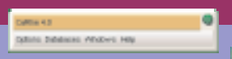
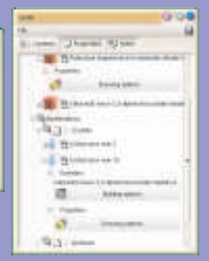
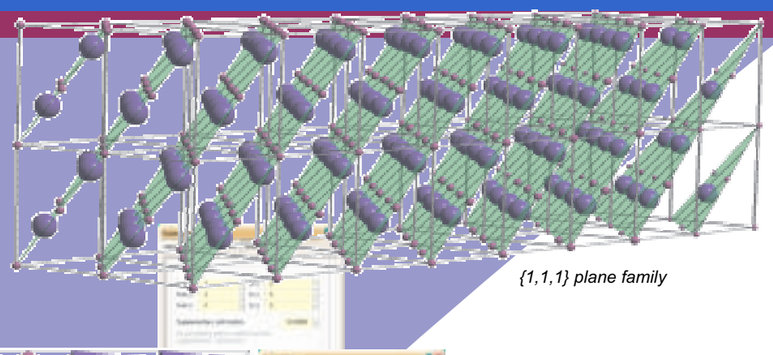
CaRIne Crystallography : 1 software, 2 complementary and compatible versions

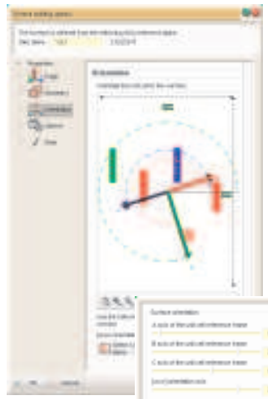


The main window, the project manager and a opened project.
(the whole project is saved by a simple click).

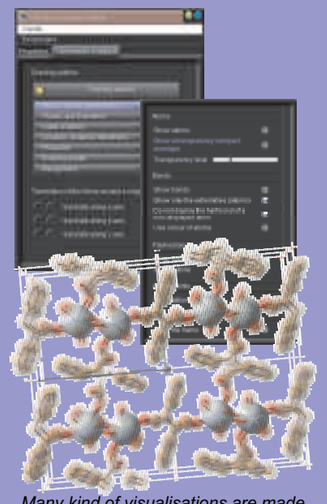




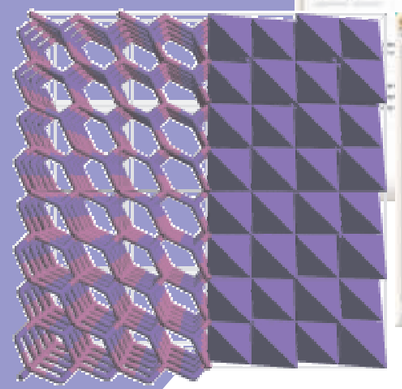
{1,1,1} plane family



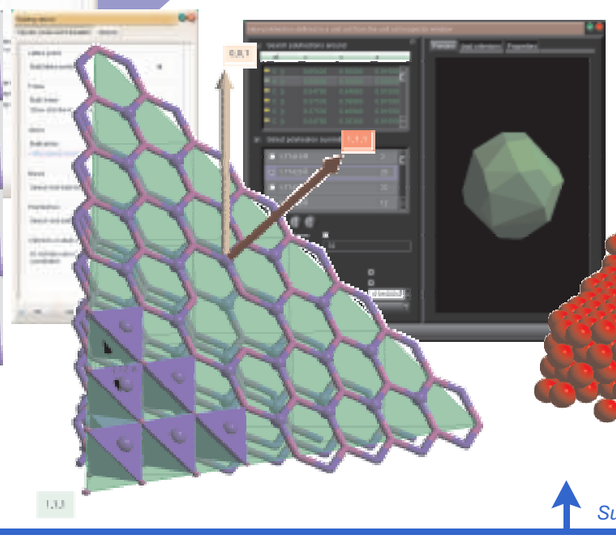
The inspector windows allow to access rapidly to the parameters and options of the crystallographic representations

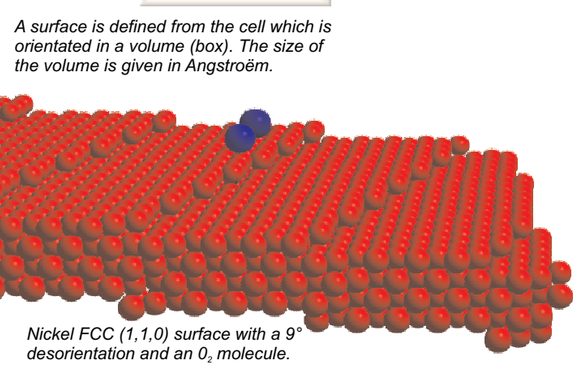


Many kind of visualisations are made possible by numerous options.



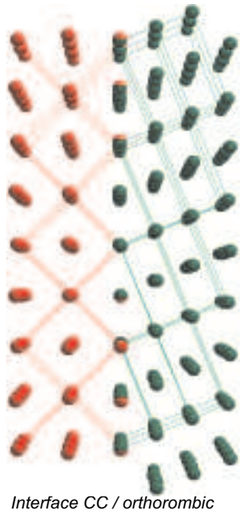
Bonds and polyhedrons can be searched interactively and automaticaly according to criterions defined by the user.





Nickel FCC (1,1,0) surface with a 9° desorientation and an 0_2 molecule.

A surface is defined from the cell which is orientated in a volume (box). The size of the volume is given in Angstroëm.



