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Thermo-mechanical behavior of clays explained from the nanoscale

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The thermo-mechanical behavior of clays is known to be quite unusual (Fig. 1). Under drained conditions, normally consolidated clays exhibit an irreversible thermal contraction, whereas over-consolidated clays exhibit a reversible thermal expansion at small temperature, followed by an irreversible thermal contraction at high temperature. In the later case, the transition from expansion to contraction occurs at a critical temperature that increases with over-consolidation. Accordingly, over-consolidation is a key property regarding the thermo-mechanics of clays.

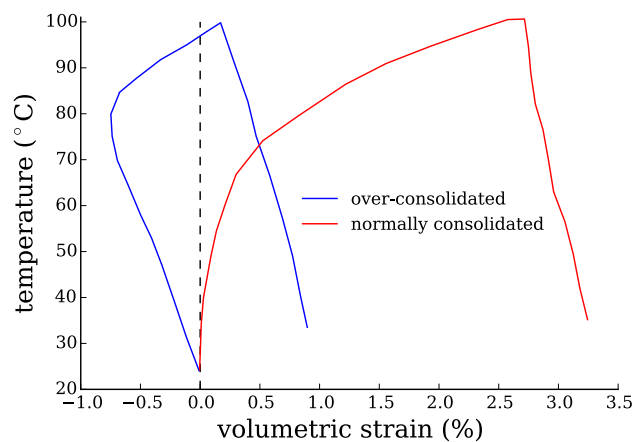


Figure 1. Volumetric deformation of Boom clay under thermal loading at constant confining stress and water pressure (adapted from Sultan et al. 2002).

The amplitudes of thermal expansion ($\sim 10^{-4} \text{ K}^{-1}$) and thermal contraction ($\sim 10^{-3} \text{ K}^{-1}$) are much larger than that of conventional solids and are closer to that of liquid water ($2 \cdot 10^{-4} \text{ K}^{-1}$ at 300 K). Accordingly, the unusual behavior of clays is usually attributed to the water, and in particular to adsorbed water which is known to significantly influence the mechanics (clay deformation under humidity changes). However, the fundamentals of clay thermo-mechanics are still poorly understood (relationship between adsorption and over-consolidation? Origin of irreversibility?), and current THM models of clays are mostly macroscopic and phenomenological and do not rely on a description of

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adsorption at the nanoscale. In this work, we propose to relate the macroscopic behavior of clays to the adsorption-induced mechanics of clay layers at the nanoscale.

At the nanoscale, clays are made of mineral layers separated by confined water. Confinement forces the water molecules to adopt a layered structure and exert a mechanical stress on the minerals that depends strongly on the basal spacing and can be much larger than the bulk pressure. The mechanical response of drained clay layer is 'oscillating' with deformation (see Fig. 2) and accordingly there exist 'forbidden' (unstable) deformations. (Meta-)stable deformations correspond to a finite number of water layers (0W, 1W, 2W etc.), which we can be viewed as different 'phases' of the material.

At the scale of ~ 100 nm, stacks of a few tens of clay layers form particles. Particles with varying orientations aggregate together to form a matrix at the micrometer scale. A clay rock is made of such a matrix mixed with mineral inclusions (silica, carbonate etc.). To relate the mechanics of clay layers to the mechanics of the rock, we follow an upscaling strategy inspired by the theory of shape memory alloys: as in martensitic materials, different phases (xW) can coexist in a stack of clay layers. Thus, the mechanics of a stack follows the convexified free energy of a single layer, which give rise to apparent plasticity. This approach is enriched to account for metastability and homogenized to the rock scale with a self-consistent scheme.

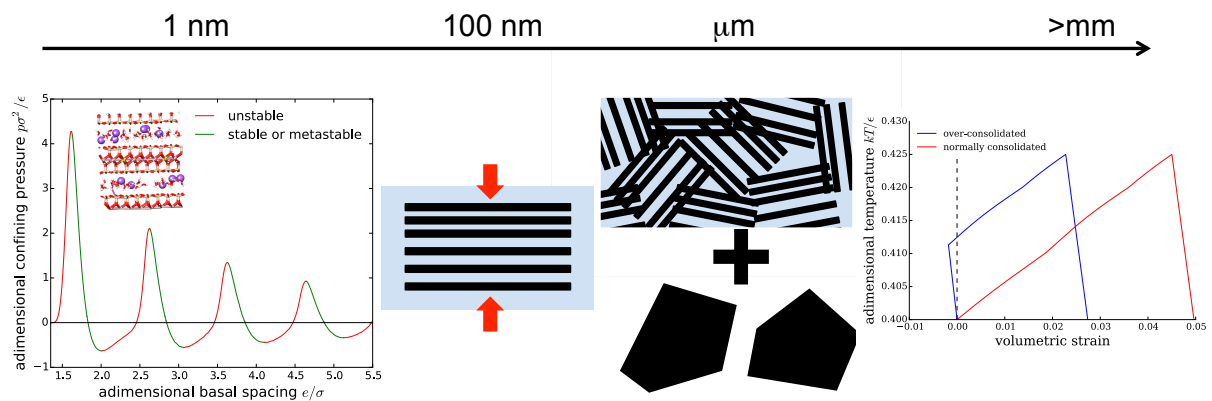


Figure 2. At the nanoscale, the mechanics of clay layers is controlled by water adsorption and exhibits different 'phases' corresponding to the number of water layers between mineral particles. At the scale of a stack of layers or particle, different phases can coexist which give rise to an apparent plasticity.

Up-scaling to the rock scale is performed with usual homogenization schemes that account for the distribution of orientation of clay particles and for the presence of mineral inclusions. The resulting mechanical model exhibits the same unusual thermo-mechanics as that observed in experiments on clays.

This upscaling approach leads to a thermo-mechanical behavior that captures all the features of the known thermo-mechanics of clays: reversible expansion / irreversible contraction depending on over-consolidation, increase of the expansion branch with over-consolidation, no effect of the magnitude of confining stress. This points to the importance of nanoscale adsorption in the thermo-mechanics of clays and call for a modeling of clay THM behavior based on the fundamentals of adsorption at the nanoscale.

References

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