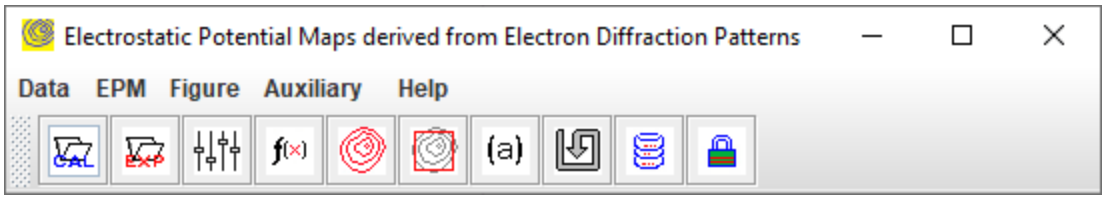
LANDYNE 蓝带软件

User Manual

Electrostatic Potential Maps derived from

Electron Diffraction Patterns



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1. Introduction

1.1 Landyne suite

The Landyne suite is a software package developed by Dr. X.-Z. Li for electron diffraction simulation and crystallography analysis since 2010. It can be used as both a research tool and a teaching aid. The current version includes 14 stand-alone software components, each designed for a specific application in simulation, analysis, or data processing. A launcher is available to conveniently access all software components. The executable codes, user manuals, and a set of crystal structural data are available on the author's https://landyne.com.

The software components were introduced in serval published papers, such as SVAT4 [2]. It provides a 3D visualization of crystal structures. SAED3 [3] is used to simulate electron diffraction patterns on a single-phase, twining and coexisted multiple phases. It has an extension for the projected atomic potential map. PCED6, as an updated version of PCED [4], is to simulate electron diffraction patterns from polycrystalline phase and phase identification. SAKI6 is used for simulation and analysis of Kikuchi patterns and simulation of double diffraction effect. A function is added recently for the precise determination of crystal orientation using an electron diffraction pattern with three Kikuchi pairs [5]. SPICA3 [6] is for stereographic projection with an application for specimen orientation adjustment using TEM holders. HOLZ3, as an upgraded version of JECP/HOLZ [7], is an interactive program for simulation of the higher-order Laue zone (HOLZ) lines using kinematical approximation and a first-order dynamic correction. QSAED6, as an updated version of QSAED4 [8], is used to quantitative retrieve/display the intensities of reflections on the electron diffraction patterns and measure line profiles on the electron diffraction pattern. QSAED6 has an extension for the projected atomic potential difference map. QPCED6, as an updated version of QPCED [9], is for processing and quantification of polycrystalline electron diffraction patterns. TEMUC3 [10] is a program to determine the unit cell of a crystalline phase in TEM using both the reciprocal unit cell reconstruction approach and the reduced cell approach.

1.2 Landyne plus ESPOT

Landyne Plus is a collection of multipurpose software that extends the capabilities of the Landyne suite. One notable component is ESPOT (ElectroStatic POTential maps), an extension of SAED6 and QSAED6. ESPOT is designed to calculate projected atomic potential maps from diffraction data generated by SAED6. These maps can be correlated with high-resolution scanning transmission electron microscopy (HR-STEM) images and high-resolution transmission electron microscopy (HR-TEM) structural images taken under Scherzer conditions. By combining the diffraction data retrieved from experimental patterns using QSAED6, users can obtain projected atomic potential difference maps to analyze and improve structural models.

This method is analogous to the approach used by X-ray crystallographers to calculate electron density maps and difference electron density maps [11]. Due to the geometry of electron diffraction, it is straightforward to obtain two-dimensional electron diffraction patterns. Consequently, ESPOT

was developed to calculate projected atomic potential maps and projected atomic potential difference maps.

ESPOT features two main interfaces: one for displaying the calculated diffraction pattern or comparing calculated and experimental diffraction patterns, and another for calculating and displaying the projected atomic potential map. It offers three types of projected atomic potential difference maps. More details of these features are described below.

