Molecular simulations and in-situ environmental x-ray diffraction experiments of clays and clay minerals

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Molecular simulations (molecular dynamics calculations:MD) and environmental in-situ experiments waere carried out to investigate the hydration, swelling, diffusion, viscosity, consolidation, etc. of clays and clay minerals.

We performed MD simulations with mxdorto and mxdtricl (Kawamura, 2003) in which all the atoms in a system are treated independently. The interatomic potential model wa newly produced to reproduce dielectric properties of water qantitativly.

Single crystal smectite (beidellite), its Cs-form and Ca form, muscovite, and pyrophyllite were investigated and compared in terms of interlayer hydration and swelling properties.

We carried out MD calculations of air-water-clay molecules three phase system to simulate real clay systems.

Environmental in-situ x-ray diffraction experiments were performd to compare with MD results. We prepared the device to keep clay sample upto 200 C and P(H2O)=1 atm. The measuremnts were made for smectite (Kunigel V1) up to 150 C and 1 atm of P(H2O) to determine the swelling properties.

We also carried out in-situ diffraction observation under uniaxial consolidation experiments of clays.

We plan to make molecular simulations with large scale systems to simulate real sytems. And also we plan to make x-ray experiments unde 200 C and P(H2O)=15 atms and up-to critical point of water conditions to simulate clays in earth's crust.