Computer practical

1. From crystal to diffraction pattern

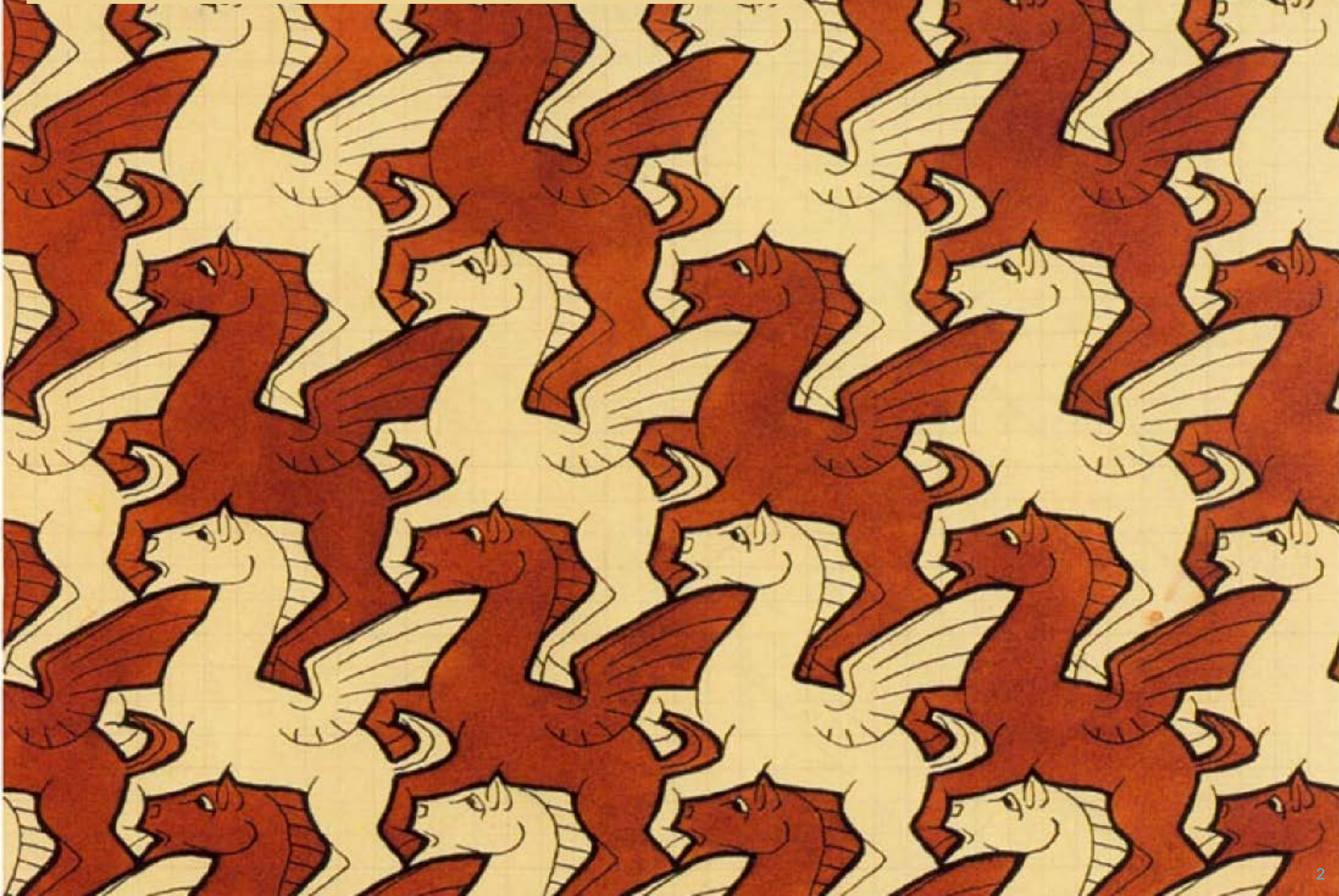Understanding a crystal lattice and how this leads to diffraction of X-rays.

