Structural refinement of Garfield nontronite

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[en] The structural transformation of Garfield nontronite, following reduction of octahedral Fe(III), was investigated by X-ray absorption pre-edge spectroscopy, polarized extended X-ray absorption fine structure (P-EXAFS), X-ray diffraction, and X-ray texture goniometry. Highly oriented, self-supporting films were prepared under inert atmosphere conditions following reduction by Na-dithionite. Quantitative texture analysis revealed an average deviation of the c* axes of individual crystallites from the film-normal to be 19.8 deg and 38 deg for the oxidized and reduced samples, respectively. Angular measurements of such oriented films greatly enhance the sensitivity of EXAFS for studying the octahedral sheet cations of fine-grained layered silicates. The partitioning of Fe between cis (M2) and trans (M1) sites within the octahedral sheet was determined from the relative intensity of the (02,11) and (20,13) scattering bands and site occupancy simulations of XRD patterns for turbostratic crystallites. In this study, pre-edge and powder EXAFS spectroscopy detected no 4- or 5-fold Fe(III) in the oxidized Garfield nontronite. Powder XRD modeling indicated that the oxidized nontronite is essentially trans-vacant within the detection limit of 5% of total iron. The in-plane and out-of-plane local structure around Fe atoms was probed by angular P-EXAFS measurements. In combination with distance-valence least squares analysis, a precise refinement of the oxidized nontronite was obtained and a structural model of reduced nontronite hypothesized. In the oxidized nontronite, Fe-Fe and (Al, Mg)-(Al, Mg) pairs are preferentially aligned along the [010] axis and Fe-(Al, Mg) pairs along the [310] and [$-^{3}$10] axes. The Fe(III) octahedra are segregated in domains separated by Al-, Mg- and vacant octahedra, which may account for the lack of magnetic ordering at low temperature

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