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JECP—a Java Electron Crystallography Project

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Introduction

JECP stands for a java electron crystallography project that includes a series of practical java stand-alone programs for electron diffraction/microscopy and crystallography applications. The aim of the JECP project is twofold, i) as teaching tools to show students the principles of electron diffraction/microscopy and crystallography, ii) as research tools to analyze experimental results. Although there are commercial and public domain computer programs available that allow a user to simulate electron diffraction patterns or processing HREM images, there are always situations when we need to perform operations that are not a feature of any of the existing programs. The programs in the JECP can be modified and extended to meet the need in experiments.

So far there are five stand-alone programs available [1-5] and additional programs are in the development stage and will be added to this project. The programs, specification files, and a set of crystal structure files are available

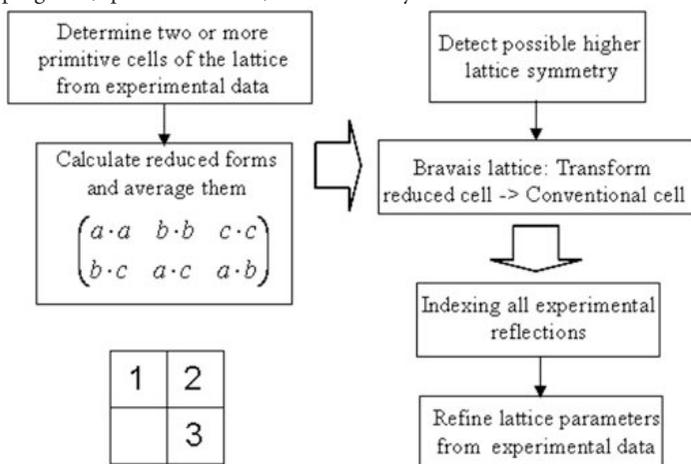


Figure 1. A general approach for the determination of the unit-cell of an unknown crystalline phase in electron diffraction experiments. Steps 1 and 2 are used to determine the lattice parameters and step 3 for refinement.

at <http://www.unl.edu/CMRACfem/XZLI/programs.htm>. A registration code can be requested via e-mail to the author. Without a registration code, the programs work in demonstration mode only. In this article, the purposes and features of these programs are introduced.

JECP/UNITCELL

Electron diffraction techniques, as a synergistically related to X-ray and neutron diffraction techniques, have been extensively used in material characterization and structure determination. Determination of the unit-cell for unknown crystalline phases is a basic requirement for materials characterization and the first step of *ab initio* structure determination.

Due to the physics of the electron diffraction method, it is natural to determine the unit-cell for unknown crystalline phases by the method of reciprocal lattice reconstruction from an electron diffraction tilt series. A simple reconstruction method was shown in the book by Vainshtein [6]: and results in a two-dimensional (2D) lattice constructed from an electron diffraction tilt series. This method is troublesome in its applicability to crystalline phases belonging to monoclinic and/or triclinic systems. General 3D reciprocal lattice reconstruction methods were discussed and implemented in computer programs [7,8].

JECP/UNITCELL adopts the concepts of a Niggli cell for the solution. A crystal lattice is characterized by a unique choice of a 'reduced' cell—a concept developed by Niggli in 1928 using reduced ternary quadratic mathematical analysis. There are 44 primitive reduced (Niggli) cells corresponding to the 14 Bravais lattices. Basically there are two steps in the determination of an unknown unit-cell: the determination of a reduced direct primitive cell

and the transformation to a conventional cell. Figure 1 shows a flowchart of a general approach for the determination of the unit-cell of an unknown crystalline phase in electron diffraction experiments.

JECP/SP

A stereographic projections (SP) plot is an important crystallographic tool for carrying out electron diffraction experiments and in the analysis of crystal structures and defects. JECP/SP was written for generating stereographic projections and was also extended as an application for specimen orientation adjustment in TEM experiments. Figure 2 shows the graphic interface of JECP/SP.

Computer assistance for specimen orientation adjustment in TEM experiments is especially useful in certain circumstances, for examples, when i) a severely stained specimen is observed and the visibility of Kikuchi line pairs is poor; ii) a beam-sensitive specimen is examined, and it is essential to shorten the time spent for specimen tilt adjustments when the electron beam is illuminating and degrading the area of interest; iii) a small-grain-size specimen is investigated, and even a small orientation adjustment may cause the corresponding diffraction pattern to disappear due to a lateral sample shift; and iv) a crystalline specimen is used in acquiring electron diffraction intensities of reachable zone axes patterns for structure determination. In these cases, the microscope can be kept in the image mode when the specimen is tilted under software guidance. The holder is tilted to the computer-predicted angles and the illuminated area of the specimen is kept at the area of interest or at some neighboring area until the target tilt angles have been obtained and then moved to the area of interest.

