doi:10.1017/S1431927613005539
Microsc. Microanal. 19 (Suppl 2), 2013

Application of Diffraction Mapping on Crystal Grain Imaging

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In the study of polycrystalline materials, the crystal size distribution is part of the critical information. The orientation mapping techniques based on diffraction indexing has been frequently used to study crystal grains [1]. To get a grain mapping, it is often beneficiary to have alternatives with relatively short data collection and process times to those indexing based techniques. This is especially important in industry, where a fast and qualitative result is often desirable. A simple grain mapping method based on tableau dark field imaging has been demonstrated [2]. In this report, we discuss some quick methods to generate grain maps based on electron diffraction patterns.

A collection of electron diffraction patterns (DP) over an area of interest can be recorded automatically with computer program interfaced to a TEM. Some commercial programs are available for this type of control [3]. Without access to a commercial program, we created our own diffraction mapping software using DigitalMicrograph® scripting language. In this study, the procedure is performed on a polycrystalline Si sample. Fig 1 shows the reference annular dark field STEM image, the DP stack, and the control program interface. The DP stack forms a data matrix from which we can generate images of different contrast using different part of the DP images. As an example, a bright field STEM image is generated using transmitted beams (Fig. 2A).

There could be different ways to create grain mapping without referring to the crystal structure. Two methods are introduced here. For all the following mapping generation, two basic processing steps are usually done: (1) the DPs are all aligned and centered on the transmitted spots; and (2) The transmitted beam spots are all filtered out during mapping calculation.

The first method is based on the similarity of DPs of neighboring steps. The intensity of a pixel in the resulting map is due to the comparison of the DP of the corresponding scan step with the one from the next step in the same row. An efficient way to quantify the similarity of two diffraction pattern is the pixel sum of the multiplication of the two DP images. With a m-row by n-column DP matrix, an image with a size of $m \times (n-1)$ is generated. Such image is shown in Fig. 2 (B). This type of image gives a good definition of crystal grains with dark grain boundaries.

The second method is to use the strongest diffracted beam (SDB) of the DP. With optional image smoothing, the strongest diffraction spot can be located for each DP. The intensity and the location of the SDB vary for different crystal orientations. This forms the basics of SDB mappings. The average of pixel intensities from an area centered on the SDB gives a value, q. This value gives a "SDB q map" (Fig. 2 C). The ratio of q value to the average annular band of the same radius as the SDB gives a q-ratio. This ratio is a quantity of the intensity of the SDB above the annular average. An amorphous region has a low q ratio. The "SDB q ratio map" (Fig. 2 D) is generated from this ratio. Each SDB has its polar coordinates (radius and angle). Each unique SDB polar position can be assigned to a unique color according to a pre-defined color scheme. This gives the "SDB orientation map" (Fig. 2 E). The multiplication of SDB q-ratio map and the SDB orientation map give a "weighted orientation map" (Fig. 2. F).

These two calculation methods are fast. For a 100x100 map, either calculation can be done in a few seconds. They do not have strong requirement of pseudo-parallel electron beam. The "similarity map" works for any convergent beam condition. The two methods are useful for grain mapping of a sample with a mixture of multiple crystal structures.

