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ICTP 40th Anniversary

SCHOOL ON SYNCHROTRON RADIATION AND APPLICATIONS
In memory of J.C. Fuggle & L. Fonda

19 April - 21 May 2004

Miramare - Trieste, Italy

1561/30

Introduction to X-ray scattering by single crystals

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X-ray scattering
Introductory talk

Basic crystallography and X-ray diffraction

A-Crystallography

1-Structure of gases, liquids and solids.

2-Structure of single crystals. Motif and mechanisms of repetition.

3-Bravais lattices. Crystallographic points, directions and planes. Unit cells. Miller indexes.

4-Reciprocal lattices. Definition and properties.

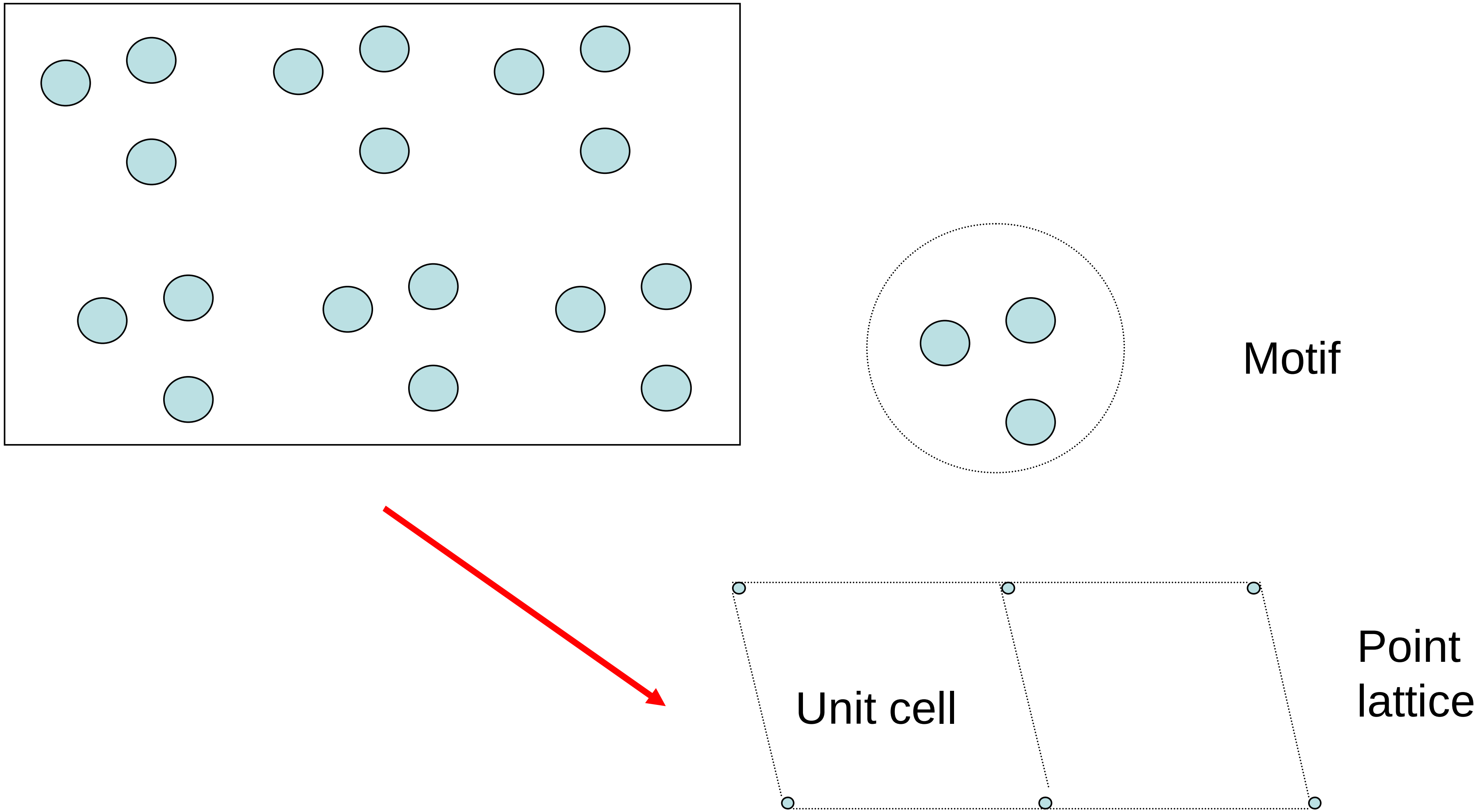
5-Crystal symmetries. Point groups and space groups.

B-X-ray diffraction by single crystals.

