TEACHING AND EDUCATION IN CRYSTALLOGRAPHY

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Interactive Web-based tools for an introductory course in crystallography

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Abstract

The new possibilities offered by the Java programming environment combined with the accessibility of the World Wide Web present new and interesting perspectives. It is thus now possible to perform simulations directly, using a Web browser, independently of the computer platform being used. Basic concepts of crystallography, *i.e.* crystal structures, point- and space-group symmetry, lattices, reciprocal lattices and diffraction principles can be illustrated utilizing interactive simulations written in Java. A number of such applications have been developed with the aim to facilitate the understanding of these crystallographic concepts to the newcomers in the field.

1. Introduction

While teaching the basics of crystallography, instructors are confronted with the need to use the third dimension to illustrate certain principles such as point- or space-group symmetry operations, the principles of diffraction by crystals or details of elaborate crystal structures. With the ubiquitous availability of computers (even in lecture halls), crystallographers can take advantage of existing software in order to illustrate specific aspects of the field. The immediate problem facing the instructor, however, is the choice of which computer platform to use. Many interesting applications have been previously written, but unfortunately no single computer can utilize all of them.

Fortunately, Web-based applications can avoid this serious drawback. The recent introduction of the Java programming language allows platform-independent development of applications which can be directly accessed by anyone connected to the Web. The current versions of most modern Web browsers are all able to handle these so-called 'Java applets'. These Java applications can then be used to illustrate specific aspects during a lecture. What is perhaps more efficient for the students is the possibility to repeat the demonstrations individually, at their own pace, with a computer linked to the network at their school or from their home.

With this universality in mind, we have developed a series of Java applications which illustrate some important concepts of crystallography: point-group symmetry, space-group symmetry and the elements of crystal diffraction. In point-group symmetry operations, the advantage of using a computer model is that we can actually perform a roto-inversion or, more generally, an improper rotation, which is not otherwise possible with a solid model. The plane-group (two-dimensional space-group) symmetry can be dynamically implemented with a Java applet and the students can quickly familiarize themselves with the concepts of general and special positions and site symmetry. Any (two-dimensional) periodic structure can be easily constructed with a minimum number of mouse clicks. Various tools can be used to perform the most elaborate periodic decorations directly. The concepts of direct and reciprocal lattices have also been implemented, based on a previously created two-dimensional periodic pattern, and can be manipulated interactively by the student. By extension into the third dimension, the very didactic concept of the Ewald sphere is used to illustrate the principles of single-crystal diffraction with a monochromatic or polychromatic incident beam.

All of the applets which have been developed in this context can be complemented or illustrated further with applications available on other Web sites. The interested user can always refer to the Web site of the International Union of Crystallography (1999) for additional pointers of interest or make use of search engines to discover other new helpful applications.

2. Web modules for crystallography teaching

The development of new computer-based teaching and multimedia tools is certainly not intended to replace the

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teacher. Its aim is rather to illustrate and improve the understanding of basic or abstract concepts and thus contribute to a better learning environment for the student. Perhaps the most important aspect of a good learning environment required by the student is a set of tools that are interactive in nature. The ultimate aim is to create intuitive tools and give the user the ability to test ideas or simulate actions in order to improve his or her understanding of the subject.

Computer-software companies have released crystallography-oriented packages [*e.g. Crystallographica*, reviewed by Siegrist (1997), and *Cerius*^{2} (Molecular Simulations Inc., 1997)], which are particularly interesting and useful in an introductory course in crystallography. The main drawbacks, however, are the costs and the lack of usability, except on specific equipment.

The rapid adoption of the platform-independent Java programming language has created a new momentum, which has already proven to be of great help for education purposes and certainly has excellent potential for the future. One of the main advantages is that the user can control his own learning process.

We have recently started to develop some basic modules, usually called 'applets' in the information technology world (Hardaker & Chapuis, 1998), which we shall describe in the following sections.

2.1. *Learning point-group symmetry*

A symmetry operation of an object is usually defined as a transformation, which leaves the object invariant. With the help of solid models, the symmetry operation can be accomplished only if the operation is a rotation. With computers, the generation of improper rotations goes beyond a 'Gedanken Experiment' and can thus be executed on virtual objects.

