

Outgassing of the magma ocean after the Giant Impact

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Catastrophic events dominated the history of the early Earth; the last Giant Impact was energetic enough to transform the proto-Earth and the impactor Theia into a protolunar disk or synestia. The Earth – Moon couple condensed upon cooling from this object. The first stage of the Earth condensation was into fully molten Magma Ocean.

Here we consider a six-component silicate melt whose composition reproduces dry pyrolite [1], the chemical and mineralogical model for the bulk silicate Earth (BSE). We explore the melts at the atomic scale, using ab initio molecular dynamics simulations. We monitor the behavior of a series of volatiles, like H₂O, CO, and CO₂, in the temperature and density ranges characteristic to the magma ocean.

We find that carbon is massively released in the first outgassing stage, mostly as CO₂. The gas, with a strong greenhouse effect, contributed to maintaining a hot dense atmosphere through a long geological time. As such, water degassed only at a later stage, when the pressure and the temperature dropped significantly. The relative proportion of released CO₂ increased with increasing oxidation state, decreasing density, and decreasing temperature [2].

The carbon fraction that remained in the melt formed oxo-carbon species in the upper parts of the magma ocean. In the deeper parts, carbon formed complex polymerized species, involving both Fe and Si [3].

Thus, our simulations offer a remarkable atomistic view in the mechanisms of magma outgassing and reactions with atmospheric gases. Our results can have extensive implications not only in understanding the chemistry of the atmosphere from the early Earth, but also in understanding volcano degassing and eruptions today.

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[1] McDonough & Sun (1995) *Chemical Geology* 120, 223-253.

[3] Solomatova & R. Caracas (2021) *Science Advances* 7, eabj0406.

[2] Solomatova & R. Caracas (2019) *Nature Communications* 10, 1-7.