Table 1. The components in the Landyne and Landyne+ software suites

Software	Description of components in the Landyne suite
PTELS	Periodic table of the elements for the Landyne suite
SVAT	Structural viewer and analytical tool including atom cluster and layer.
SPICA	Stereographic projection for interactive crystallographic analysis.
SAED	Simulation and analysis of electron diffraction (spot) patterns.
PCED	Simulation of PCED (ring) patterns and phase identification.
QSAED	Processing, quantification, and analysis of SAED (spot) patterns.
QPCED	Processing, quantification, and analysis of SAED (ring) patterns.
HOLZ	Simulation of HOLZ pattern including dynamical correction.
SMART	Simulation and measurement of rocking curve for crystal thickness.
SAKI	Simulation and analysis of Kikuchi lines and double diffraction effect.
TEMUC	Lattice determination of unknown structure in TEM/ED experiments.
ESPOT +	Electrostatic potential maps derived from electron diffraction patterns.
CTFscope +	CTF simulation and visualization for conventional and AC-TEM.
EMIPA +	HREM image processing and analysis
EMCIP +	HREM image crystallographic image processing

2. Design and features

2.1 Graphic design

The graphic user interface (GUI) of the ESPOT consists of a drop-down menu, a menu bar, a dual display panel for diffraction patterns and potential maps, and several operational dialogues. The size of the frame including the display panel can be readjusted by users. The drop-down menu provides all the options, and the menu bar offers more frequently used ones. Figure 1 shows the GUI of the ESPOT with a calculated diffraction pattern. The resolution circle in reciprocal space can be adjusted to generate a projected atomic potential map. Figure 2 shows the GUI of ESPOT with a projected atomic potential map. Multiple operational dialogues are shown in Figure 3.

2.2 Function features

Input data can be generated using SAED6 and QSAED6 in the Landyne software suite. As shown in dialogs in Figure 3, the diffraction pattern can be displayed with various options and allows it to be adjusted. The projected atomic potential maps can be calculated with user-defined grids using

input data from SAED6 only. The projected atomic potential difference maps have three types using data from SAED6 and QSAED6:

(i) 1 x calculated amplitude (phase).
(ii) 1 x calculated amplitude (phase) - 1 x experimental amplitude.
(iii) 2 x calculated amplitude (phase) - 1 x experimental amplitude.
(iv) 3 x calculated amplitude (phase) - 2 x experimental amplitude.

The various options on the contour map are available to display the projected (difference) atomic potential map.

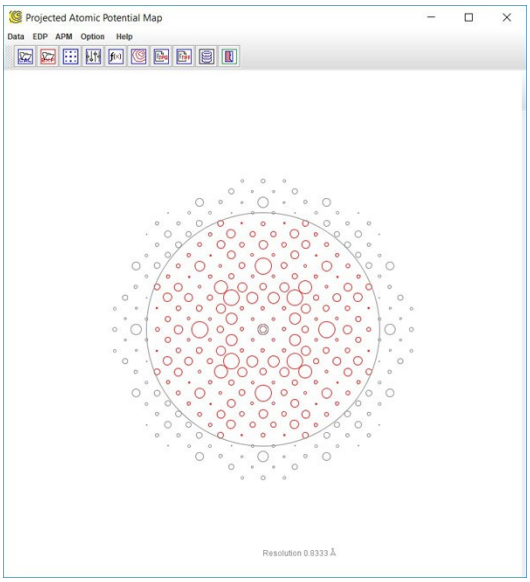

Figure 1. GUI of ESPOT with a calculated diffraction pattern. The resolution circle in reciprocal space is adjusted to generate a projected atomic potential map.

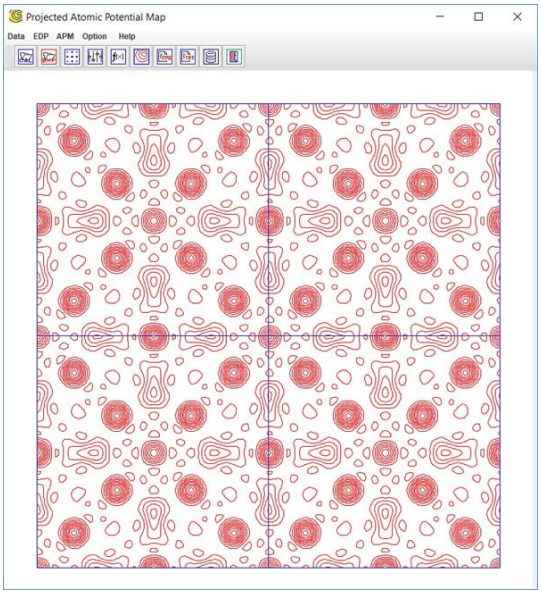

Figure 2. GUI of ESPOT with a projected atomic potential map.

