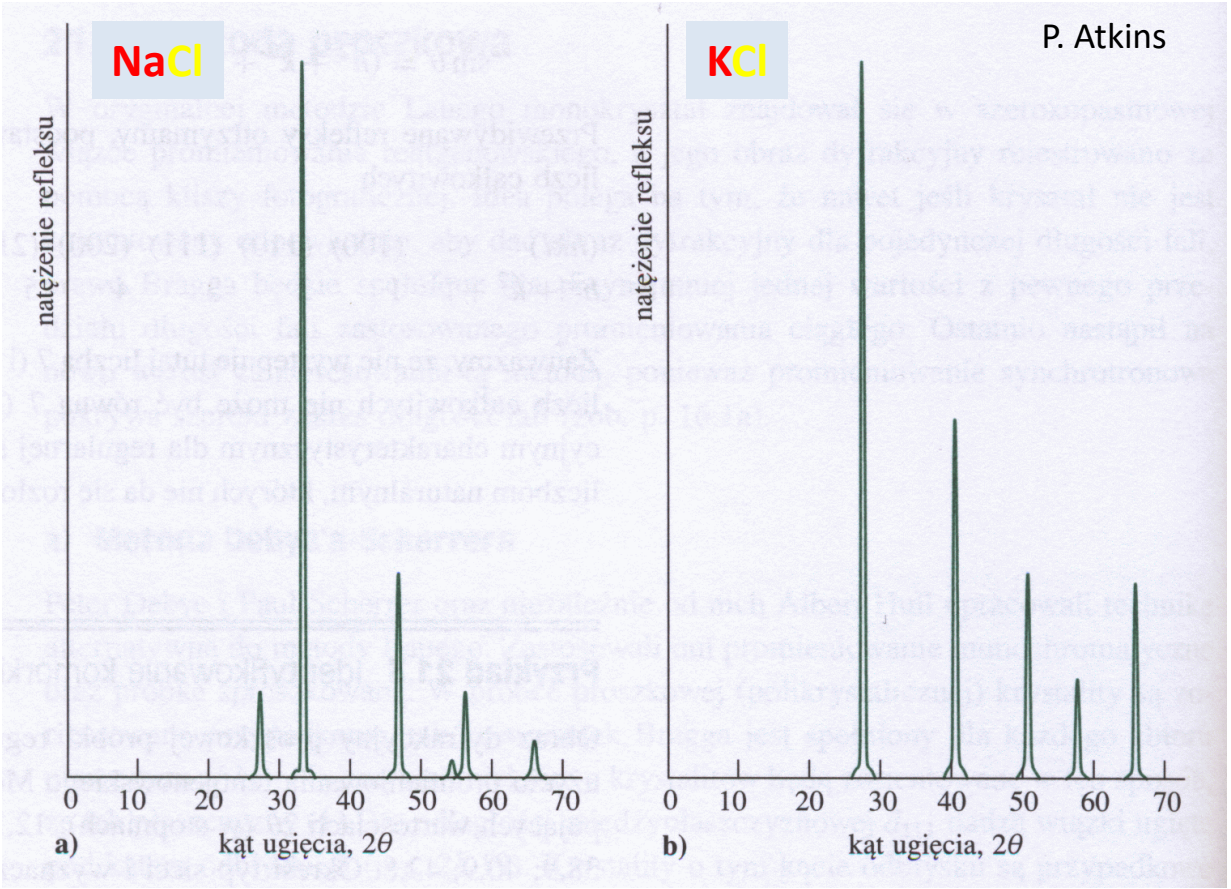


Both salts have the same crystal structure, but different diffraction, why?

Crystalography

Atomic form factor (*czynnik atomowy*)

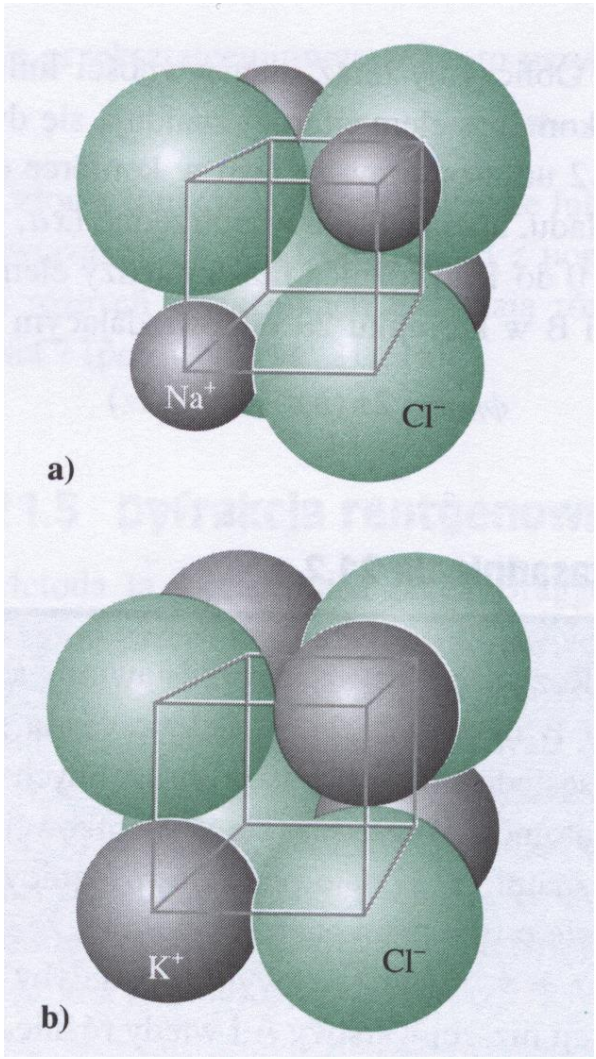




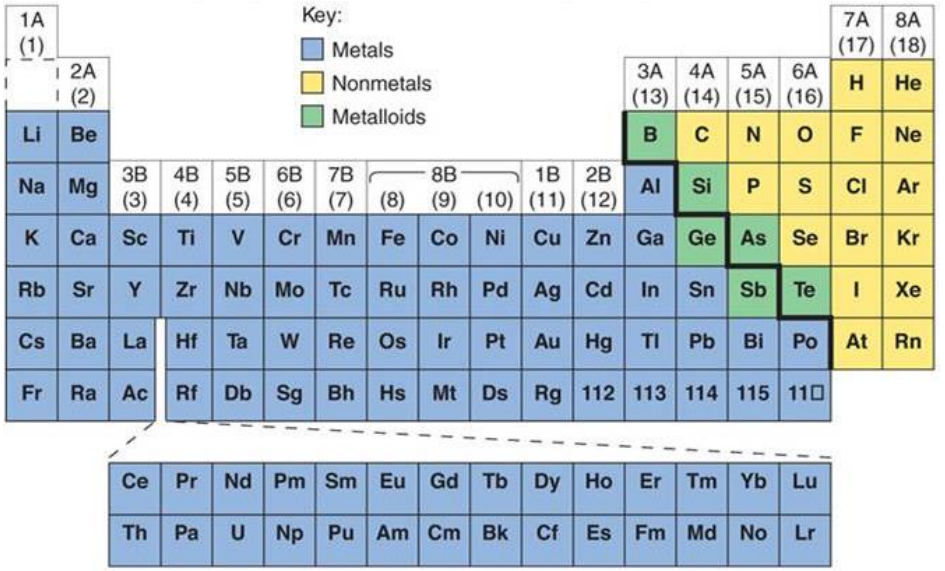
Both salts have the same crystal structure, but different diffraction, why?

