Supplementary material

(1) JECP/HOLZ specification
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(3) Simulation of ZnO HOLZ (straight and curved line) patterns
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SPECIFICATION OF
JECP/HOLZ, AN INTERACTIVE COMPUTER PROGRAM FOR
SIMULATION OF HOLZ PATTERN

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Contents:

1. Purpose of the program

JECP/HOLZ (Li, 2005a) is one computer program in the Java Electron Crystallography Package (JECP), which is designed and written by Dr. XingZhong Li. The package is developed for quantitative electron diffraction and image processing purpose,

JECP/HOLZ is an interactive program for simulation of the higher-order Laue zone (HOLZ) lines using kinematical approximation and a first-order dynamic correction.

JECP/HOLZ 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 (GUI) and program design

The selected Java classes in JECP/HOLZ are listed here:

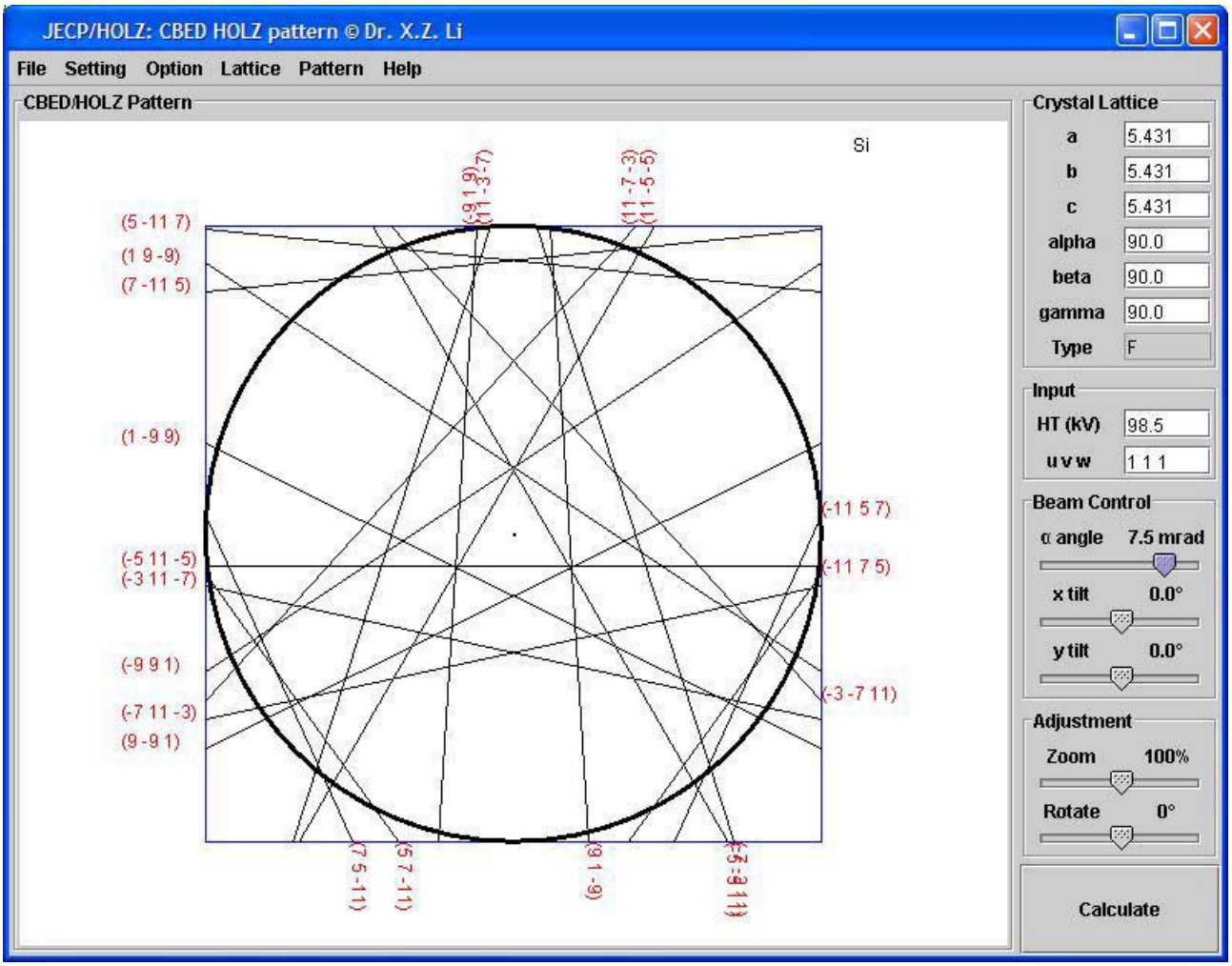
2.1 GUI

- holzGUI.java (extends JFrame and includes a JMenuBar).
- holzControlPanel.java (extends JPanel; input parameters)
- holzPattern.java (extends JPanel to show HOLZ reflections and lines)