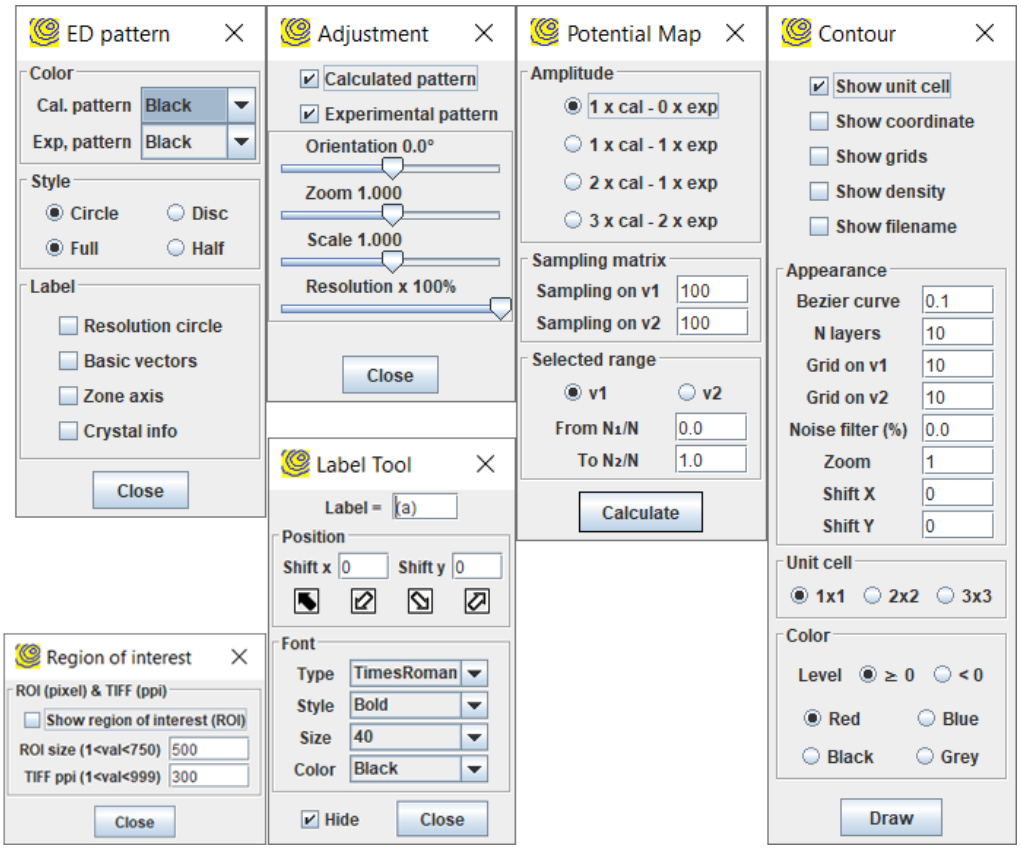

Figure 3. Multiple operational dialogues in the ESPOT.

3. Basic steps of operation

3.1 Preparation of the calculated diffraction data in SAED6

A template for the preparation of crystal structures is available in SAED6 or SVAT6. A simulated electron diffraction pattern can be generated and then saved as the input data for the ESPOT.

3.2 Preparation of the experimental diffraction data in QSAED6

The experimental diffraction data is retrieved from an experimental diffraction pattern using QSAED6. For nearly kinematical diffraction data, a thin area of the sample should be selected, and a nano-diffraction mode should be used, or a precession diffraction technique should be used.

