

ProcessDiffraction V1.2: New possibilities in manipulating electron diffraction ring patterns

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A *free* computer program was introduced recently to process electron diffraction ring patterns¹. The program (called ProcessDiffraction) produces XDR-like output from the digitized version of the measured diffraction patterns. The enhanced functionality of V1.2 is summarized in the present paper.

1. The program starts with a hint-window giving suggestions what can be done next. Hints change permanently as processing progresses. The hint-window can be switched off optionally. It is a complement to the Windows-style Help-system.
2. The center of the rings is found by manually shifting the measured pattern until it overlaps with a generated reference circle. The computer can further refine the position of the center.
3. Elliptical distortion of the measured pattern (NOT of the display, which is irrelevant) is corrected by adjusting the eccentricity and axis direction of the reference ellipse (distorted from the reference circle) until visually coincide with the measured ring. Intensity of the rings is averaged over these ellipses.
4. The distribution of circularly (elliptically) averaged intensity can also be presented as a function of scattering vector (in contrast to pixels only).
5. Effect of beam-stop (blocking part of the pattern) can be eliminated by neglecting points with zero intensity from averaging.
6. The background under diffraction peaks can be modeled and removed to get net intensities.
7. Positions and intensities of diffraction lines in the powder diffraction database can be overlaid as markers. Different phases are presented in different colors. Beside this visual presentation, a list of detected peaks (together with their net intensities) can be presented in a tabulated form in correlation with the data of markers (reference phases). Lines of the measured sample and of the reference phases falling within 1 pixel are presented in the same line of the table, helping phase identification.
8. In order to obtain a more reliable intensity for spotty rings, average intensity, calculated only for points over gross average (i.e. for pixels of the bright spots in the spotty ring) can also be calculated².
9. Calibration of camera constant can be done by clicking on corresponding lines in the measured distribution and in a marker of a reference phase.
10. Beside printing and saving, calculated distributions can also be copied to "compare" memories in order to overlay several distributions. Since each distribution can be calibrated separately, distributions recorded with different camera constants can also be overlaid.
11. Parameters of individual bright spots can be read out using a cursor function. Selection is steered by the mouse and aided by a small cursor window where a magnified image of the pixels close to the selected one is shown with maximized contrast. Correlation between the position of the selected point in the ring-pattern and its corresponding position in the distribution can also be checked visually.

The bottleneck of intensity-quantification lies in the way the intensities are recorded. In contrast to Imaging Plates and CCDs, the linearity of photographic materials is limited. Consequently, a recorded ratio of diffraction lines depends slightly on exposure. Selecting Optical Density mode during operation of the scanner (when digitizing the film) improves quantitation. Many recent scanners possess such mode of operation. Correction for the nonlinear blackening of the individual films can extend the useful range of intensity.

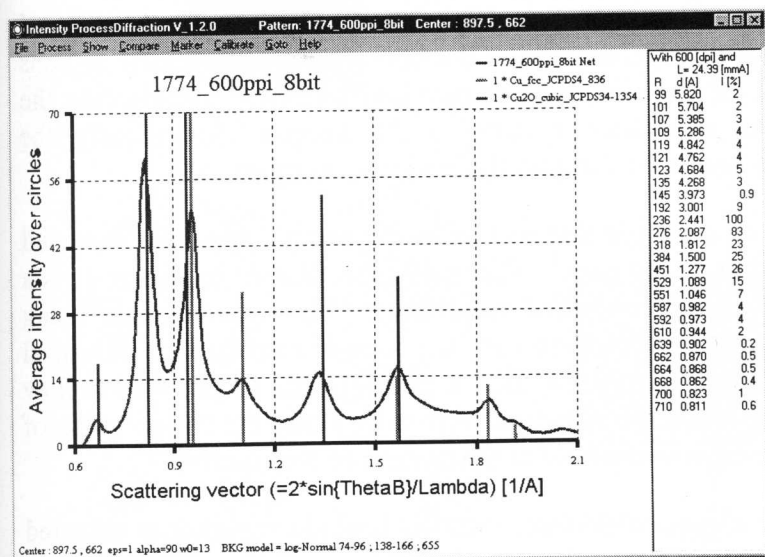


Figure 1: *Left*: Markers indicating the positions of diffraction lines for fcc Cu and cubic Cu₂O. *Below*: Cursor window.

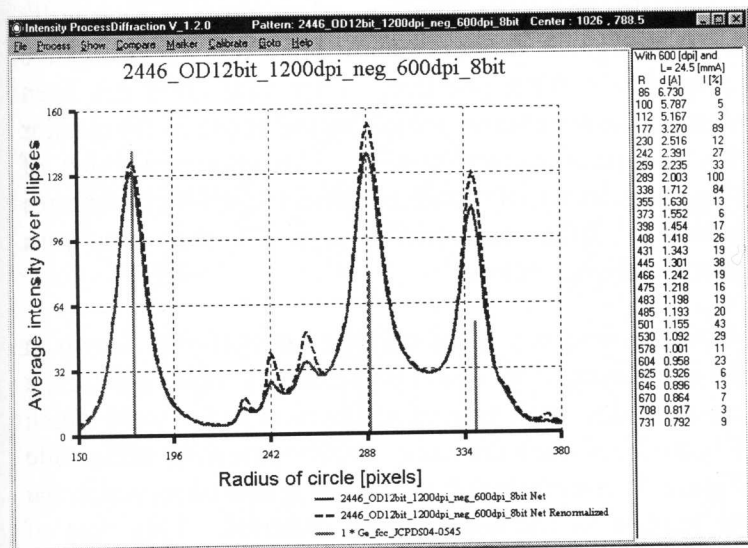
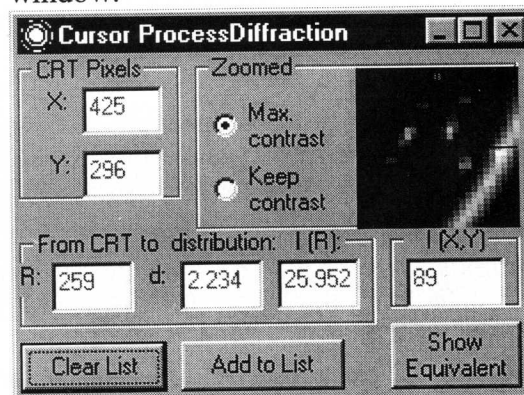
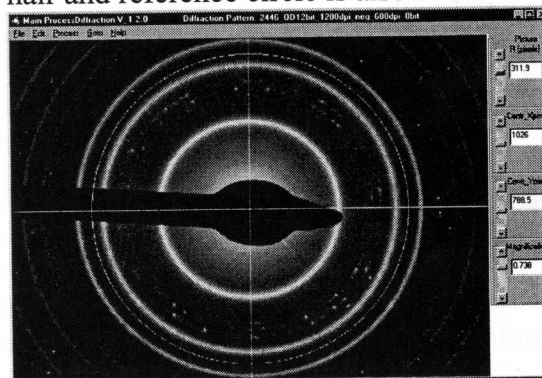


Figure 2: Effect of renormalization on the intensities of spotty rings. Corresponding parts of pattern (*below*) and distribution (*left*) are shown. Cross hair and reference circle is also seen.



The program can be download free from <http://www.mfa.kfki.hu/~labar/ProcDif.htm>.

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References:

- ¹ JL Lábár, Proceedings of 12th European Congress on Electron Microscopy, Brno, 2000, I 379
- ² Walck Scott, Proceedings of M&M, 1998