Crystalography

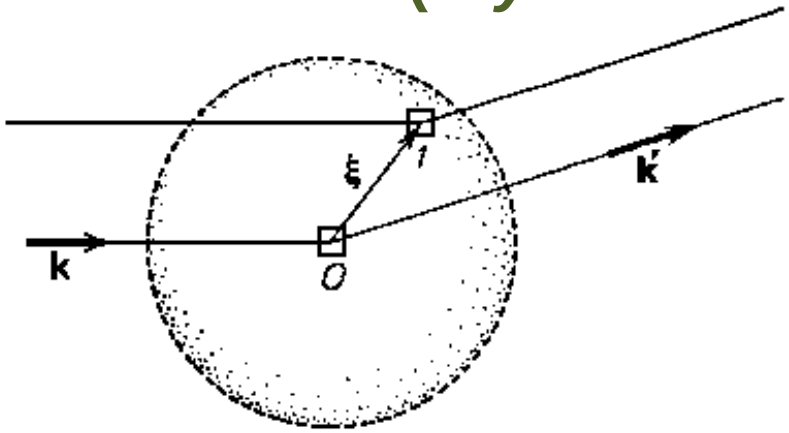
Atomic form factor (*czynnik atomowy*)



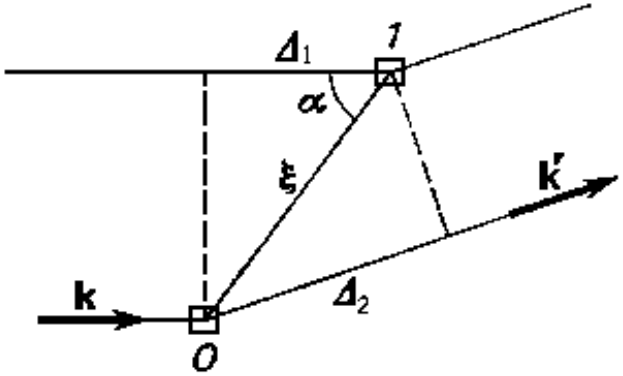
- K^+ and Cl^- have the same number of electrons. They scatter similarly X-rays.
- For certain directions the destructive interference occurs (total extinction)
- Na^+ and Cl^- - waves are scattered by atoms with different electrons, no total extinction.
- Thus there is **atomic form factor**



Atomic form factor (*czynnik atomowy*)



Rys. 8.2. Dyfrakcja fali elektromagnetycznej przez chmurę gęstości ładunku elektronów w atomie



Rys. 8.3. Oznaczenia używane w obliczeniach

Elsatic scattering of X-rays by electron cloud:
i.e. local electron concnetration $\rho(\vec{\xi})$

$$|\vec{k}| = |\vec{k}'| = k$$

$$\Delta_1 = \xi \cos\alpha = \xi \frac{\vec{k}\vec{\xi}}{k\xi} = \frac{\vec{k}\vec{\xi}}{k}$$

$$\Delta_2 = \xi \cos\alpha' = \xi \frac{\vec{k}'\vec{\xi}}{k\xi} = \frac{\vec{k}'\vec{\xi}}{k}$$

$$\Delta = (\Delta_2 - \Delta_1) = \frac{(\vec{k}' - \vec{k})\vec{\xi}}{k} = \frac{\Delta\vec{k}\,\vec{\xi}}{k}$$

$$\varphi = \frac{2\pi\Delta}{\lambda} = k\Delta = \Delta\vec{k}\,\vec{\xi}$$

Atomic form factor (*czynnik atomowy*)

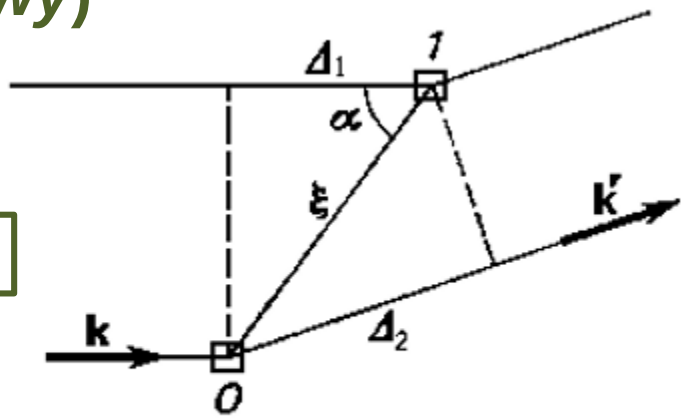
$$\Delta = (\Delta_2 - \Delta_1) = \frac{(\vec{k'} - \vec{k})\vec{\xi}}{k} = \frac{\Delta\vec{k}\,\vec{\xi}}{k}$$

$$\varphi = \frac{2\pi\Delta}{\lambda} = k\Delta = \Delta\vec{k}\,\vec{\xi}$$

Charge density in $\vec{\xi} = 0$

$$\Psi(0) = \frac{A}{r}\exp\left[i(\vec{k}\vec{r} - \omega t)\right]\rho_e(\vec{\xi} = 0)$$

$$\Psi(\vec{\xi}) = \frac{A}{r}\exp\left[i(\vec{k}\vec{r} - \omega t - \Delta\vec{k}\vec{\xi})\right]\rho_e(\vec{\xi})$$



Rys. 8.3. Oznaczenia używane w obliczeniach

Scattered wave:

$$\Psi(\vec{\xi})d\vec{\xi} = \frac{A}{r}\exp\left[i(\vec{k}\vec{r} - \omega t)\right]\rho_e(\vec{\xi})\exp\left[-i\Delta\vec{k}\vec{\xi}\right]d\vec{\xi}$$

Density of charge

Atomic form factor

$$f = -\frac{1}{e}\int \rho_e(\vec{\xi})\exp\left[-i\Delta\vec{k}\vec{\xi}\right]d\vec{\xi}$$

Atomic form factor (*czynnik atomowy*)

For instance spherical distribution of electrons

$$f = -\frac{1}{e}\int \rho_e(\vec{\xi}) \exp\left[-i\Delta\vec{k}\vec{\xi}\right] d\vec{\xi} = -\frac{1}{e} 2\pi \int \rho_e(\vec{\xi}) \exp\left[-\Delta\vec{k}\vec{\xi}\right] \xi^2 d(\cos\theta) d\xi$$

$$= -\frac{2\pi}{e}\int \xi^2 \rho_e(\vec{\xi}) \frac{\exp[\Delta k\xi] - \exp[-\Delta k\xi]}{ik\xi} d\xi = -\frac{4\pi}{e}\int \xi^2 \rho_e(\vec{\xi}) \frac{\sin \Delta k\xi}{k\xi} d\xi$$

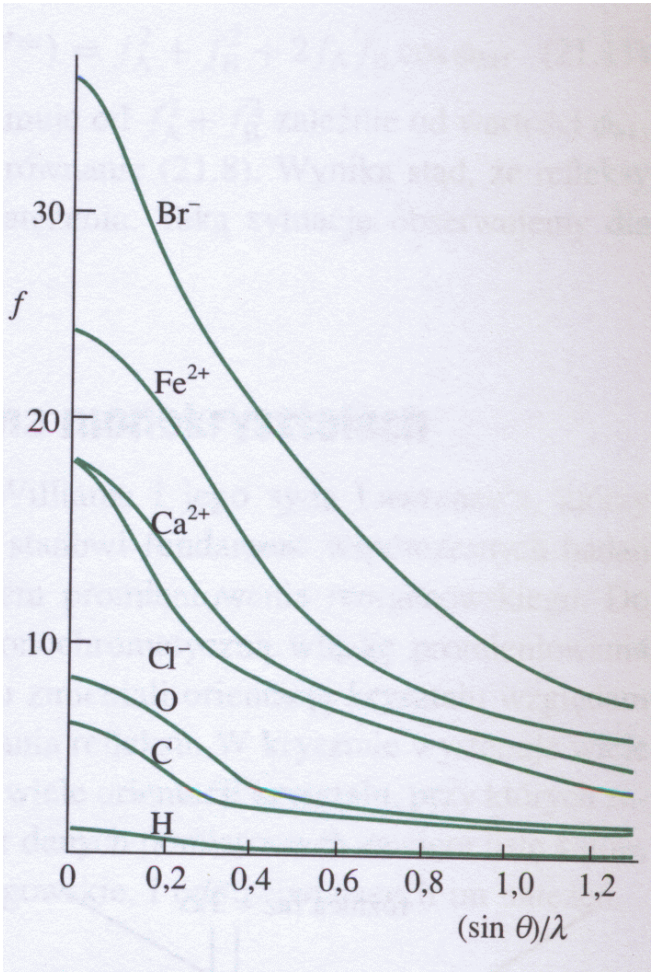
For small angles of scattering $\Delta k\xi \to 0$ and $f = -Z$

The atomic scattering factor f is the ratio of the amplitude of the radiation scattered by the actual distribution of electrons in the atom to the amplitude of the radiation scattered by one electron.

