Table of Contents

1. Purpose of the program .................................................................2
2. Graphic user interface and program design .........................................3
3. Formulas for calculating the positions of the HOLZ lines .................................4
4. Installation and user instruction ........................................................6
5. Licenses and feedback ......................................................................7
6. References ......................................................................................7

1. Purpose of the program

JECP/HOLZ (Li, 2005) is one component in the Landyne suite for simulation of electron diffraction and crystallographic analysis developed by Dr. X.Z. Li for (semi-)quantitative electron diffraction analysis and image processing. It can be used as a teaching aid for students on fundamental crystallography and a tool for scientists working on TEM experiments.

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

The main improvement in version 2 is listed below,

- A GUI for a display panel and a HOLZ dialog has been improved.
- An intensity threshold has been available for easy adjustments.
- A display system has been updated to show the index on a CBED pattern.
- A display system has been updated to show the index on a HOLZ pattern.
- A crystal constraint has been introduced for tuning of lattice parameters.
- An I/O fold system has been improved for input/output data/patterns.

The current version is HOLZ3.

- The graphic user interface (GUI) has been upgraded.
- The software has been integrated with an elemental periodic table and the space group table.
- A figure label tool is provided, together with the region of interest (ROI), allowing the user to prepare figures ready for publication.
• An integrated interface is provided for saving a file in the TIFF, JPEG, and GIF formats.

2. Software design and features

The features in the HOLZ3 are briefly listed here,
1. A window frame with a panel is used to show the simulated HOLZ pattern and convergent electron diffraction pattern.
2. Input parameters for the calculation can be initialized with an operational panel and several dialog windows.
3. Input structure data files can be easily prepared using a computer assistant.
4. Region of interest, together with a label tool, is available to prepare figures for publication.

The HOLZ3 was written and compiled in Java 8. Further code optimization (including obfuscation) was carried out for the compiled class files.

Figure 1 shows a snapshot of the HOLZ3 panel with a HOLZ pattern of silicon. In contrast, Figure 2 shows a snapshot of the HOLZ3 panel with the corresponding electron diffraction pattern with a convergent angle.

![Figure 1](image-url)

Figure 1. A snapshot of the HOLZ3 panel with Si crystal structure as an example.
Figure 2. A CBED pattern corresponding to the HOLZ pattern in Fig. 1.

Figure 3 shows the control dialogs for the HOLZ3 software. For simulation, the lattice parameters can be loaded on the drop-down menu for the calculation of the HOLZ pattern. The parameters can be changed slightly on the controlling panel and the calculated pattern will be updated immediately. The other parameters for the HOLZ pattern are TEM high voltage and the zone axis of crystal sample. Converge angle and tilt away from the true zone axis can be simulated. The appearance of the pattern can also be adjusted. Index panel provides the various position options for optimal indexing of the HOLZ and the CBED patterns. Two types of the appearance of HOLZ pattern in straight line or curve are available.
3. Formulas for calculating the positions of HOLZ lines

3.1 Formulas of the HOLZ lines under the kinematical theory

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

\[
g_1 k_x + g_2 k_y - g_3 k_z + \frac{g^2}{2} = 0 \tag{1}
\]

\[
k_z = \sqrt{k^2 - k_x^2 - k_y^2} \tag{2}
\]

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, we end up with an equation for the HOLZ line trajectory (Li, 2007):

\[ k_z = k - \frac{k_x^2 + k_y^2}{2k} \]

As shown in the early work by Tanaka and Terauchi (1985) and the book by De Graef (2003), the formation of the HOLZ is interpreted to be the intersection of a HOLZ reflection disk with the Ewald sphere. Suppose we increase the beam convergence angle to obtain a convergent beam pattern. In that case, each reciprocal lattice point becomes a disk, with each point in the disk corresponding to a different 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 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,

\[ (k_x + g_x k_x)^2 + (k_y + g_y k_y)^2 = k^2 = (k_x - g_x)^2 \] ……(3)

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

The first-order dynamical correction was developed for simplicity in the 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 as the intersection between the zero-layer dispersion surface (\(k_1 = k_0 + \gamma(1)\)), in which \(\gamma(1)\) 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 a sphere with a radius of \(k_1 = k_0 + \gamma(1)\). Thus, the dynamically corrected HOLZ-line equation is derived as (Li, 2007):

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

\[ g\Delta g = (k_1^{(0)} + \gamma(1)^2) \]

Here

When the incident beam is near or at a zone axis, the first branch of the dispersion surface can be approximately considered a flat plane with a distance of \(k_1 = k_0 + \gamma(1)\) to the origin of the reciprocal lattice. Thus, the dynamically corrected HOLZ-line equation is derived as (Li, 2007)

\[ (k_x + g_x)^2 + (k_y + g_y)^2 = r^2 = k^2 - (k_x - g_x)^2 \] ……(6)
4. Installation and user instruction

HOLZ3 is coded in Java 8 and partially coded for PC with Microsoft Windows only. A recent version of Java Runtime Environment (e.g., JRE 1.8.0_xxx or above) must be installed on a PC with an MS-Windows 10 version to run the software.

The Landyne software suite, landyn5, including HOLZ3, is packed in .z7 form. The compressed file is available at

https://www.unl.edu/ncmn-enif/xzli/computer-programs
http://landyne.scienceontheweb.net

For the latest updates and news about HOLZ3 and other Landyne components, please visit the above website. Decompress the landyne5.z7 in a selected directory and use the Landyne launcher, landyne5.exe.

The basic steps for using the HOLZ3,

i) A crystal data file can be read in the menu bar and modified in the fields of the lattice parameters in the HOLZ dialog.

ii) Select the HOLZ reflections' graphic styles, the HOLZ lines (straight or curved lines) from the menu bar Pattern.

iii) HOLZ pattern can be calculated using an interactively changing voltage, beam direction, lattice parameters, and convergent angle.

iv) There are dialogs to index the HOLZ pattern and CBED pattern.

v) A pattern in ROI, together with the figure label, can be saved to a file in TIFF, JPEG, and GIF format.

Although only lattice parameters are involved in the HOLZ, we usually use the crystal structure file for Landyne suit as the input file. A new crystal structure data file can be prepared using the New Crystal Structure File dialogue window (more details see SVAT). The dialogue window provides an automatic assistant for the user and makes sure to meet the requirement of the file format. The template is embedded with the 230 space groups in the Hermann-Mauguin notation, which list in the international table for crystallography. To save the data structure, click the Save button; or make a new one click the New button.

The crystal file can be also converted from a previous data for modification or from a crystallographic information file (CIF). If a data file in an alternative setting of space group for triclinic, monoclinic and orthorhombic systems is used, please click on the alternative settings (1~74). A tool for the transformation of files in the nonconventional notations to the standard notations is provided.

5. License and Feedback
Suggestion and comments are welcome; please send to Dr. X.Z. Li (jlandyne@gmail.com). A license is available from LANDYNE (jlandyne@gmail.com). Without a validated license, this program works in a demo mode.

6. References


Zuo, J.M., Automated lattice parameter measurement from HOLZ lines and their use for the measurement of oxygen content in YBa$_2$Cu$_3$O$_{7-\delta}$ from nanometer-sized region, *Ultramicroscopy* 41 (1992) 211.