Evaporating rocky planets: Critical vaporization of MgSiO3

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Abstract

Vaporization is an important process in Earth's earliest evolution during which giant impacts are through to have produced massive silicate atmospheres. As experimental data are very limited, little is known of the near-critical vaporization of Earth's major oxide components. We have performed novel ab initio molecular dynamics simulations of vapor-liquid coexistence in MgSiO3. The simulations, based on density functional theory, begin with a suitably prepared liquid slab embedded in a vacuum. During the dynamical trajectory in the canonical ensemble, we see spontaneous vaporization, leading eventually to a steady-state chemical equilibrium between the two coexisting phases. We locate the liquid-vapor critical point at 6600 K and 0.40 g/cm3. The critical temperature that we find is significnatly less than assumed in most hydrodynamic simulations of giant impacts (8800 K), suggesting that these simulations substantially underestimate vaporization. By carefully examining the trajectories, we determine the composition and speciation of the vapor. We find that vaporization is incongruent: the vapor is significantly enriched in O and depleted in Mg as compared with the bulk composition. Dominant vapor species are O2 and SiO; also present are greater amounts of SiO2 and free atoms than predicted by extrapolation of experimental data. These results will have important implications for our understanding of the initial chemistry of the Earth and Moon and the initial thermal state of the Earth.

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