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Xingzhong Li

University of Nebraska-Lincoln, xli2@unl.edu

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SPECIFICATION OF JECP/SP: STEREOGRAPHIC PROJECTION WITH AN APPLICATION FOR SPECIMEN ORIENTATION ADJUSTMENT USING TEM HOLDERS

by X.Z. Li

Center for Materials Research and Analysis, University of Nebraska, Lincoln, NE 68588

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1. Purpose of the program

JECP/SP is a computer program in **J**ava **E**lectron **C**ystallography **P**ackage. JECP is developed for quantitative electron diffraction and image processing, the package is designed and written by Dr. XingZhong Li.

JECP/SP provides the all necessary functions of stereographic projection for regular application and furthermore it can be used to minimized the difficulties encountered when tilting highly beam-sensitive, or small-grain-size specimens with known structures using either a double-tilt or a rotation holder.

JECP/SP can be used as a teaching aid for students on fundamental crystallography as well as a tool for scientists working on TEM experiments.

2. Graphic user interface and program design

The java classes in JECP/SP can be classified into two groups:

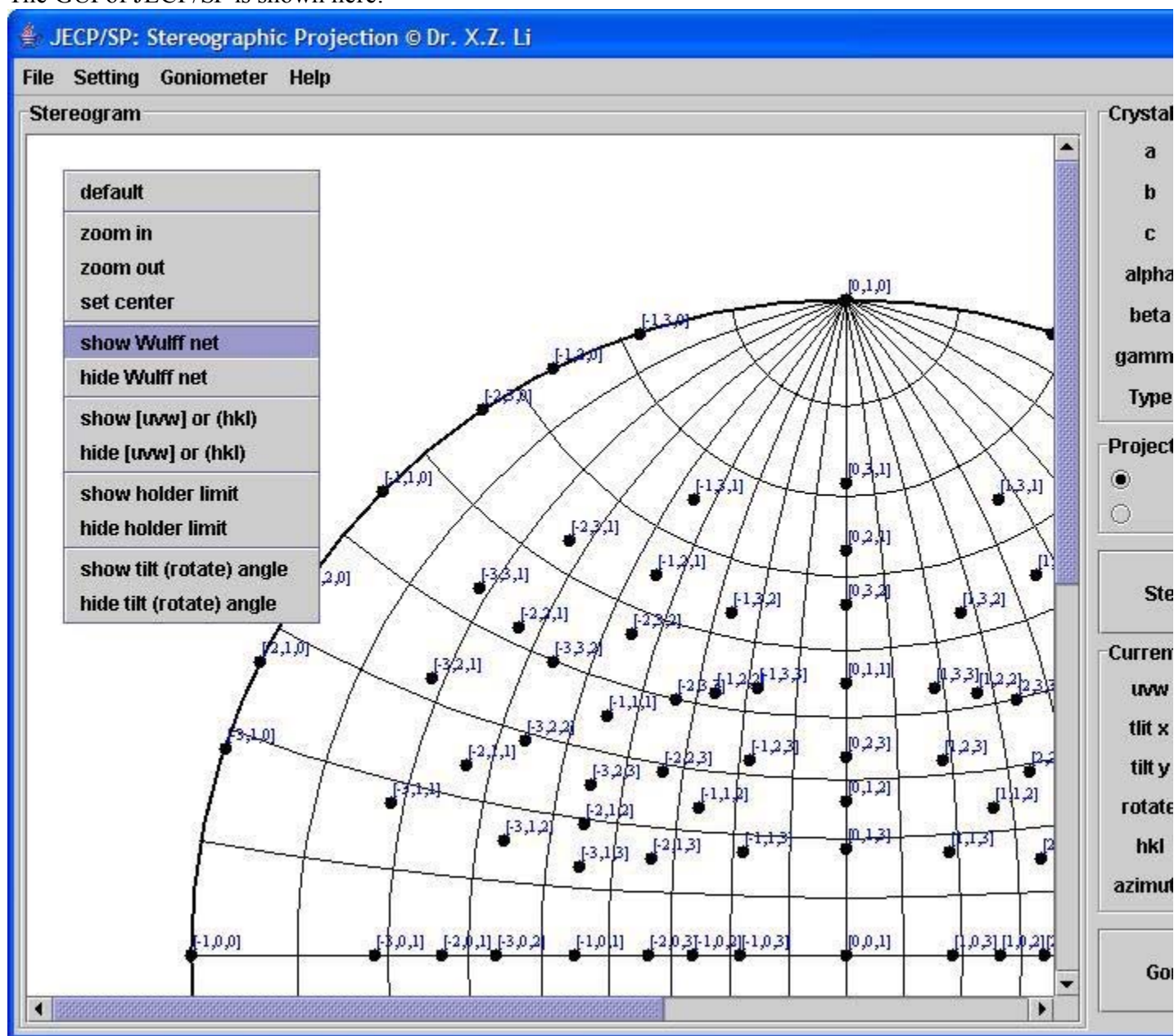
i) GUI and Wulff net

- StereogramGUI.java (extends JFrame and includes a JMenuBar).
- StereogramControlPane.java (extends JPanel with a side control pane)
- WulffNet.java (extends JPanel to show Wulff net and projection poles)
- WulffNetControlPane.java (extends JScrollPane and includes a JPopupMenu)

ii) Crystallographic calculation on stereographic projection

- CrystalLattice.java (a data structure to hold the lattice parameters and type)
- hklPole.java (a data structure for hkl pole projection)
- uvwPole.java (a data structure for uvw pole projection)
- Stereogram.java (calculation routine for stereographic projection)

The GUI of JEC/SP is shown here.



3. Crystallographic principle and implementation

3.1 Wulff net

Wulff net, or stereographic net, is a stereographic projection of the longitude and latitude lines on a sphere, which can be drawn (sphere radius = 1) as two series of circles with their center and radius defined as below:

Longitude lines:

$$y^2 + (x \pm 2/\tan(\varphi))^2 = (2/\sin(\varphi))^2 \quad (1)$$

Latitude lines:

$$(y \pm 2/\cos(\theta))^2 + x^2 = (2 \cdot \tan(\theta))^2 \quad (2)$$

The above formulae can be derived on the basis of the description of Wulff net in most books on crystallography.

3.2 Stereographic projection

There are many ways to calculate a stereographic projection map. Here we show how the routine was implemented in Stereogram.java:

i) Cartesian coordination for crystal lattice