JECP/SAED

The program is designed for full-functional selected-area electron diffraction (SAED) simulation of single crystal phases and is extended to include the animation of precession diffraction pattern simulation. The precession method [9] has been used to solve the crystal structure of the Al_mFe phase by Gjønnes, *et al.* [10]. The advantages of the precession electron diffraction method are (i) to effectively reduce dynamical multi-scattering effects, (ii) to get more electron diffraction data due to the precession of the electron beam, and (iii) the determination of the integrated intensity for each electron diffraction spot.

Figure 3 shows the graphic interface of JECP/SAED. Diffraction patterns with geometrical factor and kinematical intensities are calculated in two separate steps in the program. There are options to show the spot index, intensity, base vector, Laue center, and FOLZ. The parameters of camera length, rotational angle, and the tilt angle of the incident electron beam are needed in the calculation.

JECP/PCED

For polycrystalline or powder TEM specimens, electron diffraction ring patterns are extensively used for phase identification, where the diffraction

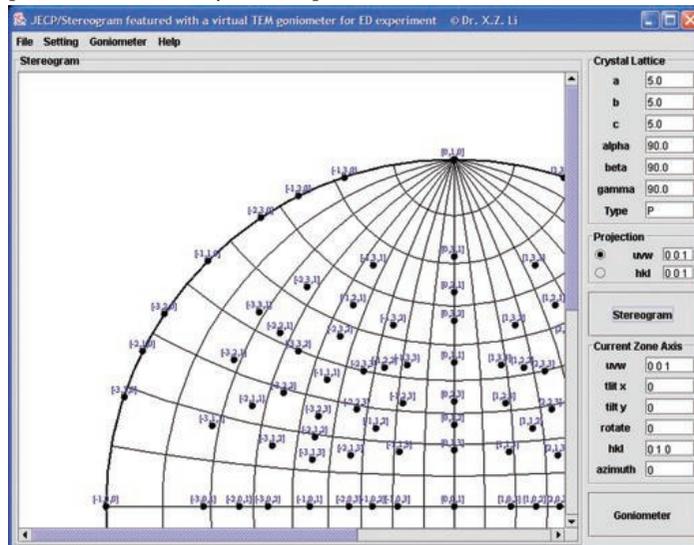


Figure 2. The graphic interface of JECP/SP and an example for a primitive cubic lattice.

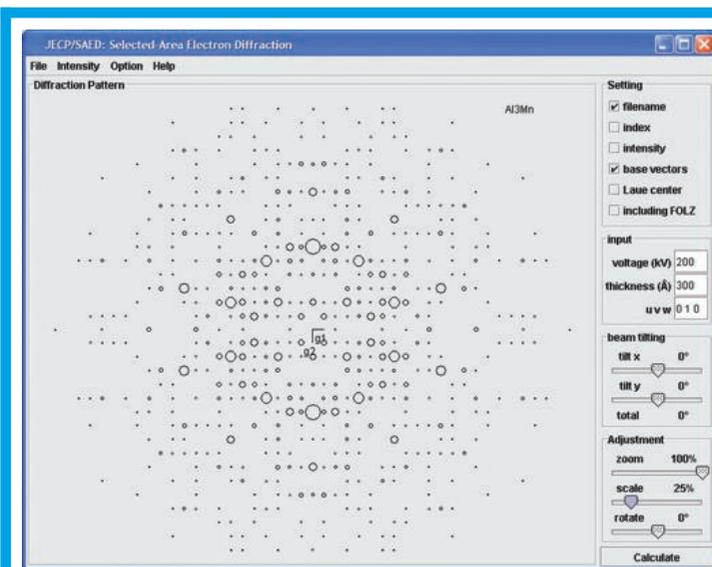


Figure 3. The graphic interface of JECPSAED and the simulated diffraction pattern of the Al_3Mn phase along the $[010]$ axis as an example.

Since electron diffraction from polycrystalline specimens is analogous to X-ray diffraction from powders, computer programs designed for powder X-ray diffraction may be used to analyze polycrystalline electron diffraction patterns for phase identification. Electron diffraction ring patterns need to be transformed into the form of integral intensity as a function of scattering angle for comparison with a powder X-ray diffractogram. The other approach is to use computer programs that implement the formula for electron diffraction intensity to analyze raw or processed polycrystalline electron diffraction patterns.

Integrated electron diffraction software packages often provide a module for simulating polycrystalline electron diffraction pattern, but rarely do they include features for direct comparison with experimental data for phase identification. JECPSAED is designed to provide a fast and accurate method for accomplishing this task. Also, it includes camera length calibration, experimental and simulated patterns matching, and the possibility of handling mixtures of two or more crystalline phases. Figure 4 shows the graphic interface of JECPSAED.

