SOME COMMERCIAL PROGRAMS FOR STRUCTURE VISUALIZATION

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Abstract
There are several programs or software packages available for structure visualization. A survey of some of them has been published in Materials Structure [1]. In this contribution, some commercial systems are mentioned. They usually include interactive graphics when the structures can be easily rotated and moved by mouse. There are many visualization options of structures, calculation of bond lengths and angles and as a rule also calculations and visualization of powder diffraction pattern. Four systems are characterized in the review - Crystal Impact software, Crystal Maker, Crystal Studio and Crystallographica including licensing options.

Crystal Impact software

Software company Crystal Impact [2] distributes molecular and crystal structure visualization software **Diamond**. In addition to structural pictures it also offers an extensive set of functions that let easily model any arbitrary portion of a crystal structure from a basic set of structural parameters (cell, space group, atomic positions). It supports both crystal and molecular structures (i.e. with and without translational symmetry). Each structure set can contain: atomic parameters, cell parameters and space-group (optional), anisotropic displacement parameters, chemical and bibliographic data (author, reference, database origin, etc.). Supports multiple structure pictures for a structure data set. It allows importing of number of different formats (e.g. CIF, SHELX, XYZ, CRYSTIN etc.). Structure pictures can be exported to 3D VRML and many graphical formats of 2D pictures. Basic screen can be seen on Fig. 1.