2.2 Crystallographic calculation on stereographic projection

- CrystalLattice.java (a data structure to hold the lattice parameters and type)
- CrystalStructure.java (a data structure to hold the atom types and positions)
- HOLZ.java (implementation of the formulas for calculation of the HOLZ lines)
- KinematicCalculation.java (electron diffraction calculation using the kinematical theory)

2.3 A Snapshoot of JECP/HOLZ



3. Formulas for calculating the positions of the HOLZ lines

3.1 Formulas of the HOLZ lines under kinematical theory

A HOLZ line in the kinematical approximation is the locus of the Bragg condition for a HOLZ reflection **g**. The incident beam **k** is described as $\mathbf{k}_n$ along **-z** and $\mathbf{k}_t$ in **(x, y)** plane. We may think of the HOLZ line as a function of K_t, a vector which originates in the center of the zone axis and extends to a point of interest in the central disk, the trajectory is described by the following two equations (Spencer and Zuo, 1992):

$$g_x k_x + g_y k_y - g_z k_z + \frac{g^2}{2} = 0 . \qquad (1)$$

$$k_z = \sqrt{(k^2 - k_x^2 - k_y^2)} \qquad (2)$$

Here $g^2 = g_x^2 + g_y^2 + g_z^2$. If we use a paraboloid equation, $k_z = k - \frac{k_x^2 + k_y^2}{2k}$ as an approximation of the sphere equation, $k_z = \sqrt{(k^2 - k_x^2 - k_y^2)}$, we end up with an equation for the HOLZ line trajectory (Li, 2005b):

$$(k_x + \frac{g_x}{g_z}k)^2 + (k_y + \frac{g_y}{g_z}k)^2 = k^2 + (\frac{g}{g_z}k)^2 - \frac{g^2}{g_z}k \qquad (3)$$

In the early work by Tanaka and Terauchi (1985) and also in a recent book by De Graef (2003), the formation of the HOLZ is interpreted as the intersection of a HOLZ reflection disk with the Ewald sphere. If we increase the beam convergence angle to obtain a convergent beam pattern, then each reciprocal lattice point becomes a disk, with each point in the disk corresponding to a difference incident beam direction. The HOLZ reflections also become disks that are parallel to the HOLZ layers. The intersection of these disks with the Ewald sphere, which is inclined with respect to the HOLZ layer, is a (curved) line segment across the disk. For the beam orientations corresponding to this line segment, electrons will be dynamically scattered out of the transmitted beam and into the HOLZ beam. Thus the equation for HOLZ trajectory is,

$$(k_x + g_x)^2 + (k_y + g_y)^2 = r^2 = k^2 - (k_z - g_z)^2 \qquad (4)$$

3.2 Formulas of the HOLZ lines under a first-order dynamical correction

The first-order dynamical correction was developed for the simplicity in calculation (Bithell and Stobbs, 1989; Lin et al. 1989; Zuo, 1992). In the first-order dynamical correction, it is assumed that only weak interactions occur between HOLZ reflections, the position of a HOLZ line in the central disc can be approximated by finding the intersection between the zero-layer dispersion surface ($k_1=k_0+\gamma^{(1)}$, here $\gamma^{(1)}$ is the distance of the topmost excited branch of the dispersion surface from the sphere at the zone axis itself) and a plane-wave sphere centered on the HOLZ reflection.

When the incident beam is far away from a zone axis, the first branch of the dispersion surface can be approximately considered as sphere with radii of $k_1=k_0+\gamma^{(1)}$. Thus, the dynamically corrected HOLZ-line equation is derived as (Li, 2005b):

$$g_x k_x + g_y k_y - g_z k_z + \frac{g^2}{2} + g\Delta g = 0 \qquad (5)$$

Here $g\Delta g = (k\gamma^{(1)} + \frac{\gamma^{(1)2}}{2})$.

