Poster Presentation

Structure determination from X-ray powder diffraction data at low resolution

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Knowledge of the structural arrangement of atoms in solids is necessary to facilitate the study of their properties. The best and most detailed structural information is obtained when the diffraction pattern of a single crystal a few tenths of a millimeter in each dimension is analyzed, but growing high-quality crystals of this size is often difficult, sometimes impossible. However, many crystallization experiments that do not yield single crystals do yield showers of randomly oriented micro-crystals that can be exposed to X-rays simultaneously to produce a powder diffraction pattern. Direct Methods routinely solve crystal structures when single-crystal diffraction data are available at atomic resolution (1.0-1.2Å), but fail to determine micro-crystal structures due to reflections overlapping and low-resolution powder diffraction data. By artificially and intelligently extending the measured data to atomic resolution, we have successfully solved structures having low-resolution diffraction data that were hard to solve by other direct-method based computation procedures. The newly developed method, Powder Shake-and-Bake, is implemented in a computer program PowSnB. PowSnB can be incorporated into the state-of-the-art software package EXPO that includes powder data reduction, structure determination and structure refinement. The new combination could have potential to solve structures that have never been solved before by direct-methods approach.

Keywords: Direct methods, Powder diffraction, Low resolution data