

POWDER X-RAY DIFFRACTION

I – CRISTALLOGRAPHY

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CENTRE NATIONAL
DE LA RECHERCHE
SCIENTIFIQUE

Faculté des Sciences
Fondamentales
et Appliquées



Outline of the course



I – CRISTALLOGRAPHY

II – X-RAY DIFFRACTION

III – POWDER DIFFRACTOMETRY

Outline of the course

1. – POINT LATTICES

1.1. - Crystal space lattice

1.1.1. - Definitions

1.1.2. - Lines and planes

1.1.3. - Set of planes - Miller indices ($h\ k\ l$)

1.2. - Reciprocal lattice

1.2.1. - Diffraction condition

1.2.2. - Properties of the reciprocal lattice

1.3. - Applications of reciprocal lattice

1.3.1. - Miller indices of a set of planes defined by two lines

1.3.2. - Indices $[u\ v\ w]$ of a line defined by two planes

1.3.3. - Angle between two planes (or faces of a crystal)

1.3.4. - Building the reciprocal lattice

1.3.5. - d-spacing determination

1.4. - Axis changes

Outline of the course

2. – CRYSTALLOGRAPHIC GROUPS

2.1. - *Crystal lattices*

2.2. - *14 Bravais lattices*

2.3. - *Space groups*

2.3.1. - 7 one-dimensional space groups

2.3.2. - 17 two-dimensional space groups

2.3.3. - 230 three-dimensional space groups

INTRODUCTION

Cristalline state: defined by a 3-D periodic ordering of atoms

- perfect (no defect)
- infinite

Crystal: limited part of crystalline state

- smooth faces
- regular geometric shapes: set of equal faces (cube, octahedron, prismatic...)
- possibility of cleavage (not possible for amorphous solids)

Geometric model of crystalline state

- infinite point lattices
- 3 non-coplanar vectors: **a**, **b**, **c** (in bold) or $\vec{a}, \vec{b}, \vec{c}$ (with arrows)

1. – POINT LATTICES

1-D → line lattice: **a**

2-D → plane lattice: **a , b**

3-D → space lattice: **a, b, c**

1. – POINT LATTICES

1.1. - Crystal space lattice (or direct space)

1.1.1. - Definitions

- three vectors + origin point
- lattice translations from origin to any point P_i

$$\mathbf{OP}_i = u_i \mathbf{a} + v_i \mathbf{b} + w_i \mathbf{c} \quad \text{or}$$

$$\vec{\mathbf{OP}} = u_i \vec{\mathbf{a}} + v_i \vec{\mathbf{b}} + w_i \vec{\mathbf{c}}$$

- u_i , v_i and w_i are relative integers

Translation vector between two lattice points: $\mathbf{P}_1\mathbf{P}_2$ (see figure)

- $\mathbf{OP}_1 = u_1 \mathbf{a} + v_1 \mathbf{b} + w_1 \mathbf{c}$
- $\mathbf{OP}_2 = u_2 \mathbf{a} + v_2 \mathbf{b} + w_2 \mathbf{c}$
- $\mathbf{P}_1\mathbf{P}_2 = \mathbf{OP}_2 - \mathbf{OP}_1 = (u_2 - u_1) \mathbf{a} + (v_2 - v_1) \mathbf{b} + (w_2 - w_1) \mathbf{c}$

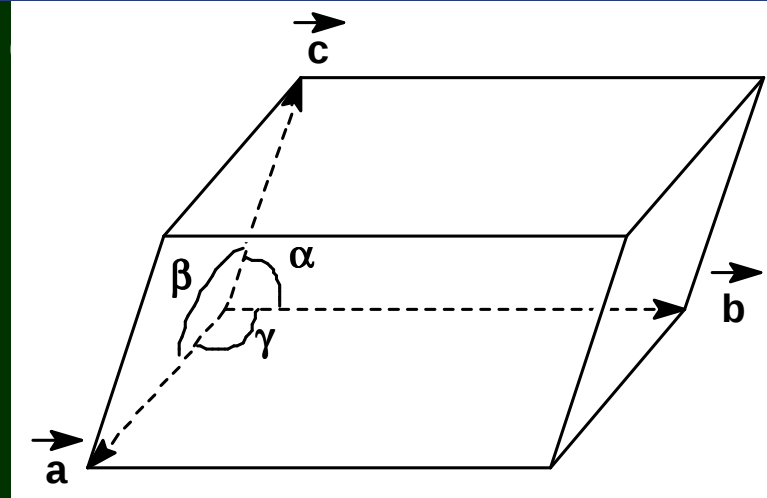
1. – POINT LATTICES

The vectors **a**, **b** and **c** define the **unit cell**

6 cell or lattice parameters :

a b c α β γ

a = $|\mathbf{a}|$ = modulus of **a**



The unit cell must be **right-handed** (like corkscrew)

This corresponds to a **direct rotation**

Different vector products

- scalar product
- cross product

Volume of unit cell:

$$V = (\vec{a} \times \vec{b}) \cdot \vec{c} = (\vec{a}, \vec{b}, \vec{c})$$

$$\vec{OP}_i = u_i \vec{a} + v_i \vec{b} + w_i \vec{c}$$

With any 3 vectors (non-coplanar) we can build a cell:

Exercices

Ex. 1. Determine the multiplicity of the cell based on the following vectors:

$$\text{a) } \vec{a} - \vec{b}, \vec{a}, -\vec{a} + \vec{c} \quad \text{b) } \vec{a}, 4\vec{a} + \vec{b}, 3\vec{a} - \vec{c}$$

Ex. 2. The angle between the perpendicular lines to the two faces $(h \ k \ 0)$ and $(h \ -k \ 0)$ has been determined for a tetragonal (quadratic) crystal. The experimental value is $53^\circ 10'$. What are the values of the indices h and k ?

Ex. 3. Determine the indices of the line going through the points $3 \ 2 \ 1$ et $2 \ -4 \ 0$.

Ex. 4. Is the line $[-2 \ 1 \ 0]$ contained in the plane $(1 \ 2 \ 3)$?

Ex. 5. What are the indices of the plane which contains the lines $[1 \ 1 \ 1]$ and $[3 \ 2 \ 1]$?

Ex. 6. Determine the indices of the line common to the planes $(3 \ 2 \ 1)$ and $(1 \ 2 \ 3)$.

Exercices

Ex. 7. What is the value of the angle between the lines $[1\ 1\ 1]$ and $[1\ 1\ 0]$ for a tetragonal lattice with cell parameters $a = 5.00\text{ \AA}$ and $c = 3.00\text{ \AA}$?

Ex. 8. Determine the value of the angle between the planes $(1\ 1\ 1)$ and $(1\ 1\ 0)$ for a cubic lattice with cell parameter a . Same question for the planes $(1\ 0\ 0)$ et $(1\ 1\ 0)$.

Ex. 9. Can you show that the lines $[-1\ 0\ 1]$, $[-1\ 1\ 0]$ and $[-2\ 1\ 1]$ are lying in the same plane, whatever the lattice? Determine the indices of this plane.

Ex. 10. Determine the indices of the line defines by two planes, the first going through the lattice points $3\ 2\ 1$; $2\ -4\ 0$ and $3\ 3\ -1$, and the second one through the lattice points $-1\ 2\ 1$; $1\ 1\ 1$ and $-2\ 1\ 2$.

Ex. 11. Draw the seven 1-D space groups, using a rectangular triangle as asymmetrical unit.