Pyrolite melts during and in the aftermath of the Giant Impact

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We study realistic six-component pyrolite melts over an extended range of pressures and temperatures that cover the protolunar disk from its outskirts down to the bottom of the Magma Ocean. For this we employ first-principles molecular dynamics as implemented in the VASP package.

Under pressure we find an increase of the coordination number of all atomic species, as a mechanism for accommodating compression, and a linear decrease of the self-diffusion. Iron atoms exhibit a gradual reduction of their magnetic moment. The presence of volatile species does not change the compressibility, but considerably affects the diffusion, the melt being less viscous by almost one order of magnitude.

At low pressures, i.e. densities below 1.5 g/cm^3, temperature-dependent, we identify the region of coexistence of vapour and liquid. The vapour is formed mainly of isolated ionized clusters of atoms. When volatiles are present they are the first one populating the bubbles.

We constrain the position of the supercritcal point. In the supercritical regime, at 7500K, the fluid is homogeneous even down to low densities. Si is in 3-fold coordination. At least 10% of O atoms bond to form molecules.

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