# „ProcessDiffraction" : A computer program to process electron diffraction patterns from polycrystalline or amorphous samples

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**Summary:** Digital versions of electron diffraction ring-patterns are transformed into integral intensities as a function of scattering angle, producing the same presentation that is usual for powder X-ray diffraction patterns. First, the point corresponding to the exact direction of the non-scattered beam is identified by visual image manipulation. Then, the intensities over concentric rings are averaged as a function of the radius of the ring (i.e. scattering angle). Advantages of the method include good angular resolution, quantified intensities, reproducible identification of discontinuous and/or faint rings and easy and fast operation. Comparison of electron- and X-ray-diffractogramms also becomes much easier and quantitative with the program. The program runs under Windows operating system and is available ***free***.

## 1 Introduction

Two main types of samples that produce ring-patterns in selected area electron diffraction (SAED) are polycrystalline and amorphous samples. For polycrystalline samples phase identification is the main task and comparison to X-ray-based data bases is essential. Measurement of the positions of either broad or faint or discontinuous rings is difficult from the electron diffraction patterns. Assessment of intensities presents an even worse problem. Direct comparison of these SAED patters to X-ray diffractogramms of known phases is also difficult due to the different forms of presentation for the two methods. For amorphous samples both phase identification and determination of the next-neighbor distances also require the distribution of intensities over scattering angles. In spite of the obvious need for such re-presentation of the information present in the SAED ring patterns, the author does not know of the existence of such a program. The several available programs for processing images and diffraction patterns do not do the same (for a catalog of programs see e.g. [1]). Measuring intensity along a single line (diameter of the ring pattern) does not give either the required sensitivity or accuracy (furthermore, it can miss rings from spotty rings of textured samples). Present contribution summarizes the first version of a ***free*** program that averages over the entire rings to get both position and intensity.

## 2 Main functions of the program

The program communicates through the usual Windows graphical interface, where the diffraction pattern is manipulated as a picture and the distribution is presented as a line diagram.

### *2.1 Input*

Images stored in grayscale (8bits), non-compressed Bitmap format are accepted by the program. This standard image format is supported by most of the scanners, so the pattern can be directly stored in this format. Resolution of the scanner and magnification of the print should be adjusted so that one pixel in the digital pattern correspond to about 50 micrometers on the original film. For instance magnification around 1.6x and resolution of 300 dpi (dots per inch) is not far from this value. Reduced magnification and/or resolution deteriorates the accuracy, while excessive magnification (resolution) increases computer requirements without any benefit. For CCD, the compromise between angular resolution and the number of available pixels gives image size.

### 2.2 *Finding the center*

The pattern can be magnified and shifted over a reference circle to find the direction of the non-scattered beam (center of the distribution). The radius of the reference circle can also be adjusted independently. The reference circle should overlap a continuous ring completely.

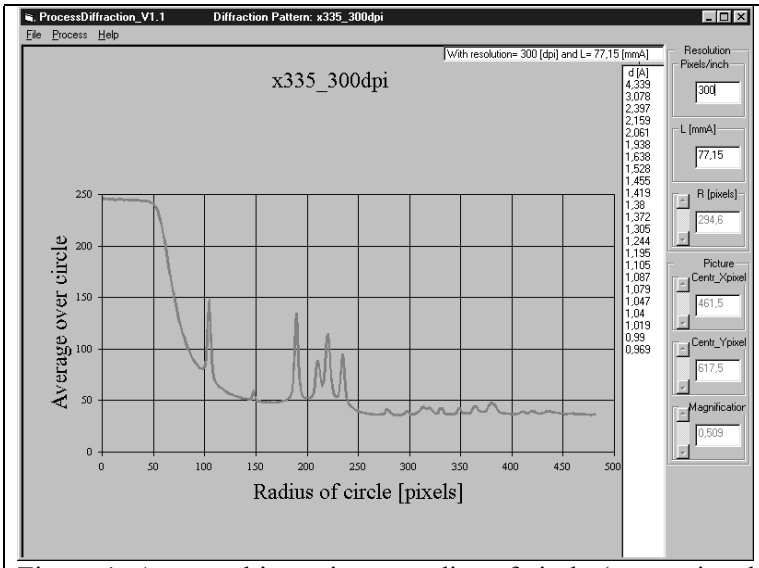


Figure 1: Averaged intensity vs. radius of circle (proportional to scattering angle)

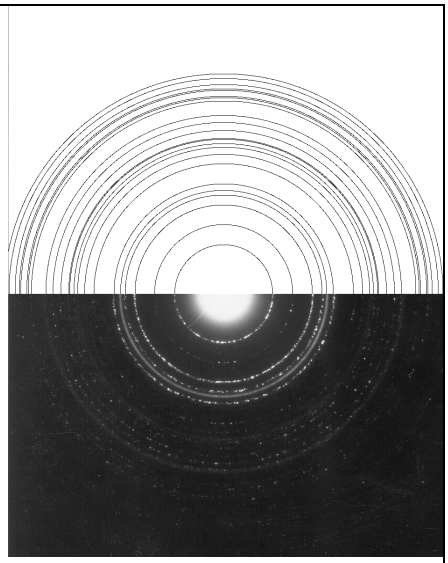

Figure 2: Measured SAED with detected circles

### 2.3 *Menu Process Distribution*

Calculates the average of intensity over a circle as a function of the radius of the circle. This provides the XRD-like distribution as a function of scattering angle. The numerical values can be stored in a text file (.DAT extension) compatible with other graphical programs (Excel, Origin, etc.). Alternatively, it can also be printed (*Fig. 1*). After this step, the center can also be automatically refined (within 2 pixels to the true position). The distribution becomes the sharpest possible and reduces the chance to find false "rings" due to artificial split (caused by a shifted origin that is closer to one of the sides of the circle than to the other).

### 2.4 *Menu Process Schematic Half-circles*

In place of the half of the original SAED pattern half-rings are generated at the positions where the automatic procedure identified the presence of a diffraction ring (irrespective of the fact if the ring was complete or only spotty). This image is also saved in Bitmap format (*Fig 2*).

## 3 Conclusions

A procedure realized in a form of a graphical computer program is presented to process electron diffraction ring patterns and show them in XRD power diffraction style. Identification of weak or incomplete features is more reliable with this method and the result is quantitative (can be easily compared to XRD results). The computer program is ***free***. The result lends itself to both Rietveld-type quantitative phase identification [2] and for texture analysis (among others, see [3]). Later versions of the program are planned to include elements of such further processing. Financial support of the Hungarian National Science Found is acknowledged (contract number OTKA 030432).

**References**:

[1] Williams DB and Carter CB: Transmission Electron Microscopy, Plenum Press, 1996, pp. 14-16
[2] Rietveld H., Acta Cryst. **20** (1966) 508
[3] Hono K, Wong B and Laughlin DE, JAP **68** (1990) 4734