The c axis of crystal lattice is chosen as the z axis of the coordinate system, the a axis is in x - z plane, and the b axis can be calculated.

ii) Stereographic projection

Stereographic projection was firstly calculated using (001) or [001] as default projection direction. Stereographic projection with the selecting (hkl) or [uvw] projection direction was obtained by rotating the generated projection map so that (hkl) or [uvw] becomes the projection direction.

3.3 Application for specimen orientation adjustment

The following parameters needed for the application of JEC/SP for specimen orientation adjustment:

- Lattice parameters
- Tilting or rotating angles (ϕ , θ) for an observed zone axis [uvw]
- Indices of selected reflection (hkl) in the zone pattern
- Angle between (000)-(hkl) and the projection of the holder on the fluorescent screen.

The application of stereographic projection for specimen orientation adjustment was also described in the paper by C.T. Chou (1987).

4. System requirement

For executing JEC/SP, a Java virtual machine, i.e., J2RE, must be installed on the computer.

5. The installation and user instruction

The executable bytecodes in compressed form (jecp_sp.zip) including this specification file is available at <http://www.unl.edu/CMRAcfem/programs.htm>. For the latest updates and news about JEC/SP and other JEC/SP programs are available in the above site.

Unzip the installation file jecp_sp.zip in a selected directory and execute jecp_sp.jar (mouse double click or type 'java -jar jecp_sp.jar' or click jecp_sp.bat for MS win9x or winXP).

i) A GUI is shown as above. Crystal Lattice file can be read in menu bar or directly input in the text field in right side of GUI.

ii) Select the type of stereographic projection: uvw or hkl and input the projection direction.

iii) Click 'Stereogram' button, a stereographic projection map is generated. A pop-up menu can be selected by right click on mouse, which provides options

- to zoom the map

- to show or hide indices of the poles
- to show or hide Wulff net
- to show or hide the tilt/rotate angle to reach the zone axis if applicable.
- to show or hide the limitation of the TEM holder.

iv) Using a TEM holder to tilt/rotate crystal to get a zone axis pattern. Input the tilt/rotate angles and selected one reflection and its azimuth angle. Click 'Goniometer' button, a stereographic projection map is generated with the information about the tilt/rotate angles to get the selected zone axis pattern.

6. How to contact the author

Suggestion and bug reports are welcome (xli2@unl.edu).

A registration code can be obtained by e-mail from the author. Without registration code this program works in demo mode.

7. References

Chou, C.T. (1987). J. Elec. Micros. Tech. 7, 263-268.

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