3.3 Display of the calculated and experimental diffraction data

Load the input data in ESPOT; Click [display] in EDP to show the diffraction pattern with many options. [adjustment] in EDP allows to rotate, zoom, scale the diffraction pattern, and set the resolution for generating the projected atomic potential map. If the experimental data were also

loaded, the two diffraction patterns could be displayed side by side in different colors for comparison, as shown in Figure 4.

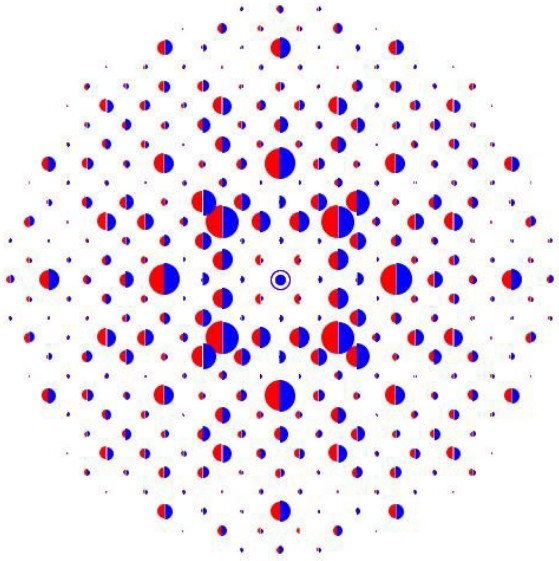

Figure 4. Comparison of two diffraction patterns, calculated pattern, and (simulated) experimental pattern.

3.4 Calculation and display of a projected atomic potential map

Only a calculated diffraction pattern is needed to generate the projected atomic potential map. Click [Calculation] in AMP to set up the number of grids and the region for a contour map. Calculation of the map data using option 1: the amplitude 1 x – 0 x mode. Click [Draw] to display the projected atomic potential map.

If both calculated and experimental diffraction data are loaded, the projected atomic potential difference map can be calculated using the amplitude in 1x - 1x, 2x - 1x, or 3 x – 2x modes. These maps can be used to check why the calculated pattern is different from the experimental one and then make the improvement. It should be pointed out that this method doesn't work if the structural model is wrong initially, and the ESPOT will not lead to the correct structural model.

3.5 Analysis and output of the ESPOT contour map

The contour map can be shown in 1x1, 2x2, 3x3 unit cells. Multiple display options of the contour maps are available, e.g., color, the number of layers, zoom, shift, to show grides, etc.

The coordinates in the two-dimensional unit cell can be listed using the mouse pointer. Region of interest (ROI) can be set up and adjusted. A tool is also available for generating a figure label. The output can be saved in TIFF, PNG, JPEG, GIF formats.

4. Examples

4.1 Example 1

As an example, using In_7Ni_3, cubic, a = 0.918 nm, space group 299 Im-3m. Suppose the structure with the In atoms removed as a good structural model and the intensities calculated from the original structure as the measured intensities. We can deduce the positions of the missing In atoms from the phase from the structural model and the measured intensities, as shown in Figure 5. It is noticeable that negative regions on the contour map, the negative regions in the dot curves correspond to the positions of the missing atoms.

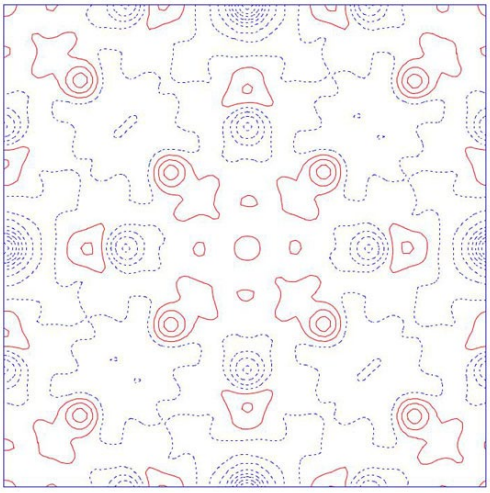

Figure 5. Atomic electrostatic potential difference map based on the diffraction data in Figure 4. The possible missing atoms are revealed in the dot line peaks.