When the incident beam is near or at a zone axis, the first branch of the dispersion surface can be approximately considered as a flat plane with a distant of $k_1=k_0+\gamma^{(1)}$ to the origin of reciprocal lattice [2, 8]. Thus, the dynamically corrected HOLZ-line equation is derived as (LI, 2005b):

$$(k_x + g_x)^2 + (k_y + g_y)^2 = r^2 = k^2 - (k_z + \gamma^{(1)} - g_z)^2 \qquad (6)$$

4. System requirement

For executing JECP/HOLZ, a Java virtual machine, i.e., the J2SE Java Runtime Environment (JRE), must be installed on the computer. Any computer capable of supporting J2RE should be suitable for running JECP/HOLZ. No special hardware is required.

5. Installation and user instruction

The executable bytecodes in compressed form (jecp_holz.zip), including this specification file in PDF format, is available at http://www.unl.edu/CMRAcfem/XZLI/programs.htm.

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

Tips:

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 graphic mode for the HOLZ reflections, the HOLZ lines (straight or curve lines) from menu bar Pattern.

iii) HOLZ pattern can be illustrated while an interactively changing of high voltage, beam direction, lattice parameters, convergent angle.

iv) There is an option to index the HOLZ pattern in menu bar Option.

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

Bithell, E.G. and Stobbs, W.M. (1989). *J. Microscopy* **153**, 39-49.
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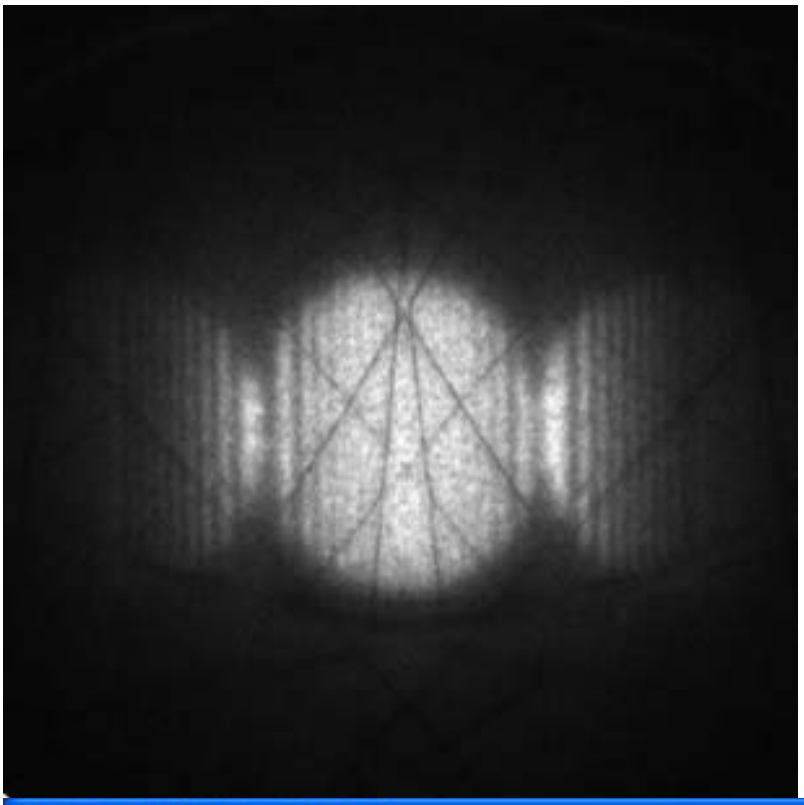
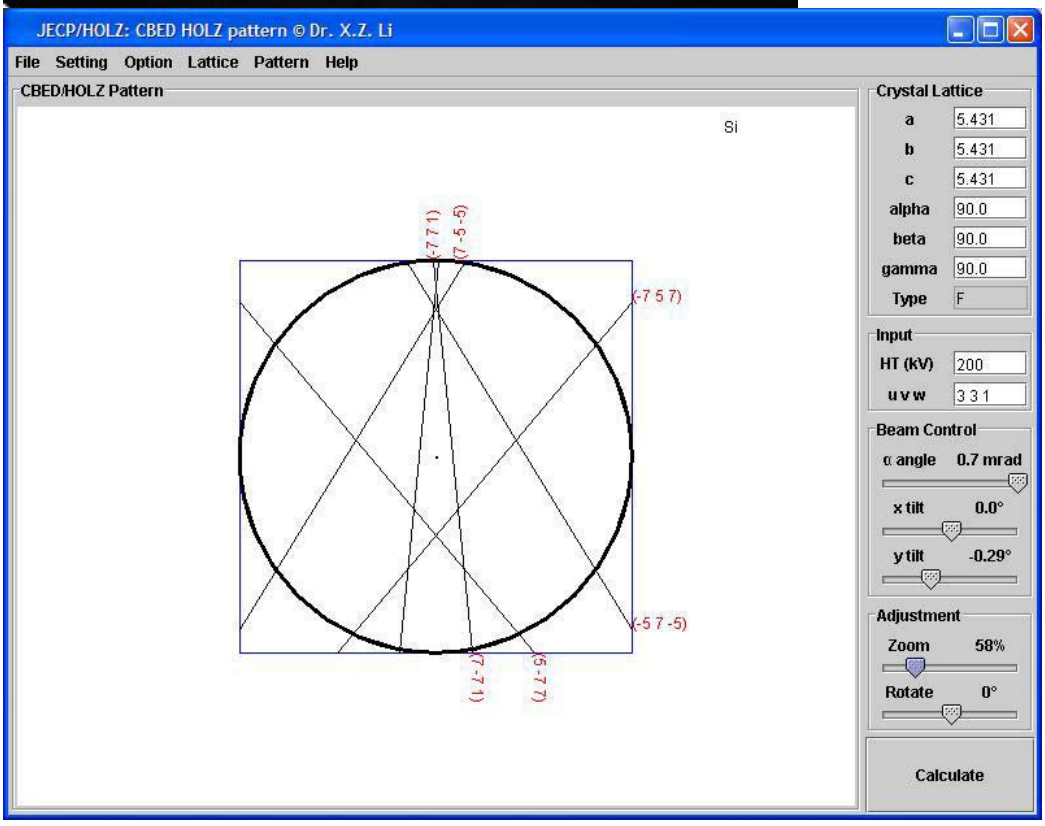
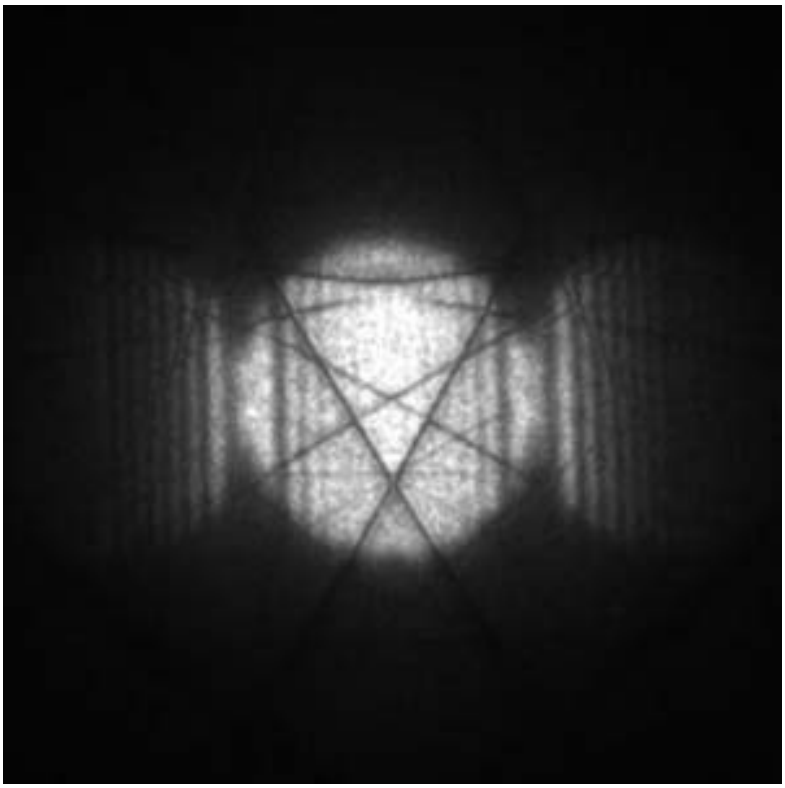
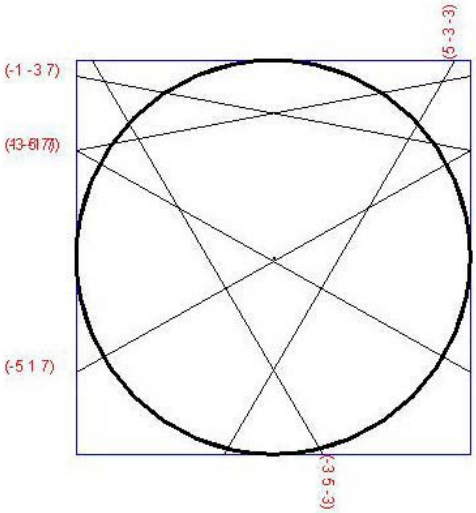
Experimental and simulated HOLZ patterns of Si [331]



