

Is H₂O-NaCl fluid enough to explain high electrical conductivity in the earth's crust?

SAKUMA, Hiroshi^{1*} ; ICHIKI, Masahiro²

¹National Institute for Materials Science, ²Tohoku University

Old continental crust has a high electrical conductivity layer at 20 to 30 km in depth [1]. Presence of aqueous fluids is a plausible hypothesis for explaining the high conductivity zone [2]. Therefore the electrical conductivities of aqueous fluids under high pressure (P), temperature (T) conditions should be investigated in order to evaluate the hypothesis. The phases of water and aqueous NaCl solutions at the P - T conditions of the Earth's crust correspond from liquid to supercritical states.

Experimental approaches to measure the electrical conductivities at high P , T and salt concentration (c) conditions are limited and the data at $P < 400$ MPa, $T < 1073$ K and $c < 0.6$ wt% for aqueous NaCl solutions is only available [3]. Classical molecular dynamics (MD) simulations are useful to obtain the electric conductivities at high P , T and c conditions and for understanding the underlying mechanism controlling the conductivities.

We used the flexible and induced point charge (FIPC) H₂O model [4] for MD simulations of aqueous NaCl solution. The technical details of the model and computational methods are explained in the literature [4]. The unit cell contained 2222 H₂O and 4 NaCl, 2035 H₂O and 22 NaCl, and 2035 H₂O and 66 NaCl for $c = 0.6, 3.4,$ and 9.6 wt% NaCl solutions, respectively.

The isotherms indicate that the conductivity increases with increasing pressures and saturated at high pressures. The conductivity decreased with increasing temperature. This behavior may seem to be strange, since the ionic mobility should be high at high temperatures. This can be explained by the mixed effects of the change of (i) the density, (ii) ionic mobility, and (iii) dielectric constant of water as discussed in Quist and Marshall (1968) [3]. We concluded that the change of the conductivity of H₂O-NaCl fluids along with a geotherm model can explain one order of the increased magnitude at the high conductivity layer in depth, but more change observed by the Magnetotelluric method should be explained by the additional mechanism such as the connectivity of the fluids and the conductivity of H₂O-CO₂ fluids.

References

- [1] T. J. Shankland and M. E. Ander (1983) *J. Geophys. Res.* **88** 9475-9484.
- [2] B. E. Nesbitt (1993) *J. Geophys. Res.* **98** 4301-4310.
- [3] A. S. Quist, and W. L. Marshall, (1968) *J. Phys. Chem.* **72** 684-703.
- [4] H. Sakuma, M. Ichiki, K. Kawamura and K. Fuji-ta (2013) *J. Chem. Phys.* **138** 134506.

Keywords: salt water, electrical resistivity, supercritical fluid, molecular dynamics, static dielectric constant