

Poster Presentation

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Single-crystal diffraction data from powder samples via SFX

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With the serial femtosecond crystallography (SFX) [1] using hard X-ray free-electron laser as light source, it is possible to obtain three-dimensional single-crystal diffraction data from powder samples consisting of submicron crystal grains. This offers two advantages. First, complicated crystal structures far beyond the ability of powder X-ray diffraction analysis now can be solved easily; second, mixtures of two or more crystalline components can be examined in a single experiment. The percentage of each component can be determined accurately and the crystal structure of them can be solved readily. Simulating calculations were performed with a mixture of two different kinds of zeolites. The program suite CrystFEL [2] was used for simulating SFX diffraction patterns, diffraction indexing and Monte-Carlo integration of diffraction intensities. The program suite SHELX [3] was used for structure determination. Satisfactory results have been obtained and will be discussed in detail.

[1] H. N. Chapman et al. (2011). *Nature* 470, 73-77., [2] T. A. White et al. (2012). *J. Appl. Cryst.* 45, 335-341., [3] G. M. Sheldrick (2008). *Acta Cryst. A* 64, 112-122.

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