Using Transmission Electron Microscopy (TEM) to Complement Powder Diffraction Data

Fabian Gramm, Lynne B. McCusker, Christian Bärlocher, *Laboratory of Crystallography, ETH Zürich, Switzerland.* E-mail: fabian.gramm@mat.ethz.ch

In recent years, a number of different approaches to structure solution from powder diffraction data have been developed, and they have been applied successfully to increasingly complex problems. Nonetheless, the structures of some polycrystalline materials remain intractable. In attempt to address such problems, we are currently investigating how electron microscopy techniques can be used to complement those of powder diffraction.

Not only can selected area electron diffraction (SAED) be used to facilitate the indexing of complex powder diffraction patterns, but the electron diffraction intensities themselves can sometimes be used to obtain a more correct partitioning of the intensities of reflections that overlap in the powder diffraction pattern. However, the effects of dynamical scattering can distort the intensities to the extent that this is no longer a reliable approach. In this case, a reconstructed potential distribution map from a high-resolution electron microscopy (HREM) image can be used to obtain the phases of the stronger reflections in that projection, and these, in turn, can be used to generate a structure envelope that defines where atoms are likely to be located within the unit cell. This envelope can then be used in conjunction with any direct-space structure determination algorithm. A test of this approach with the complex zeolite ZSM-5 showed that FOCUS (a zeolite-specific structure determination program) runs approximately five times faster with an envelope (generated from a single HREM image) than without it. Thus, even more complex structures become accessible.

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