IUCr-UNESCO Bruker OpenLab Albania

Lectures by Gervais Chapuis, EPFL, Lausanne, Switzerland

1. **Symmetry in crystallography. Point groups and space groups. Introduction to Vol. A of the International Tables for Crystallography (2h course, 2h exercises)**

   In crystallography, the concept of symmetry is fundamental to understand crystalline forms, crystal architectures and all physical properties arising from them. We shall first introduce the notion of translation as well as the symmetry properties that result. The concept of group is introduced along with point and space groups. Finally, we show how the concepts of symmetry can be used to solve the crystal structures using the International Tables of Crystallography

2. **Introduction to the phenomenon of diffraction. Fourier transform. Structure factor. Direct and reciprocal space. Diffraction conditions. (2h course, 2h exercises)**

   The phenomenon of diffraction is fundamental in the study of crystal structures. Thanks to this property, practically any crystal structure whether periodical or not can be solved. The laws of the Fourier transform allow to understand the phenomenon of diffraction and to study its consequences. The reciprocal lattice concept will be introduced for a better understanding and interpretation of diffraction phenomena and their properties.

3. **Methods to solve crystal structures. Patterson function, direct methods, Charge flipping and other iterative methods based on alternating direct space and reciprocal space. (2h course)**

   The evolution and development of diffraction methods are closely linked to our ability to interpret the diffraction measurements. Since its discovery a century ago, many structure solving methods have been proposed but only a limited number are now in use. In this course, we will present the theoretical justifications and the limitations of using each method.

4. **Structure completions and methods of refining crystal structures (1h course)**

   The methods of solving crystal structures often give a partial picture of the overall structure. Since the X-ray diffraction power is proportional to the atomic number of each atom, the light atoms, that is to say those having a small atomic number, might not be detected by some solution methods. In a first step, it is necessary to identify the full set of atoms in a structure and ultimately optimize the atomic parameters so that the resulting model fit best to the measured intensities. This is called the structure refinement.

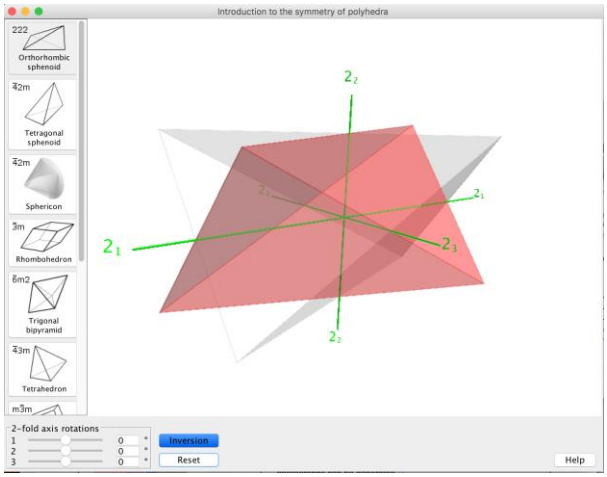
5. **Anisotropic tensor properties of atomic displacements. (1h course)**

   In addition to the atomic positions, the refinement of a crystal structure is also able to characterize the displacements of each atom, either thermally induced or caused by other effects such as impurities, defects, etc. These displacements can be isotropic or even anisotropic. We will give the theoretical basis justifying the model of anisotropic displacements and give an interpretation of the atomic or molecular mechanisms that can be associated with them.

Most of the lectures will be illustrated in practical sessions by solving exercises with the aid of dedicated applets, i.e. small applications, which can be freely downloaded from Internet for a better understanding of numerous crystallographic aspects. In particular we shall use the applets listed below.

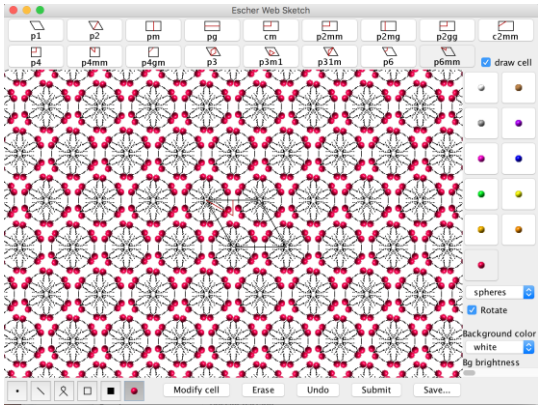
Sufficient time will be given to the students in order to clarify some basic crystallographic concepts, solve exercises and ask questions.

