Investigation of Smectite Structure Heterogeneities: an XRD Profile Modelling Approach.

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Because of its high ability for cation and water retention, smectite clay mineral plays an important role in water mobility and retention in soil or in waste repositories. As a function of relative humidity and under non-saturated conditions, smectite typically shows a stepwise hydration behaviour corresponding to the intercalation of 0, 1 or 2 discrete sheets of water molecules in its interlayer. However, heterogeneities of charge location (between octahedral and tetrahedral sheets) and/or of charge amount (from one interlayer to the other or within a given interlayer) most often lead to the coexistence of different hydration states within smectite crystals. In addition strong positional disorder of interlayer water and cations has most often to be considered when attempting to reveal the structure of such disordered layered systems. The presentation will be devoted to the characterization of these structural defects by comparing experimental X-ray diffraction (XRD) patterns with calculated profiles for (00L) reflections.