

DAFS Study of Site-specific Local Structure of Mn in Manganese Ferrite Films

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Manganese ferrite (MnFe_2O_4) is a well-known magnetic material widely used in electronics for many years. It is well established that its magnetic behavior is strongly influenced by local structural properties of Mn ions, which are distributed between crystallographically inequivalent tetrahedral and octahedral sites in the unit cell. In order to understand and be able to tune properties of these structures, it is necessary to have detailed site-specific structural information on the system. Here we report on the application of diffraction-anomalous fine structure (DAFS) spectroscopy to resolve site-specific Mn local structures in manganese ferrite films. The DAFS measurements were done at undulator beamline 4-ID-D of the Advanced Photon Source at Argonne National Laboratory. The DAFS spectra (Fig. 1) were measured at several Bragg reflections in the vicinity of the Mn absorption K-edge, having probed separately contributions from tetrahedrally and octahedrally coordinated Mn sites.

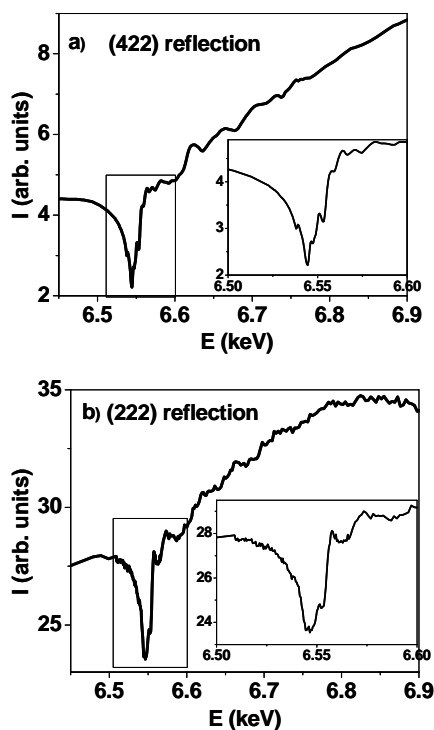


Fig. 1. Raw DAFS spectra obtained from Bragg reflections probing different site contributions: (a) purely tetrahedral site contribution measured at (422) reflection, (b) purely octahedral site contribution taken at (222) reflection.

The DAFS data analysis done with an iterative Kramers-Krönig algorithm made it possible to solve separately the local structure around different inequivalent Mn sites in the unit cell. The reliability of the data treatment was checked carefully, and it was showed that the site-specific structural parameters obtained with DAFS allow us to describe fluorescence EXAFS spectrum measured independently. Fig. 2 shows individual site contributions to the imaginary part of the resonant scattering amplitude obtained from the treatment of the data of Fig. 1.

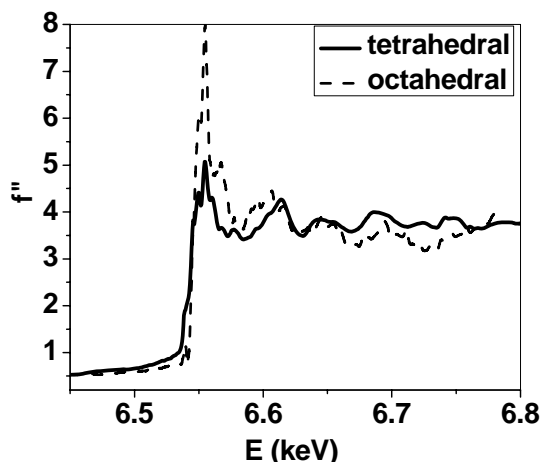


Fig. 2 Refined $f''(E)$ for Mn atoms located at tetrahedral and octahedral sites in MnFe_2O_4 film.

The analysis of the refined site-specific absorption spectra was done using EXAFS methods based on theoretical standards. We provided direct evidence for the tetrahedral Mn-O bond distance being increased relative to the corresponding Fe-O distance in bulk manganese ferrites. The first coordination shell number was found to be reduced significantly for Mn atoms at these sites. This finding is consistent with the well-known tendency of Mn to be tetrahedrally coordinated in these compounds.

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