Symmetry



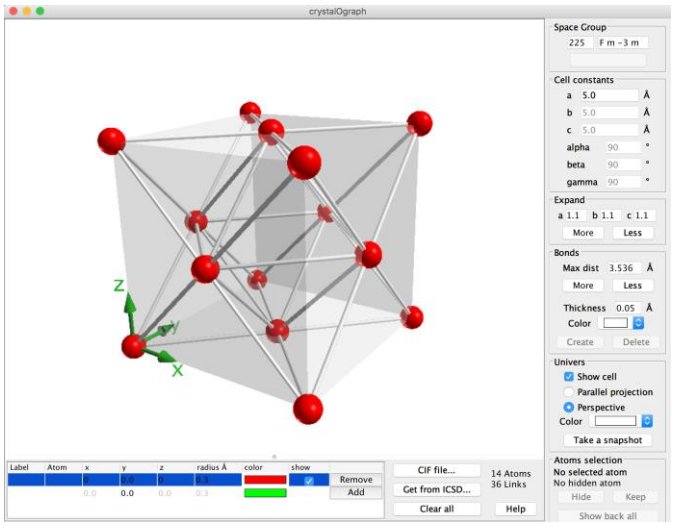
Initiation to the discovery of point symmetry groups

An applet to explore the point group symmetry of polyhedra including platonic ones. In particular, rotations, inversion and combinations of them can be simulated.



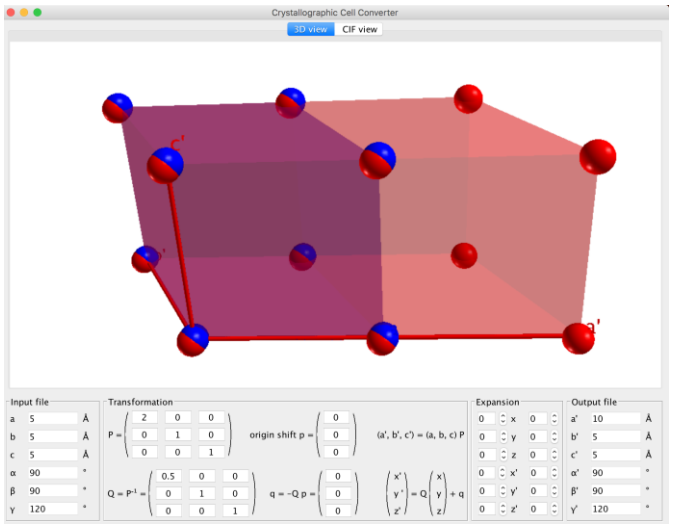
Escher Web Sketch 2

An applet to simulate any periodic pattern corresponding to one of the 17 possible two-dimensional symmetry groups (17 planar groups).



crystalOgraph

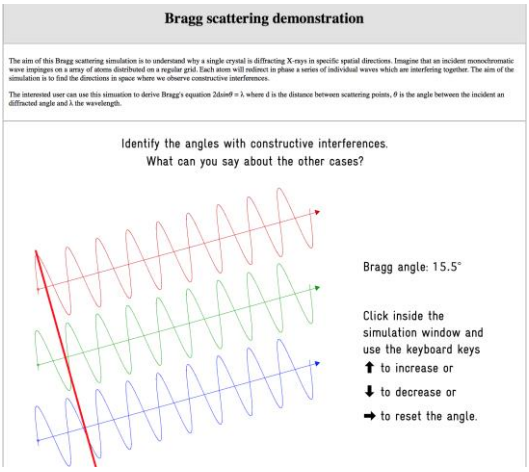
An applet to represent any type of crystalline structure given the lattice parameters, the space group and the atomic coordinates of symmetry independent atoms. It is also possible to import directly a structure from the ICSD database or from a CIF file.



