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# The magma ocean of the early Earth: compressibility, structure, and volatile content

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As the protolunar disk formed by the giant impact with the incoming asteroid Theia started to cool, the Earth condensed in its center as a molten planet. The outer layer, rich in lithophile oxides, formed the magma ocean, whose dynamical behavior heavily influenced the entire evolution of the early Earth. Here, we employ first-principles molecular dynamics simulations to characterize the magma ocean in its initial stage. We consider molten pyrolite, which best approximates the bulk silicate Earth composition. With an extensive set of calculations, we span its entire relevant pressure-temperature range.

First, we provide a detailed analysis of its athermal and thermal equations of state.

Then, we analyze the evolution of the structure of the liquid as a function of pressure and temperature. The melt structure is formed on a backbone of silica and alumina polyhedra. The other cations, like Na, Mg, and Ca, freely float in between these large polymers. Iron plays a special role in that it may participate in the polymerization or may just lie in between these polymers. We follow the enlargement of the first-coordination sphere with pressure, and identify the fundamental role played by the collapse of the second coordination sphere in accommodating compression.

We investigate the dissolution of various volatiles in the magma ocean. We find that noble gases and CO2 are profoundly incompatible in silicate melts. They easily degas under lower pressure conditions, particularly when they are present jointly in the melt.

We relate the geochemical evolution of the magma ocean to the formation of the atmosphere and the development of deep reservoirs of volatiles, which remained isolated from the surface throughout the entire evolution of our planet.