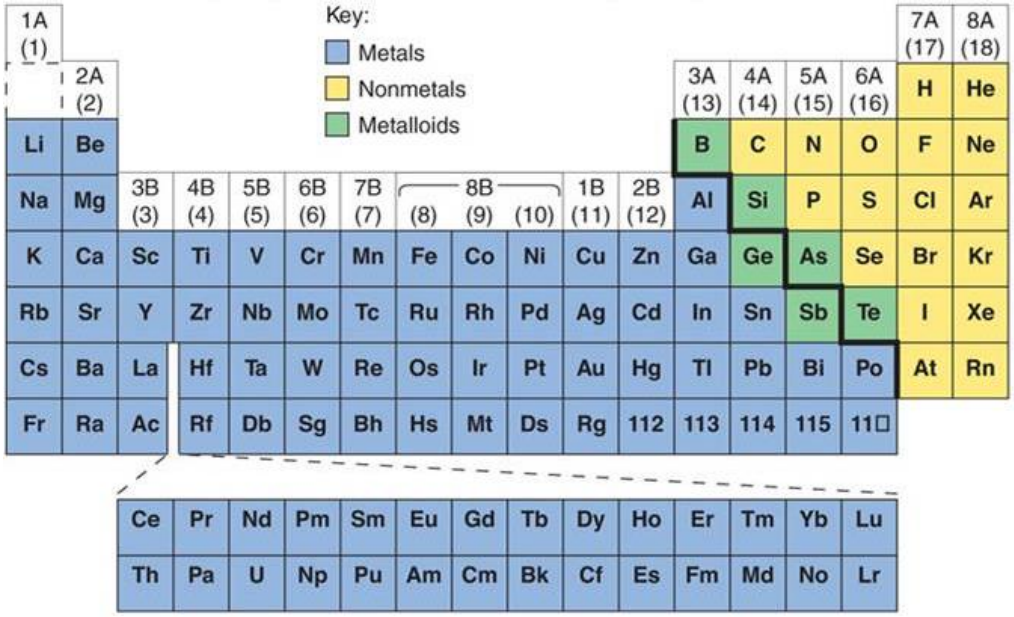
Atomic form factor $$f = -\frac{1}{e}\int \rho_e(\vec{\xi}) \exp\left[-i\Delta\vec{k}\vec{\xi}\right] d^3\xi$$

Crystalography

Atomic form factor (*czynnik atomowy*)



For small angles of scattering
$ef = Q$ (total charge)



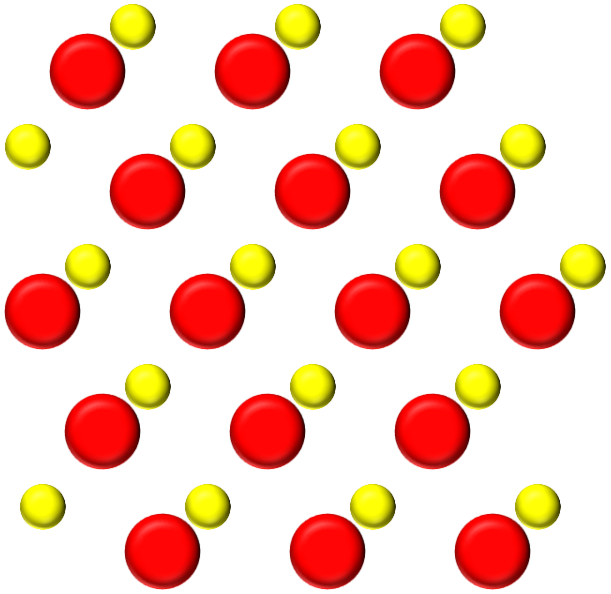
$$f = -\frac{1}{e}\int \rho_e(\vec{\xi}) \exp[-i\Delta\vec{k}\vec{\xi}]\, d^3\xi$$

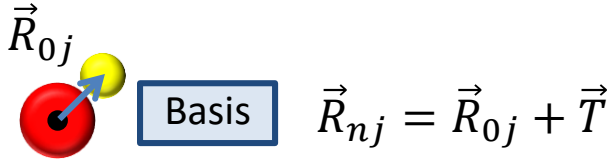
Crystalography

Wave scattered on one of the atoms (j)

$$\Psi = A\, e^{i(\vec{k}'\vec{r}-\omega t)} f_j$$

Wave scattered on all atoms (in direction $\vec{k}'$):





Crystalography

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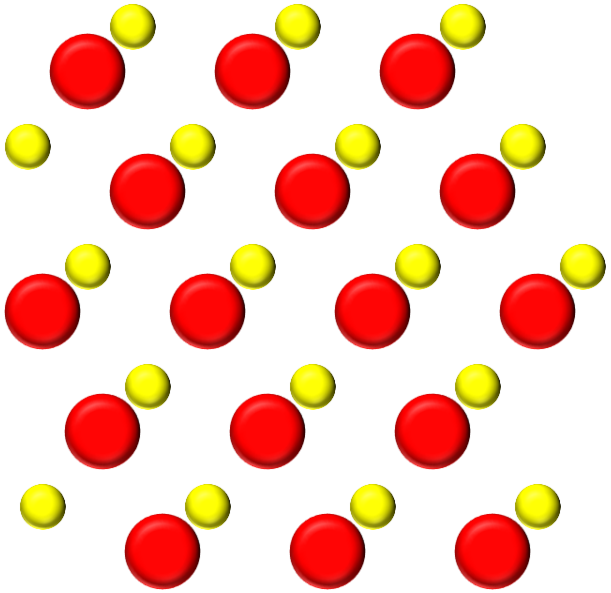
Wave scattered on all atoms:

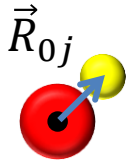
$$\Psi = A \sum_n \sum_j e^{i(\vec{k}'\vec{r}-\omega t)} f_j e^{-i\Delta\vec{k}\vec{R}_{nj}}$$

$\Delta\vec{k} = (\vec{k}' - \vec{k})$

Atoms in basis

Period of the lattice





Basis

$$\vec{R}_{nj} = \vec{R}_{0j} + \vec{T}$$

Crystalography

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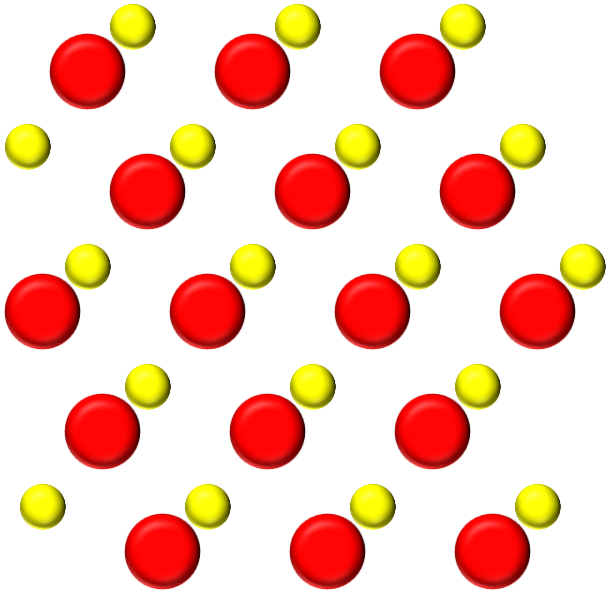

