Microsymposium

Why powder diffractionists need help from electron crystallography

<u>D. Xie</u>¹, S. Zones¹, T. Rea¹ ¹Chevron Energy Technology Company, Richmond, CA, USA

Although X-ray powder diffraction (XPD) is used as a routine tool for solving crystal structures of polycrystalline materials, its weakness is obvious: not only is the phase information lost during the diffraction experiment, but reflections with similar d-spacings, which are well-separated in a single-crystal measurement, overlap in a powder pattern. These effects increase the difficulty of structure solution especially when dealing with complex structures. Compared to XPD, the advantages from electron microscopy are: (1) single-crystal electron diffraction data, either in 2-dimensional or 3-dimensional form, can be obtained from a very tiny crystallite in a powder sample; and (2) high-resolution images can be collected and used to extract phase information in reciprocal space or to provide a direct view of structural features (ordered and disordered) [1]. With the extra information supplied by electron microscopy, the limits of structure determination for polycrystalline materials can be extended [2]. Here we will present a few examples to demonstrate why powder diffractionists need help from electron microscopy and how to integrate these two techniques into the structure determination process.

[1] T. Willhammar, X.D. Zou, Z. Kristallogr., 2013, 228, 11-27, [2] L.B. McCusker, Ch. Baerlocher, Z. Kristallogr., 2013, 228, 1-10

Keywords: Structure Determination, X-ray Powder Diffraction, Electron Microscopy