Powder neutron diffraction studies of ferrihydrite, a nanocrystalline material

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Due to the nanoparticulate nature of ferrihydrite and the lack of a crystalline analogue, structure determination has eluded researchers for over 50 years. Over the years, various structural models have been proposed; the one with the greatest longevity was put forward by Drits *et al*. in 1993 [1], This suggested ferrihydrite to be an intergrowth of two separate phases, one ordered and one highly disordered with variable composition. Recently, using high energy x-ray diffraction collected at the APS coupled with PDF analysis, Michel *et al*. proposed a single phase model [3], based on the structure of the mineral akdalaite, $Al_{10}O_{14}(OH)_2$.

The model proposed by Michel *et al*. [2] is incomplete, however, as the hydrogen atoms are neglected due to their weak scattering of x-rays. We have conducted neutron powder diffraction experiments on deuterated samples using the NPDF diffractometer at Los Alamos to further investigate and test the robustness of this structural model. The model proposed by Michel *et al*. [2] fits the PDF derived from the neutron diffraction better than any other model proposed in the literature to date. Details of the hydrogen positions and defects in the sample are also possible using this technique.

[1] V. A. Dritis *et al*. (1993), *Clay Minerals*, **28**, 185-207. [2] F. M. Michel *et al*. (2007), *Science*, **316,** 1726-1729.

Development of a dynamic Mercury cycling model for the Gulf of Mexico

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The vast majority of the mercury exposure for people in the United States is from consumption of marine fish. The Gulf of Mexico (GOM) is a major source of fish from both recreational and commercial fishing (40% and 14% of the national totals, respectively). Many of these fish species have elevated levels of mercury, and the Florida Department of Health has issued consumption advisories for dozens of fish species from the GOM. We have developed a screening level dynamic mercury cycling model for the Gulf of Mexico with the following objectives: (1) simulate mercury cycling and bioaccumulation in the Gulf of Mexico, (2) examine the relative importance of mercury inputs from the atmosphere, watersheds, Atlantic Ocean, and in the case of methylmercury, internal production, and (3) examine how the importance of these sources varies regionally within the Gulf of Mexico to explain elevated mercury levels in commercially and recreationally important fish species. The primary model components include: (1) simulation of water circulation in the Gulf of Mexico by the Navy Coastal Ocean Model (NCOM), (2) a multi-cell adaptation of EPRI's Dynamic Mercury Cycling Model (D-MCM) to simulate mercury cycling and bioaccumulation, and (3) a simple box model representation of estuarine mercury dynamics.