Strategies for indexing big datasets of electron diffraction patterns for nanostructure orientation and phase mapping

Zuo, J.[1], Meng, Y.[1], Yang, Q.[1] and Yuan, R.[1]

[1] University of Illinois at Urbana-Champaign, United States

Fine-grained and nanostructured materials are very much at the core of materials research. Significant properties arise in nanostructures from surface/interface effects. Since the chemical bonds of surface or interface atoms can differ significantly from interior (or bulk) atoms, interfacial atoms give rise to distinct chemical, mechanic, thermodynamic, electronic, magnetic and optical properties. However, nanostructure characterization is challenging because of the small sizes and the difficulty of characterizing small interfaces. Electron Backscatter Diffraction (EBSD) is commonly used to characterize the microstructure of granular materials, such as metals and alloys, down to the sub-micron scale. However, the spatial resolution of the EBSD technique is limited by the relatively large electron probe size in a SEM and the interaction volume, as well as the need to tilt the sample to a high angle.

For very fine grains, electron nanodiffraction techniques, such as scanning electron nanodiffraction (SEND) performed in a TEM, offers the spatial resolution of ~1 to 5 nm. The major limitation to the use of electron nanodiffraction for orientation mapping is diffraction pattern indexing, which for a long time was mostly manual and thus was not as fast as the EBSD technique. The ability to extract structural information from a big dataset of electron nanodiffraction patterns is thus critical for orientation and phase mapping of nanostructured materials. With the development of fast electron detectors, a large number of nanodiffraction patterns can be acquired over a short time for a region of interest. Indexing of such large diffraction dataset in future also requires a fast and robust approach to diffraction pattern indexing. Automatic DP indexing is usually achieved by comparing an experiment diffraction pattern with a set of simulated diffraction patterns and by searching for the best match. However, these techniques face significant challenges when the quality of experimentally acquired DPs is poor, especially, when the diffraction spots are weak or overlapping with diffraction patterns from different grains.

Here we will introduce a correlation based strategy for automatic sorting and indexing of diffraction patterns. The aim of the correlation analysis method is to identify similar diffraction patterns, average these similar patterns and obtain a correlation map where the distribution of similar diffraction patterns is identified. This correlation image is further processed to form the orientation map image. The similarity of DPs is quantified by the value of normalized cross correlation coefficient (NCC) calculated for two individual diffraction patterns. The value of an NCC calculation between two DPs will range from -1 to 1 with NCC = 0 indicating complete dissimilarity and NCC = 1 indicating complete similarity. Next, the DPs are grouped using the values of NCC between the pairs of diffraction patterns. A group is defined as one with all DPs belonging to the group having values of the NCC values amongst themselves to be equal to or greater than a fixed, pre-defined, threshold value. Using an iterative procedure, the group diffraction pattern can be averaged and further correlated with the experimental pattern to improve diffraction pattern grouping. In this talk we will demonstrate how such correlation analysis can be combined with the automatic indexing algorithm we developed for orientation mapping [1] in nanostructured Au films and porous Fe3O4 samples [2].

[1] Meng Y, Zuo J-M. Improvements in electron diffraction pattern automatic indexing algorithms. Eur Phys J Appl Phys 2017, 80(1): 10701.

[2] This work is supported by U.S. Department of Energy under contract DEFG02-01ER45923.