4.2 Example 2

Demczyk & Cheng (1991) reported an orthorhombic phase in the Zr_2Co_{11} and $HfCo_7$ alloys. Ivanova, Shchegoleva & Gabay (2007) classified that there is a rhombohedral phase at high temperature region and the same phase as reported by Demczyk & Cheng (1991) but in different lattice parameters at lower temperature region. Li *et al*. (2014) revisited the orthorhombic phase in the Zr_2Co_{11} and $HfCo_7$ alloys, an incommensurate modulated structure was observed, and the lattice parameters can be viewed an approximation of an orthorhombic phase with lattice parameters close to result by Demczyk & Cheng (1991). Table 1 lists these crystal lattice parameters. X. Zhao, *et al*. (2014) proposed a structural model for the rhombohedral phase by an adaptive genetic algorithm and the first principle calculation. Figure 6 shows the structure model and the comparison to the experimental results.

A stable rhombohedral phase was late synthesized in $Zr_2Co_{11-x}(MoSiB)_x$ alloy. The selected-area electron diffraction (SAED) data was collected, and a structure model has been developed using the ESPOT. Figure 7 shows the experimental SAED pattern and intensity data. Figure 8 shows the

projection along the c axis for the structural model by Zhou *et al*. (2014) and the modified structure. Figure 9 shows the electrostatic potential map of the modified structure which can be used to interpret the local image of the high-resolution electron microscope image of Zr_2Co_{11} in Figure 10.

Table 1. Crystal lattice parameters in the Zr_2Co_{11} and $HfCo_7$ alloys.

Reference	Type	a (nm)	b (nm)	c (nm)
Demczyk & Cheng (1991)	Orthorhombic	0.48	0.82	3.6
Ivanova, Shchegoleva & Gabay (2007)	Orthorhombic	0.471	1.67	2.42
Ivanova, Shchegoleva & Gabay (2007)	Rhombohedral (h.t.)	0.476	-	2.42
X.Z. Li, *et al.,* J. Alloy Compd. (2014)	Orthorhombic*	0.476	0.82	(3.58)*

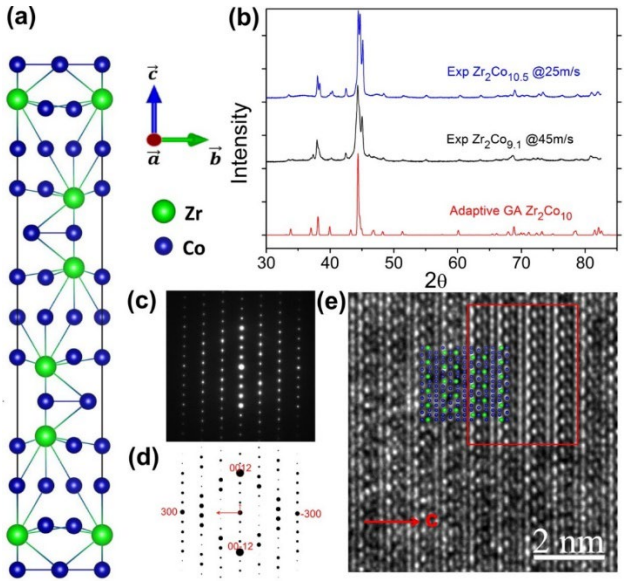

Figure 6. The rhombohedral structure has space group R32 with lattice parameters a = 0.469 and c = 2.40 nm, which match well with experimental data. The structural model was proposed by Adaptive Genetic Algorithm and the first principle calculation (Zhao *et al*. 2014).

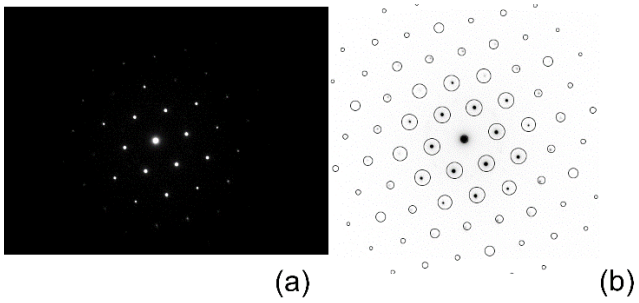

Figure 7. Selected-area electron diffraction pattern of the rhombohedral structure in $Zr_2Co_{11-x}(MoSiB)_x$, (b) the intensity data retrieved using QSAED.