2. Viewing electron density and building an atomic model.

Learn how to use Coot to view and manipulate crystal structure data.
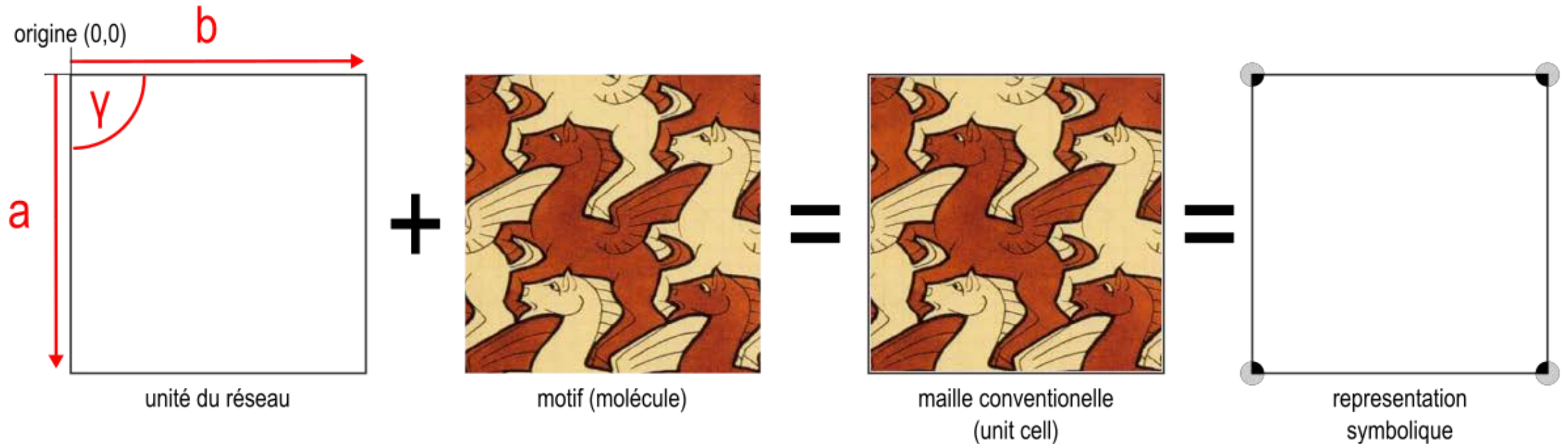
3. Analyzing and rendering crystal structures.

Learn how to use PyMol to dissect and render crystal structures.

2D crystal: The 'Flying Horses" by Maurits Cornelis Escher

The unit cell is the basic repeating unit of the crystal

| unité du réseau | motif (molécule) | maille conventionelle (unit cell) | representation symbolique |

- **The unit cell** comprises of the geometry of the lattice and the motif (building block, molecule, protein) of the crystal.

- The crystal can be reconstituted in its entirety by translational operations of the unit cell.

- The unit cell is defined by **geometric parameters**:

  - Length of the axes (a, b, c)
  - Angle between axes(α, β, γ)
  - Origin of the coordinate system.
  - Internal symmetry of the unit cell.

- The motif is often intersected by the unit cell planes. However, putting together all of its pieces contained in the unit cell will reconstitute the entire molecule.

Le crystal amplifies diffracted waves when they are perfectly in phase

- Each unit cell emits radiation as the X-rays interact with its electrons. Under conditions where the waves overlap in phase with the waves from neighbouring unit cells strong constructive interferences emerges:

$$\Delta\varphi = 2\pi \mathbf{S} \cdot \mathbf{r} = n2\pi$$
$$\mathbf{S} \cdot \mathbf{r} = n$$

- The distance between atoms in neighbouring unit cells is $\mathbf{r} = \mathbf{a} + \mathbf{b} + \mathbf{c}$, and based on these geometric considerations, **Max von Laue**, one of the pioneers in X-ray research formulated the following conditions:

$$\mathbf{S} \cdot \mathbf{a} = h2\pi$$
$$\mathbf{S} \cdot \mathbf{b} = k2\pi$$
$$\mathbf{S} \cdot \mathbf{c} = l2\pi$$

