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JECP/SP: A computer program for generating stereographic projections, applicable to specimen orientation adjustment in TEM experiments

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1. The crystallographic problem

Stereographic projection (SP) is an important crystallographic tool in carrying out electron diffraction experiments and in the analysis of crystal structures and defects. There are several commercial or public-domain computer programs available that allow users to draw stereographic projections of direct and reciprocal space. While these programs are often sufficient for regular use, there are always situations when the user will need to perform a certain operation that is not a feature of any of the existing programs. In the present work, a computer program was written for generating stereographic projections and was also extended as an application for specimen orientation adjustment in TEM experiments.

Computer-assisted specimen orientation adjustment in TEM experiments would be especially useful under certain circumstances, for example, when (i) a severely stained specimen is observed and the visibility of Kikuchi line pairs is thus poor; (ii) a beam-sensitive specimen is examined, and thus it is essential to shorten the time spent on specimen tilting when the electron beam is illuminating the area of interest; (iii) a small-grain-size specimen is investigated, for which even a slight orientation adjustment may cause the corresponding diffraction pattern to disappear due to a lateral sample shift; and (iv) a crystalline specimen is used in acquiring electron diffraction intensities of reachable zone-axis patterns for structure determination. In these cases, under the guidance of this software, the microscope can be kept in the image mode when the specimen is tilted. The holder is tilted to the computer-predicted angles and the illuminated area of the specimen is kept in the area of interest or in some neighboring area until the target tilt angles have been obtained, afterwhich it is moved to the area of interest.

2. Method of solution

Chou (1987) developed a computer program for specimen orientation adjustment using a double-tilt or rotation holder (implemented on microcomputers with 32 kbyte RAM). The design of *JECP/SP* is greatly influenced by Chou's work. A slightly different algorithm was adapted in the present work and a concise graphic user interface is provided.

JECP/SP is a fully functional tool for generating stereographic projections in direct and reciprocal space. To generate a stereographic projection, the user needs to provide the crystalline lattice parameters, a, b, c, α, β, γ, and the projection direction, [uvw] or (hkl). As an option, the Wulff net can be drawn in the generated stereographic projection. Details of the construction and usage of stereographic projections can be found in most books in crystallography. Methods of implementation of stereographic projections in computer programs can be found in the books by De Graef (2003) and Edington (1975).

JECP/SP has been extended as an application for specimen orientation adjustment using a TEM holder. To generate a stereographic projection as a guide map in TEM experiments, the user also needs to provide information about the currently observed electron diffraction pattern: the zone axis [uvw], tilting (or rotating) angles of the TEM holder, and the angle between one selected reciprocal vector $\mathbf{g}(hkl)$ and the projection of the TEM holder on the fluorescent screen of the microscope. With these input parameters, the user obtains a stereographic projection with a projection zone axis calculated under the condition of the TEM holder in its initial status (tilting and/or rotating angles are zero). The guide map provides all zone axes with computer-predicated tilting/rotating angles. As an option, the tilting limitation of the TEM holder can also be drawn in the generated stereographic projection.

JECP/SP can be used as a teaching aid for students in crystallography as well as a practical tool for scientists performing TEM experiments.

3. Program specification

The program is written in Java using JDK1.3 (Java Development Kit) from Sun Microsystems (Sun Microsystems, 2000). The program was designed and tested under Microsoft Windows 98 and XP.

4. Software and hardware environment

For executing *JECP/SP*, a Java virtual machine, *i.e. J2RE*, must be installed on the computer. Any computer capable of supporting *J2RE* should support *JECP/SP*. No special hardware is required.

5. Documentation

Documentation on the design and implementation of *JECP/SP*, together with a user manual, is provided in the form of an HTML file. An online version of this documentation is available at http://www.unl.edu/CMRAcfem/XZLI/programs.htm .

6. Availability

The program in compressed form (jecp_sp.zip) including a specification file is available at http://www.unl.edu/CMRAcfem/XZLI/programs.htm . A registration code can be obtained by e-mail (xli2@unl.edu) from the author. Without a registration code, this program works in demonstration mode only.

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