A Java module has been developed with the intention to perform symmetry transformations on a number of specific objects, in particular crystal forms (Hardaker & Chapuis, 1997*a*). After selecting the model for which we would like to study the symmetry properties, a copy of the object on which the transformations will be performed is generated first. With this copy available, the student can always refer to the original object for comparison purposes. By using specific buttons, the user can execute rotations about various axes or perform an inversion of the object ($\bar{1}$). By selecting an object with point-group symmetry $\bar{4}$, the student can perform the inversion and will soon realise that this operation is not a symmetry operation of the object because the two copies cannot be superimposed. The combination of inversion followed by a rotation of 90° is, however, a symmetry operation of the object and is specifically the $\bar{4}$ operation. Fig. 1 illustrates the interactive windows from which many transformations can be executed. Other geometrical forms like the cube, the octahedron and the tetrahedron are also available for exercising point-symmetry operations.

2.2. *Creating two-dimensional periodic patterns*

The understanding of periodic structures is so fundamental to crystallography that a basic knowledge of space groups is unavoidable. The description of space groups presented in the *International Tables of Crystallography* (1996) is well suited for reference purposes but certainly not for didactical purposes. What is implicit in the definition of atomic coordinates is that the space-group properties provide for the generation of an infinite number of equivalent positions in space. Computers can conveniently play this role and act as an instantaneous generator of a large amount of symmetrically equivalent atoms or points. Examples of plane groups can already illustrate most of the concepts needed for a better understanding of periodic structures. The module *Escher Web Sketch* (Hardaker & Chapuis, 1997*b*) has been developed for the training of students. It provides interactive tools that permit not only the creation of any type of periodic pattern (Fig. 2) but it also provides the ability to test interactively the effects of space-group symmetry by displacing an object on the screen. The choice of the two-dimensional space groups, the choice of the object, and the choice and size of the drawing tools all contribute to the manifold offered for creation of periodic patterns.

Escher Web Sketch (*EWS*) is able to differentiate between general and special positions (*International Tables of Crystallography*, 1996). It is thus possible to study the properties of site symmetry and identify all the possible cases associated with a specific plane group. Cooperative phenomena can also be simulated from a simple oscillation of the computer mouse.

The creation of two-dimensional crystalline structures can be accomplished easily by placing atoms and bonds using simple mouse clicks. The interested user will discover one of the interesting properties of space groups by creating a parquet floor from a single line provided the correct choice of the space-group symmetry has been made.

2.3. *Introduction of the reciprocal-lattice concept*

In an introductory course on crystallography, the presentation of the reciprocal lattice is the most challenging task facing the teacher. Understanding the constant interplay between the direct and reciprocal spaces requires some practice, which can only be acquired by training. The aim of the reciprocal-lattice module is to introduce the subject using a graphical method instead of an algebraic method. For this purpose, the starting element is a periodic pattern, which has been previously generated by *EWS*. In a first step, the applet attempts to identify the (two) translation periods characteristic of the specific pattern by scanning the pattern. After successive steps of abstraction, only a periodic array of lattice points remains and the generation of lattice planes (or rather, lattice lines in two dimensions) can be started interactively. Following the selection of a series of parallel lines, the applet creates a series of equidistant lattice points normal to the lines and with distances inversely proportional to the distance between the lines. The process can continue further with other series of lattice lines until the student realises that he or she has generated the reciprocal lattice of the original pattern. The student can return at will to previous steps for better understanding and finally ask the module applet to complete the task (Fig. 3). With the basic understanding of reciprocal-lattice points and reciprocal-lattice vectors, the principles of crystal

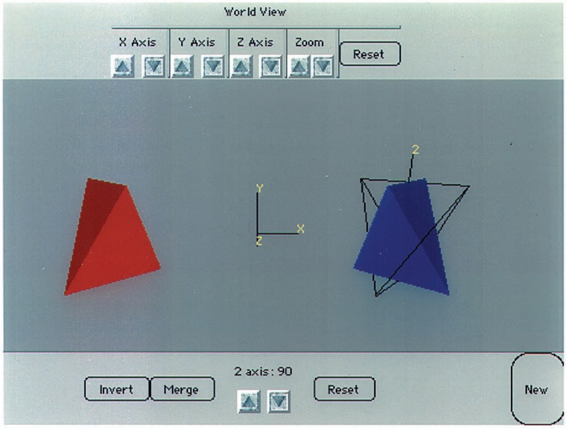

Fig. 1. Learning and testing point-group symmetry. This simulation allows the user to perform proper and improper rotations. Inversions or, more generally, roto-inversions can be performed on a screen but not with physical objects.