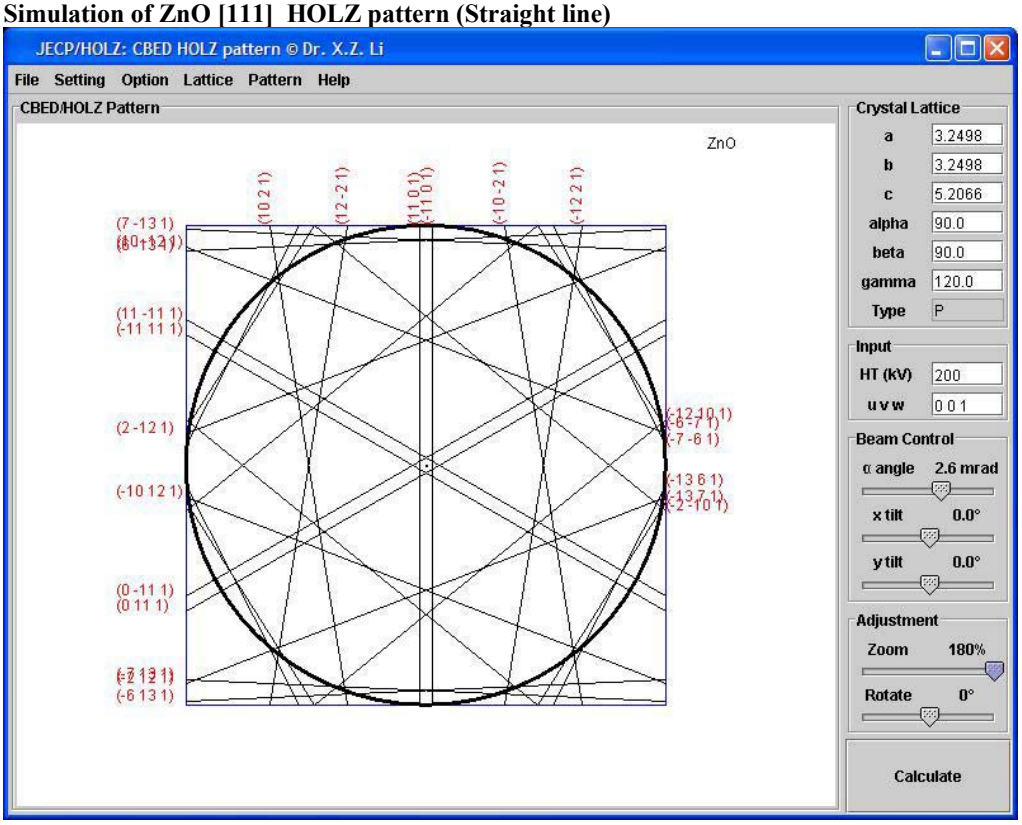


Experimental and simulated HOLZ patterns of Si [553]

