Teaching Biophysics

XRayView: A Teaching Aid for X-Ray Crystallography

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ABSTRACT A software package, *XRayView*, has been developed that uses interactive computer graphics to introduce basic concepts of x-ray diffraction by crystals, including the reciprocal lattice, the Ewald sphere construction, Laue cones, the wavelength dependence of the reciprocal lattice, primitive and centered lattices and systematic extinctions, rotation photography, Laue photography, space group determination and Laue group symmetry, and the alignment of crystals by examination of reciprocal space. *XRayView* is designed with "user-friendliness" in mind, using pull-down menus to control the program. Many of the experiences of using real x-ray diffraction equipment to examine crystalline diffraction can be simulated. Exercises are available on-line to guide the users through many typical x-ray diffraction experiments.

INTRODUCTION

In the early 1900s, Max von Laue, W. L. and W. H. Bragg, and others laid the groundwork for what has become a powerful method of visualizing complex molecules, x-ray crystallography. Students often are intimidated by this method's apparent complexity, and I have found that experience in observing diffraction effects greatly facilitates students' appreciation of key concepts. A firm grasp of Bragg's law and the wavelength dependence of the diffraction (Bragg, 1913; Bragg and Bragg, 1913) and the reciprocal lattice (von Laue, 1913; Ewald, 1913a) and its symmetry (Ewald, 1913b) is central to an understanding of crystallography. The Ewald sphere construction (Ewald, 1921), the sphere of reflection and the limiting sphere (Bernal, 1926), and the effects of mosaicity are also key concepts that must be mastered before x-ray crystallography can be understood and applied.

Increasingly, area detectors are replacing film and diffractometers, especially for studies on macromolecules. Their ease of use has produced a tendency of students to use them as "black boxes," and often experiments are done in less than optimal ways because of lack of appreciation of basic diffraction concepts. It is true that usually crystals can be put on instruments in arbitrary orientations and the data can be indexed automatically. Data taken in this "wild West" style (shoot first and ask questions later) can be perfectly usable, but often better use can be made of the crystals and instrument time if a better understanding of the reciprocal lattice is at hand.

Modern x-ray diffraction equipment is also expensive, especially area detectors, and access is often limited to only the most sophisticated users. Safety issues are also a factor: new students must be trained properly in radiation safety before he or she can be left to explore diffraction from real crystals.

A software package, *XRayView*, has been developed that uses interactive computer graphics to introduce basic concepts of x-ray diffraction by crystals, including the reciprocal lattice, the Ewald sphere construction, Laue cones, the wavelength dependence of the reciprocal lattice, primitive and centered lattices and systematic extinctions, rotation photography, Laue photography, space group determination and Laue group symmetry, and the alignment of crystals by exploration of reciprocal space. *XRayView* allows beginning crystallographers a safe and convenient way to develop their intuitions about complicated diffraction effects without the expense or danger of real experiments.

METHODS

XRayView is designed with "user-friendliness" in mind, using Motif style (Open Software Foundation, 1991) and pull-down menus to control the program. The program is written in C, using interactive, object-oriented paradigms. Although supported at present only on Silicon Graphics, Inc. computers, it is expected that as Silicon Graphics supports it's OpenGL graphics language on more hardware platforms, *XRayView* will be made more widely available.

The real-time simulations require significant graphics computational power. For this reason, this version is restricted to use on the Silicon Graphics workstations, including the entry level Indy's, although future releases may be available for other X-based platforms.

USING *XRayView*

Once the *XRayView* main menu is on the screen (Fig. 1), the menus at the top can be "pulled down" by placing the pointer on the desired item with the mouse, pushing and holding down the left mouse button, moving the cursor down to expose the choices, and then letting go of the left mouse button when the pointer is positioned over the de-

