Molecular dynamics simulation of the water structure in nano-pores between kaolinite (001) surfaces

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It has long been found that the structure and chemical activity of the water in nano spaces are significantly different than those of bulk water. In order to obtain the possible behavior of the geofluids in argillaceous rocks, molecular dynamics (MD) simulations of liquid water held in one-dimensionally confining space by two parallel surface of kaolinite (001) was carried out. The simulation cell consists of four kaolinite platelets of eight unit cells each (2 in x-dimension and 4 in y-dimension) and one slit pore is placed in the middle. As the initial state, 200 water moleculars were placed randomly in the space. The basal surface area is about 21.12×18.28 $Å^2$. In the simulations, the periodic boundary condition is imposed on three dimensions. All simulations were undertaken by using the LAMMPS package (version 10 Nov_2005) [1], and clayff force field was used to describe the interatomic interactions. NPT (298 K, 1 atm) simulations were firstly performed to acquire the equilibrium height of the slit pore. Then, the NVT simulations were executed to get the detail structure of the confining waters.

The structure of the entire water volume is substantially perturbed compared to bulk water. The density profile for oxygen of water is not symmetrical on either side of the water layer, which is attributed to the difference between the surface of octahedral sheet and that of tetrahedral sheet. The surface hydroxyl on the octahederal plays crucial roles. The oxygen atoms of the waters near the octahederal sheet generally form hydrogen bond with the surface hydroxyl, whereas the interaction between the waters on the other side of the water layer with the tetrahedral one is likely expulsion. In addition, the radial distribution function (RDF) reveals three regions of the water layer with different degrees of water orderings.

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Re-Os dating from Dongou Molybdenum ore Deposit in East Qinling orogenic belt, North China

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The Nangou molybdenum deposit is located in east Qinling orogenic belt tectonically belonging to the south edge of north China Craton. In fact this area is rich in molybdenum mineralization and may be one of the largest molybdenum mineralization districts in the world, where a series of molybdenum ore deposits have been discovered. The Nangou molybdenum deposit is newly discovered. These ore deposits retain the largest capacity of molybdenum in China. The most important mineralization of these molybdenum ores are porphyry type genetically forming with the Yanshan granites (Mesozoic) in Qinling orogenic belt [1]

In this study, 10 molybdenum samples from Donggou ore were collected for Re-Os precise dating analyzed by the ICP-MS method in National Research Center of Geoanlysis, Chinese Academy of Geological Sciences. The isochron age is 103±17Ma to 107±1.1 Ma with an initial Os ratio of 0.62±2.2 to 0±0.20 (MSWD=0.84 to 0.41). We believe these ages represent the ore-forming time of the Nangou molybdenum deposit, indicating that the uplifting Yanshanian magmatism after the collision of north and south China plates since the Triassic is of great significance for molybdenum mineralization belt in Qinling orogenic belt.

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[1] Du XW, Yang XY, Li ML, Lu XX (2007) *Geochemica Cosmochemica Acta* **71** (Suppl) A239.