

Processing and Quantification of Polycrystalline Electron Diffraction Patterns

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Polycrystalline electron diffraction is an important technique of crystalline phase analysis, especially in the studies of thin film and particle samples. The quantitative analysis of polycrystalline electron diffraction patterns requires digital experimental data and dedicated computer software. Two computer programs have been developed for this purpose - one is designed for the quantification of experimental patterns, e.g., retrieving the positions and intensities of diffraction peaks, and the other is for the advanced simulation using the Blackman formulas on integral intensities, the March model of textures and the pseudo-Voigtian function for peak shapes [1]. Here we introduce the computer program for quantification of polycrystalline electron diffraction patterns.

Previous computer programs, QPCED and APCED [2], were developed for processing polycrystalline electron diffraction patterns in order to achieve better angular resolution, quantified intensities, and reproducible identification of discontinuous and/or faint rings. The two programs have been rewritten and merged into a single program - QPCED2.0 with a lot of enhanced and extended functions. Although the procedure for the quantification of polycrystalline electron diffraction patterns is easily understood, the implementation in computer programs can be in various ways. The methods adopted in QPCED2.0 are outlined here.

When a polycrystalline electron diffraction pattern is loaded in QPCED2.0, a pair of intensity profiles of the diffraction pattern is generated instantly from two orthogonal scan lines, which intersect at the center of the display panel. The orientation of the scan lines, being horizontal and vertical by default value, can be set to any azimuth angle. For an ideal polycrystalline electron diffraction pattern, the two profiles are identical and each has a mirror-symmetry. The rules should be applied to experimental patterns although there may exist some imperfections here and there. By shifting the image while comparing the intensity distributions in the two profiles, the center of the diffraction pattern is accurately located. The profile pair can also be used to determine the ellipticity (ϵ) and the orientation of the elliptic ring in case $\epsilon \neq 1$. QPCED2.0 provides a function to easily correct the distorted rings into perfect circles with the determined ellipticity. Figure 1 shows the graphical user interface (GUI) of QPCED2.0 with an example of a diffraction pattern and the intensity profiles of horizontal and vertical line scans.

Two types of integral intensity profiles can be converted from a diffraction pattern, (i) an integral intensity distribution of the diffraction pattern as a function of radius; (ii) an integral intensity distribution of a diffraction ring as a function of azimuth. The background of an integral intensity profile can be estimated either automatically using the algorithm proposed by Brückner [3] or manually. In the manual method, the background curve can be defined by selecting points and then connecting the points into line segments. Two types of peak functions in QPCED2.0 are pseudo-Voigtian and Pearson VII, both of which are commonly considered the most practical and useful functions in evaluating polycrystalline electron diffraction patterns for peak fitting. The Levenberg-Marquardt algorithm [4], a powerful method for non-linear least-squares fitting, is used to determine the positions and shapes of peaks. Figure 2 shows the integral intensity profile with its background subtracted and the diffraction peaks described in a set of pseudo-Voigtian functions

after a least-squares refinement. A camera-length calibration can be done in QPCED2.0 using an experimental diffraction pattern of a crystalline phase with a known structure. Finally, a data file containing a list of the lattice spacings and normalized intensities can be saved for further analysis. The integral intensity profiles can also be exported and used as the input data in PCED2.0 for qualitative or semi-quantitative analysis.

Both of QPCED2.0 and PCED2.0 were written in Java SE6. Java runtime environment is needed to execute the two programs. QPCED2.0 also needs the support of Java Advanced Imaging API. The executable jar files, user manuals and example data files can be downloaded from the author's webpage.

References

- [1] X.Z. Li, Ultramicroscopy, 110 (2010) 297.
- [2] X.Z. Li, Microsc Microanal. 13 (Suppl 2) (2007) 966 CD.
- [3] S. Brückner. Appl. Cryst. 33 (2000) 977.
- [4] W.H. Press et al. (1992) Numerical Recipes in C: The Art of Scientific Computing (2nd ed.), Cambridge university press, New York, USA.

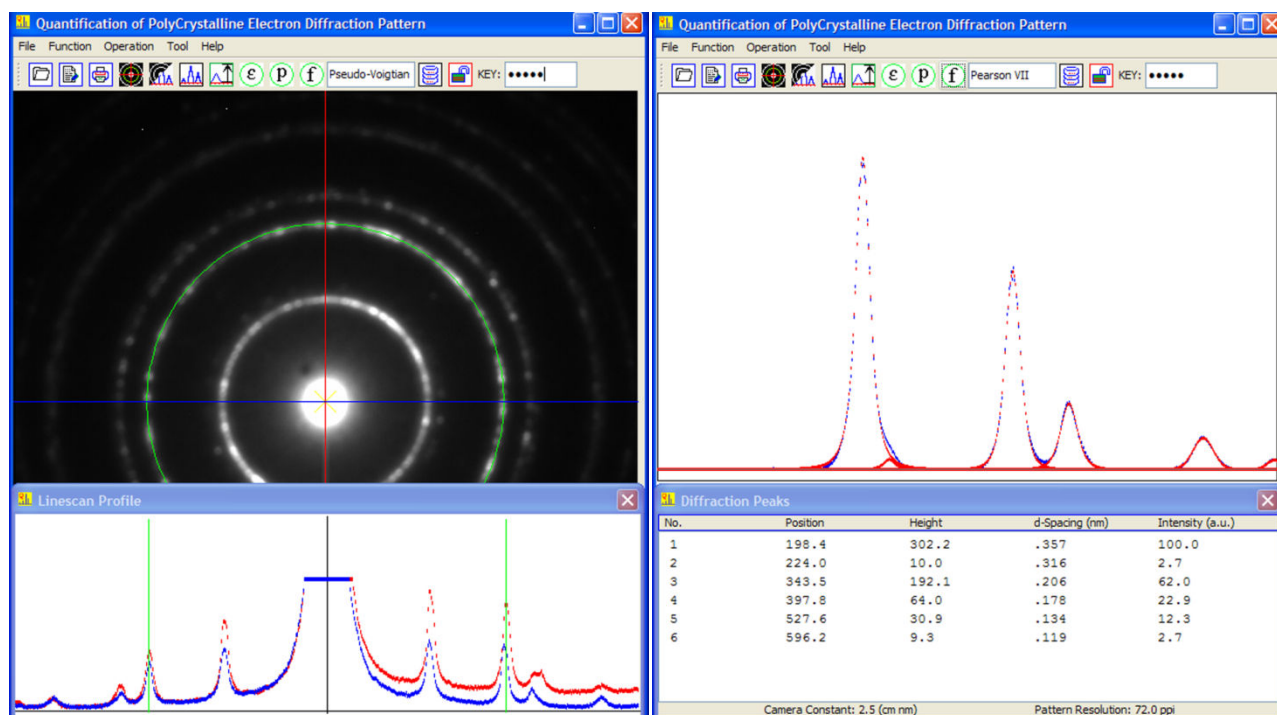


Figure 1

Figure 2

Figure 1. A screen shot of QPCED2.0 with a SAED pattern of a (001)-orientated ZnO film. Inset is two intensity profiles of the pattern along horizontal and vertical lines, respectively.

Figure 2. The analysis of the intensity profile retrieved from figure 1. Peak positions and shapes were refined using the Levenberg-Marquardt algorithm. Inset shows selected important parameters.