Usage Report for Fiscal Year 2019

Project Title:

Magma from the early Earth to the current Earth

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1. Background and purpose of the project, relationship of the project with other projects

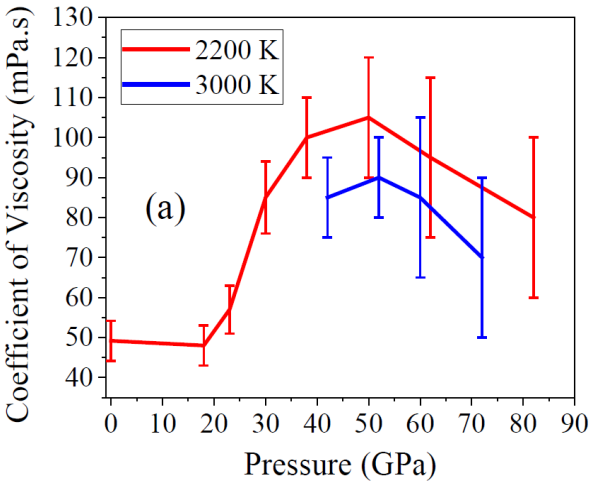
Transport properties such as diffusivity and viscosity of melts not only dictated the evolution of the early Earth's magma ocean but also control many geological processes from the dynamics of mantle convection to magma migration and volcanic activity. However, experimental measurements of melt diffusivity and viscosity at most of the mantle conditions remain impossible due to technical challenges. Here we focussed on providing reliable viscosity information on basalt melt, a major mineral component of the magma from ambient pressure to 80 GPa from First Principles molecular dynamics simulation on model ($Ca_{11}Mg_7Al_8Si_{22}O_{74}$).

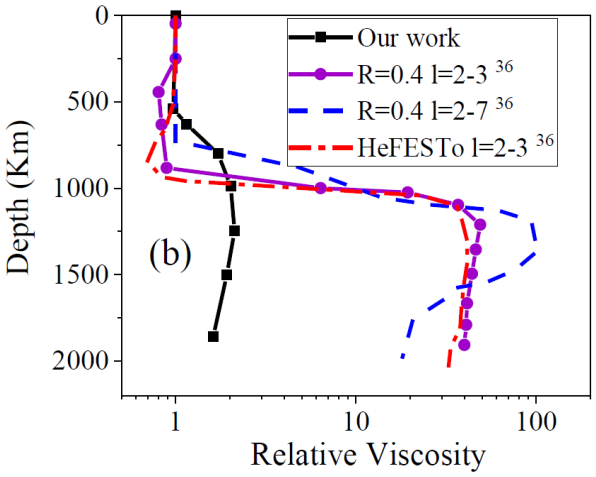
2. Specific usage status of the system and calculation method

Ab initio Molecular dynamics simulations were carried out on a model of liquid basalt. The computational protocol is as follow. The melt was produced by melting of basalt at 0 GPa. At each pressure, the melt was first computed using *NpT* ensemble for at least 10,000 steps using the *NpT* ensemble. The density at this pressure was then computed rfrom the equilibrated trajectory. For the ease of the calculation of viscosity using the Green-Kubo method, the system is constrained to be orthorhombic and *NVT* ensemble calculation was performed. Depending on the system, simulation up to 50000 – 10000 ps were performed. The simulations were carried using the VASP program, expanding electron orbitals in the plane wave (PAW) basis set. PBE functional was used keeping the kinetic energy cut-off of the plane wave 400 eV. One k-point (Γ) was used to sample the Brillouin Zone. For the melt system, simulations were performed at 0, 18, 23, 30, 38, 50, 62, 68 and 82 GPa and 2200/3000 K, similar to the experimental conditions. At each pressure, the melt was first equilibrated using constant-pressure-constant temperature (*NPT*) molecular dynamics at the desired temperature. Atomic trajectories from the MD calculations was used in the analysis.

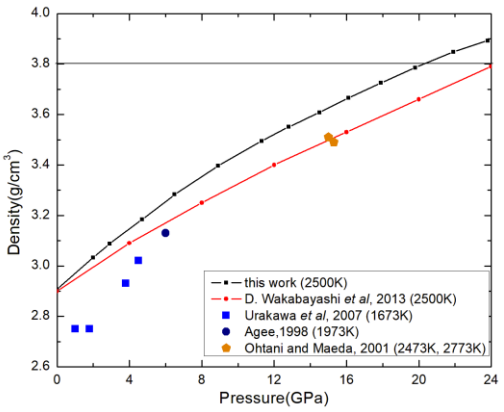
3. Result

In last year reported, we observed an anomaly in the transport properties (diffusion coefficients, electrical conductivity and viscosity) around 60 GPa and 2200K (Fig.1a and b). Additional calculations were performed at 3000K and the results confirmed this finding. The theoretical prediction supports the most recent inferences about the mantle's viscosity structure (M. Rudolph, *et.al., Science*, 350, (2015)).suggest that viscosity increases with depth by several orders of magnitude, with effects from temperature, melt fraction, mineral phase transitions and other compositional variations such as the water content. For example, based on an analysis of the long-wavelength nonhydrostatic geoid, it was suggested a significant increase in viscosity occurs at 800 to 1000 km depth, which matches the *P-T* condition of the MD calculations (Fig 1b).





Recently, we shift the focus to the structure and properties of basalt glass and melt at low pressure. The research is motivated by a recent report of a basaltic glass under pressure (T. Ohashi, *et.al.* J. *Mineral. Petrol. Sci.,* 113, 286–292 (2018) suggesting that the intermediate–range order structure of glass becomes more compact, indicating that the tetrahedral glass is permanently polymerized and densified Preliminary result on the computed equation of state is compared with a simple phenomenological model and selected experimental observations in Fig .2.



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4. Conclusion

Transport properties such as diffusivity and viscosity of melts not only dictated the evolution of the early Earth's magma oceans but also govern many dynamic processes on the present-day Earth, from mantle convection to plate tectonics, magma migration and volcanic activity as well as global climate changes. Unfortunately, experimental measurements of melt diffusivity and viscosity at most mantle conditions remain impossible due to technical challenges. Herein, we computed the structure, density, diffusivity, electrical conductivity and viscosity of a model basaltic ($Ca_{11}Mg_7Al_8Si_{22}O_{74}$) melt from first-principles molecular dynamics calculations at temperatures from 2200 and 3000K, and pressures from 0 to 80 GPa. Results on the melt structure and viscosity at low pressure agree well with experiments and previous theoretical predictions. A key finding is that, although the density and coordination numbers around Si and Al increase with pressure, the Si-O and Al-O bonds become more iconic and weaker. The temporal atomic interactions at high pressure are fluxional and fragile, making the atoms more mobile and reversing the trend in transport properties at pressures near 50 GPa. This remarkable result provides an alternative explanation for decreasing viscosity below the mid-lower mantle towards the core and mantle boundary. The reduced melt

viscosity under lower mantle conditions also has important implications for the timescales of the early Earth's magma oceans.

5. Schedule and prospect for the future

This project has been successfully completed. A paper has been submitted to *Nature Comm.* and currently under review.

6. If no job was executed, specify the reason.