SAXS-WAXS studies of Amorphous, Mesoporous and Nanomaterials

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High energy x-rays (>50 keV) are extremely penetrating and provide a bulk probe of a material's structure. A wide region of reciprocal space is reduced to a small angular cone allowing access to high momentum transfers and high real space resolution in the associated pair distribution function. Here we describe a dual detector system for high-energy x-ray, simultaneous, small and wide-angle x-ray scattering (SAXS and WAXS). The instrumentation provides continuous reciprocal space coverage over many length-scales (0.01 to 20 nanometers), opening the door to *in-situ* and time-resolved studies of atomic to mesoscopic scale processes. The varying resolution, splicing of data and normalization on an absolute scale are discussed with a focus on applications to amorphous, mesoporous and nanomaterials. Examples will include glassy itraconazole and the amorphous mesoporous silicas MCM-41 and SBA-15.

The combination of SAXS and WAXS theory is considered with a view to enabling Fourier transformation of the structure factor spanning multiple length-scales in reciprocal space into real space, to obtain an extended-range pair distribution function. Several examples are used to illustrate that when the SAXS intensity in the structure factor, S(Q), is similar to the WAXS intensity, the contributions to the extended-range pair distribution functions are minimal. However, when the SAXS intensities are significantly stronger than the WAXS, the observed density fluctuations can provide unique information on the local, intermediate and nanometer length-scales. Most notably, the method strongly reflects the periodicity associated with intense low-Q reflections and is useful in obtaining direct information on maximum particle sizes and their distributions.