Exploring Novel Synchrotron Approaches to Structure Determination by Single-crystal XRD

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Introduction of modern area detector equipped high-pressure crystallographers in an important new tool and opened possibilities for new types of experiments. So far, however, the exploration of benefits of these detectors has been restricted only to monochromatic experiments. Polychromatic radiation has been used in high-pressure studies for almost two decades, but has never been demonstrated to be competitive with monochromatic experiments in terms of full structure determination. In this presentation it will be shown that single-crystal polychromatic diffraction (pSXD) can be successfully used for full structure determination at high pressure, and at the same time offers such advantages, as ultrashort data collection time, ability to collect diffraction data without rotating the sample and depth-resolution. By combining recent solutions developed in protein Laue crystallography, materials science, and novel detector technology, unique approaches, optimized to meet the demands of ultrahigh pressure experiments can be developed. I will describe the theory of polychromatic microdiffraction, computational and experimental methods developed to deal with its limitations, and compare pSXD to alternative methods. Special emphasis will placed on discussing aspects of working with microcrystals and multigrain aggregates (with depth-resolution), and experimental approaches to peak energy determination, and harmonic deconvolution. It will be shown that in pSDX experiments x-ray absorption near-edge spectra can be obtained at the same time as the structural data, providing additional information about the local environment of individual ions as well as their electronic state. The status of on-going development of the discussed techniques at beamline 16BMB, APS and efforts to coordinate the development of SXD techniques at other high-pressure synchrotron beamlines in the US will be presented.

Keywords: phase transitions, XAS, polychromatic diffraction