Structure, thermodynamics and transport properties of Mg_2SiO_4 liquid under high pressure from molecular dynamics

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Melting is an ubiquitous process in planetary interiors and one of the dominant mechanisms for thermal transport and chemical differentiation in planets. The properties of silicate liquids are thus essential for understanding a wide range of geophysical phenomena related to the Earth and its origin and evolution. Forsterite is a major component of the Earth's upper mantle and is thus of considerable importance in controlling its properties, rheological and thermal structure.

In the present study, we have used large-scale molecular dynamics simulations to compute structure, thermodynamics, and transport properties of Mg_2SiO_4 liquid up to 32 GPa and over a temperature range of 2600 to 3200 K. The interactions between the atoms are modeled by an aspherical ion model (AIM). The parameters of the potential are fitted to ab initio results. Simulations were performed using a cubic simulation box with 2016 ions (288 formula units), a time step of 1 fs, in the NVT ensemble. The equilibration is done using an isotropic barostat coupled to the thermostat for 50 ps before the production run of 150 ps length is started.

We find that the coordination of Mg and Si increase with pressure. There is also a large redistribution of bond angles. Under compression the Si-O-Si distribution is shifted to smaller angles, allowing for more dense packing of the SiO_4 tetrahedra. Contrary to solids under pressure we find thermal pressure and the Grüneisen parameter to increase with compression. We find that diffusivity decreases uniformly with pressure, and viscosity increases uniformly with pressure. Both transport properties can be readily fit with closed Arrhenius expression over the whole pressure and temperature range considered. The independent estimates on diffusivity and viscosity allow us to examine their relation through the Eyring equation: the proportionality factor between them, the translation distance for a diffusion event, is determined as 18 Å at 0 GPa, and decreasing with pressure. Combining thermodynamic results with the viscosity fit we compute a magma ocean adiabat and the associated viscosity profile. We find that viscosity in the magma ocean is ~ 2. 10^{-2} Pas near the surface, and that it decreases by less than 0.1 log-unit up to 32 GPa.

Colder NADW leads to salty deep water formation in the South

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Today the deep ocean is filled with a mixture of warm/salty North Atlatnic Deep Water (NADW) and cold/fresh Antarctic Bottom Water (AABW). While NADW is more dense at the surface of the ocean, its relative warmth means that it is less dense than AABW at 3,000 meters deep, and as a result there is substantial mixing of the two water masses. However, there is growing evidence that at the Last Glacial Maxiumum (LGM) this arrangement was very different. Cold-salty waters from the south filled much of the deep Atlantic at the expense of cold-fresh waters from the north. In this configuration temperature and salinity do not oppose each other in the two water masses, and LGM AABW can be isolated from LGM Northern Source waters. I will show how this LGM water mass architecture can be a natural result of cooling NADW.

The densest componenet of AABW forms in winter time on continental shelves where sea ice formation and export leaves the remaining water enriched in salt. However, continental ice shelves impinge in these regions and provide a degree of ‘pre-freshening’ due to contact with the relatively warm ocean waters and subsequent melting. As the source of this ocean heat is largely NADW itself, I will explore a feedback mechanism where cooling NADW leads to less ‘pre-freshening’ of proto-AABW and eventually salty-cold waters forming in the south that are denser than all other open ocean water masses. Contrary to popular belief, cooling of NADW could sow the seeds of its own demise and lead to the LGM arrangement of very dense, isolated waters forming around Antarctica.