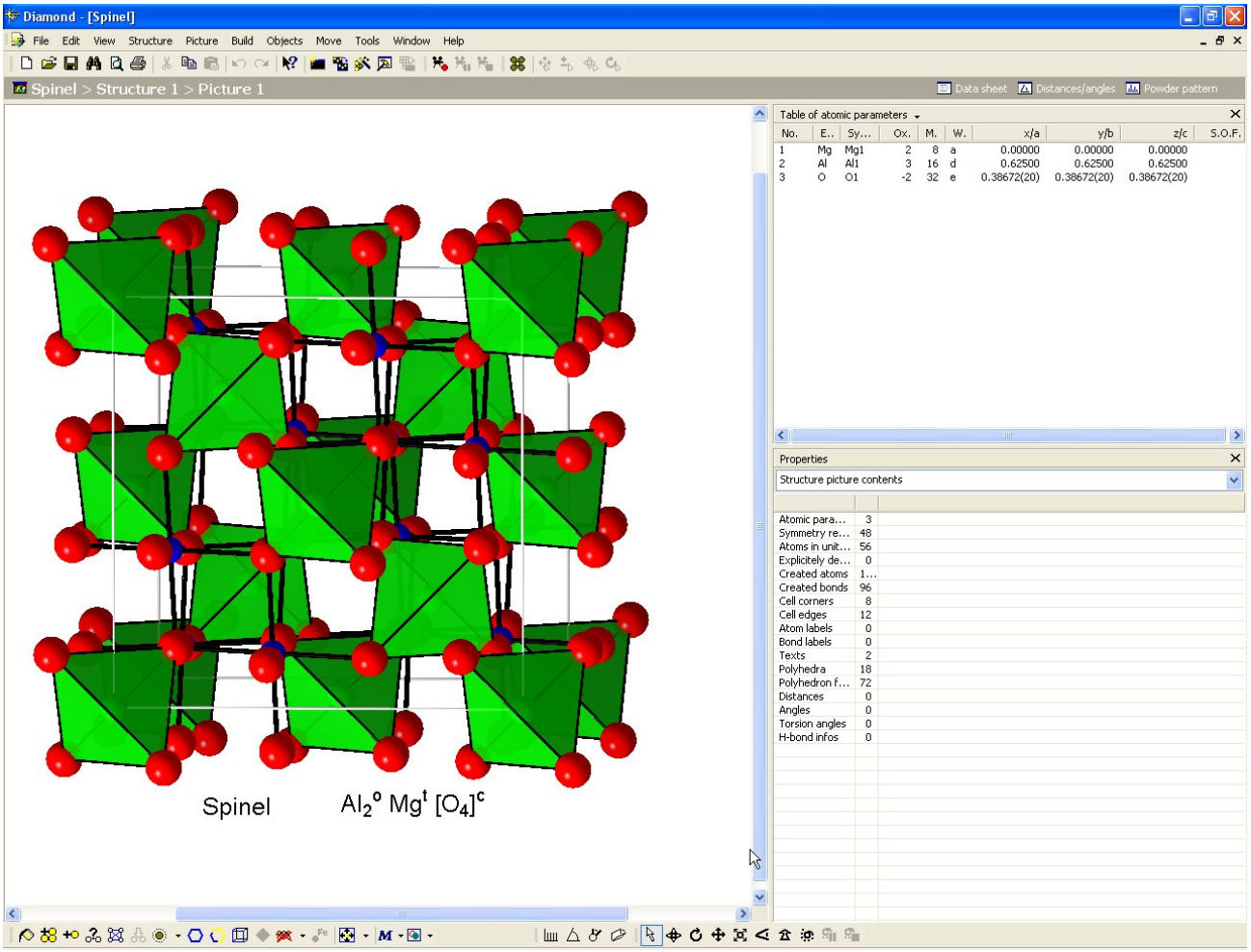

Figure 1. Basic screen of Diamond software

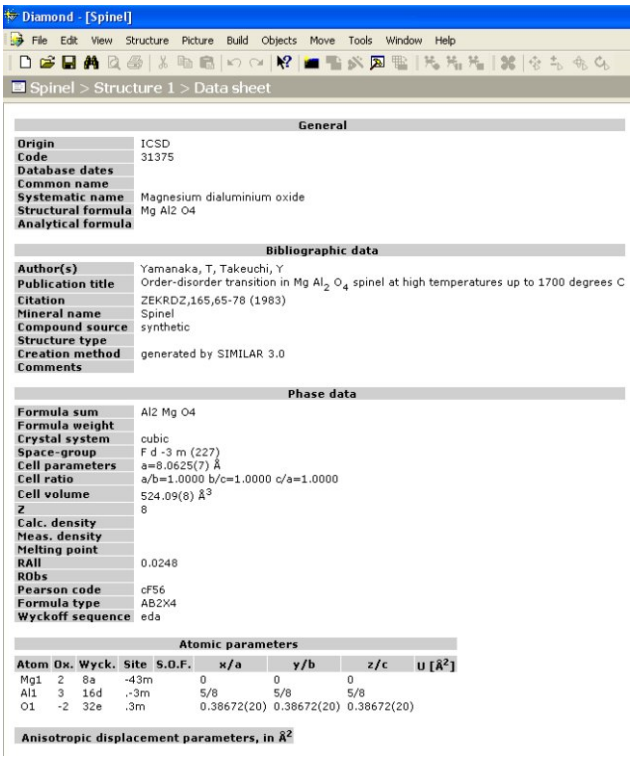

Figure 2. Data sheet window

For each structure several windows can be open - picture, data set (atomic parameters - Fig. 2), distances and angles, powder pattern. Options for building model and work with structural picture can be found in the bottom toolbar. They are also accesible in the top menu. If the rotation of structure is slow on the particular computer, on-line rendering (shading) should be switched off.

The features can be subdivided into several categories (see [2]).

Structure construction has the following options:

- Optional assistant that helps to create a structure picture from scratch or to modify a picture.
- Optional "Auto-Builder" that creates pictures automatically or according to a user-defined strategy ("scheme"). Useful when visualizing a lot of similar structures.
- Conversion between "crystal" and "molecular" structures, i.e. adding or removal of cell and symmetry information.
- Filling of unit cell, multiple cells, any cell range, or boxes or spheres around selected central atoms.
- Filling of user-defined rectangular areas within the screen.
- Filling of slabs along a plane (hkl or least-squares) or between a plane and the walls of the coordinate system. Selection of atoms to construct sublattices.
- Discussion of connectivity assisted by histograms showing the distribution of distances between selected atom types, together with automatic calculation and checking of distance ranges.
- Creation of bonds automatically, basing on connecitivity, or manually by inserting bonds between two atoms each.
- Generation of atoms from parameter list serving as initial atoms for building up complex frameworks.
- Completion of coordination spheres around selected atoms.
- Automatic generation of molecules or completion of fragments which has been clipped at cell edges.
- Creation of "broken-off" bonds to signal infinitesimal chains, layers, or 3D-frameworks.
- Cut, copy and paste of structural parts between structure pictures: A fragment of a structure picture (or the whole picture) can be copied. The copied fragment can be pasted into a blank or another picture of the same data set.

Visualization mode

- Variable zoom factor
- Models, assigned globally or individually to single or groups of atoms (allows mixing of different models in one and the same picture - Fig. 3): Ball-and-stick (regular), ellipsoid, space-filling, sticks or wires (depending on bond radius).

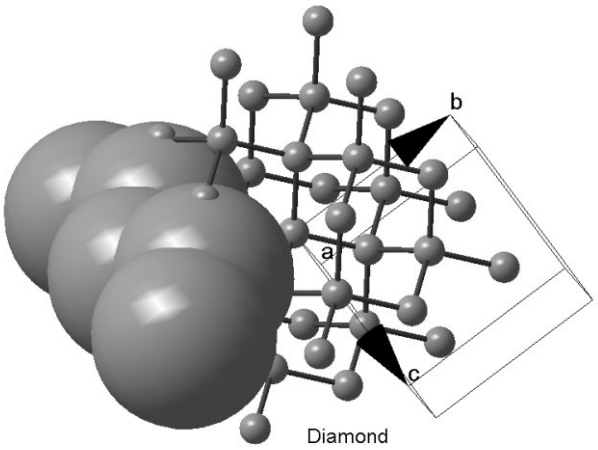

Figure 3. Diamond structure visualized in different way in different parts (standard, space filling), units cell and axis drawn.

