Characterization of nanocrystalline mineral precipitates using PDF analysis from X-ray total scattering.

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Evaluating atomic structure in nanocrystalline materials using traditional powder diffraction analysis techniques (e.g., Rietveld method) is often hindered by the broadening of diffraction maxima resulting from the effects of particle size and disorder. These effects are manifested as a significant diffuse scattering component in a diffraction pattern which contains important information regarding the local atomic arrangement in the structure. Total scattering and pair distribution function (PDF) analysis is therefore a valuable tool for evaluating nanocrystalline materials because the diffuse scattering, as well as the Bragg component, are included in the analysis and therefore information regarding the short-, medium-, and long-range atomic ordering is attainable.

We have recently used the PDF method to probe the atomic structures of a number of nano-sized metal sulfides (e.g., FeS and MnS) and oxides (ferric and aluminum hydroxides). These compounds are abundant in certain near-surface environments and often play important roles in geochemical processes and the fate of contaminants. The atomic structure of a material has implications on its reactivity and other unique properties and is therefore an essential component for completing a fundamental characterization study.