Goldschmidt 2021 Abstract
https://doi.org/10.7185/gold2021.5879

Hot supercritical MgO melt in the context of the giant impact

TIM BÖGELS[1] AND RAZVAN CARACAS[1,2]

[1]CNRS

[2]University of Oslo

Presenting Author: tim.bogels@ens-lyon.fr

The giant impact hypothesis is the currently accepted model to explain the formation of our moon. Here, a collision of a mars-sized impactor collides with the proto-earth. This giant impact vapourized a significant portion of the impactor and the proto-earth, creating a large accretionary disk from which the moon formed. Currently, there is a large effort to build reliable thermodynamic descriptors for the building materials of the two bodies involved in the impact. Understanding the behavior of major rock-forming minerals under these extreme conditions is vital for increasing the accuracy of these models.

Magnesium oxide, MgO, is one of the fundamental building blocks for rocky planets. It is an archetype material of ionic solids and a well-known refractory material. Because of its relevance it has been studied extensively. The phase transformation of the face-centered B1 phase to the body-centered B2 phase and its associated melting curves have been approximated often. These pressure and temperature regions are of great interest for the planetary sciences, studying planetary interiors. In contrast, we know very little of the liquid behaviour of MgO under pressure, let alone at the low pressures of accretionary disks.

Here we investigate the subcritical and supercritical regimes of MgO using ab initio molecular dynamics. We determine the critical point and examine its structural and transport properties in the sub- and supercritical regimes. We find an elevated critical temperature in comparison to previously studied magnesium-silicates, due to the refractory nature of MgO. Furthermore, we provide insight into the speciation of liquid MgO and the liquid-gas separation. We see a shift in Mg-O speciation towards lower degrees of coordination as the temperature increases from 4000K to 10000K. This shift in speciation is less pronounced at higher densities. The majority of the chemical species forming the incipient gas phase consist of isolated Mg and O ions and some MgO and O_2.

This research was supported by the European Research Council under EU Horizon 2020 research and innovation program (grant agreement 681818–IMPACT to RC). This research was performed by access to supercomputing facilities via eDARI stl2816 grants, PRACE RA4947 grant, Uninet2 NN9697K grant.