- Definition of views along special axes or toward special planes.
- Central or parallel projection, depth cueing, and stereo display.
- Photorealistic rendered models with user-defined light source and material properties (OpenGL- POVRay, Fig. 4).
- Variation of colors, styles and radii of atom groups and bonds. Individual design of each single atom is possible.
- ORTEP-like atom styles (ellipses, octants) in both flat and rendering mode.
- Optionally fragmentated and two-colored bonds.
- Labelling of atoms and bonds. User-defined text, can be placed at arbitrary position of picture.
- Generation of coordination polyhedra: Around central atoms of selected groups or around individually selected

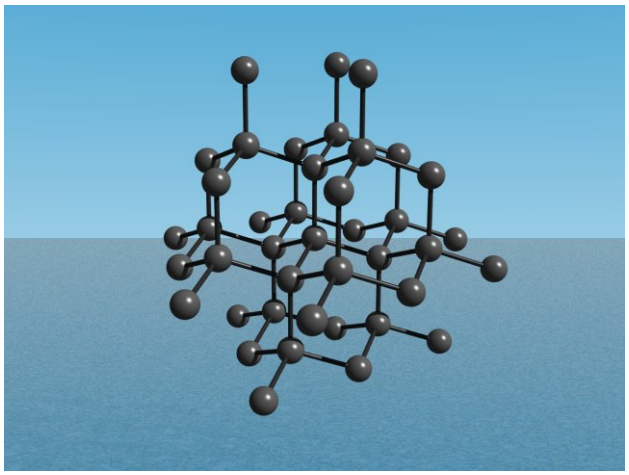

Figure 4. Rendering with external ray tracing program POVRay.

atoms, built up from selected ligand atoms, optionally with transparent or hatched surfaces.
- Definition of (transparent) lattice planes and (best) planes or lines through selected atoms.
- Adding of vectors to atoms to indicate e.g. a magnetic moment.
- Generation of H-bonds.
- Alternative color differentation to visualize oxidation numbers, site occupation factors etc.

Animation:
- Movement of structure picture: Modes: rotation along x-, y-, and/or z-axis, horizontal and/or vertical shift within drawing area, variation of enlargement factor (from Angstroems to centimeters),
- variation of camera distance (perspective impression). Controlled by: Mouse (the faster the mouse the faster the rotation etc.), keyboard (e.g. one degree rotation per keystroke), numerically (input through dialog).
- Optional "Spin" function, i.e. acceleration of movement.
- Continuous movement, which can be interrupted and continued.
- Walk-through mode, enabling the camera/viewer to navigate through the structure picture.
- Recorder that helps to create video sequences, e.g. as AVI files.

Exploration:
- Calculation of powder pattern: Variation of diffraction parameters: Radiation type: X-ray (laboratory, synchroton), neutron, electron, wavelength, LP correction, 2theta range, optional profile functions - pseudo-Voigt, width. Table of reflection parameters with zoom in/zoom out and tracking through 2 range - Fig. 5.
- Calculation of distances and angles (incl. standard uncertainties): in a configurable table, for selected atom types and a sizeable distances range, around the atom(s) currently selected in structure picture, graphical repre-

