THERMOCHEMICAL STATE OF THE PROTOLUNAR DISK AFTER THE GIANT IMPACT.

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Introduction: Giant and large-scale impacts are ubiquitous features of early solar systems. They dominate the end of the accretion stage, where the number of bodies decreases but their size increases. The last major accretion event in Earth's history was the Moon-forming giant impact. Depending on the impact parameters, the outcome of this impact was the formation of a traditional protolunar disk or a synestia. Eventually the protolunar disk/synestia evolved to condense a large central hot body: the Earth, and a smaller satellite: the Moon.

Here we study the behavior of a multi-component silicate fluid with bulk silicate Earth composition [1], called pyrolite, at conditions typical for the giant impact. For this, we employ molecular dynamics simulations based on *ab initio* calculations.

Results from *ab initio* molecular dynamics simulations. We used 153 atoms in a cubic periodic simulation box to mode the system with $NaCa_2Fe_4Mg_{30}Al_3Si_{24}O_{89}$ composition. First, we monitor the variation of the pressure as a function of density along various isotherms. This procedure helps us determine the limits of stability of the molten silicate and the position of the critical point. Then we analyze the chemical speciation as a function of density and temperature.

We cover the 0.75 – 7.5 g/cm^3 density range and 2000 – 10000 K temperature range. With respect to Earth, this allows us to investigate the entire protolunar disk (from which the Earth and the moon formed), from the interior of the molten core to the outer regions of the vaporized disk.

At high density, the liquid is highly polymerized and viscous. At low densities and low temperatures, in the 2000 to 4000 K range, we hit the liquid-vapor dome: the melt is mechanically unstable. At these conditions only a mixture of gas and melts is stable; and our simulations are long and large enough to capture the nucleation of gas bubbles. The bubbles contain a low-density gas phase rich in individual alkaline and calc-alkaline cations and SiO_x groups. When volatiles are present in the system, such molecular species are the first ones to evaporate and be present in these bubbles. We interpret the bubble nucleation in terms of the liquid-vapor equilibrium. At high temperature, we identify the supercritical region characterized by one homogeneous fluid, featuring peculiar chemical speciation and short lifetimes.

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.

We also compute the Hugoniot equations of state for the bulk silicate Earth [2] and discuss its position with respect to the thermal-pressure profile inside the protolunar disk.

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References:

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