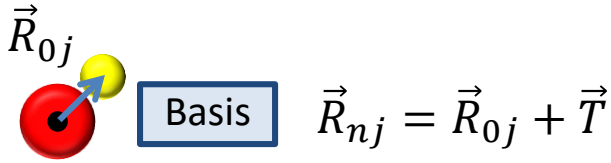

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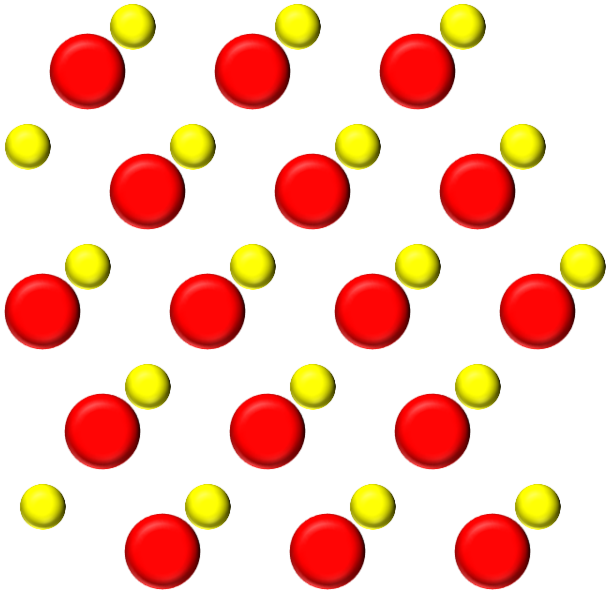
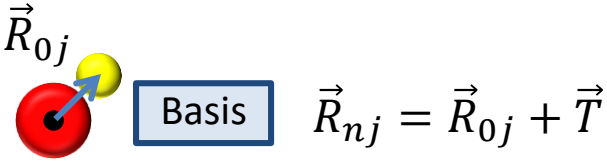
Atoms in basis

Period of the lattice





Crystalography

Wave scattered on one of the atoms (j)

$$\Psi = A\, e^{i(\vec{k}'\vec{r}-\omega t)} f_j$$

Wave scattered on all atoms:

$$\Delta\vec{k} = (\vec{k}' - \vec{k})$$

$$\Psi = A \sum_n \sum_j e^{i(\vec{k}'\vec{r}-\omega t)} f_j\, e^{-i\Delta\vec{k}(\vec{R}_{0j}+\vec{T})}$$

Atoms in basis

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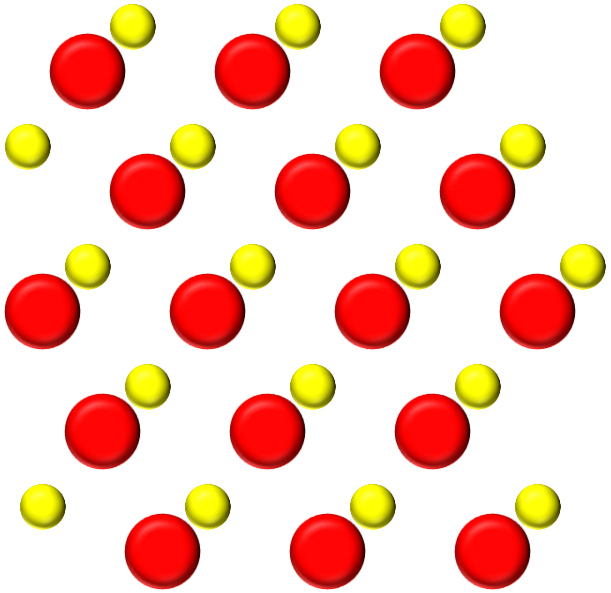

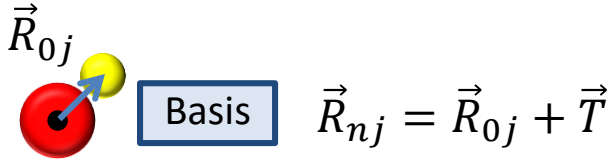

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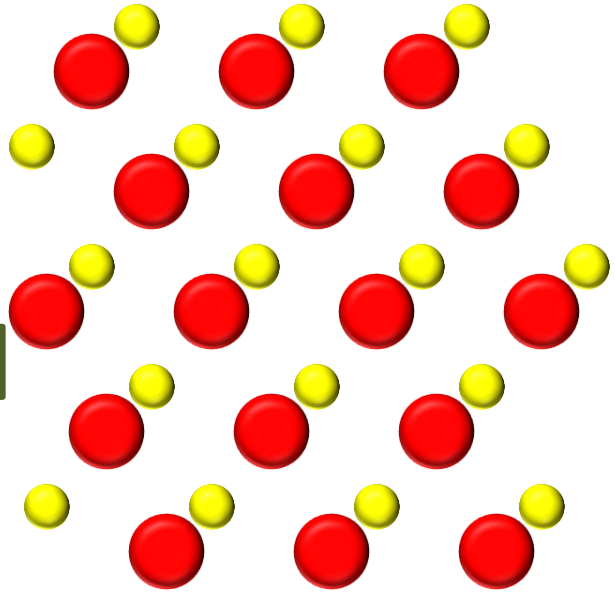

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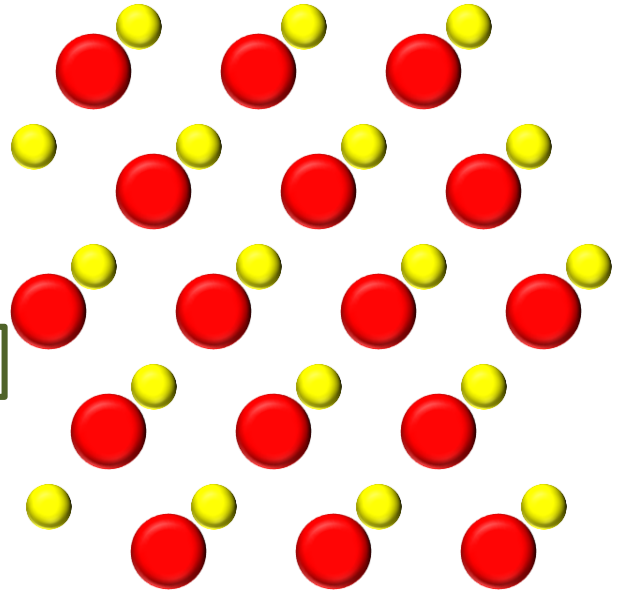

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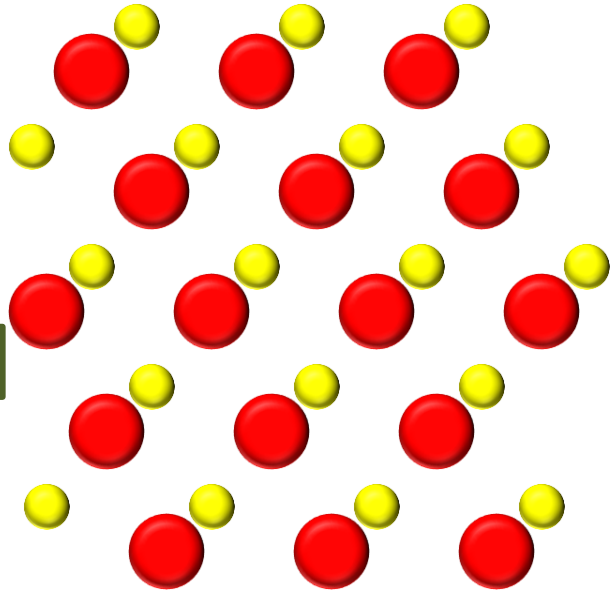