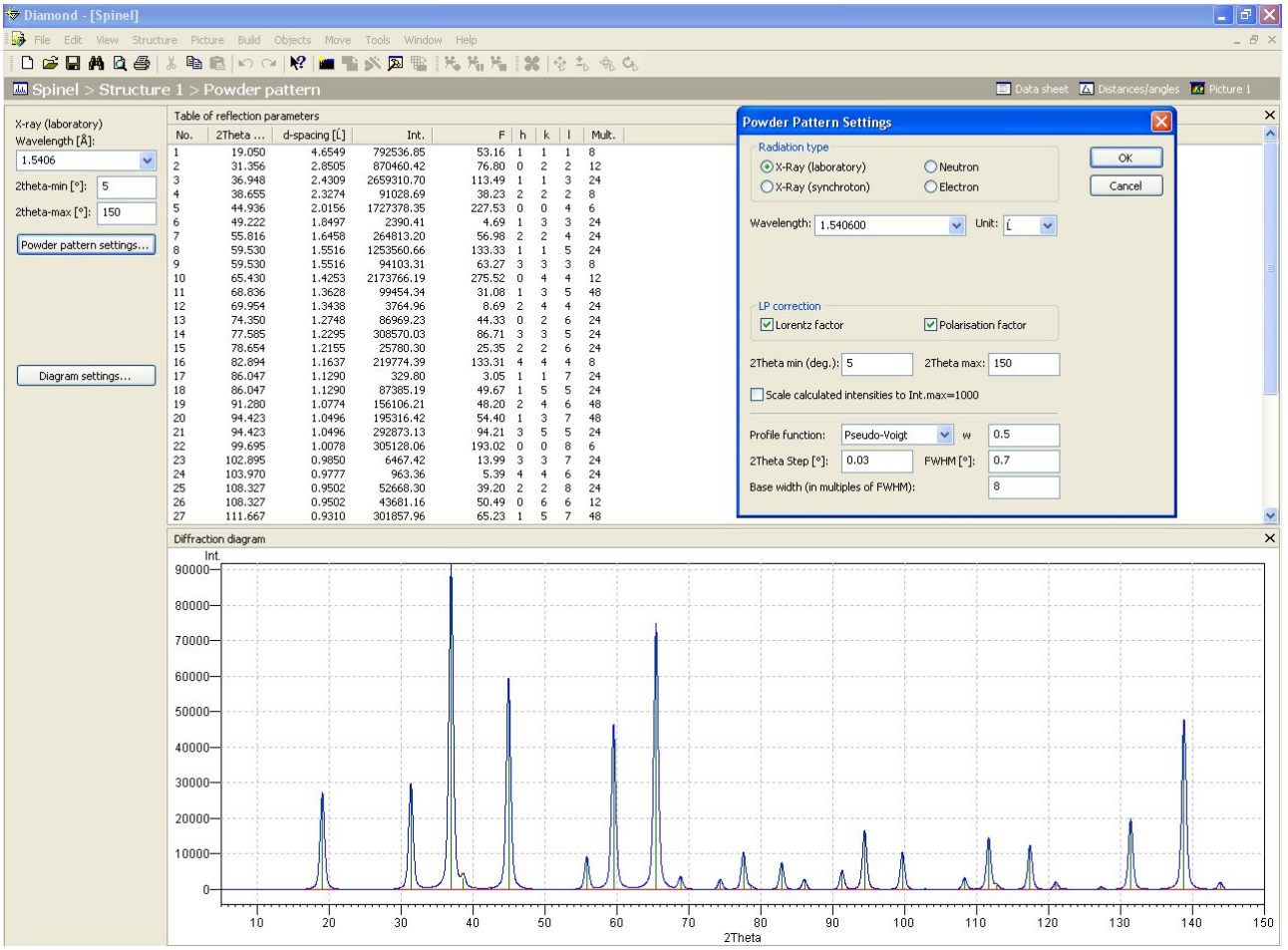

Figure 5. Diffraction pattern window of Diamond

sentation of distances as histogram with color-coded distances.
- Measuring of distances, angles, and torsion angles interactively (incl. standard uncertainties).
- Measuring of extended geometric features (incl. standard uncertainties): Angle between two planes (by hkl or (best) plane through 3 or more atoms), angle between two lines, angle between a normal of a plane and a line, distances of atoms from a plane or a line, centroid of a set of atoms, planarity or linearity of a set of atoms (distances of constituent atoms from plane/line).
- New Properties panel, displays information about: Contents of the structure picture (how many created atoms, bonds, polyhedra, etc.), the current "formula sum", that means the number of created atoms associated to atom groups, table of the currently selected objects, distances around the selected atom(s), distances between the selected atoms, the center of the selected atoms (centroid), planarity or linearity of the selected atoms and the deviations of the atoms from that plane or line, rsp., table of atoms assigned to the selected atom of parameter list or selected atom group, table of bonds assigned to the selected bond group (i.e. atom group pair), ligand, edges, and faces informations of the selected polyhedra.

Price of single academic licence is 500 Euro, site licence (one institute or department) 1000 Euro, campus licence 2000 Euro.

Other useful software offered by Crystal Impact is *Endeavour* designed for the solution of crystal structures from powder diffraction data. The concept implies a combined global optimization of the difference between the calculated and measured diffraction pattern and of the potential energy of the system.

Match! is an easy-to-use software for phase identification from powder diffraction data. It compares the powder diffraction pattern of your sample to a database containing reference patterns in order to identify the phases which are present. Both ICDD products can be used for database source.

Pearson's Crystal Data is a new crystallographic database (see also [3]).

All the above Crystal Impact software can be found on demo CD distributed for all the conference participants.

Crystal Maker Software

Crystal Maker software is distributed in two versions for Mac an PC, respectively [3].

CrystalMaker visualizing software for molecular and crystal structures is by features similar to Diamond. The interactive graphics is significantly faster on slower computers. It has the ability to display massive structures (up to 2 billion atoms). Bonds and polyhedra are automatically calculated, with the option of bond distance output and error propagation, as well as direct visualization of cluster shells and coordination networks.

In general, the program may have not all the possibilities of Diamond but it seems to be very user-friendly and nice to work with. Everything is smooth. Main window is shown on Fig. 6. One can easily switched on/off individual types of atoms from the picture and history of different views is quickly accesible.