- 1-X-rays. Classical and synchrotron sources and setups.
- 2-X-ray diffraction amplitude produced (i) by an electron (Thompson scattering, (Ae), (ii) by an atom (atomic factor, f(s)), (iii) by an unit cell (structure factor, Fhkl), and (iv) by a crystal (Fourier transform).
- 3-General relationship between the scattering amplitude (defined in the reciprocal space) and the electron density (defined in the direct space). Particular case of single crystals.
- 4-Determination of the direct lattice and unit cell from X-ray scattering experiments. Ewald construction.
- 5-Determination of the atomic position of the atoms inside the unit cell from experiments that only provide the scattering intensity, I(s), instead of the scattering amplitude, A(s): The phase problem.

- 6-X-ray scattering theory, procedures and examples of applications to be presented in next talks along the week: single crystal methods (diffraction by protein crystals), scattering by isotropic materials (polycrystals, amorphous and composite materials), low resolution scattering by nanoheterogeneous materials (SAXS), inelastic scattering and magnetic scattering.

Periodic structures



The structure can be described by a motif generally of a few atoms and a point lattice.

General equations

$$A(\vec{s}) = A_e \int\limits_{Total\ .volume} \rho(\vec{r}) e^{-2\pi i \vec{s}\vec{r}} d\vec{r}$$

$$\rho(\vec{r}) = \frac{1}{A_e} \int A(\vec{s}) e^{2\pi i \vec{s}\vec{r}} d\vec{s}$$

We can see that A(s) and ρ(r) are simply related by a mathematical Fourier transformation.

For a single crystal:

$$f(s) = \frac{A_a}{A_e} = \int\limits_{Atom\ .volume} \rho(\vec{r}) e^{-2\pi i \vec{s}\vec{r}} d\vec{r}$$ (Atomic factor)

$$F_{hkl} = \frac{A_{u.c.}}{A_e} = \sum_{j=1}^{n} [f(s)]_j e^{-2\pi i \vec{r}^{*}_{hkl} \vec{r}_j} = \sum_{j=1}^{n} [f(s)]_j e^{-2\pi i (hx_j + ky_j + lx_j)}$$

(Structure factor)

$$A_{crystal} = A_e . N . F_{hkl}$$ (Scattering amplitude by a crystal)

$$I_{crystal} = A_{crystal} A^{*}_{crystal} = \left| A_{crystal} \right|^2 \qquad \left(I_{crystal} \right)^{1/2} = \left| A_{crystal} \right|$$

but $$\left[A_{crystal} \right]_{hkl} = \left| A_{crystal} \right|_{hkl} e^{2\pi i \varphi_{hkl}}$$

so φ_{hkl} **cannot be determined from scattering experiments !!**

This is the so-called "phase problem".

On the other hand:

$$I(\vec{s}) = V \int_{Total\ .volume} \gamma(\vec{r}) e^{-2\pi i \vec{s}\vec{r}} d\vec{r} \qquad \gamma(\vec{r}) = \frac{1}{A_e} \int I(\vec{s}) e^{2\pi i \vec{s}\vec{r}} d\vec{s}$$

The correlation function is given by: $$\gamma(\vec{r}) = \frac{1}{V} \int \rho(\vec{r}\,') \rho(\vec{r}\,' + \vec{r}) d\vec{r}\,'$$

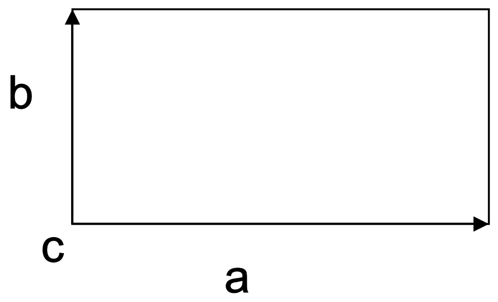
Definition of the reciprocal lattice

$$\vec{a}^* = \frac{\vec{b} x \vec{c}}{V_c}$$

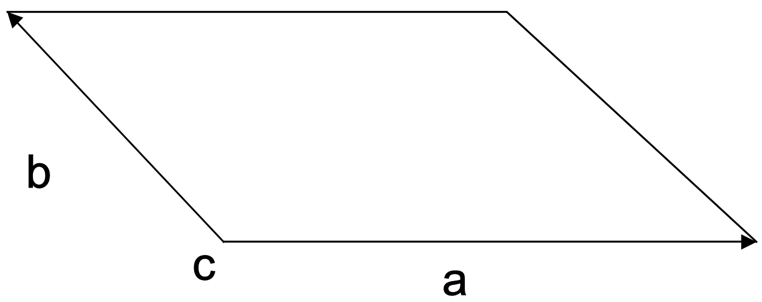
$$\vec{b}^* = \frac{\vec{c} x \vec{a}}{V_c}$$