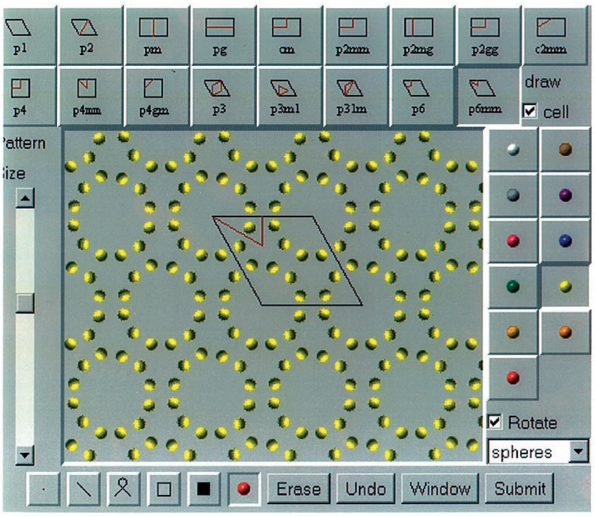

Fig. 2. Plane groups (two-dimensional space groups) can be simulated interactively with this applet. The concepts of general and special positions, and site symmetry can be easily illustrated. Simple structures can be rapidly obtained from the tools using a few mouse clicks.

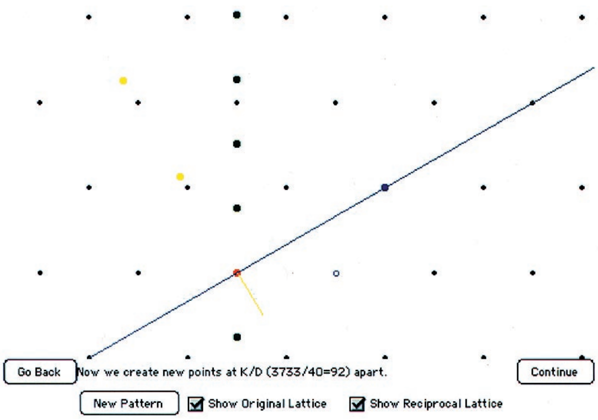

Fig. 3. Starting from a plane group two-dimensional periodic pattern, this applet can extract the lattice periodicity and construct interactively the corresponding reciprocal lattice. The figure represents one step in the interactive creation of the reciprocal lattice.

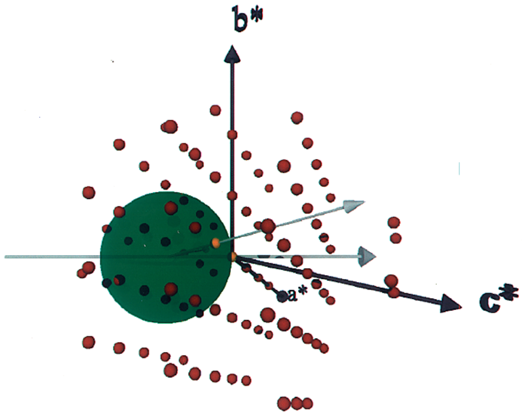

Fig. 4. Screen shot of the Ewald sphere simulation with a reciprocal-lattice point cutting the sphere and giving rise to a diffracting beam.

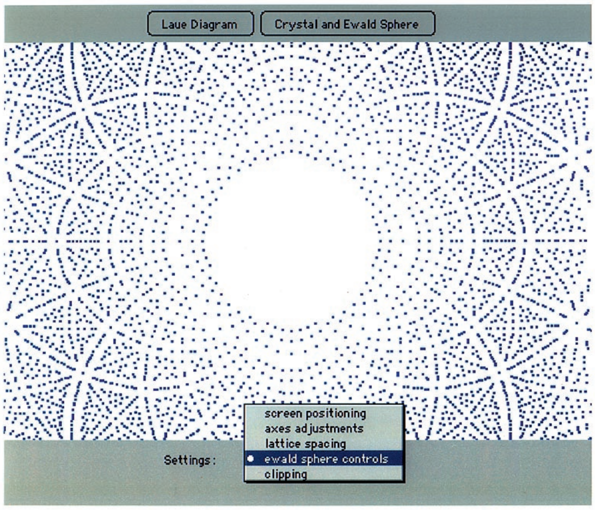

Fig. 5. Interactive simulation of Laue diffractograms. The user can directly observe the effect of various crystal-, orientation- and diffraction-parameter changes on the diffractogram.

diffraction can then be introduced to the student as a next step in the learning process.

