Japan Geoscience Union Meeting 2013
(May 19-24 2013 at Makuhari, Chiba, Japan)

SCG63-12 Room:104 Time:May 23 11:00-11:15

Electrical Conductivity of Highly Concentrated Salt Solution at Elevated Temperature and Pressure

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Introduction: Aqueous fluids in the Earth's crust would have large effect on the occurrence of earthquake and volcanic eruptions. To understand the effect of aqueous fluids, it is necessary to delineate their distribution in the Earth's crust. The distribution of the fluids has been expected to be revealed by electromagnetic observation, e.g. magnetotellurics. Electrical conductivity distribution in the crust is considered to roughly correspond to the fluids distribution because of the high electrical conductivity of fluids relative to solids. To develop a plausible model of the fluids distribution to explain the electromagnetic observations, we have to construct a database of the electrical conductivities of fluids over a range of pressure (p), temperature (T), and electrolyte concentrations (c). Classical molecular dynamics (MD) simulations are useful to obtain the physical properties of fluids at a range of p, T and c and to understand the underlying atomic-scale mechanism of the electrical conduction. Liquid and spuercritical phases of water and aqueous NaCl solutions are dominant at the p-T conditions of the Earth's crust. The aims of this study are (1) to develop a database of electrical conductivity of aqueous NaCl solution at a range of temperature, pressure, and salt concentrations and (2) to understand the physics and chemistry of the electrical conductivity of NaCl solution at extremely supercritical conditions.

Computational Methods: We used a flexible and induced point charge (FIPC) water model [1]. The point charges are fluctuated during the MD simulations. The MD simulations were performed using the code MXDORTO with some modifications. The database of electrical conductivity was developed for NaCl solution at $T < 2000$ K, $p < 2$ GPa, and $c < 9.5$ wt%

Results and Discussion: The electrical conductivity was almost constant at $T > 673$ K, $p > 0.5$ GPa, and low salt concentration c = 0.6 wt%. This is because the association of ions canceled out the mobility of ions at these conditions. At the salt concentration c = 3.3 wt%, which corresponds to the concentration of sea water, the electrical conductivity showed large temperature and pressure dependences at $T > 1000$ K and $p < 1.0$ GPa. The values were a function of temperature and density of the solution. The maximum conductivity was ~25 S/m. The behavior of highly concentrated salt solution c = 9.5 wt%, which is a few times higher than the sea water, will be discussed in the presentation. In this study, we explain the underlying mechanism of the change of the electrical conductivity of aqueous NaCl solution in the supercritical phase from atomistic view and try to construct the useful equations for the electrical conductivity of aqueous NaCl solution in the supercritical phase.

[1] Sakuma, H., Ichiki, M., Kawamura, K., and Fuji-ta, K., under revision.

Keywords: NaCl, geofluid, MT, static dielectric constant, water, viscosity