

PRESSURE-INDUCED SMOOTH STRUCTURAL EVOLUTION IN A TERRESTRIAL MAGMA OCEAN.

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Introduction: Rocky planets in the Solar System are widely thought to go through magma ocean phases in their violent early times (e.g. [1]). Silicate melts, that make up magma oceans, play a key role in the evolution of terrestrial planets, because their structure and properties at depth control how the metallic core segregates from, and the early atmosphere is degassed by, the magma ocean [2, 3]. However, due to the challenging nature of characterizing melts under extreme conditions inside planet interiors, their structure and properties remain largely elusive [4, 5]. Here, we combine acoustic velocity measurements and molecular dynamics simulations on the silicate Earth-like pyrolite glass/melt, to imitate the terrestrial magma ocean under mantle conditions (up to ~ 160 gigapascals) in the laboratory.

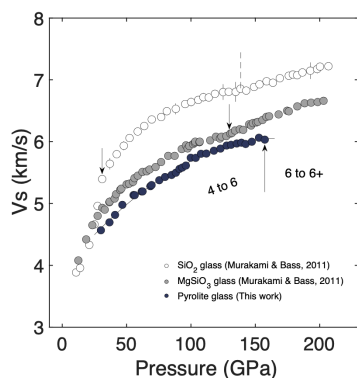


Figure 1: Transverse acoustic wave velocities V_s of SiO_2 , MgSiO_3 and pyrolite glass. Number denotes the inferred Si-O coordination under relevant pressure range.

Melt Structure Changes in Pyrolite Glass/Melt at Mantle Conditions:

We respectively performed in situ Brillouin scattering measurements and ab initio molecular dynamics simulations on pyrolite glass and melt. Over the entire mantle pressure range, the acoustic wave velocity changes continuously (Fig. 1), corroborating the predicted smooth structural modifications (Fig. 2). By comparing with previous studies on silicate glasses with varying compositions (e.g. [6–11]), we find that in less polymerized silicate, the pressure-induced transition from four- to six-coordinated Si is more protracted. Unlike instantaneous phase transitions in minerals that mark the discontinuities in the present-day mantle, gradual densification and coordination increase are expected in early terres-

trial magma oceans.

Our results highlight composition-structure-property relationships of the terrestrial magma ocean at varying depths, i.e. in a realistic magma ocean with complex components, silicate melt structure evolves continuously and gradually over the entire mantle conditions [12]. As a result, many magma ocean properties, e.g. density, diffusivity, viscosity, thermal conductivity and element partitioning, should behave in the similarly smooth fashion in response to pressure, which, when incorporated into magma ocean models, may change the picture of early evolution of the Earth and other rocky planets.

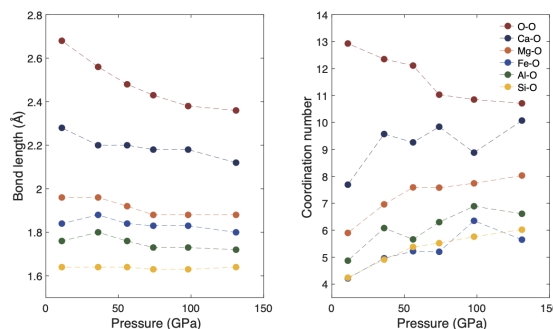


Figure 2: Bond length and coordination number of cation-O in pyrolite melt at 4000 K from ab initio simulations (details in [12]).

References: [1] Elkins-Tanton L. T. (2012) *Annual Review of Earth and Planetary Sciences*, 40(1):113–139. [2] Huang D. et al. (2020) *Proceedings of the National Academy of Sciences*, 117(45):27893–27898. [3] Huang D. et al. (2022) *Geophysical Research Letters*, 49(7):e2021GL095546. [4] Sanloup C. et al. (2013) *Nature*, 503(7474):104–107. [5] Bajgain S. et al. (2015) *Nature Communications*, 6(1):8578. [6] Stixrude L. and Karki B. (2005) *Science*, 310(5746):297–299. [7] Karki B. B. et al. (2007) *Phys. Rev. B*, 76:104205. [8] Murakami M. and Bass J. D. (2010) *Phys. Rev. Lett.*, 104:025504. [9] Murakami M. and Bass J. D. (2011) *Proceedings of the National Academy of Sciences*, 108(42):17286–17289. [10] Prescher C. et al. (2017) *Proceedings of the National Academy of Sciences*, 114(38):10041–10046. [11] Petitgirard S. et al. (2019) *Geochemical Perspectives Letters*, 9:32–37. [12] Huang D. et al. (2022) *Earth and Planetary Science Letters*, 584:117473.