Interface CC / orthorombic centered :(1,1,0) // (1,0,1)
[0,0,1] // [0,1,0]

An interface is defined via the definition inspector window as a crystals stacking.

The orientation relationships within an interface are defined quickly and easely by many interactive tools.

The search for coincidences can be activated for lattice points and atoms.

Crystals

Surfaces

Interfaces, grain boundaries, multi-layers

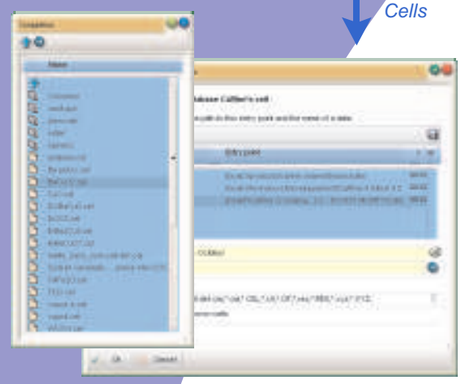
Cells

3D Modeling with CaRIne 4-0

Simulation, calculation and analysis with CaRIne 3-1

New interactive tools allow to create crystals, surfaces and interfaces from one or several cells, inside a same project.

The relations between the different geometrical representations of crystals are exposed in a clear way with CaRIne 3.1.



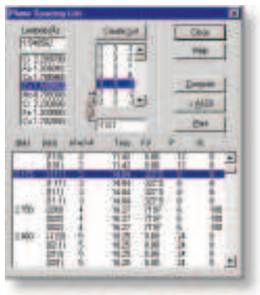
Selection and insertion of a cell in a project from the database.

Selection of the equivalent positions generator : Bravais lattice or space groups.

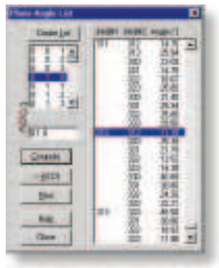
Integrated and automatic exportation of cells from CaRIne 4.0 to CaRIne 3.1.

The cell inspector window (atoms, lattice points, bonds and polyhedrons).

Calculation lists

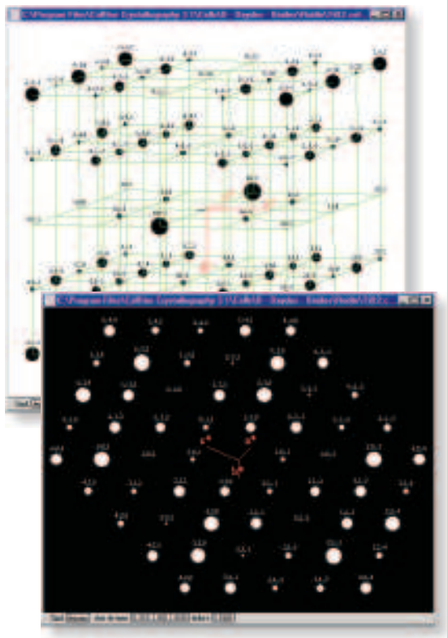


Ordered interplanar distance list (dhkl, indices, $h^2+k^2+l^2$, Bragg angle, structure factor, multiplicity, XRD intensity)



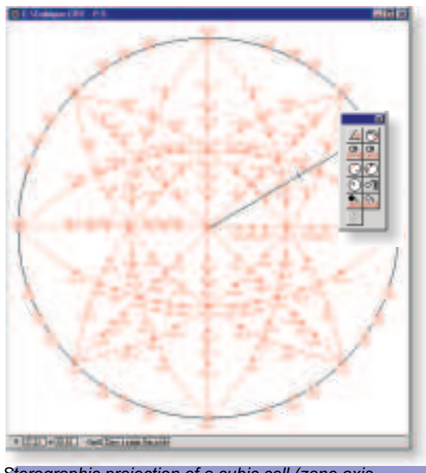
Interplanar angle list ($h_1k_1l_1$, $h_2k_2l_2$, angle)

3D reciprocal lattice, and plane cut of the reciprocal lattice



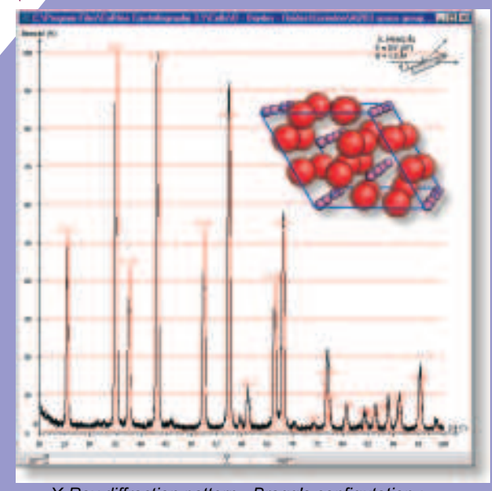
TiO_2 : Reciprocal lattice in 3D and a plane cut (zone axis [111])

Stereographic projection



Sterographic projection of a cubic cell (zone axis [0,0,1]). Any orientation is possible even by moving spots with the mouse.

X-Ray diffraction patterns



X-Ray diffraction pattern - Bragg's configutation : Comparison of calculated and experimental X-Ray diffraction patterns (Al_2O_3).

Multi-tasks and multi-platforms

Take advantage of the power of nowadays operating systems and processors. The same software is animated around the same graphic user interface whatever the operating system you use (Windows, Linux, Mac OS X *).

** Version available second term of 2005*

For research and teaching

Use the same tool to make your presentations, your research and to train your students.

A modular and evolutive software

The new organisation of the 4.0 version allows the futur development of a new range of fonctionnnalities inside the same user interface.