The conditions postulate that diffraction from a crystal will produce very strong reflexions, which are distributed on a regular lattice in 3D with indices hkl.
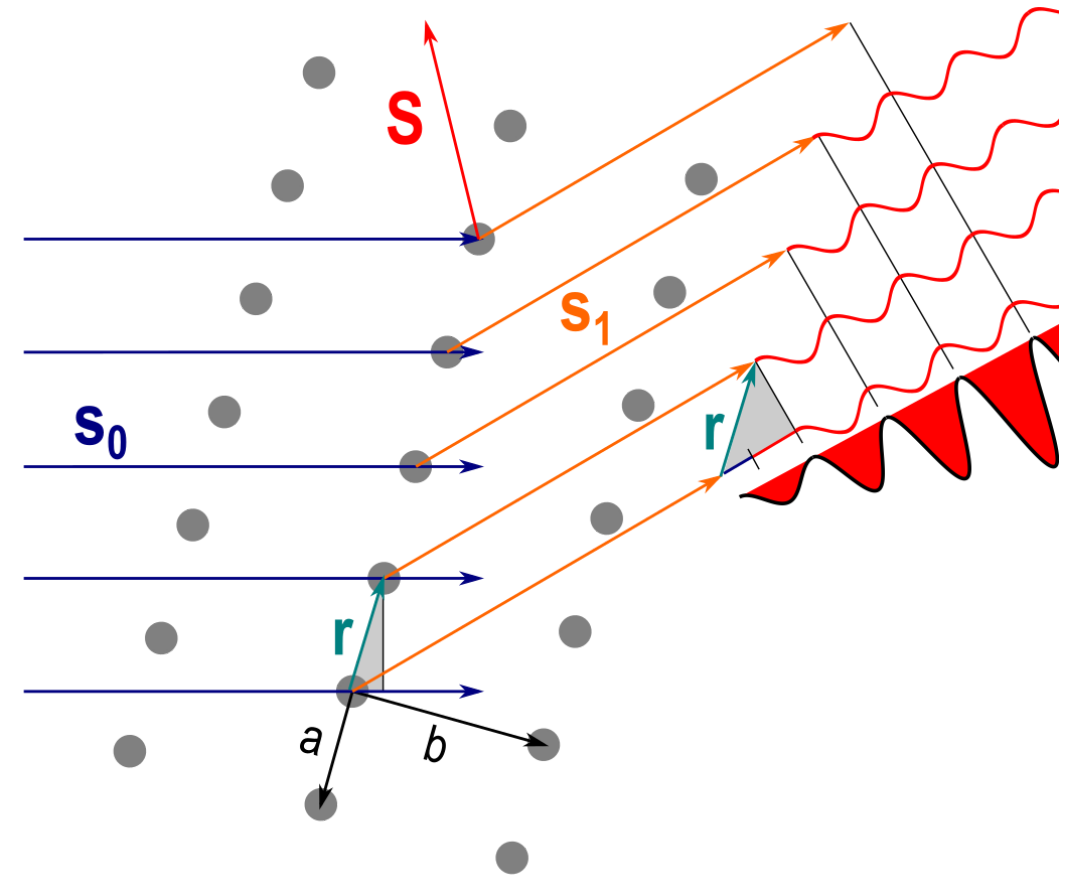
Bragg's law relates the crystal planes with the reciprocal lattice

- **Sir William Bragg** had the idea to treat diffraction as reflection from crystal planes.

- To calculate the path difference Δc between incoming and reflected wave on a plane we can use **trigonometric analysis of the triangle ABC**:

$$\overline{BC} = d \sin \theta$$

- The total path difference is:

$$\Delta c = 2\overline{BC} = 2d \sin \theta$$

- **Bragg's law** postulates that constructive interference is only produced when Δc corresponds to an integral multiple of the radiation wavelength.

$$\Delta c = n\lambda = 2d \sin \theta$$

$$d^* = \frac{1}{d} = \frac{2 \sin \theta}{n\lambda}$$

- The distance between the planes d corresponds to **dimension of the resolved detail** by this family of planes. Bragg's law shows that d has an inverse relationship with θ, which means that **high-resolution reflexes are diffracted further away from the beam than low resolution reflexes!**

