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Electron Diffraction Phase Analysis and Pattern Simulations Using the ICDD Powder Diffraction File (PDF-4+)

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The Powder Diffraction File ™ (PDF®) is a comprehensive materials database that is the key source of reference powder diffraction data for identification and analysis of materials; from natural minerals and high-tech ceramics, to metals and alloys, and pharmaceuticals. New developments in X-ray analysis, and advances in scientific research, have dramatically influenced the range of data present in the PDF. ICDD's premier database, PDF-4+, contains d-spacing, intensity, and hkl data used for phase identification, as well as atomic coordinates for more than 223,000 phases. In addition to being a reference database used for the analysis of traditional single phase X-ray diffraction data, the PDF-4+ also supports electron diffraction (ED) based analyses. Often in materials characterization, X-ray, electron and neutron diffraction are used to complement one another. Given the complimentary character of these techniques, it seemed only logical to compile this data into one comprehensive database, the PDF-4+. As a result, a suite of electron diffraction based simulation tools have been designed. Research scientists often use electron diffraction as a method for obtaining higher diffraction intensities of a material when X-ray scattering is limited. The increased intensity of an electron beam allows the user to investigate smaller samples and utilize a more focused beam to determine the atomic arrangement of crystals. However, the high energy beam can often promote multiple scattering interactions; making structure solution by electron diffraction alone relatively difficult compared with X-ray diffraction structure analysis. In support of the diffraction community, the ICDD has developed tools that enable users to stipulate the type of diffraction they want to reference.

The PDF electron diffraction tools currently consists of selected area electron diffraction (SAED) patterns, electron backscatter diffraction (EBSD) patterns, 2-D ring patterns, and 1-D powder diffraction patterns (Figure 1). In addition, several data analysis features have been included that allow the user to obtain zone axis, spatial orientation, and crystallinity information (Figure 2). The simulations are derived using calculations based on the atomic parameters, electron scattering factors, and/or X-ray scattering factors specified in the PDF entry of interest [1]. Each simulation is interactive and allows the user to perform instantaneous alterations to the pattern by adjusting dynamic parameters such as zone axes, camera length, electron voltage, etc. The PDF-4+ electron diffraction tools streamline comparisons and contrasts of X-ray and electron diffraction data in one place.

PDF-4+ offers a variety of algorithms and simulation options that allow users to analyze electron diffraction data. In many cases, this provides a unique capability to analyze the difficult material analysis problems. This presentation depicts the capabilities of the various electron diffraction simulation tools and describes the process of identifying phases from electron diffraction data in PDF-4+. Currently, PDF-4+ data mining capabilities provide extensive filtering options to enhance the identification process, and the search/match engine, SIeve+, enables users to carry out vital search/match analyses using ED data [2].

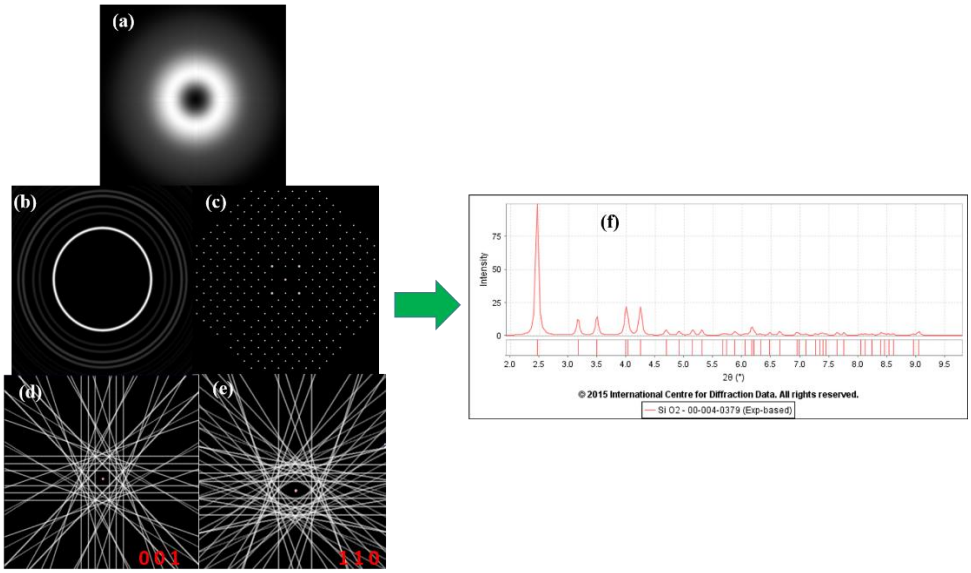

Figure 1: Electron diffraction simulations of (a) an amorphous, (b) a polycrystalline (ring pattern), or (c) a single-crystal (SAED pattern) material showing the variation of ED patterns due to crystallinity. EBSD simulations in (0 0 1) orientation (d) and (1 1 0) orientation (e) are depicted, as well as a 1-D simulated powder pattern (f).

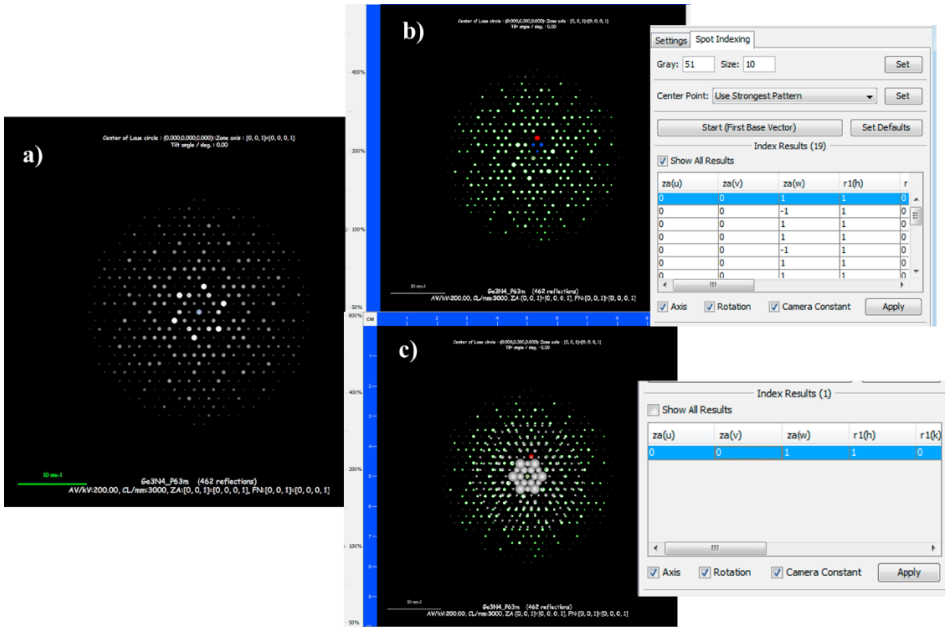

Figure 2: Various displays encountered when performing zone axis auto-indexing. Screen (a) shows the user's imported data, (b) shows the location of the center of the pattern and the list of possible choices for zone indexing (*box on the right*), and (c) shows the simulated data points (based on the indexed zone axis; *box on the right*) compared to the user's original data.

References

[1] Reid, J. *et al.*, Microscopy Today, **January** (2011), p**.** 38.

[2] Kabekkodu, S. N. *et al.*, Acta Crystallographica Section B: Structural Science **B58** (2002), p. 333.