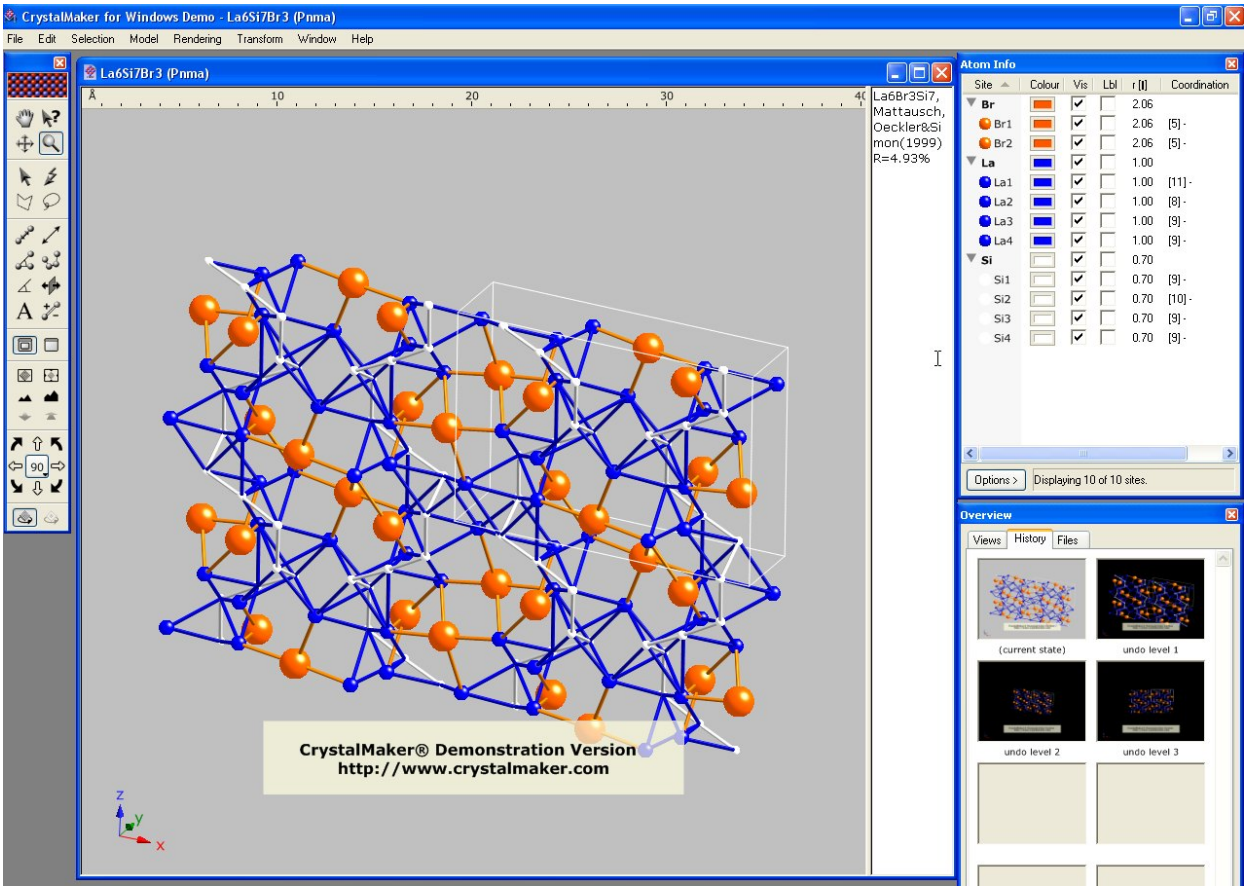

Figure 6. Main window of Crystal Maker

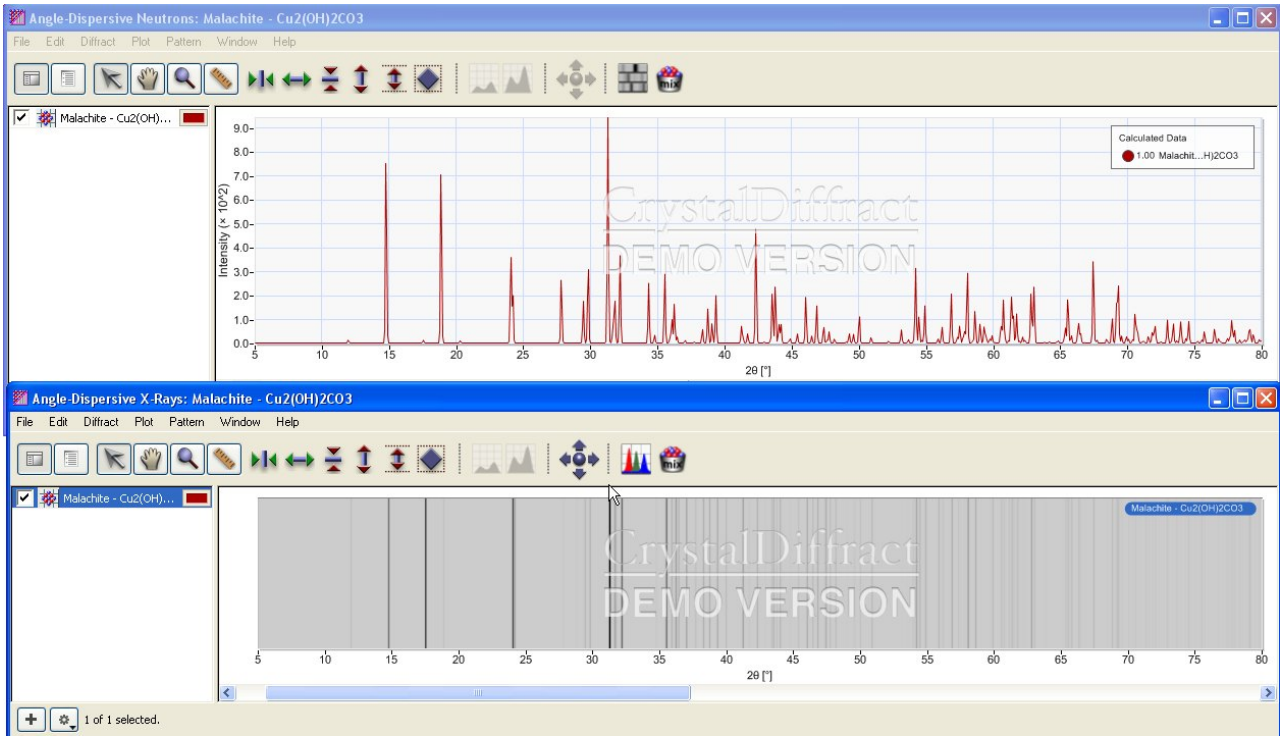

Figure 7. Two windows of CrystalDiffract - simulation of powder diffraction pattern obtained by the detector (top) and film record (bottom).

