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Supercritical silicate melts during the Giant Impact and in the protolunar disk

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We investigate the physical and chemical behavior of the molten protolunar disk, at the atomic level from first-principles molecular dynamics simulations. We consider the average composition of the Earth's mantle as proposed by Sun and McDonough (1995). We cover the 0.75 – 7.5 g/cm3 density range and 2000 – 10000 K temperature range.

At high density, the liquid is highly polymerized and viscous. At low density and low temperatures, in the 2000 to 4000 K range, we capture the nucleation of bubbles. These bubbles contain a low-density gas phase dominated by atomic species, alkaline and calc-alkaline cations, and SiOx groups. When volatiles are present such molecular species are the first ones to evaporate into these bubbles.

At high temperature, we identify the supercritical region characterized by one homogeneous fluid, rich in ionic species with short lifetimes. Its chemical speciation is very different from the one at ambient pressure conditions.

The nucleation of the bubbles corresponds to the spinodal instability of the melt phase in the van der Waals description of the liquid-gas equilibrium. The spinodals are reached consistently regardless of the thermodynamic path we chose to obtain the low densities. The critical curves, inferred from the spinodals, are necessary to understand the separation and degassing of volatiles during the recovery from a giant impact. As such we obtain that the largest part of the disk was in the supercritical state for a long time.

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