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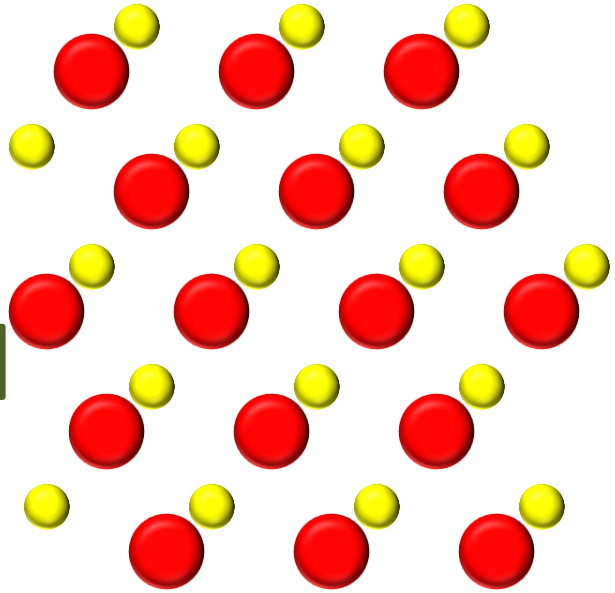
Structure factor S_G

$$S_G = \int_{cell} dV\rho(\vec{R})e^{-i\Delta\vec{k}\vec{R}}$$



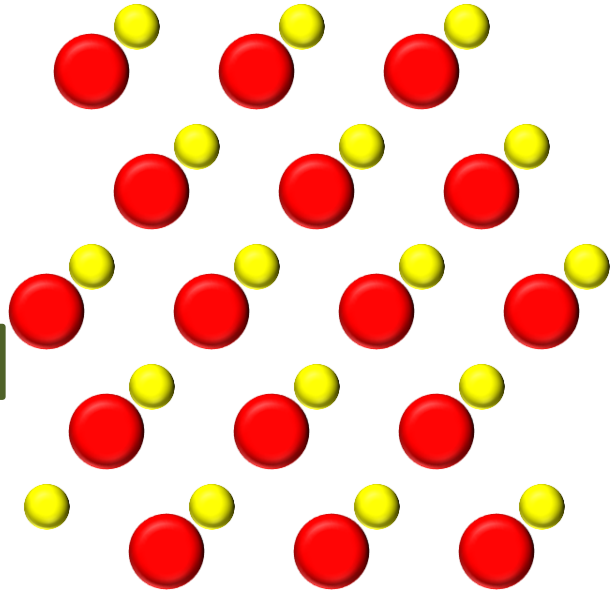
Crystalography

Maximal value of the intensity

$$\left[\sum_{n_1} e^{-i\Delta\vec{k}(n_1\vec{t}_1)}\right]\left[\sum_{n_2} e^{-i\Delta\vec{k}(n_2\vec{t}_2)}\right]\left[\sum_{n_3} e^{-i\Delta\vec{k}(n_3\vec{t}_3)}\right]$$

When?

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



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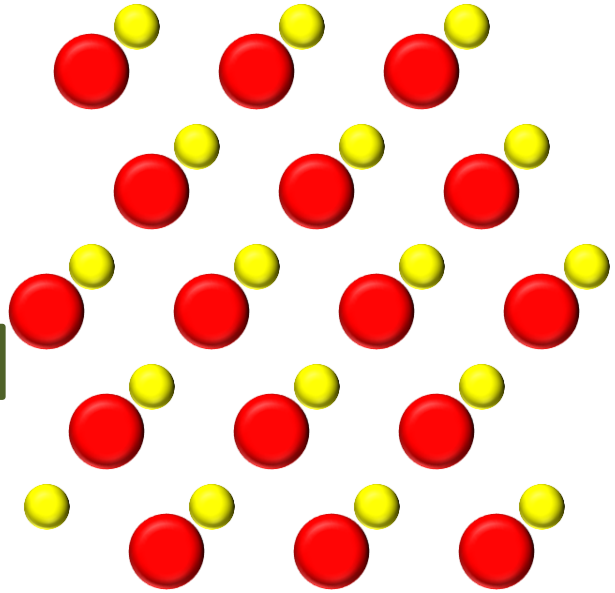
When $e^{-i\Delta\vec{k}(n_1\vec{t}_1)} = 1$

$$\begin{aligned}\Delta\vec{k}\vec{t}_1 &= 2\pi h\\ \Delta\vec{k}\vec{t}_2 &= 2\pi k\\ \Delta\vec{k}\vec{t}_3 &= 2\pi l\end{aligned}$$

Laue conditions

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



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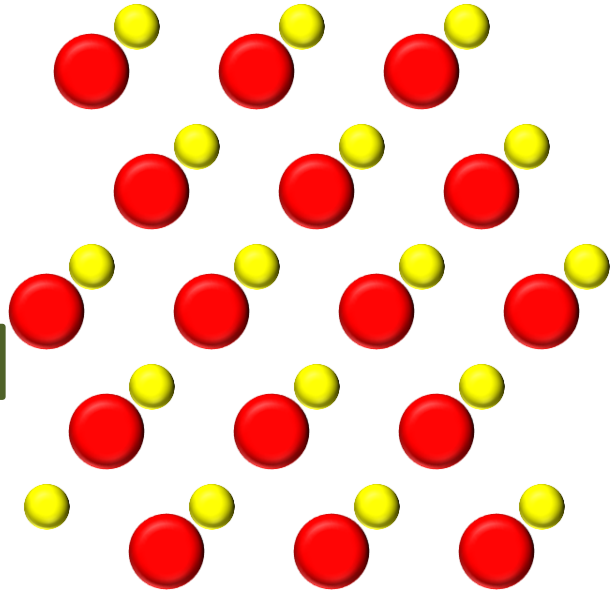

$$\Delta\vec{k} \equiv G = h\vec{g}_1 + k\vec{g}_2 + l\vec{g}_3$$

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

$$|\vec{g}_i| = \frac{2\pi}{a_i} \qquad \vec{g}_i = 2\pi\,\frac{\vec{t}_j \times \vec{t}_k}{\vec{t}_i(\vec{t}_j \times \vec{t}_k)}$$

reciprocal lattice

Structure factor S_G

$$S_G = \int_{cell} dV\rho(\vec{R})e^{-i\vec{G}\vec{R}}$$

Crystalography

$$\Delta\vec{k}\vec{t}_1 = 2\pi h$$
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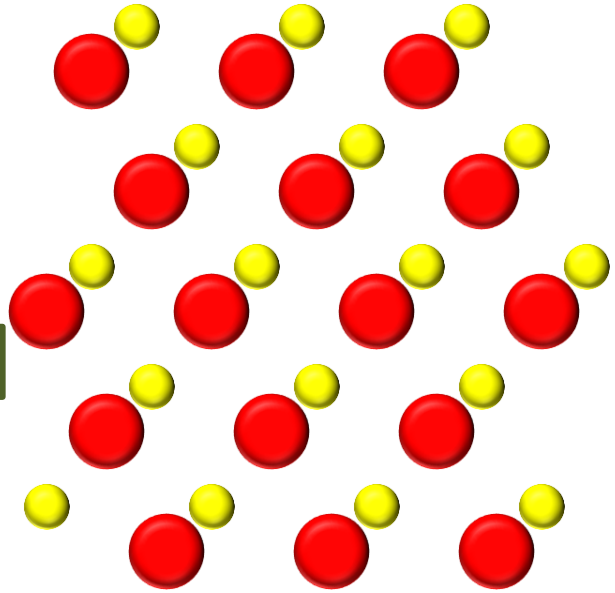


Structure factor S_G

$$S_G = \int_{cell} dV\rho(\vec{R})e^{-i\vec{G}\vec{R}}$$

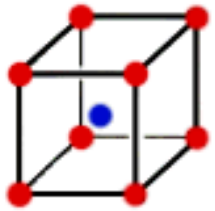
Geometryczny czynnik strukturalny S_G

$$\left[\sum_j f_j\, e^{-i\Delta\vec{k}(\vec{R}_{0j})}\right] = \left[\sum_j f_j\, e^{-i\vec{G}(\vec{R}_{0j})}\right] = \sum_j f_j\, e^{-i2\pi(n_1h+n_2k+n_3l)}$$

Crystalography

Structure factor

$$F(h,k,l) = \sum_j f_j \, e^{-i2\pi(n_1 h + n_2 k + n_3 l)}$$



The crystal of Li and TlBr (bcc lattice - body centered cubic) – find the possible values of the structure factor

