

The structure and transport properties of diopside supercritical fluid from ab initio calculations

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Subduction is one of the unique geological features of the Earth that carry water to the deep mantle. The slab-derived fluids could melt the surrounding mantle and generate the hydrous melt and the aqueous fluid with a miscibility gap. In the deeper subduction zones with higher temperature, the miscibility gap diminishes to form the supercritical fluid. The supercritical fluids with fluid-like viscosity and melt-like element carrying ability play a fundamental role in the chemical transport in the subduction zone. Yet, the atomic structures and their effect on transport properties of supercritical fluids remain poorly understood.

Here, we perform the first-principle molecular dynamic calculations on supercritical fluid of the composition of diopside with 0 ~ 78 wt.% water ($\text{CaMgSi}_2\text{O}_6\text{-xH}_2\text{O}$) at 3000 K. We find that all the cation-anion coordination numbers decrease with water content, while bonding O (BO) and non-bonding O (NBO) change to free O as the water content increases. H occurs mostly as hydroxyl at water-poor condition and switches to H_2O molecule at water-rich condition. The diffusion coefficients appear as $D_H > D_{Mg} \sim D_{Ca} > D_O > D_{Si}$ and $D_H > D_O > D_{Mg} \sim D_{Ca} > D_{Si}$ for water-poor and water-rich condition, respectively. We find diffusivities of all elements ($\text{Log}D_i$) reduce linearly with the amounts of Si-related BO proportions. Similarly, the viscosities of diopside supercritical fluid increase linearly with the BO proportions. Our results suggest the presence of water has an equivalent effect as decompression, and the corresponding changes of BO proportion are responsible for the unique transport properties of supercritical fluid.