CrystalMaker is shipped with over 600 structures files, including the major rock-forming minerals plus important technological phases such as zeolites, superconductors and organic molecules. Each file is fully-annotated, with views and model types carefully chosen to highlight the salient structural features, and ready for immediate display. Animations can be saved as Quick Time movies. CrystalMaker provides photo-realistic graphics, including 3D stereo graphics (red/blue stereo glasses included with the program package).

Diffraction patterns are generated by stand-alone program **CrystalDiffract** that can be used unlike Diamond as a separate tool for simulation of powder patterns. CrystalDiffract lets simulate also patterns for multi-phase mixture; switch between x-ray or neutron radiation including time-of-flight or energy scale; visualize intensities as "films" or graphs (Fig. 7); choose different diffraction techniques; interactively edit structural and experimental parameters, and export detailed diffraction information. For shape function pseudo-Voigt function is used. Constant value of instrumental broadening can be given and in simple way also size and strain broadening.

CrystalDiffract lets edit aspects of a selected pattern's underlying crystal's structure, so one can determine how this affects diffraction. You can edit lattice parameters and site occupancies—and also omit sites from the diffraction calculation. The Edit Crystal sheet can be resized horizontally and vertically, in order to show a range of sites and their atomic displacement parameter data (Uij and Uiso).

In Graph mode one can use the Stack command to stack multiple diffraction patterns without danger of overlap. For a complex diffraction pattern there may be many overlapping peaks. The Overlay Peak Positions submenu allows you to identify the positions of individual diffraction peaks. One can superimpose a series of peak markers showing the peak centres, and their relative intensities.

Of course, very important feature is a possibility to load experimental data (in xy format) and compare them with the simulation. CrystalDiffract work well together with CrystalMaker.

The third part of the software package is **SingleCrystal**. It lets simulate electron diffraction patterns, display sections of the reciprocal lattice and work with stereographic projections. One can manipulate diffraction patterns in real time, changing the orientation of a crystal, the scale or intensity saturation. It is possible to measure intensities, distances and angles on screen. There is even a unique option of visualizing the phases of diffracted beams, via colour-coded diffraction spots.

Educational pricing of the software is the following: single licence - CrystalMaker 350 Euro, CrystalDiffract 150 Euro, SingleCrystal 99 Euro.

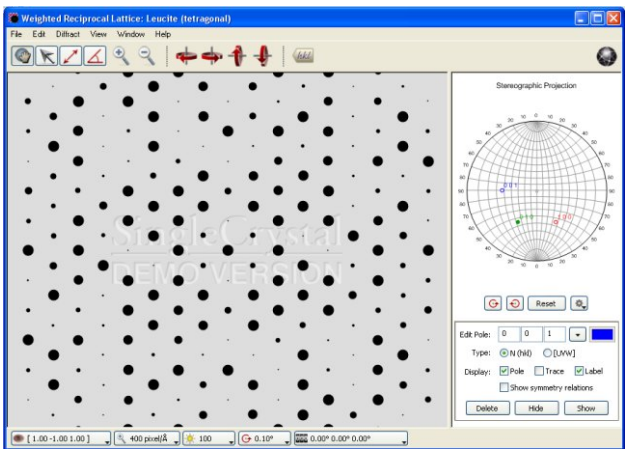

Figure 8. Screen of the program SingleCrystal.

Crystallographica

The package is distributed by Oxford Cryosystems [4, 5] and it includes structure and reciprocal lattice display, powder simulation, graphing (including common x-ray data formats) and a unique crystallographic scripting language, all supported numerous example scripts and structures as well as free unlimited technical support.

Crystallographica is essentially a visualisation program, consisting of a series of tools for setting and displaying a multitude of properties of a crystal structure. Some of these tools are highly visual in nature: the program incorporates a structure drawing package, reciprocal lattice display and powder pattern simulation. A set of dialogs allow not only crystal properties to be set, but also provide quick and easy methods for viewing crystal properties.

All these features are shared by the Lite and Full versions of Crystallographica. The Full version adds a unique crystallographic scripting language based on pascal syntax which allows a whole new level of flexiblity and power to the program. This language is fully integrated with the other tools, and may be used for anything from calculating simple properties to creating animations. Four typical windows are shown on Fig. 9.

Integrated crystal structure drawing package allows a number of views of the same structure or else comparison of different structures. Plots can be examined using the mouse and keyboard to rotate and zoom the image, or controlled precisely from the Interpreter.

