

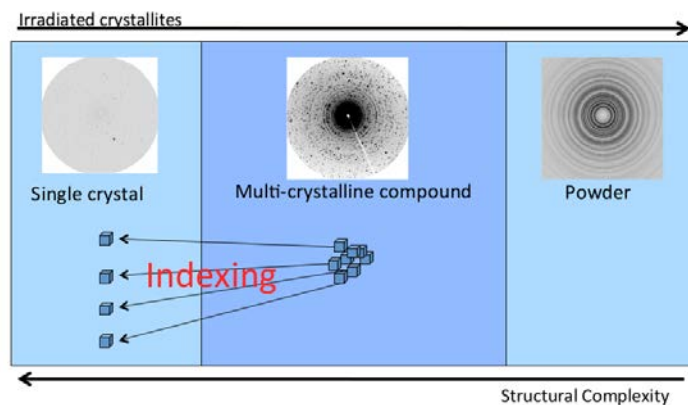
08th January 2013 - 02:00 pm
CFEL – Building 99, seminar room IV (O1.111)

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Multi-crystal indexing

The ability to index individual crystals embedded in multi-crystalline materials has been widely used within the synchrotron community for the past decade. Through indexing, each crystallite can be treated as a single crystal (1,2,3), thus enhancing the information content with respect to powder, as illustrated in the figure below:



Conventional indexing relies on the fact that the crystallography of the material is known (unit cell and space group), and that overlap among the recorded diffraction spots are not too severe. In the talk, new indexing approaches are discussed for known and unknown crystallography (4), as well as, for cases with severely overlapping diffraction spots (5). In addition, an overview of recent applications within the fields of Neutron scattering and Electron microscopy (6) is given.

References

1. S. Schmidt, H.F. Poulsen, G.B.M. Vaughan, Structural refinements of the individual grains within polycrystals and powders, *J. Appl. Cryst* (2003) 36, 326-332.
2. G.B.M. Vaughan, S. Schmidt, H.F. Poulsen, Multicrystal Approach to Crystal Structure Solution and Refinement, *Zeitschrift für Kristallographie* (2004), 219 (no. 12), 813-825
3. H.O. Sørensen, S. Schmidt, J.P. Wright, G.B.M. Vaughan, S. Techert, E.F. Garman, J. Oddershede, J. Davaasambu, K.S. Paithankar, C. Gundlach, H.F. Poulsen, Multigrain Crystallography, *Zeitschrift für Kristallographie* (2012), 227, 63-78
4. S. Schmidt, *GrainSpotter*, in prep.
5. S. Schmidt, N.F. Gade-Nielsen, M. Høstergaard, B. Dammann, I.G. Kazantsev, High Resolution Distribution Function, *Mat. Sci. Forum*, 702-703 (2012), 536-539.
6. H.H. Liu, S. Schmidt, H.F. Poulsen, A. Godfrey, Z.Q. Liu, X. Huang, Three-Dimensional Orientation Mapping in the Transmission Electron Microscope, *Science* (2011), 332, 833-834.