References:
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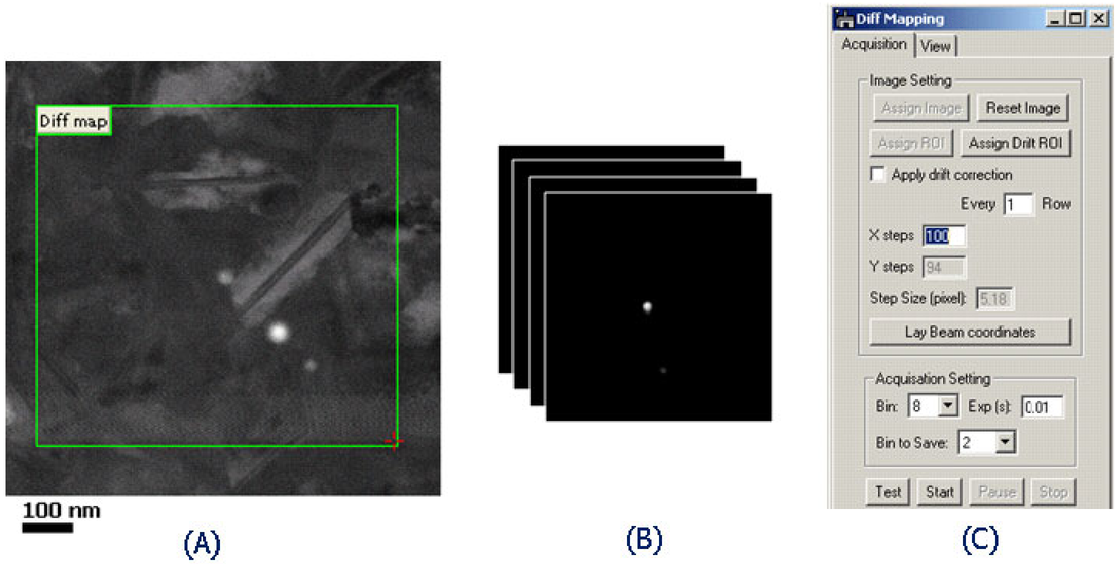

Fig. 1. (A) STEM image. The box marks the area for the diffraction scan. (B) A stack of diffraction patterns collected at each step when the electron beam scans over the boxed area. (C) Program interface for data collection.

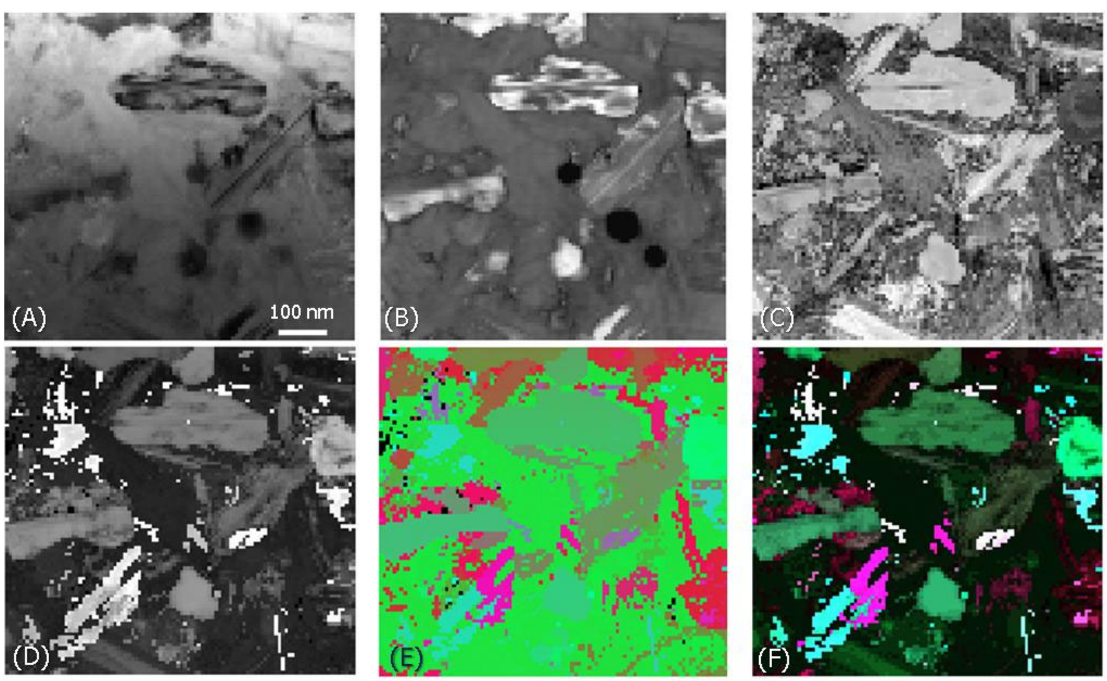

Fig. 2. (A) Transmitted beam map, (B) Similarity map, (C) SDB *q* map, (D) SDB *q* ratio map, (E) SDB orientation map, (F) Weighted SDB orientation map.

https://doi.org/10.1017/S1431927613005539 Published online by Cambridge University Press