Molecular Dynamics Simulations of NaCl-H_2O fluid: Prediction of Electrical Conductivity of Salt Water in the Crust

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Presence of water reduces the strength of rock fracture and the frictional strength of faults, and the distribution of water in the crust, therefore, should be revealed for understanding the mechanism of earthquake occurrences. Water in the crust is considered to be salt water dissolving various ions. The electrical conductivity of such salt water shows six orders magnitude higher than that of common rocks at ambient conditions. In this context, electrical conductivity measurements have been performed for determining the distribution of salt water in the crust. Available conductivity data of NaCl-H_2O fluid, however, was limited to low pressure (<0.4 GPa) [1,2]; thus, it was difficult to discuss whether the presence of salt water can explain observed highly conductive zones in the crust.
In this study, we performed classical molecular dynamics (MD) simulations for predicting the electrical conductivity, density, and molecular behavior of NaCl-H_2O fluid at elevated temperatures and pressures in the crust. Our H_2O interaction model used for the MD simulations has succeeded in reproducing the density and permittivity of H_2O at temperatures and pressures over the critical point [3]. This H_2O model has been applied for reproducing and predicting the density and isothermal compressibility of NaCl-H_2O fluid [4]. Finally, we have derived the electrical conductivity of NaCl-H_2O fluid in the *pT* conditions of the crust [5].
In this talk, we discuss the behavior of NaCl-H_2O fluid in the crust as a function of temperature, pressure, and salinity. The salinity and fluid fraction of NaCl-H_2O fluid are discussed for explaining the observed highly conductive zone in the crust.

References

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