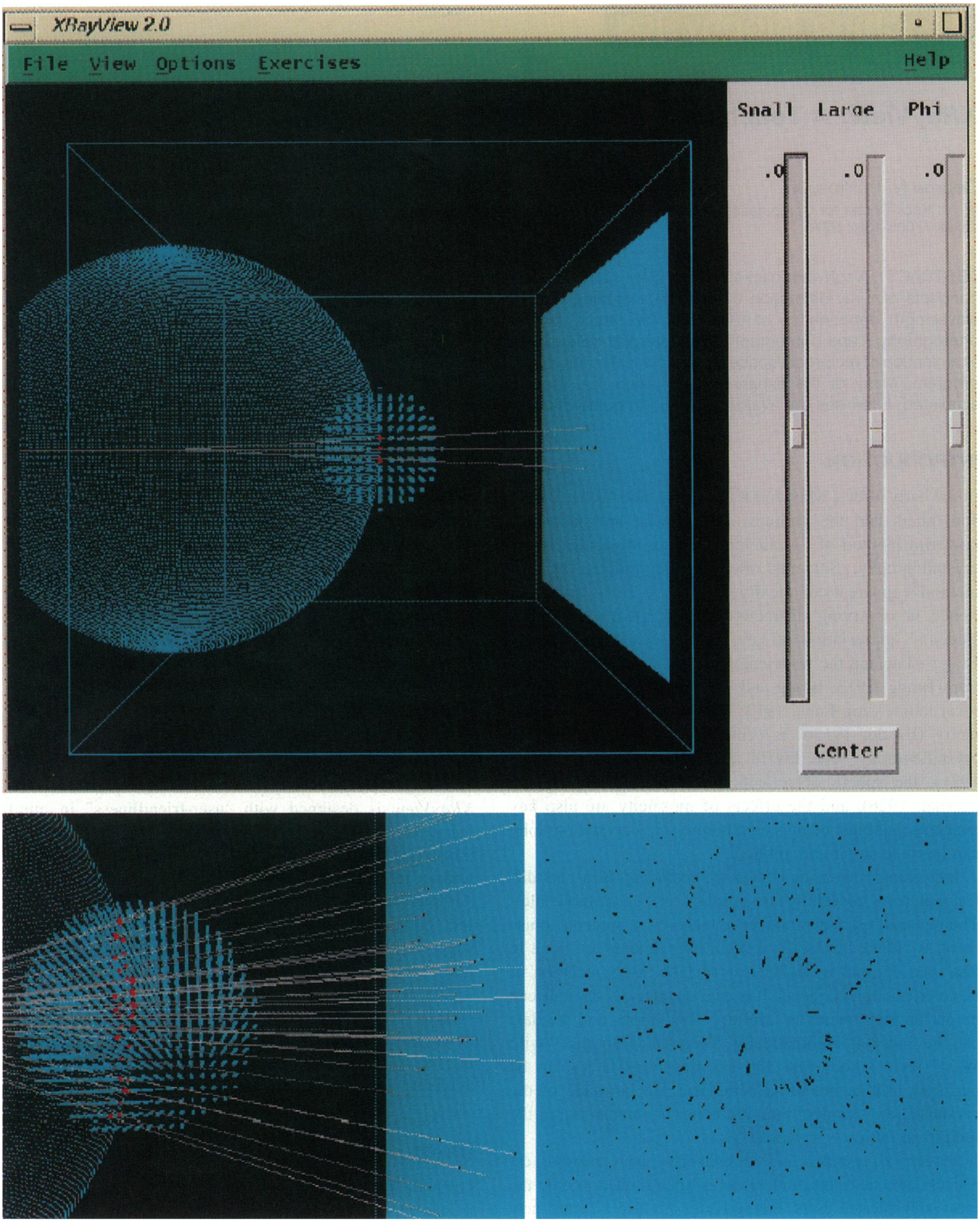

FIGURE 1 View of the main window (*top*). Pull-down menus (only headers shown) across the green bar allow the unit cell, wavelength, and other parameters to be changed. There are also a series of exercises that can be called on to guide the student. As the slide bars on the right are moved up and down, the crystal is reoriented and the resulting diffraction pattern is redrawn quickly in the window, thus providing interactive involvement. A close up of one of the key features of the program, the visualization of the reciprocal lattice and the Ewald construction, is shown at the lower left. Monochromatic

sired option. The pull-down windows are largely self-explanatory. The buttons at the bottom will either apply the constants and keep the window open ("Apply") or apply the constants and close the window ("OK").

The slide bars at the right control rotations of the crystal, with the rotations also corresponding to real-time reorientations of the reciprocal lattice. Definitions of the angles are consistent with a variety of area detectors and goniometer heads.

ON-LINE EXERCISES

Exercises are available on-line that can be assigned as homework in classes or used just for browsing. They begin simply and gradually increase in difficulty, with the goal of teaching the students how to control many experimental parameters often encountered in real data collection situations. Exercise 1 in the current version of the program includes introduction of the reciprocal lattice and the Ewald construction, the inverse relationship of the real and reciprocal lattices, and the wavelength dependence of the diffraction pattern (Fig. 1, *lower left*). Exercise 2 shows how Laue circles result from the intersection of reciprocal lattice planes with the Ewald sphere and how to achieve an alignment along a crystal zone by recognizing the Laue circles and moving the crystal in appropriate directions. Exercise 3 illustrates the effect of mosaicity on the diffraction pattern and explains both the common definitions of the Ewald sphere and the reciprocal lattice, i.e., one with the radius of Ewald sphere as 1, and the other with radius of 1 divided by the wavelength.

Simulations of rotation photographs can be achieved by turning on "integration" under the View menu as in Exercise 4. This exercise allows students to recognize why overlap of diffraction spots requires finite angular ranges and also teaches how exploring small regions of reciprocal space can be more helpful in seeing the reciprocal lattice than are still photographs.

Space groups of "unknowns" can be determined in Exercise 5 by examination of the reciprocal lattice in "rotation" photographs. By hiding the reciprocal lattice and the Ewald sphere during this exercise and just looking at the diffraction patterns, this exercise closely mimics the determination of space groups in real structural analyses. Laue photographs can also be simulated (Exercise 6) by gradually changing the wavelength while integrating the diffraction pattern (Fig. 1, *lower right*).

USE OF *XRayView* ON RESEARCH PROJECTS

XRayView is also useful for research purposes, allowing "simulation" of many real diffraction effects. In my laboratory, we have found it useful for guiding the reorientation of crystals from being aligned along one zone to another and for verifying reciprocal lattice symmetry effects in real "unknowns."

HOW TO OBTAIN *XRayView*

XRayView is available free to universities and other educational institutions and by special arrangement with other organizations. Any proceeds are used for further development of educational software for teaching purposes, including improvements to *XRayView*. Executables of the program are available via the World Wide Web at http://www-bioc.rice.edu/XRayView. Source code is available by special arrangement.

For information not available from the web site, or for additional information or comments please contact:

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x-rays strike the surface of the detector or film only if reciprocal lattice points "touch" the sphere of reflection (*red dots*), defined by a radius equal to 1 and centered at the crystal (*large sphere at left*). Layers of the reciprocal unit cell lattice can be seen on the surface of the detector. Multiwavelength Laue photographs (*lower right*) can also be simulated by varying the wavelength with the program in "integration mode." The critical role of mosaicity and wavelength range in Laue photography can then be appreciated easily.