Combining Laue Diffraction with White-beam Single-crystal EXAFS

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Polychromatic radiation has been used in high pressure x-ray diffraction studies for almost two decades, but has never been demonstrated to be competitive with monochromatic experiments in terms of applicability of it's results in full structure determination. This presentation will summarize the outcomes of new development efforts located at the HPCAT 16BMB beamline of APS. It will be shown that by combining the experience and ideas from such fields as high-pressure crystallography, protein Laue crystallography, microdiffraction, and EXAFS, new crystallographic methods, offering unique advantages and optimized for high pressure applications can be developed.

Transition elements control the oxidation-reduction process and magnetism of the Earth. The theoretically predicted and observed magnetic collapse in Fe_2O_3 and other Fe-containing oxides are usually associated with distortive structural transitions that can be definitively understood only by high-pressure SXD. Moreover, since conventional XRD techniques are not sensitive enough to detect continuous electronic transformations, such as spin crossover, complementary information from techniques such as conventional and synchrotron Mossbauer spectroscopy, X-ray emission spectroscopy or EXAFS, is needed. In our white beam SDX experiments diffraction data are obtained at the same time as x-ray absorption near-edge information, providing additional information about the local environment of individual ions as well as their spin state. As examples, data obtained for Cr_2O_3 and (Fe,Mg)O will be demonstrated.

Keywords: phase transitions, spin crossover, polychromatic diffraction