

Molecular dynamics simulations of dielectric constant of salt water at elevated temperatures and pressures

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Fluids in the crust have large effects on the mass transfer, heat transport, and physicochemical properties of rocks. Static dielectric constant of solution is one of the most required properties for understanding the dissolution and precipitation of minerals in the Earth's crust. The dielectric constant of pure water has been measured at elevated temperature and pressure; however, the experimental values of salt solution is, in our knowledge, limited at temperature lower than 50°C. Most equation of state of fluid used in geochemical modeling can be applied at less than 350°C. One of the reason of such limitation is the lack of adequate molecular-scale behavior of fluid at elevated temperature [1]. Molecular simulation is a powerful tool for estimating the macroscopic thermodynamic properties of fluid based on the intermolecular interaction.

Here, we calculated the static dielectric constant of NaCl solution at 573 K and 100-200 MPa using the classical molecular dynamics (MD) simulations. The dipole moment of water molecules, degree of dissociation of NaCl in water and hydration structure were calculated and the relationship with the dielectric constant was discussed. The static dielectric constant of salt water was obtained by the method proposed by Caillol *et al.* (1986) [2].

The degrees of dissociation of NaCl at 1.0 mol/kg, 573 K were 72% at 100 MPa and 76% at 200 MPa. The relationship with the dielectric constant is discussed in the talk.

References

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- [2] Caillol, Levesque, Weis, *J. Chem. Phys.* **85** (1986) 6645.

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