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ADVANCED PHOTON SOURCE

A New Tool for Structure Studies at High Pressures with a DAC

A scanning angle energy-dispersive x-ray diffraction (SA-EDXD) technique employing an energy-dispersive solid-state detector and white synchrotron radiation has been developed for high-pressure structure studies using a diamond anvil cell (DAC). The main feature of the technique is well-defined collimation of the diffracted beam path into the detector, which improves the signal-to-noise ratio significantly compared to routine monochromatic angle-dispersive powder diffraction. This is particularly useful and essential for materials with low-scattering cross section and/or amorphous and liquid diffraction/scattering studies using a DAC.

The diamond anvil cell is one of the most common devices used for high-pressure structure studies. Due to the thin sample used in a DAC at high pressure, the background from the diamond and from pressure-transmitting media is often significant for routine angle-dispersive powder diffraction. Combining a solid-state point detector with a scanning diffraction angle, one can establish good collimation to measure only the diffraction signals from a sample (Fig. 1). A group at the High Pressure Collaborative Access Team (sector 16 at the APS) has extended the technique—making it suitable for DAC experiments—by employing high-precision stages with a sphere-of-confusion that is less than 5 μm. Together with software developed for automation control and data analysis, this technique is now available for APS general users. The diffraction intensity is sorted to 4,000 channels by the energy-dispersive detector. When the multichannel energy data is converted to constant-energy angle-dispersive data, only a coarse 2θ scan is required to achieve the regular angle-dispersive diffraction resolution. One can achieve an angle-dispersive diffraction pattern at certain energies (and energy-dispersive diffraction pattern at other angles) for structure analysis and refinement.

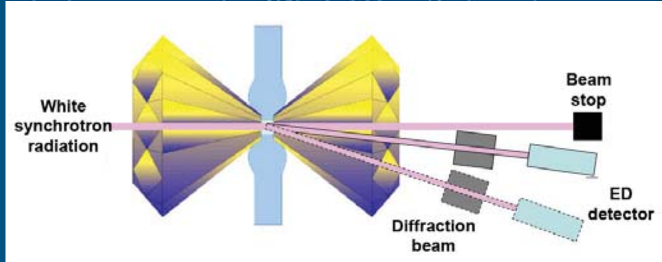

Fig. 1. Schematic of data acquisition with the SA-EDXD technique.

The SA-EDXD technique provides an important new tool for amorphous and liquid structure studies under extreme conditions. The well-defined collimation ensures the necessary signal-to-noise ratio for weak signals from amorphous and liquid materials in DAC. The use of white beam up to 110 keV covers a large Q-range (>20 Å^{-1}). The intensity data collected by the SA-EDXD technique are a function of energy and angle, from which one can obtain angle-dispersive data from different energies, and energy-dispersive data at different angles as well. The structure factor, S(Q), can be calculated from the angle-dispersive pattern at different energies (Fig. 2), while each one has different Q-range. A combined S(Q) can be obtained for a large Q-range. The work for partial structural factors is in progress.

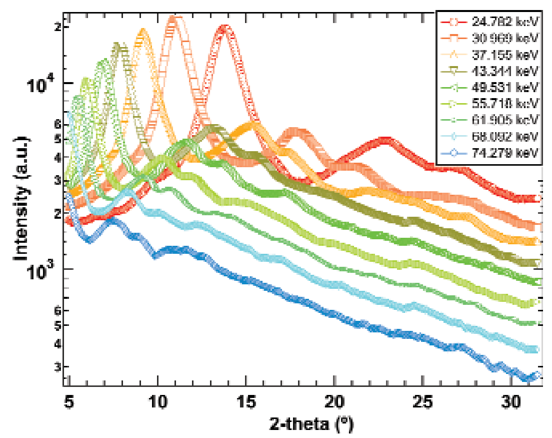

Fig. 2. Nine angle-dispersive data (a), with energies from 24 keV to 74 keV, are used to obtain the full structural factor S(Q).

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See: Y. Wang et al., J. App. Cryst. (2004) **37**, 947-956.

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