cellConverter

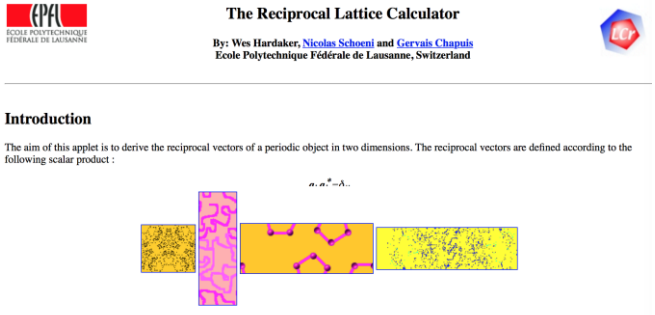
An applet to transform any unit cell ant its content to another cell. Based on the original CIF file, the applet generates a new CIF file resulting from the transformation specified by the user.

Diffraction



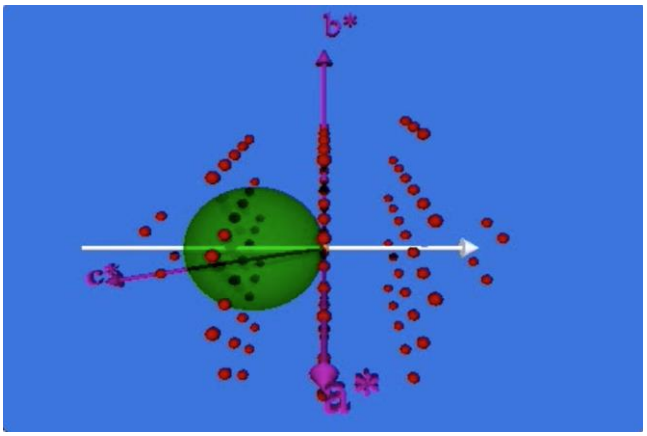
Bragg scattering

A Flash animation to illustrate constructive or destructive interferences as expressed by Bragg's law



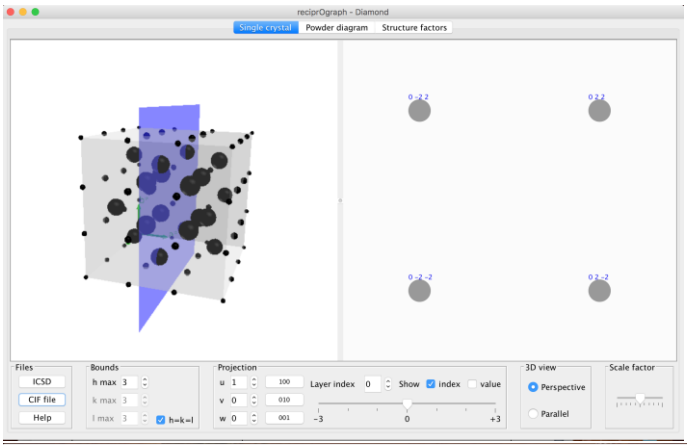
Reciprocal lattice generator

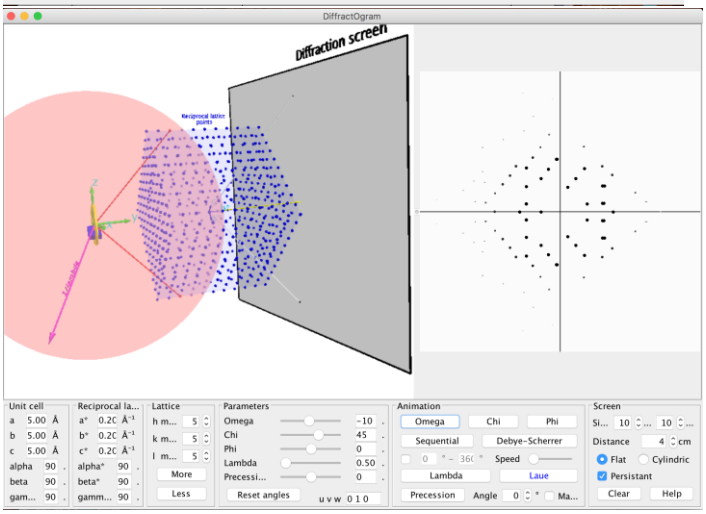
From a periodic diagram generated by Escher Web Sketch, the user is guided step by step by the applet in order to create the reciprocal lattice corresponding to the periodicity of the initial periodic pattern.



