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Vaporization of $MgSiO_3$ from First Principle Molecular Dynamics Simulations and Implications for Planetary Impacts

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During the planetary impacts, large amounts of vaporized debris can be generated by releasing highly compressed materials adiabatically and intersecting the liquid-vapor phase envelope. They have long been recognized to be important for the chemical equilibrium and dynamics in the aftermath of giant impacts. However, present knowledge of the liquid-vapor phase equilibria and vapor phase speciation of silicates is extremely scarce or completely unknown over much of the relevant range, which makes the degree of impact-induced vaporization impossible to estimate accurately and therefore hinders our understanding of planetary formations and evolutions.

In this study, we have studied the vaporization of liquid $MgSiO_3$ from first principle molecular dynamics simulations over unprecedentedly high temperature regime (from 4000K to 8000K). Heterogeneous simulations involving two coexistence phases have been carried out with initial conditions prepared by first running a one-phase liquid simulation and then embedding the final snapshot in a large simulation cell that consists mostly of vacuum. The interfaces between the phases were then identified via the Gibbs criterion, which allows us to determine the densities and compositions of liquid and vapor phases in each snapshot. Speciations in the gas phase were inspected through bond-length criteria and analysis of the charge densities. The location of the critical point was finally estimated.

While the finite-size effects and phase behaviors of the other systems await further investigations in our subsequent studies, the *ab initio* simulation results in this study provide new constraints on silicate vaporizations and substantially reduce current uncertainties on the critical temperature and speciation. These may greatly affect the amount of vapor produced in giant impact, the composition of the first atmosphere overlaying the hadean magma ocean and potentially alter the accretion history of terrestrial planets.

キーワード: vaporization, first principle, impact, heterogeneous, phase equilibrium, silicate
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