Japan Geoscience Union Meeting 2010
(May 23-28 2010 at Makuhari, Chiba, Japan)

SCG004-10 Room: 302 Time: May 25 11:30-11:45

Prediction of electric conductivity of salt solutions in the earth's crust studied by a molecular simulation

Hiroshi Sakuma[1*], Katsuyuki KAWAMURA[1]

[1]Tokyo Tech. Depart. Earth Planet. Sci.

Geofluid is a key element to understand the physics and chemistry of earthquakes and volcanos. To know the distribution of the geofluid in the earth's crust, we have to decode the observed seismic and electric waves which include the information about the distribution of the geofluid. The development of material science for fluids in the earth's crust is necessary to translate the results of observations to materials. Here we focused on the electric conductivity of aqueous NaCl solution in the earth's crust and calculated the conductivity using classical molecular dynamics simulations.
We have used the full flexible atom model proposed by Kawamura (2008) for the aqueous salt solutions and minerals. This model successfully reproduces the thermodynamic, spectroscopic, dynamic properties and structure of ice and liquid water, salt solutions and minerals. To apply this water model at high pressure and temperature conditions, we have to check the reliability of the model under super critical conditions. We compared the electric conductivity of 0.1 m NaCl solutions calculated by this model with an experiment [2] at P = 1-4000 bar and T = 298-1100K. We discuss the applicability of this model to the NaCl solutions at high pressure and temperature conditions and the possibility of the development of the model.

Keywords: Water, Specific resistance, MD, Geofluid, Solid-liquid interface, Electric conductivity