$$\vec{c}^* = \frac{\vec{a} x \vec{b}}{V_c}$$

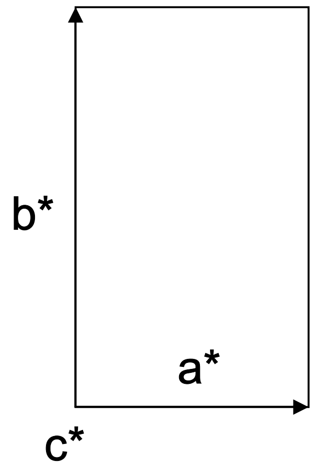
Direct unit cell

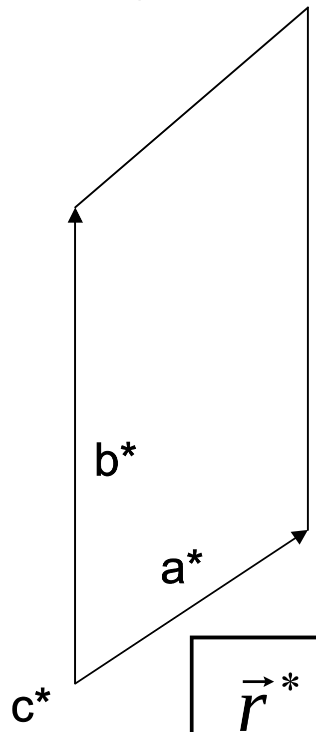


$$\vec{r}_{uvw} = u\vec{a} + v\vec{b} + w\vec{c}$$



Reciprocal unit cell





$$\vec{r}^{\,*}_{hkl} = h\vec{a}^{\,*} + k\vec{b}^{\,*} + l\vec{c}^{\,*}$$

Properties of the reciprocal lattice

i)

$\vec{a}^{\,*}$ **is perpendicular to** $\vec{b}$ **and** $\vec{c}$ ...

so as $\vec{a}.\vec{b}^{\,*} = \vec{a}.\vec{c}^{\,*} = \ldots = 0$

ii)

$$\vec{a}.\vec{a}^{\,*} = \vec{b}.\vec{b}^{\,*} = \vec{c}.\vec{c}^{\,*} = 1$$

iii)

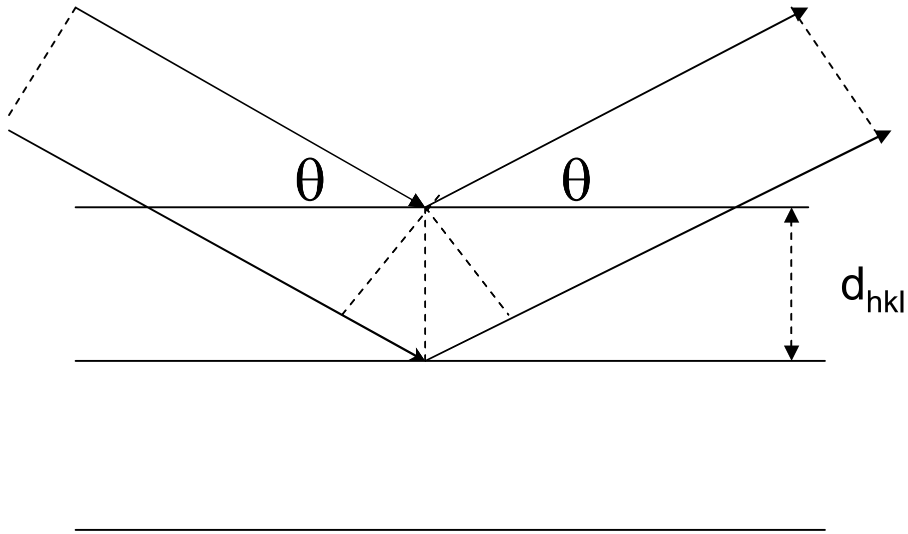
$$\left|\vec{r}^{\,*}_{hkl}\right| = \frac{1}{d_{hkl}}$$

iv) $\vec{r}^{\,*}_{hkl}$ **is perpendicular to the family of planes (hkl)**

Bragg law

Direct space:

$$\boxed{2d_{hkl} \sin\theta_{hkl} = \lambda}$$



Reciprocal space:

$$\vec{s} = \frac{\vec{S}}{\lambda} - \frac{\vec{S}_0}{\lambda}$$

$$\boxed{\vec{s} = \vec{r}^{\,*}_{hkl}}$$