le vecteur de diffusion
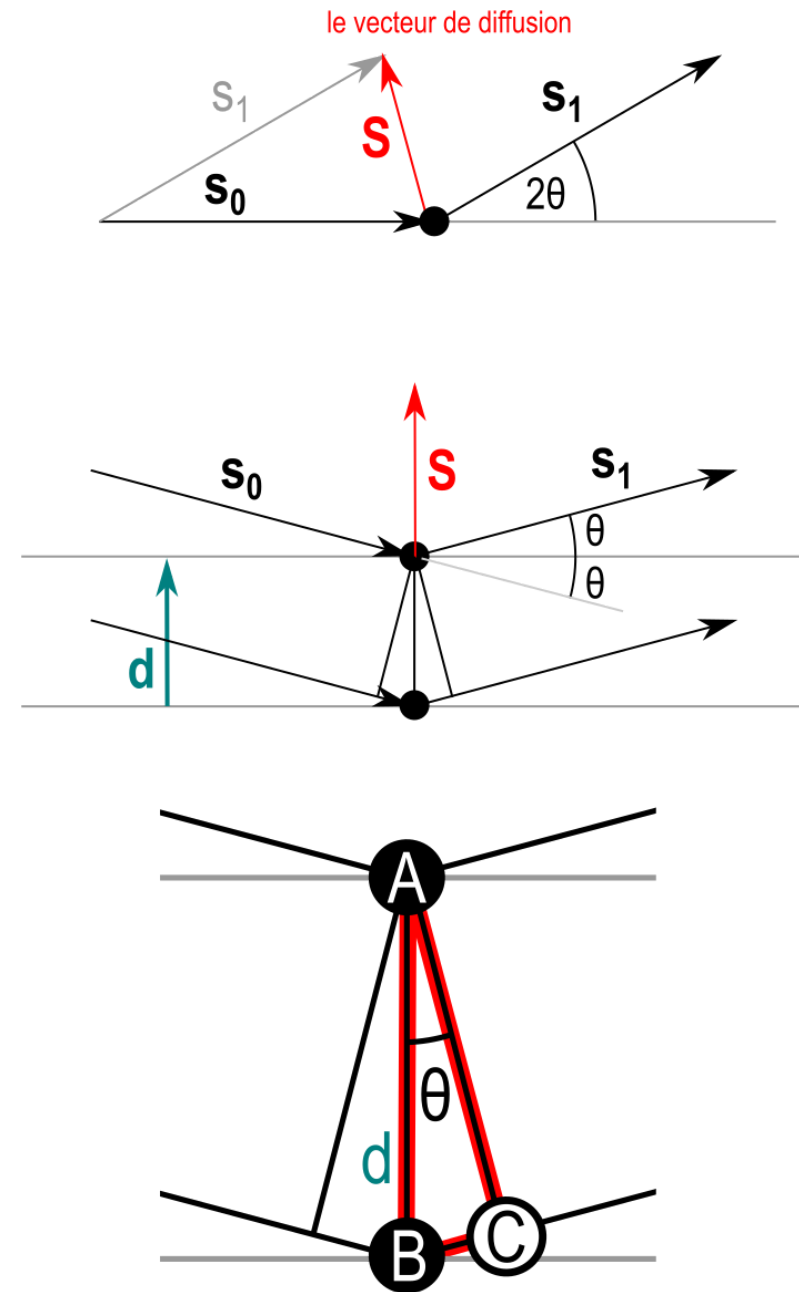
Lysozyme diffraction pattern reveals lattice parameters and symmetry
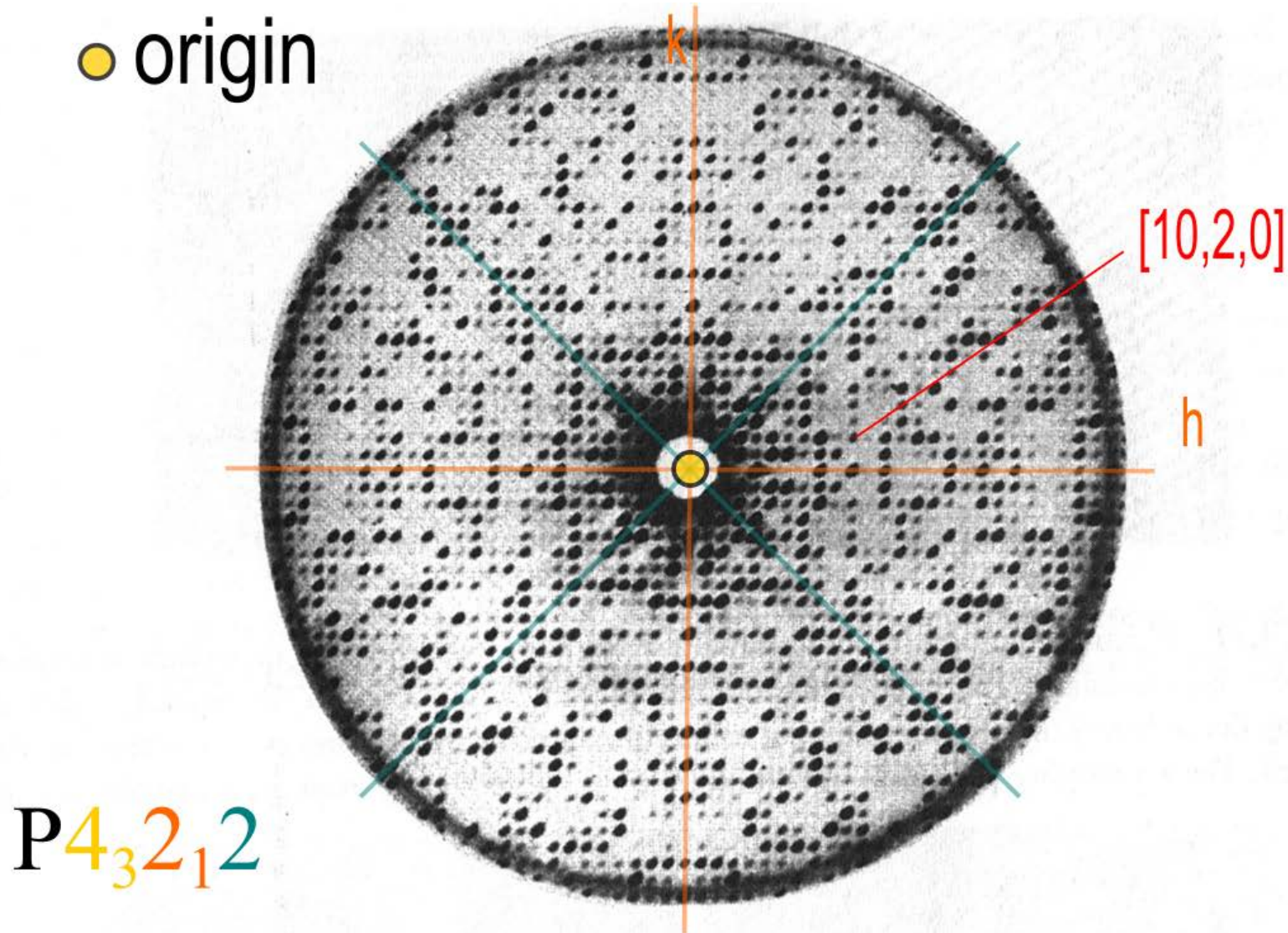
FIGURE 1.13 The *hk*0 zone diffraction image from a tetragonal crystal of lysozyme, an enzyme from hen egg white. Here, the fourfold symmetry of the pattern is striking, and it reflects the fourfold symmetry of the arrangement of the protein molecules in the unit cells of the crystal. Again, the intensities fall on a very regular, periodic net, or reciprocal lattice. The net is based on a tetragonal axis system (see Chapter 3).