2.4. *Introducing the Laue conditions of diffraction and the Ewald sphere*

The mathematical derivation of the Laue conditions of diffraction is beyond the scope of the present series of modules. For our purpose, we shall accept them without proof and use them to construct the Ewald sphere. The intersection of the reciprocal-lattice points with a sphere of which the radius depends on the wavelength of the incident beam is an elegant method to illustrate the principles of single-crystal diffraction. A video sequence has been prepared representing a three-dimensional array of reciprocal-lattice points rotating around a specific axis. Each time one of the reciprocal-lattice points crosses the sphere, a vector representing a diffracted beam is generated during the time the point is intersecting the Ewald sphere. This demonstration illustrates nicely the fact that the diffracted beam can point in all directions of space, including directions opposite to the incident beam. Examples of multiple scattering can also be observed with this demonstration when at least two reciprocal-lattice points intersect simultaneously the Ewald sphere (Fig. 4). With the standard video tools available for current Web browsers, the interested user can interact with the video by inverting some sequence or by controlling the flow of frames in order to clarify aspects of the simulations.

2.5. *Simulation of Laue diffractograms*

Laue diagrams (the oldest diffraction method) have recently regained some interest since the availability of modern area detectors. By interacting with a series of a few control buttons, the user can select the wavelength range of the spectrum, the orientation of the single crystal relative to the incident beam, and generate in real time the corresponding Laue diffraction pattern (Fig. 5). An interesting feature of this applet is that the position of the detector can be arbitrarily selected around the vertical axis. This feature illustrates nicely the differences between Laue diffraction in transmission and reflection (back scattering) or any other arbitrary orientation.

The possibility to select the lattice constants and angles of the crystal gives the student the opportunity to study the effect of crystal parameters on the Laue diffractogram. The effect of varying one of the lattice constants can then be immediately observed on the diffractogram.

3. Conclusions

The possibilities offered by the new Web-based programming environment in order to create interactive applications which are directly available on the network are very impressive. Specialists interested in the development of curriculum materials in crystallography can take full advantage of the new programming languages, which leaves each user with the freedom of selecting the hardware platform of his or her choice without any limitation on the choice of the application he or she wishes to access. From the didactical point of view, the possibilities offered by the interactivity between the user and the applications will greatly facilitate the learning ability of the student interested in crystallographic concepts and methods. To cite just an example, the possibility to move interactively an object on a screen subject to the symmetry constraints of a space group is, without doubt, an excellent complement to the description of the same space group in a textbook. New concepts described by lengthy explanations that are not immediately evident can be quickly illustrated and consequently better understood with the help of an interactive simulation.

Other sources of interactive modules can be found on the Web, which can complement the applets developed locally. The increased power of Internet search engines facilitates the identification of useful modules at large, which can be retrieved for practical use. Some interactive modules can already be found dealing with other fundamental aspects of crystallography, *e.g.* stereographic projection and the generation of crystal forms, Laue diffractograms, the Bragg interpretation of diffraction and the effect of wavelength (Weber, 1997; Shields & Lukin, 1997). Space groups and its generalization can also be generated interactively directly from some Web sites (Thiers *et al.*, 1997). Interactive modules to familiarize the user with the concept of quasicrystals can be used to introduce more advanced topics (Durand, 1994).

The synergies that can be gained from independent developers concerned with developing teaching aids in the same field are promising. It is easy to include new pointers in an application referring to recent developments in order to complement the subject or to present other aspects. Without doubt, the continuous development of new applets will greatly contribute to the world of learning and distance learning and possibly help to improve the quality of the simulations from the development of new tools and techniques which are offered to the developers.

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