JECPSAED

Because high-order Laue zone (HOLZ) lines correspond to a HOLZ reflection with a long reciprocal lattice vector, the position of the line will be very sensitive to lattice parameters. HOLZ line patterns have been used in many areas in microanalysis of materials, e.g., lattice parameters, strain,

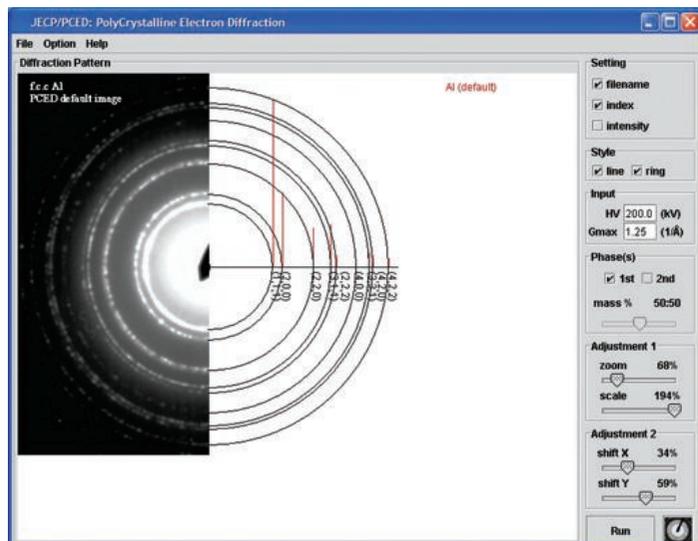


Figure 4. The graphic interface of JECPCED and the example of matching the experimental and simulated diffraction pattern of the Al phase.

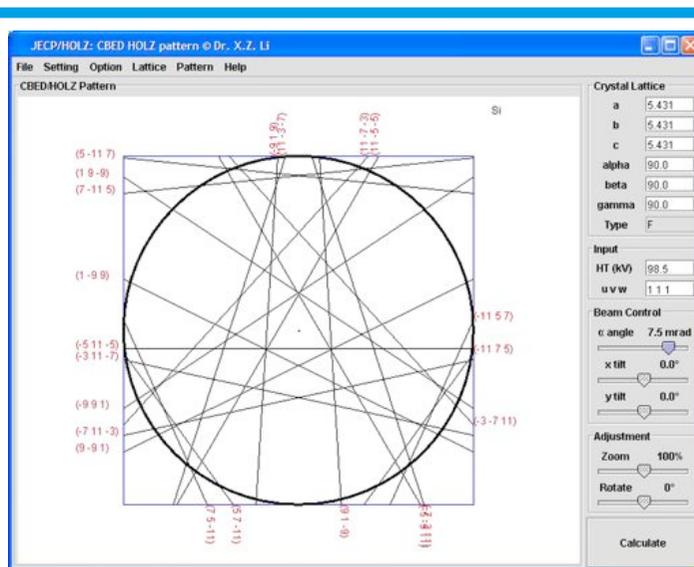


Figure 5. The graphic interface of JECPSAED and the simulated HOLZ pattern of the Si phase along the $[111]$ axis as an example.

local chemical composition, and electron potential. These applications are aided by computer programs for the simulation of HOLZ line patterns. Software packages providing for the simulation of HOLZ patterns can be found, in references [11-13].

A HOLZ line, in a kinematical approximation, is the locus of the satisfied Bragg condition for a HOLZ reflection. The position of a HOLZ line calculated from the kinematical approximation shows a slight deviation when compared to a corresponding experimental line due to the effect of dynamical electron scattering. Early computer programs for HOLZ lines were written under the kinematical approximation and only later was a first-order dynamic correction applied to take account of the dynamic line shift effect [11,14,15].

JECPSAED is an interactive computer program for simulation of HOLZ line patterns. Figure 5 shows the graphic interface of JECPSAED. The feature of this program is the integration of the simulation of the HOLZ (curved and straight) lines under kinematical approximation and a first-order dynamic correction. The program is interactive with respect to changes in lattice parameter, accelerating voltage, zone axis, and beam tilt.

Summary

A series of practical java stand-alone programs for electron diffraction/microscopy and crystallographic applications have been developed. The programs were designed to include not only the routine functions for crystallographic simulation but also additional features to address problems that may happen in experimental work. Besides the five programs introduced here, more practical programs will be soon added in this project. The next programs are JECPSAED and JECPSAED, which are designed to retrieve diffraction intensities from electron diffraction patterns of single/poly crystals. ■

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