$r_1 = (0,0,0)$ $\qquad$ $r_2 = \left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$

$$F_{Li}(h,k,l) = \sum_j f_j \, e^{-i2\pi(n_1 h + n_2 k + n_3 l)} = f_{Li} e^{-i2\pi(0+0+0)} + f_{Li} e^{-i2\pi\left(\frac{1}{2}h + \frac{1}{2}k + \frac{1}{2}l\right)}$$

$$F_{Li}(h,k,l) = f_{Li}\left(1 + e^{-i\pi(h+k+l)}\right)$$

odd

even

$$F_{TlBr}(h,k,l) = \sum_j f_j \, e^{-i2\pi(n_1 h + n_2 k + n_3 l)} = f_{Tl} e^{-i2\pi(0+0+0)} + f_{Br} e^{-i2\pi\left(\frac{1}{2}h + \frac{1}{2}k + \frac{1}{2}l\right)}$$

$$F_{TlBr}(h,k,l) = f_{Tl} + f_{Br} e^{-i\pi(h+k+l)}$$

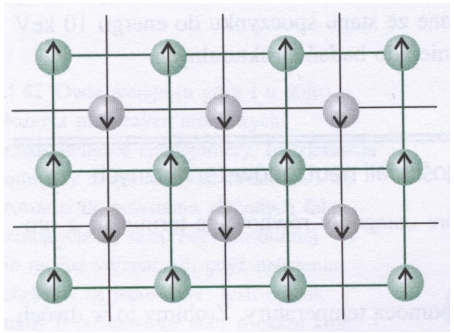
odd

even

Neutrons

Neutrons - generated in the reactor are slowed down by collisions with the moderator (graphite) to v = 4 km/s, which corresponds to the energy E = 0.08 eV and that energy that corresponds to λ = 1 Å

The neutrons interact with: nuclei (one can determine the density of the probability of finding nuclei), determine the phonon dispersion curves, the magnetic moments of nuclei.

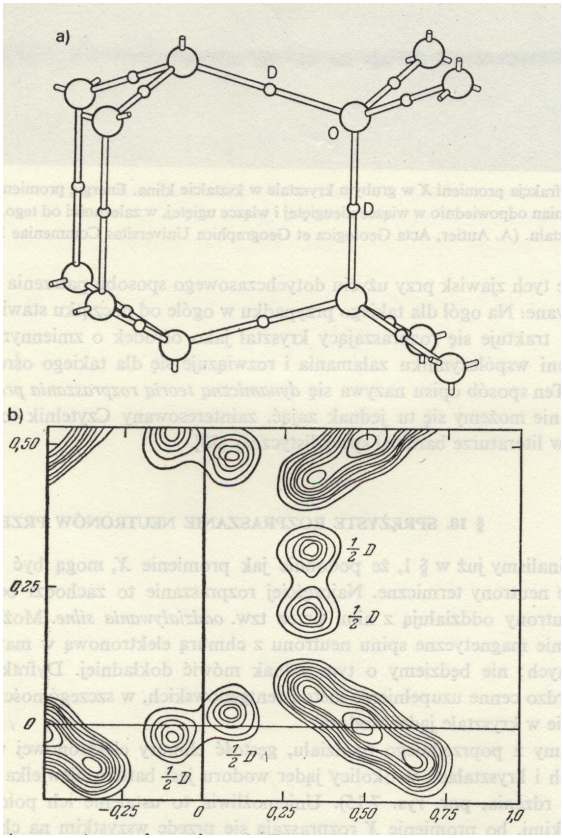


$$E = \frac{\hbar^2}{2M\lambda^2}$$

$M = 1{,}675 \times 10^{-24}\ \mathrm{g}$

$$\lambda(\mathrm{\AA}) = \frac{0{,}28}{\sqrt{E(\mathrm{eV})}}$$

1 Å for E=0,08 eV



J. Ginter

Crystalography

Electrons

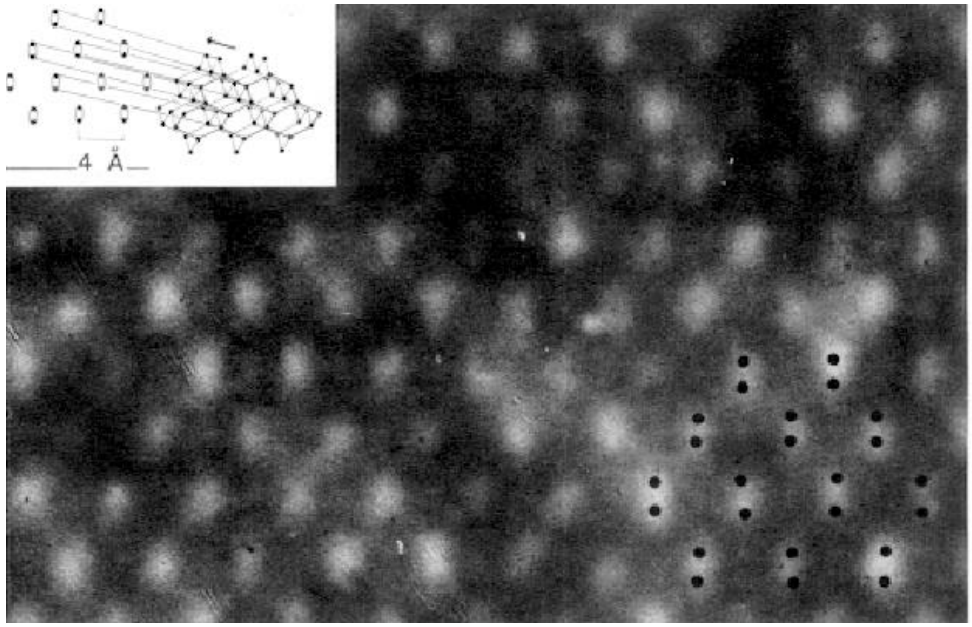
Electrons have an electric charge and interact strongly with matter, penetrate it very shallow.
The phenomenon of diffraction of electrons allows for structural studies of surfaces and very thin layers