Ewald sphere animation

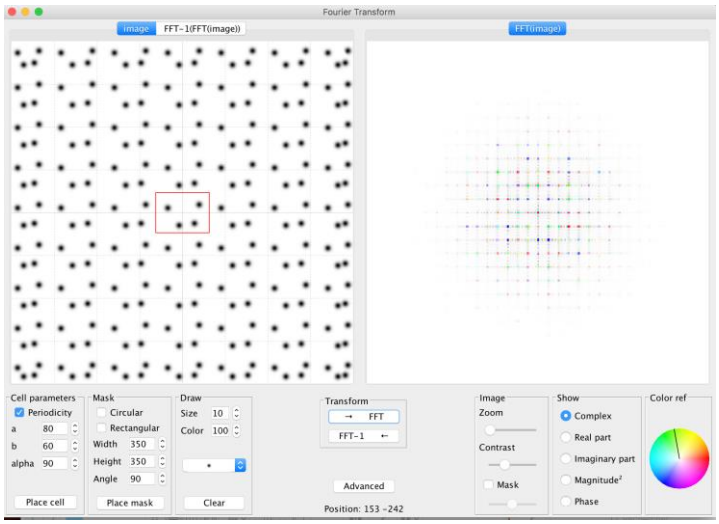
Video sequence illustrating the diffraction phenomenon based on the Ewald sphere





diffractOgram

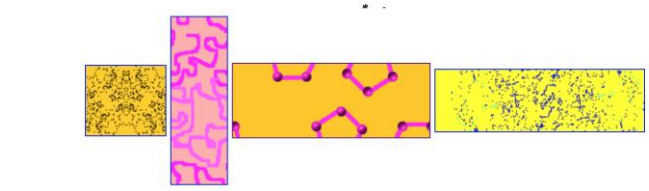
An applet to simulate any type of diffraction pattern based on the Ewald sphere and the reciprocal lattice. In particular, Laue patterns, Debye Scherrer diagrams, rotating crystals and even precession photographs can be generated.



Diffraction and Fourier Transform

An applet to calculate the Fourier transform of a density function ρ(**x**) yielding the complex magnitude G(**S**). The density function can be either periodic or non-periodic.

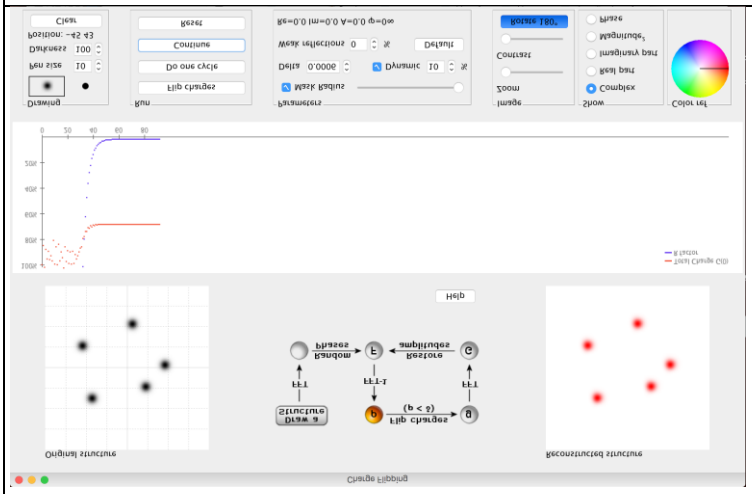
The applet is also able to calculate the inverse Fourier transform of G(**S**). Numerous tools can be applied in order to understand the role of amplitudes and phases, which are of particular importance in diffraction phenomena.



reciprOgraph

An applet to simulate the X-ray diffraction intensities for single crystal in reciprocal space and powder diffraction patterns. Structures can be selected from from CIF files.

Structure resolution



Charge flipping

An applet to solve the phase problem in diffraction by the charge flipping algorithm. The user can create a 2D crystalline structure and follow the evolution of the algorithm in solving the structure.