Molecular dynamics simulations of NaCl-H_2O fluid at elevated temperatures and pressures

*Hiroshi Sakuma[1], Masahiro Ichiki[2]

1. National Institute for Materials Science, 2. Tohoku University

Fluids in the crust have large effects on the mass transfer, heat transport, and physicochemical properties of rocks. We have investigated the physical properties of aqueous fluids for developing the database used to model the distribution of fluids based on the geophysical observations. This study contributes to understanding the fundamental physical chemistry for characterizing the properties of aqueous fluids. Major components of fluid in the crust are estimated to be H_2O, NaCl and CO_2. Here we discuss the properties of NaCl-H_2O fluid.
Density and electrical conductivity of NaCl-H_2O fluids were calculated by classical molecular dynamics (MD) simulations from 673 to 2000 K, 0.2 to 2 GPa, and 0 to 10 wt% NaCl (to 22 wt% for the density) [1, 2]. These wide ranges of temperature, pressure, salt concentrations can be sufficient to discuss the fluids in the crust. Some highly conductive zones in the crust observed by the magnetotelluic technique can be interpreted by the presence of NaCl-H_2O fluid with the salinity lower than 7.0 wt%.
Our MD simulations can provide a plausible model to explain the density, electrical conductivity, dielectric constant of the fluid by the behavior of ions and H_2O molecules in the fluid. The behavior is discussed for developing the physical chemistry of aqueous fluids at elevated temperatures and pressures.

References
Sakuma and Ichiki (2016) *Geofluids*, **16**, 89-102.
Sakuma and Ichiki (2016) *J. Geophys. Res. Solid Earth*, **121**, 577-594.

Keywords: Supercritical fluid, Electrical conductivity, Density, Dielectric constant, Salt water