VRML files can be exported, showing crystal structure and including anisotropic displacement ellipsoids, polyhedra and crystal planes.

Integrated viewer allows the reciprocal lattice to be displayed in a variety of styles. Viewing direction may be synchronised with other such windows and with structure display.

Flexible X-ray and neutron powder diffraction pattern simulation including Rietveld-style control over peak shape and width area available. Simulated pattern may be compared with experimental data in the graphing tool. Profile and peak data may be exported to file. Scripting language includes utilities for combining plots to form multi-phase patterns or residuals.

A set of simple and easy-to-use dialogs provides a powerful user interface to access atom properties, contents of asymmetric unit, cell parameters, bond lists, crystal symmetry (via space group or list of generators), radiation, reflection lists, powder simulation and VRML options.

Pascal interpreter supportes variables, arrays, records, sets, functions and procedures. Extensions to core Pascal include exponential operator, dynamic sizing of arrays and enhanced string handling. The interpreter may be

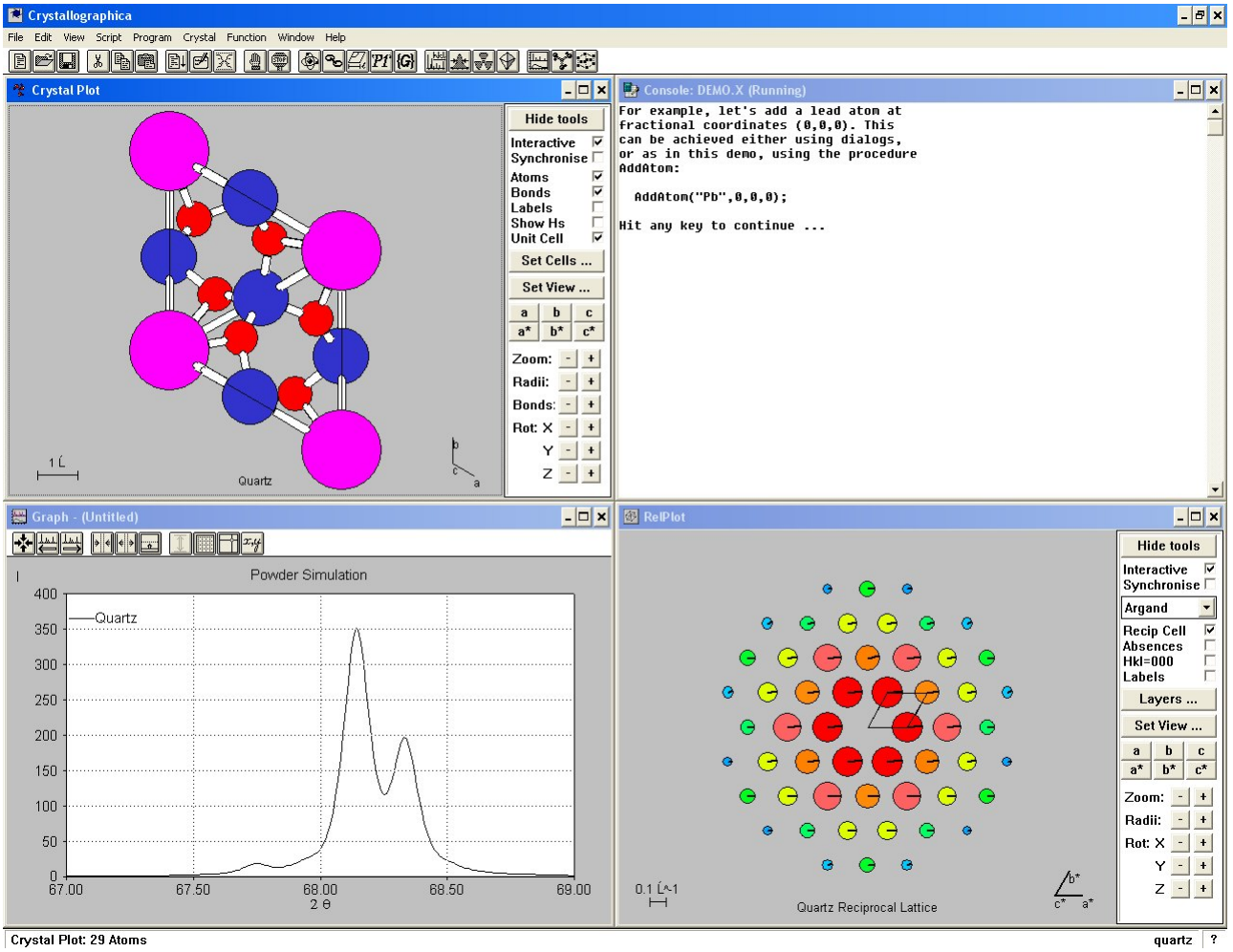

Figure 9. Crystallographica windows showing interactive structure picture (top left), command line window of the scripting language (right top), part of diffraction pattern (left bottom) and reciprocal lattice (right bottom).

used interactively or called to run scripts contained in text files.

A *library* of several hundred crystallographic routines covering atom properties, bonding, cell parameters, symmetry, radiation, reflections, powder simulation, crystal structure drawing and graph plotting.

