2010 GSA Denver Annual Meeting (31 October –3 November 2010)

Paper No. 18-4

Presentation Time: 8:50 AM-9:05 AM

STRUCTURAL STUDY OF BIOTIC AND ABIOTIC NANOCRYSTALLINE MANGANESE OXIDES USING ATOMIC PAIR DISTRIBUTION FUNCTION TECHNIQUE

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Atomic pair distribution function (PDF) analysis is a powerful technique to determine crystal structures of nanoparticulate, poorly crystalline and amorphous materials. The PDF technique recently has been applied in the structural characterization of several disordered environmental minerals, such as ferrihydrite and imogolite. In this study, we used PDF analysis to investigate the structures of nanophase manganese (Mn) oxides. Mn-oxides, including both layered and tunnel structures, are strong oxidants and extraordinary metal sorbents in nature. Naturally-occurring Mn-oxides often have poor crystallinity as determined via XRD, and neither XRD nor EXAFS techniques are able to fully interpret, or even differentiate, their structures. For example, amorphous todorokite (3×3 tunnel structure) and birnessite (layered structure) cannot be differentiated by XRD and EXAFS if they are so disordered that 7 or 10 Å d-spacing is not observed. δ-MnO_2, polymeric MnO_2 and biogenic Mn-oxides are most often used as analogues to investigate the environmental behaviors of natural poorly crystalline Mn-oxides. Our PDF results indicate that δ-MnO_2, polymeric MnO_2 and a biogenic Mn-oxide sample are layered structures with nearly hexagonal symmetry. The particle size and shape are refined during the structural modeling for the PDF simulation. The best model accurately allowing simulation of the PDFs is a monoclinic structure with the C2/m space group using a disk-like shape factor with a high degree of stacking disorder. These results help in understanding the reactivity and mineralogy of several naturally-occurring Mn-oxide minerals.

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General Information for this Meeting

Session No. 18
Structure, Properties, and Geochemistry of Nanoparticles, Nanoclusters, and Nanocomposites in Biogeochemical Systems I: In Honor of Benjamin Gilbert, Recipient of the 2010 MSA Award
Colorado Convention Center: Room 111/113
8:00 AM-12:00 PM, Sunday, 31 October 2010

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