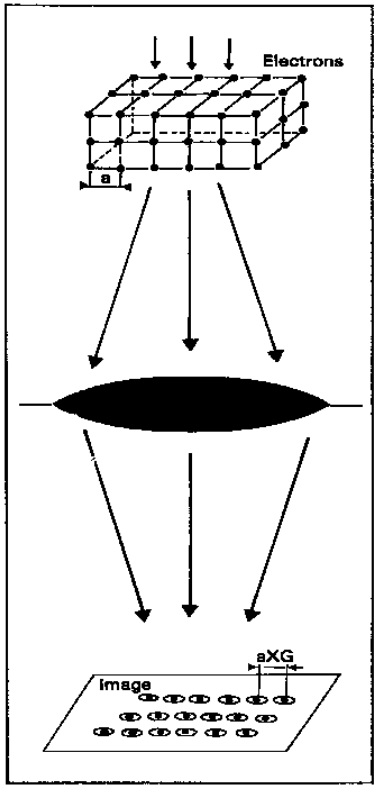
$$E = \frac{\hbar^2}{2M\lambda^2}$$

$M = 0{,}911 \times 10^{-27}\ \mathrm{g}$

$$\lambda(\mathrm{\mathring{A}}) = \frac{12}{\sqrt{E(\mathrm{eV})}}$$

1 Å for E=144 eV

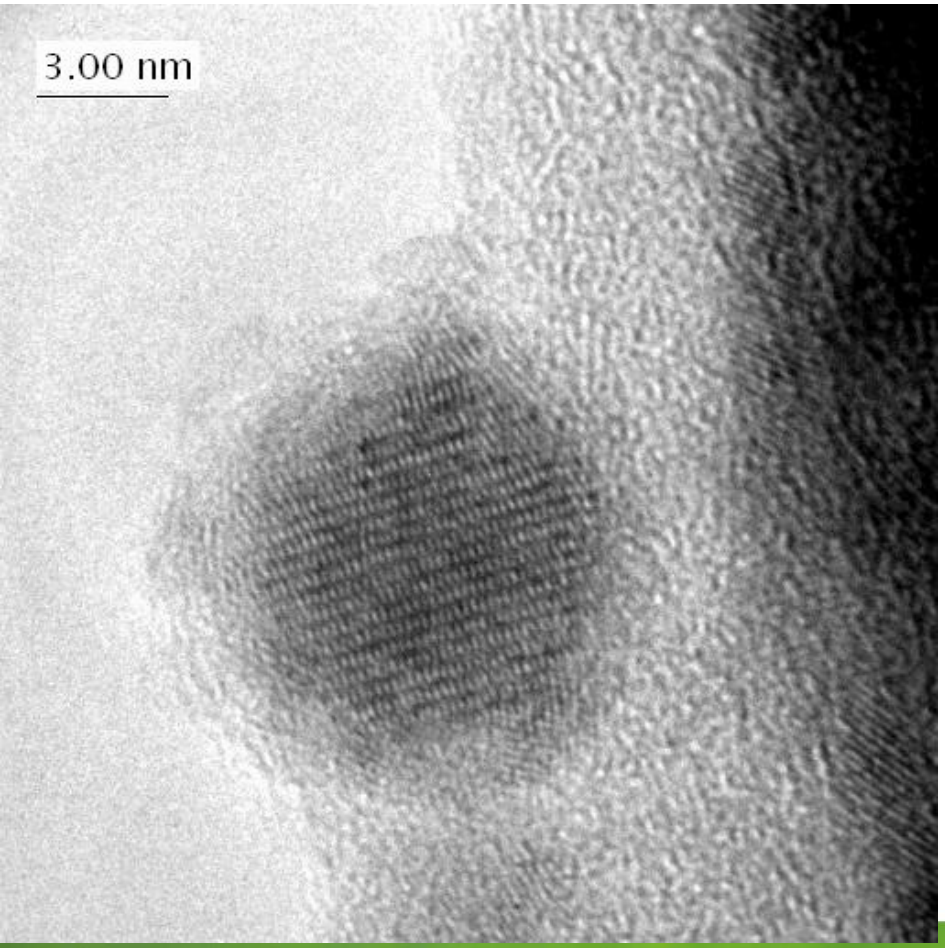


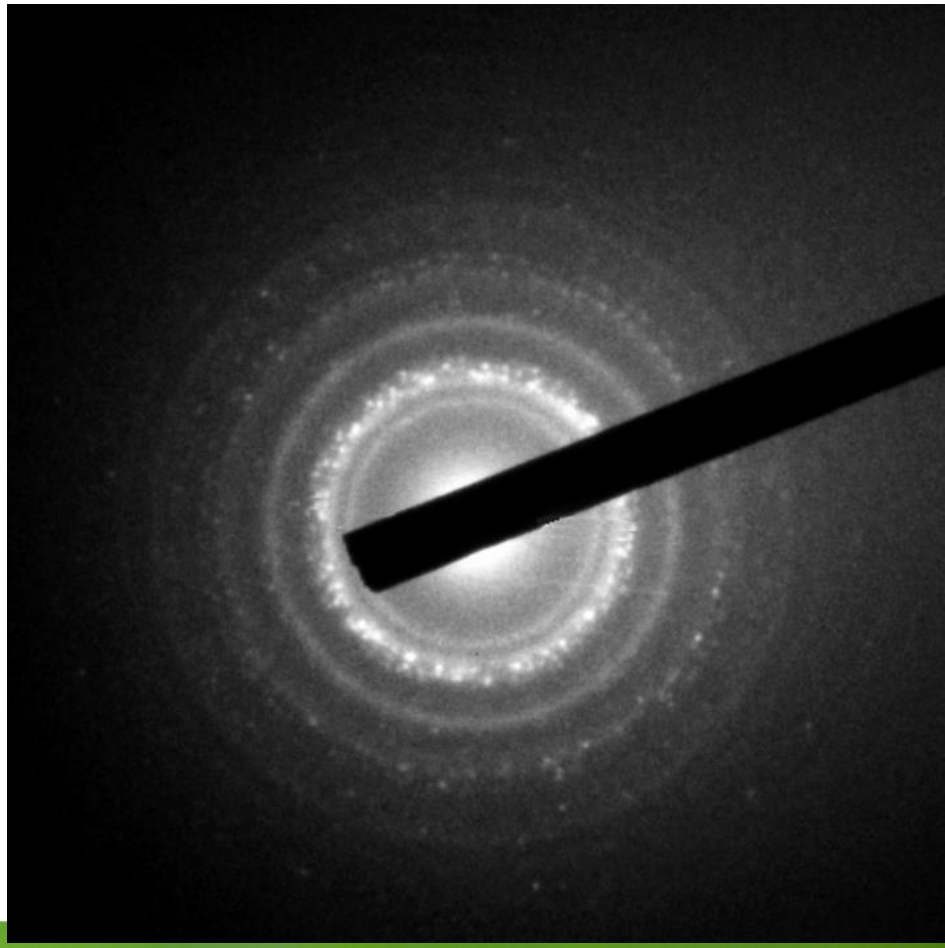


T. Stacewicz & A. Witowski

Crystalography

Electrons





Crystalography

Electrons

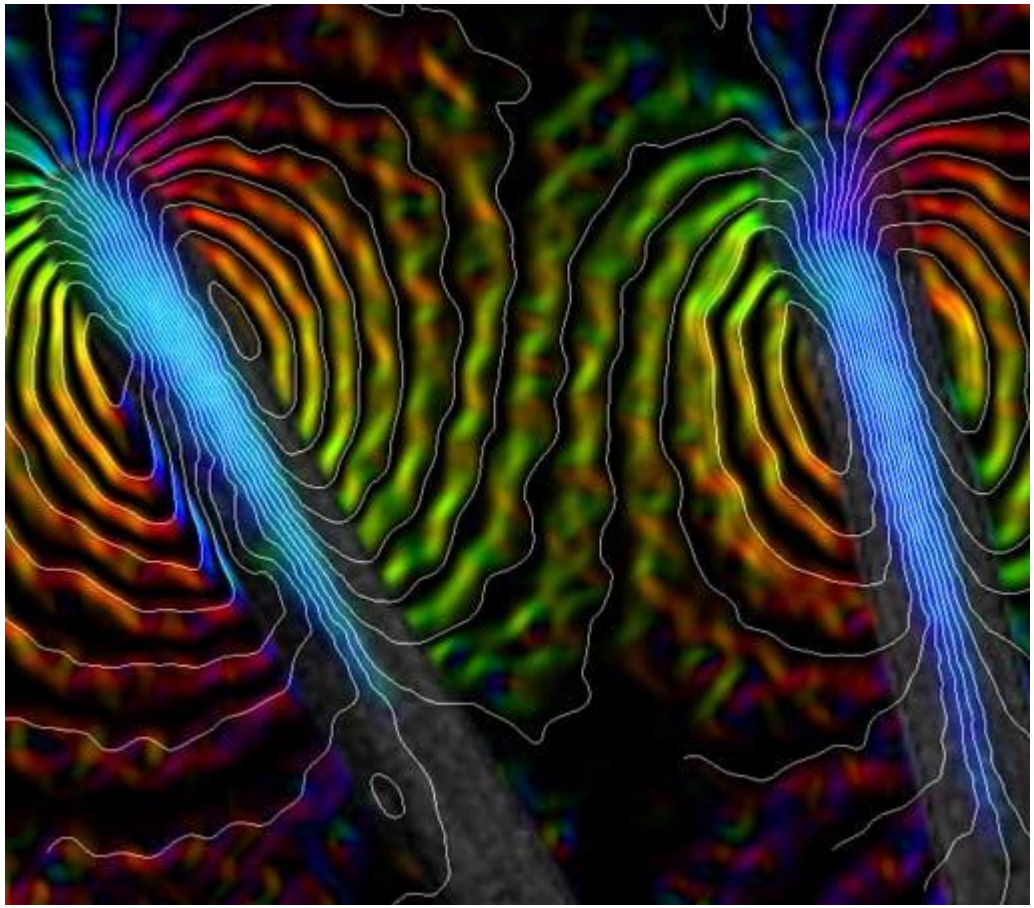
Rafał Dunin-Borkowski

Magnetic domains in a thin cobalt film The colors in the image show the different directions of the magnetic field in a layer of polycrystalline cobalt that has a thickness of only 20 nm. The field of view is approximately 200 microns

http://www.rafaldb.com/pictures-micrographs/index.html

Electrons

Rafał Dunin-Borkowski



Magnetic nanotubes. The nanotubes were fabricated in the University of Cambridge Engineering department by Yasuhiko Hayashi, who grew them using a Cobalt-Palladium catalyst. This alloy remains present in the ends of the nanotubes, and is magnetic. The nanotubes you see here have a 70-100 nm diameter.