Simulating X-ray diffraction from a crystal with DiffractOgram

Use DiffractOgram from IPHYS at EPFL in Lausanne, Switzerland [1]

- Slide Omega, Chi and Phi. What are those angles? What happens on the right side screen?

- In Animation, tick box and enter 0-5° for the rotation range. Clear screen and press on Phi. What happens?

- Set Lambda to 1 (should be Å, not °). What is Lambda and what happens?

- Press "More" in the Lattice box until you have an 8x8 lattice and change unit cell dimensions to 10 Å for a, b and c. Clear Screen and press Phi. What do you observe? [2]

- [1] https://www.epfl.ch/schools/sb/research/iphys/teaching/crystallography/diffractogram
- [2] https://www.youtube.com/watch?v=DFFU39A3fPY

Load and fix a crystal structure with Coot

based on "Problems in crystal structures" from G. Vriend, CMBI [3].

- Use "Fetch PDB&MAP using PDB-REDO" to load pdb structure 1LEE. What are we looking at here?

- Navigate to Lys238. What do you observe there?

- How would you fix the structure? Give it a try.

Analyze and render a crystal structure with PyMol

- Use "Get PDB" to load the pdb structure 1LEE or "Open..." to load the corrected version that you saved.

- Separate protein from ligands by using create command:

```
PyMOL> create plasmepsin, c. A and not r. HOH and not r. R36
PyMOL> create R36, r. R36
PyMOL> create SO4, r. SO4
```

- Show surface for protein.

- Change colors for R36 ligand and protein.

- Render structure using "Ray".

- Select R/K 238

```
PyMOL> select R238, i. 238
```