Study of self diffusion of noble ases in magma ocean

Adrien Saurety

Presented at IMA 2022 conference

Abstract

The source of the primordial isotopes of noble gases remains a matter of debate amongst geoscientists. Recent computational studies tend to agree on a reservoir in the deep mantle, though questions remain with respect to its actual formation, or the role played by the core.

Here, we study the diffusivity and the partial molar volume of the noble gases in the magma ocean. We work with pyrolite, with composition NaCa2Al3Fe4Mg30Si24O89 [Caracas et al., 2019], close to the bulk silicate Earth, and 2 atoms of the noble gas. Our calculations follow the magma ocean adiabat. We perform ab initio molecular dynamics simulations, as implemented in the VASP package. We perform the analysis of the results using the UMD package [Caracas et al., 2021].

The difference in Birch-Murnagham equations of state yields the partial molar volume for the gas. The relative order of partial molar volumes strictly follows the size of the noble gas atoms, as expected. At high pressure He is almost one order of magnitude more compressible than the rest of the noble gases.

With the exception of He, the diffusion coefficients of the noble gases are comparable to Mg. The lifetime of the coordination polyhedra formed by O around the noble gases are about half those of Mg. We analyze in detail a series of other structural parameters of the melt.

Acknowledgements

The Research Council of Norway through projects 223272 and 325567, the ERC (grant agreement 681818 – IMPACT), and supercomputing access via eDARI stl2816, PRACE RA4947, and Uninet2 NN9697K grants.

Reference

R. Caracas, K. Hirose, R. Nomura, and M.D. Ballmer. EPSL 516, 202–211 (2019)
R. Caracas, et al. J. Vis. Exp. 175, e61534. arXiv:2109.02916 (2021)