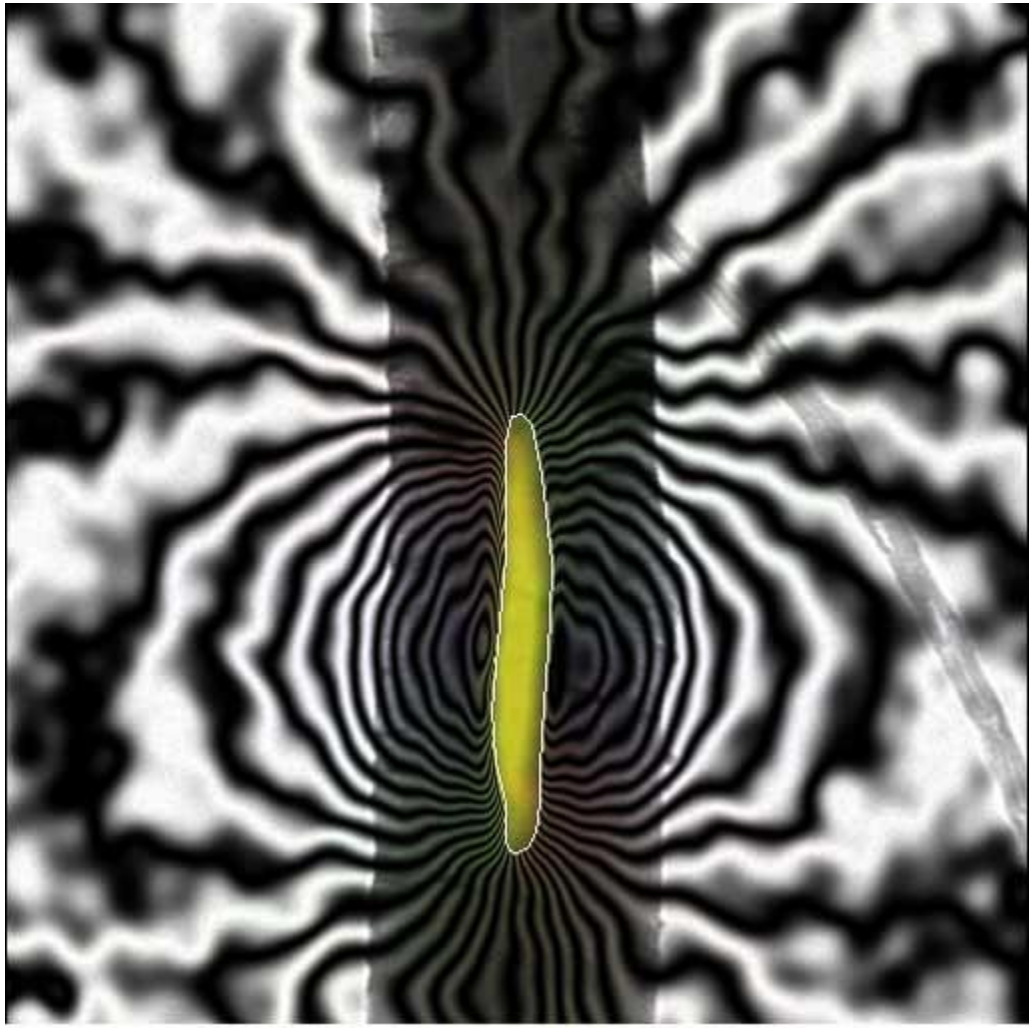
http://www.rafaldb.com/pictures-micrographs/index.html

Crystalography

Electrons

Rafał Dunin-Borkowski

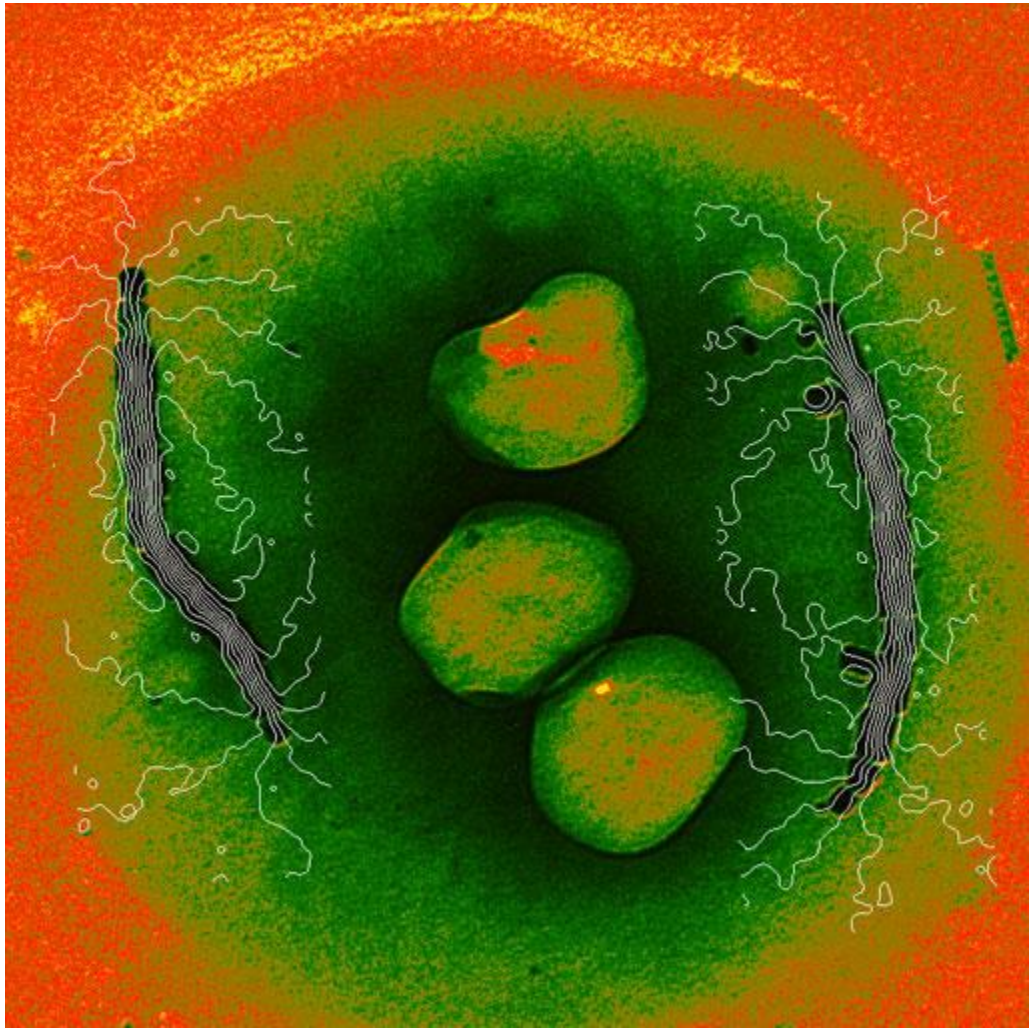
This image won First Prize in the "Science Close-Up" category in the Daily Telegraph Visions of Science competition. The image shows a **multi-walled carbon nanotube**, approximately 190 nm in diameter, containing a 35-nm-diameter **iron crystal** encapsulated inside it. Electron holography has been used to obtain a map of the magnetic field surrounding the iron particle, at a spatial resolution of approximately 5 nm.



http://www.rafaldb.com/pictures-micrographs/index.html

Electrons

Rafał Dunin-Borkowski



The image shows the magnetic field lines in a single **magnetosome chains** in a **bacterial cell**. The fine white lines are the magnetic field lines in the cell, which were measured using off-axis electron holography.

http://www.rafaldb.com/pictures-micrographs/index.html