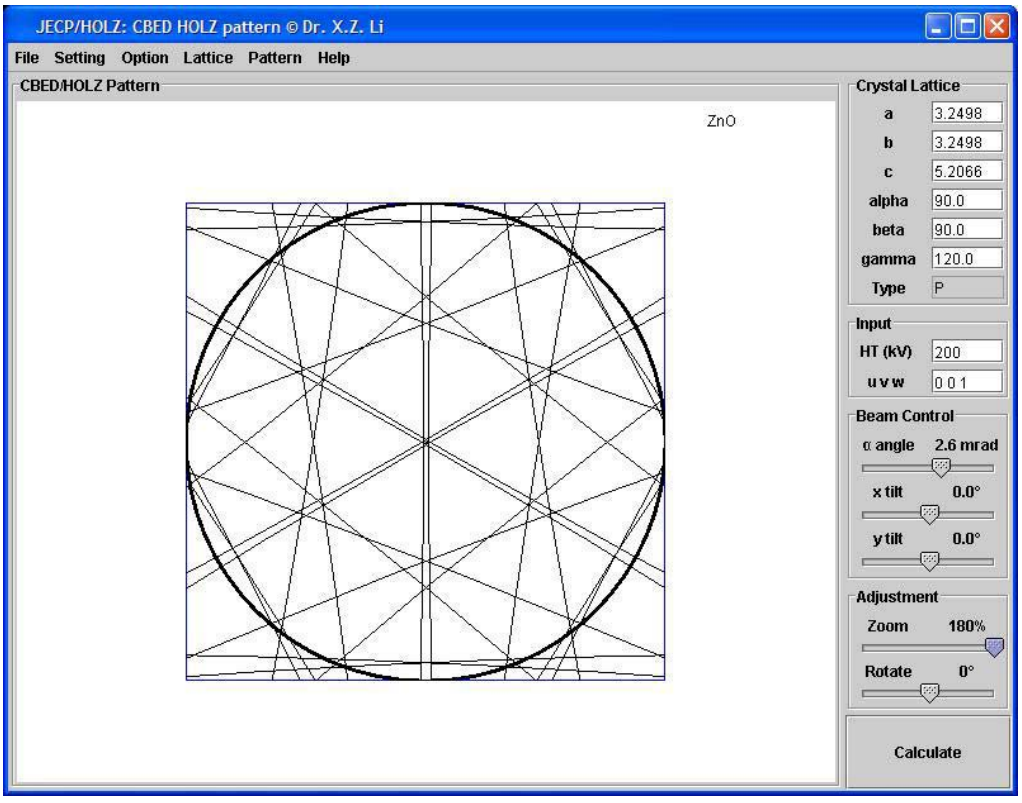




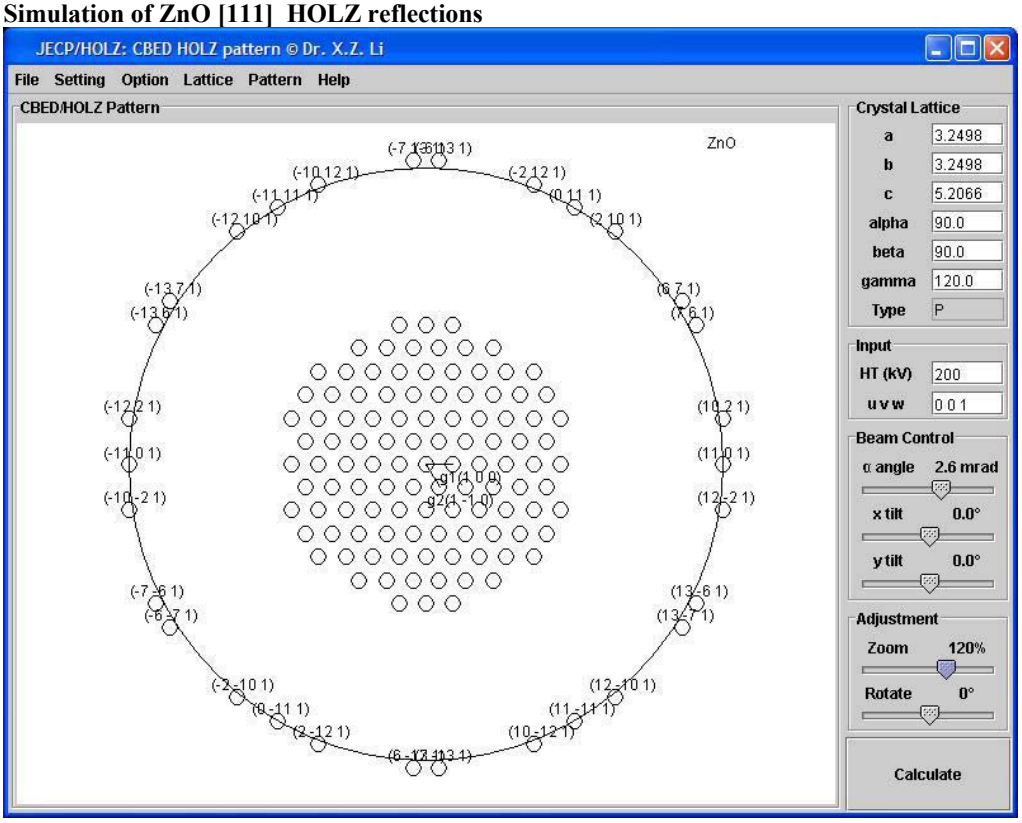
Simulation of ZnO [111] HOLZ pattern (Straight line)



Simulation of ZnO [111] HOLZ pattern (Curved line)



Simulation of ZnO [111] HOLZ reflections



Simulation of ZnO [111] HOLZ pattern (Straight line under beam tilt)