JECP/HOLZ, an Interactive Computer Program for Simulation of HOLZ Pattern

(Version 2t)

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1. Purpose of the program

JECP/HOLZ (Li, 2005) is one computer program in the Java Electron Crystallography Package (JECP), which is designed and written by Dr. X.Z. Li. The package is developed for (semi-)quantitative electron diffraction analysis 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/HOLZ2a is the second version of JECP/HOLZ. HOLZ2a has improvement over HOLZ including but not limited to the following,

- improved GUI with a display panel and a HOLZ dialog.
- add intensity threshold in HOLZ dialog for easy adjustments.
- a new display system to better show the labels for CBED pattern.
- a new display system to better show the HOLZ index.
- crystal constraint for fine tuning of lattice parameters.
- allow to save the HOLZ pattern to .jpg and .tif.
- improved i/o fold system for easy input/output data/patterns.
- incorporate with Landyne launcher.

JECP/HOLZ2t is the current version of JECP/HOLZ. HOLZ2t updates the GUI menu and upgraded with the elemental periodic table and the space group table, HOLZ2t 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

A snapshots of the JECP/HOLZ2t panel with a HOLZ pattern.

This is snapshots of the JECP/HOLZ2 panel with a CBED pattern.
This is the HOLZ dialog and index dialogs for HOLZ and CBED patterns.
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 \( \mathbf{g} \). The incident beam \( \mathbf{k} \) 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 \( \mathbf{K}_t \), 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):

\[
g_x k_x + g_y k_y - g_z k_z + \frac{g^2}{2} = 0 \quad \text{......(1)}
\]

\[
k_x = \sqrt{\mathbf{k}^2 - k_y^2 - k_z^2} \quad \text{......(2)}
\]
Here \( g^2 = g_x^2 + g_y^2 + g_z^2 \).

If we use a paraboloid equation, as an approximation of the sphere equation, \( k_z = k - \frac{k_x^2 + k_y^2}{2k} \), we end up with an equation for the HOLZ line trajectory (Li, 2007):

\[
(k_x + \frac{g_x}{g_z} k)^2 + (k_y + \frac{g_y}{g_z} k)^2 = k^2 + (\frac{g_y}{g_z})^2 - \frac{g_x^2}{g_z} k \quad \ldots \ldots (3)
\]

In the early work by Tanaka and Terauchi (1985) and also in a 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,

\[
(k_x + g_x)^2 + (k_y + g_y)^2 = r^2 = k^2 - (k_z - g_z)^2 \quad \ldots \ldots (4)
\]

### 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, 2007):

\[
g_x k_x + g_y k_y - g_x k_x + \frac{g_x^2}{2} + g \Delta g = 0 \quad \ldots \ldots (5)
\]

\[
g \Delta g = (k \gamma^{(0)} + \frac{\gamma^{(0)2}}{2})
\]

Here

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, 2007)
\[(k_x + g_x)^2 + (k_y + g_y)^2 = r^2 = k^2 - (k_x + g^{00}_x - g_z)^2 \quad \ldots\ldots (6)\]

4. Installation and user instruction

JECP/HOLZ2t is coded mainly in Java and partially coded for PC with Microsoft windows only. To run the software, a recent version of Java Runtime Environment (e.g., JRE 1.8.0_60), must be installed on a PC for XP or up version of Microsoft window.

The executable bytecodes (holz2.exe and jecp_holz2.jar) are packed in .z7 form. The compressed file is available at http://www.unl.edu/ncmn-cfem/xzli/computer-programs. For the latest updates and news about JECP/HOLZ2 and other Landyne programs, please visit in this website.

Decompress the installation file holz2.z7 in a selected directory and execute holz2.exe by double click or use Landyne launcher.

The basic steps for using JECP/HOLZ2,

i) Crystal data file can be read in menu bar and modified in the fields of the lattice parameters in HOLZ dialog.
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 displayed while an interactively changing of high voltage, beam direction, lattice parameters, convergent angle.
iv) There are dialogs to index the HOLZ pattern and CBED pattern.

5. Feedback and license

Suggestion and comments are welcome, please send to Dr. X.Z. Li (jlandyne@gmail.com). License can be purchased from LANDYNE (jlandyne@gmail.com). Without validated license this program works in demo mode.

6. References