

Partial core vaporization during the Giant Impact

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The most widely accepted model today for the Moon formation is that of a Giant Impact. The energy during this impact was high enough to melt and partially vaporize the two bodies. Due to poorly constrained equation of state and thermodynamic properties of iron in low density region, to what extent a planet's iron core is vaporized is still undetermined.

Here we investigate thermodynamic properties, liquid-vapour equilibrium line and the supercritical point of iron using first principles molecular dynamics simulations. Our calculated liquid-vapour equilibrium line is in a good agreement with available experimental data. We compute the vibrational spectrum using the velocity autocorrelation function and eventually obtain the entropy along the spinodal and the Hugoniot lines. They suggest that partial core vaporization may be achieved during giant impacts. We also characterize the atomic speciation at high temperature and show the presence of a strong atomic component in the supercritical fluid, with little or no clusterization. We provide new information on equation of state and thermodynamic properties of iron that may be used in future hydrodynamic simulations of Giant Impacts.

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