User-scripted routines are easily integrated, so that the system can be customised.

A set of databases holding information on X-ray and neutron scattering factors including dispersion corrections, absorption factors, X-ray wavelengths, bonding radii, elemental properties and space group symmetry.

Academic single user pack costs 500 GBP (lite version without interpreter - 250 GBP), teaching pack - site licence is for 1000 GBP.

Crystal Studio

This is a software by Australian CrystalSoft corporation [6]. Apart from providing normal crystallography functionalities like 3D graphics etc. as other packages, **Crystal Studio** offers ample functions for *defects like dislocations, twin boundaries and stacking faults, interfaces and surfaces and two phase coherent combinations*. It also covers XRD, neutron and electron diffraction simulations and reciprocal lattice. Moreover it especially simulates the combined zone axis diffraction patterns for twins and two phase coherent combinations.

As in the preceding programs different visualization options are available: ball and stick model, stick model, space filling model, ellipsoid and stick model, ball and stick plus translucent space filling model, mixed model, *ribbon model*, perspective or orthographic projection. Vectors can be added to the atoms.

Crystal Studio is integrated with a crystallographic database. The database contains information about all 530 space group specifications from various versions of International Tables for (X-Ray) Crystallography, information on all elements in the Periodic Table including valence, radii etc. and latest data for atomic scattering amplitude and Debye-Waller factors for diffraction calculations. The database also include a crystal structure database and a layer/cluster database. Non-standard space group specifications can be created and added to the database by user. The 530 existing space group specifications can also be modified by users. Crystal structures without space group specifications can also be created, built and stored in the database.

The program is distributed in several versions - Lite, Standard, Professional, Enterprise with academic pricing starting from 450 to 1300 US$ for single licence and 1900 US$ for 5 user site licence.

Acknowledgement

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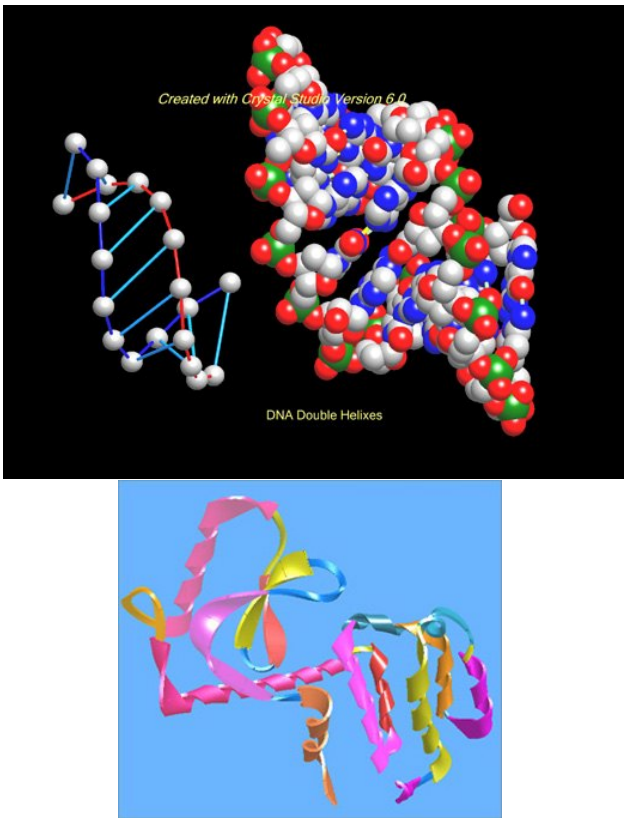

Figure 10. Different models for visualization in CrystalStudio.

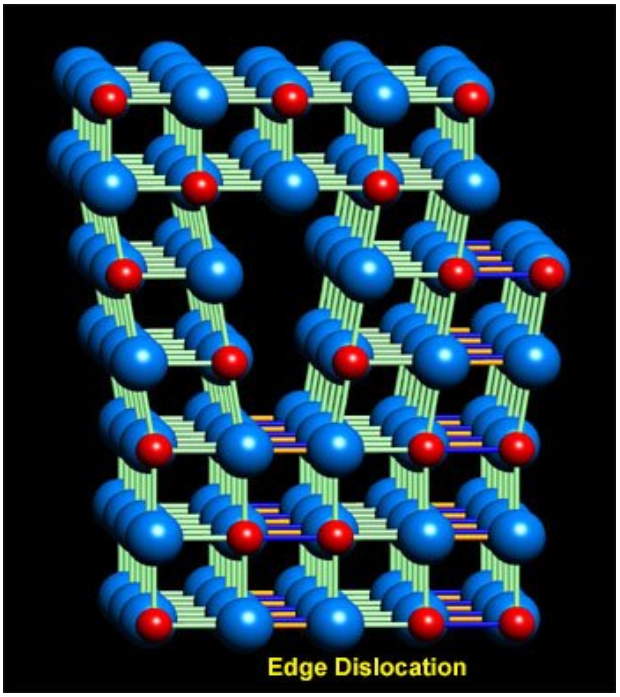

Figure 11. Visualization of dislocation in the lattice by CrystalStudio.