Resolving Structure and Size of Amorphous Mineral Precipitates by PDF Analysis

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Amorphous, or X-ray amorphous, is a common term used to describe mineral precipitates lacking long-range order. Earth materials, such as amorphous FeS, silica, and Fe(III)-hydroxide, are abundant in natural environments and play an important role in geochemical processes and the fate of contaminants. While use this term persists in the Geosciences community, it is important to resolve the short- to medium-range structure and fundamental size of these solids to deepen our understanding of their role in geochemical processes. In this study, we report on the structure and size of so-called amorphous FeS, the first Fe-S phase formed in anoxic sediments which, over time, will convert to pyrite (FeS_2). Amorphous FeS can also sequester metals and metalloids, such as cadmium and arsenic and react with contaminants, such as Cr^{6+}. High-energy X-ray scattering data for freshly precipitated and aged FeS (7 days at 70°C) were collected at the Advanced Photon Source and analyzed using the PDF method. Results indicate that amorphous FeS has short- to medium-range order consistent with that of crystalline mackinawite. Further, the range of structural coherence (i.e., fundamental particle size) as can be obtained from PDF [1] is initially about 2 nm, but increases to 4.5 nm for the aged sample. Hence, the initial FeS precipitate is better described as a nanocrystalline material with mackinawite structure. This technique holds great promise for further study of nanocrystalline earth materials lacking long-range order.

[1] Page et al., *Chemical Physics Letters*, 2004, **393**, 385-388.

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