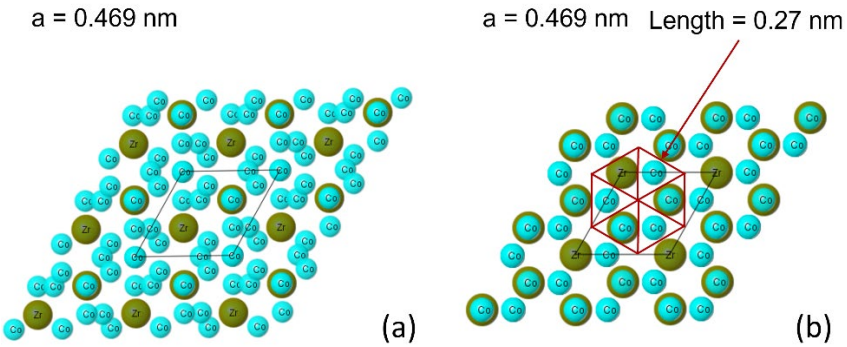

Figure 8. (a) the structural model proposed by Zhou *et al*. (2014) and (b) the modified model proposed using ESPOT and the experimental SAED data.

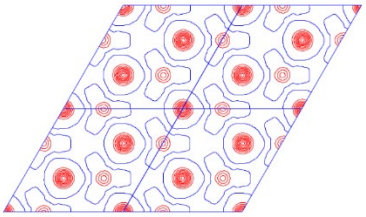

Figure 9. The electrostatic potential map of the modified model for the rhombohedral structure.

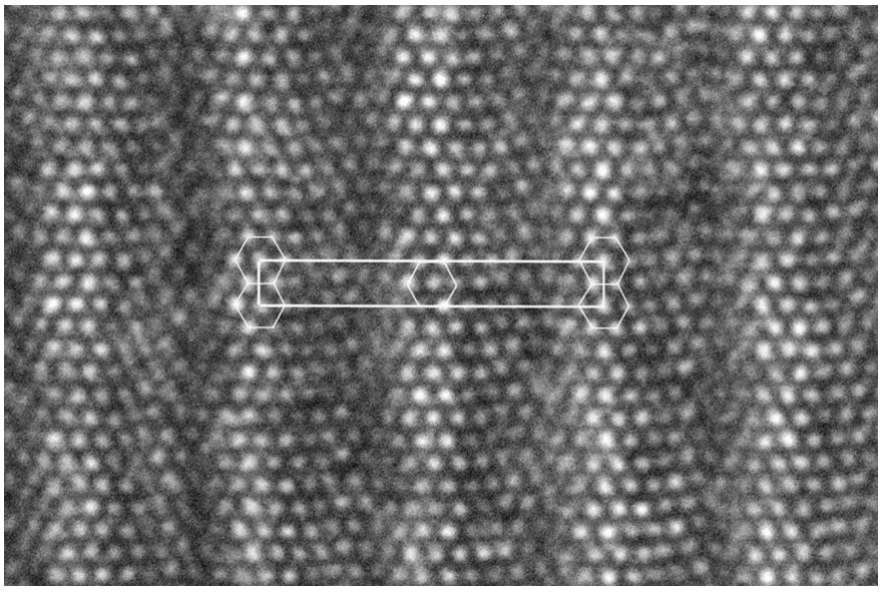

Figure 10. The high-resolution electron microscope image of the Zr_2Co_{11} modulated structure.

5. Installation

5.1 Installation

ESPOT requires support from OpenJDK 21 or later versions. The executable bytecodes, along with data files for testing and the specification file, are available in a compressed form (landyne6.7z) from https://landyne.com. To install, decompress landyne_plus.zip into a user-defined directory (e.g., `C:\landyne6\`) and execute `landyne6.exe`.

5.2 Feedback and license

The software works in two modes, demo mode and license mode. The software is fully operational at demo mode but limited to the demo input file (alumnium.txt in SAED6).

Both short-term and perpetual licenses are available at LANDYNE (jlandyne@gmail.com). Suggestions and comments are welcome.

6. References

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