

Title : Numerical modelling of the transformation of clay minerals under hydrothermal conditions.

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Summary :

The aim of this simulation internship is to apply the NANOKIN code to the transformation of clay minerals under hydrothermal conditions : smectite-type minerals in interaction with aqueous solutions at various concentrations (from dilute surface waters to sea water or thermal waters composition) and their evolution to chlorite- or illite-type compositions. The code NANOKIN allows to predict the nucleation and growth of secondary phases in fluid-mineral interaction with description of the crystal size distribution of secondary formed particles. The major objective of the stage will be to consider the effect of a thermal gradient on the interaction between clay minerals and aqueous solutions as it occurs in natural systems (diagenetic conditions or hydrothermal systems) between 60 and 150°C.

Duration of the stage : 5 months (february to june 2014).

Recent publications related to NANOKIN :

Noguera C., Fritz B., Clément A. et Baronnet A (2006) - Nucleation, growth and ageing in closed systems II : dynamics of formation of a new phase. *J. of Crystal Growth*, 297, 187-198.

Fritz B., Clément A., Amal Y., Noguera C.(2009) Simulation of the nucleation and growth of simple clay minerals in weathering processes : the NANOKIN Code. *Geochimica et Cosmochim. Acta*. 73, 1340-1358. Doi : 10.1016/j.gca.2008.11.043

Noguera C., Fritz B. and Clément A. (2011) - Simulation of the nucleation and growth of clay minerals coupled with cation exchange. *Geochim. et Cosmochim. Acta*, 75, Issue 12, 3402-3418.

Fritz B., Clément A., Montes-Hernandes G. and Noguera C. (2013) - Calcite formation by hydrothermal carbonation of portlandite: complementary insights from experiment and simulation. *CRYSTENGCOMM*, 15, 3392-3401, DOI:10.1039/C3CE26969H.