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Landyne - a Software Suite for Electron Diffraction Simulation and Analysis

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Landyne software suite is the 2.0 version of the previous JECP—a java electron crystallography project [1]. The software suite currently includes eight stand-alone programs for electron diffraction simulation and crystallographic analysis. Each of them was designed for one topic of application in simulation, analysis or data processing. It hopes that the programs are grouped into a suite to increase the total usefulness. A launcher was developed recently for the software suite, which is a tool for the user to conveniently access all of the programs.

The purpose of this software suite is twofold: i) as research tools to analyze experimental results, ii) as teaching tools to show students the principles of electron diffraction and crystallography. Each program in this software suite provides some unique features for electron diffraction simulation and analysis. The executable codes, user manuals, specifications and a set of crystal structural data are available at http://www.unl.edu/ncmn-cfem/xzli/programs.htm. In this paper, the purposes and features of this software suite are briefly introduced. More details about each program can be found in the user manuals and specifications.

JECP/SVAT provides a 3D display of the crystal structure in a unit-cell, including the chemical bonds and magnetic moments. The structure can be analyzed (i) as a projection in a user-selected [uvw] direction or layer-by-layer, (ii) as a local structure (or polyhedral cluster) by defining a center atom and a radius of spherical range.

SPICA is the upgraded version of early JECP/SP [2], which was designed for stereographic projection with an application for specimen orientation adjustment using TEM holders; see a snap shot in Figure 1(a). SPICA inherits JECP/SP functions and expands many new functions, e.g. Kikuchi map, for crystallographic analysis with a more user-friendly GUI design.

SAED2s, as the successor of the previous JECP/ED [3], can be used to simulate electron diffraction patterns of a single phase, twining and coexisted multiple phases with fixed orientation and also to find the zone axis of the experimental diffraction pattern and indexing.

PCED2s is the updated version of PCED2.0 [4], which was for electron diffraction simulation of polycrystalline phase and for phase identification. The features include (i) an integral two-beam dynamical theory for intensity calculation, (ii) out-of-plane and in-plane texture and (iii) peak profile of diffraction ring. A snap shot of PCED2s is in Figure 1(b)

JECP/HOLZ2a is the upgraded version of JECP/HOLZ [5], which was 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 an improvement with an intensity threshold in HOLZ dialog for easy adjustments and a new display system to better show the labels for CBED and HOLZ patterns.

JECP/QSAED2a is an updated version of JECP/QSAED [6]. It can quantitatively retrieve/display the intensities of reflections in selected-area electron diffraction (SAED) patterns and precession electron diffraction (PED) patterns and to display/measure line profiles at SAED and PED pattern.

QPCED2t is an updated version of QPCED2.0 [7]. It was designed for digitization and quantification of polycrystalline electron diffraction patterns. It can also be used for correction of pattern with elliptical rings and display enhancement for a pattern with weak diffraction rings.

JECP/UC2b is an upgraded version of JECP/UnitCell [8], which was a program to determine unit cell of crystalline phase in TEM using both the reciprocal unit cell reconstruction approach and the reduced cell approach. The first approach is suitable for cubic, tetragonal, hexagonal, orthorhombic phases, but hard for monoclinic and impossible for triclinic phases. The second approach works for all seven types of crystalline lattices. However, it requests more accurate tilt angle comparing to the first approach.

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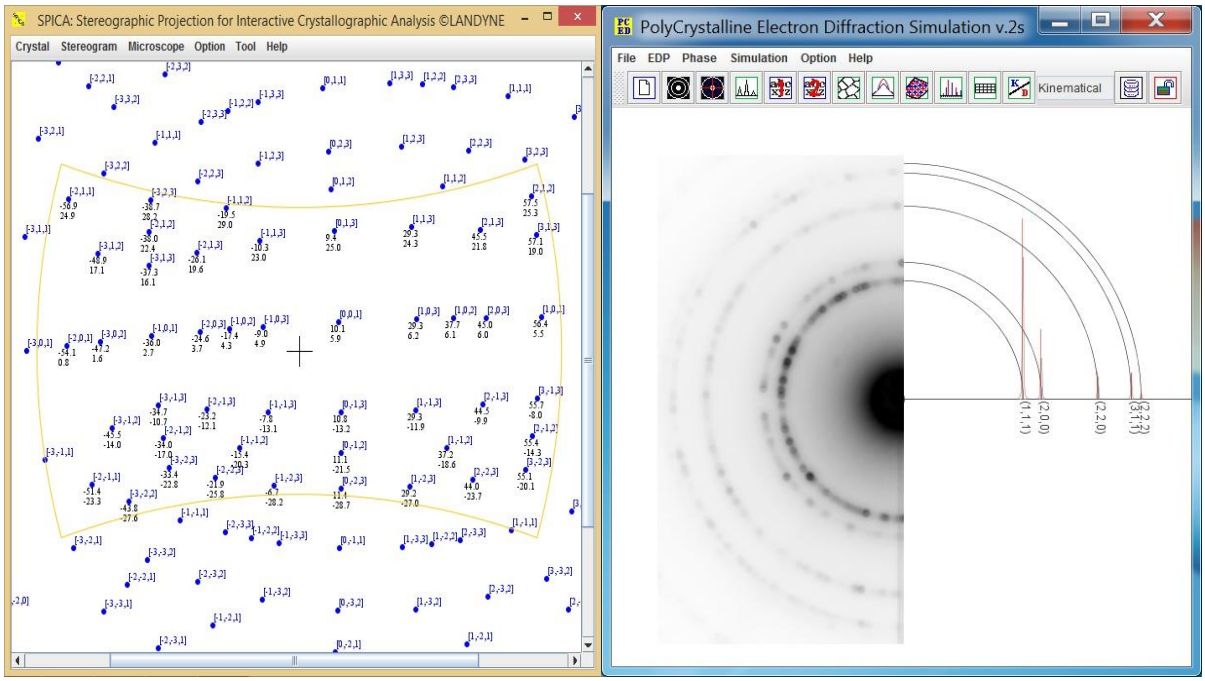

(a) (b)

Figure 1. Examples of Landyne software suite, snap shots of (a) SPICA and (b) PCED2s.

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