Silicate fluid thermodynamics in the aftermath of giant impacts

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Modelling of the aftermath of giant impacts entails assumptions about the phase relations of silicate materials and properties of the resulting system. Yet, the relevant low-pressure, high-temperature conditions are barely accessible by experiment, leading to huge uncertainties on such assumptions. As the first step in addressing this limitation, we present results of first principles molecular dynamics simulations on low density (100-1800 kg/m^3) SiO_2 fluid at 4000-5000 K. Our low-density simulations reveal a molecular liquid structure (Si-O coordination number <2).

In parallel with our simulations, we have parameterised a modified Redlich-Kwong (MRK) equation of state (EoS) for the Si–O fluid system, built on the species {Si, O, SiO, O_2, SiO_2} subject to simple mixing rules. The model is well supported by the structural and equilibrium properties drawn from our simulations, and shows remarkable consistency with independently determined phase relations at 0.1 MPa [1]. Notably, the MRK model predicts that liquid of bulk SiO_2 composition boils incongruently, with an Si-enriched negative azeotrope becoming apparent above ~10 MPa. The model differs in a number of predictions from the commonly used EoS of Melosh [2] for SiO_2 fluid, which, crucially, omits explicit speciation, imposing congruent boiling.

We expect our better supported model to put more accurate thermodynamic limits on the modelling of giant impact-related processes: for example, on the silicate-liquid maxcondentherm (generalised critical temperature), which defines the lowest temperature at which mass exchange can take place between a proto-planet and its debris disc without chemical fractionation. Future work will see the simulations and modelling extended to the MgO-FeO-SiO_2 system.

[1] Schnurre *et al*. (2004) *J Non-Cryst Solids* **336**, 1-25. [2] Melosh (2007) *Meteorit Planet Sci* **42** 2079-2098.