Usage Report for Fiscal Year 2020

**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

Basaltic melts that form the oceanic crusts and large igneous provinces and layered mafic intrusions in continents are the most common magmas on Earth, Moon and Mars [1]. They are generated mostly in the asthenosphere in the upper mantle and mantle plumes at greater depths, possibly down to the core-mantle boundary. Therefore, information on the structures and properties of basaltic melts under high pressures and high temperatures is indispensable to understand the origin and activity of magmas in the Earth's interior and the evolution of the Earth and other planets. Much effort has been devoted to exploring the structures and properties of melts, including basaltic liquids [2-9]. However, there are tremendous technical challenges associated with experimental measurements of melt properties at high pressures and high temperatures. To date, most measurements on silicate melts were restricted to less than 10 GPa, and only a few have been successfully carried out above 10 GPa [10]. Since solid glasses are much easier to handle at high pressures, they are often used as analogs of the corresponding melts to infer the structures and properties of the latter under mantle conditions [11-18]. Thus, many high-pressure experiments on silicate glasses quenched from melts have been performed. . In this work, Ab initio Molecular Dynamics (AIMD) calculations have been performed to investigate pressure-induced structural changes of a model basalt melt and its corresponding glass consisting of CaO, MgO, $Al_2O_3$ and $SiO_2$. The primary focus of this study is the pressure range relevant to the upper mantle and the transition zone where experimental results are available for comparison. In particular, results from this study are anticipated to shed new light on the long-standing assumption that glasses quenched from melts can be used as models for probing structural characteristics of the latter under mantle conditions.

## 2. Specific usage status of the system and calculation method

All calculations were performed on the Hokusai system. The VASP code [19] was used for the First Principles Molecular Dynamics calculations using the PBE functional and the projected Augment wave (PAW) potential [20] to replace the core electron of the atoms. A 244 atom model with the stoichiometry 22CaO, 14MgO, $8Al_2O_3$ and $44SiO_2$) was used. The P-T conditions from ambient pressure to 90 GPa were investigated. The initial melt structure was generated by melting of the solid model and cooled slowly to room temperature at 0 GPa. At each pressure, an isobaric-isothermal (NPT) MD was performed on the cubic supercell to relax the structure. This was followed by a lengthier constant-volume constant temperature (NVT) simulation employing the Langevin thermostat [21]. An integration time-step of 1fs was used. Following the work from last year, we paid special attention from 0 to 25 GPa for the glass at 300 K and from 0 to 23.8 GPa at 2500 K on the melt. For the latter, we investigated the transport properties such as

diffusion, viscosity and the electrical conductivity.

3. Result

The results for the melts at pressure from 0 – 90 GPa has been reported in last year report and published in a recent paper and, therefore, will not be repeated here [22]. This report focuses on the recent work at the low-pressure region.

The new results show that the local structures of the melt and glass are similar over a broad pressure range, but there are subtle but distinct differences. The pressure trends on the average Si-O, Ca-O, Mg-O, Al-O, O-O and Si-Si distances for the glass and melt are found to be very close. At ambient pressure, both are composed primarily of Si-O and Al-O tetrahedra. As expected, the Si-O coordination increases from four to fivefold and subsequently to sixfold. However, changes in the nearest neighbor Si-O and O-O are found to behave quite differently between the glass and melt. The most significant differences are in the distributions of the Si-O-Si and O-Si-O angles, which lead to different local structures and packing of the polyhedra. These differences demonstrate that caution must be exercised in the use of glasses as models for probing pressure-induced structural changes in the mantle. The consequence of the structural changes to the viscosity of the basaltic melt in the pressure region of 0-25 GPa is is comparable with available experimental data.

4. Conclusion

The results show that structural changes predicted for the basaltic glass over a wide pressure range are consistent with available experimental data. Moreover, the calculated bulk properties, such as the EOS and sound velocities, are similar between the basaltic melt and glass. However, there are significant differences in the local distortion trends of the Si-O and Al-O coordination shells. In particular, a large decrease in the Si-O-Si angle occurs in the pressure range from 0 to 13 GPa. The change in the Si-O distance is not noticeable and the mean O-Si-O angle is relatively constant. Compaction is largely achieved by changing the packing of the SiO4 tetrahedra and compressing the large Ca-O and Mg-O polyhedra. At pressure above 13 GPa, the Si-O-Si angle decreases substantially. This is accompanied by a concomitant increase in the Si-Si and Si-O distances. When pressure exceeds 16.9 GPa, the Si-O distance increases while the O-O distance decreases and the $SiO_4$ tetrahedra transform into fivefold- and sixfold-coordinated polyhedra. From detailed comparison of the basaltic glass structure and melt, we can conclude that, in both cases, the mean Si-O coordination number increases with more fivefold, and subsequently sixfold-coordinated species replacing the $SiO_4$ tetrahedra when pressure increases. However, the pressure trends in the T-O and O-O distances (T = Si or Al) are not the same between these two states. They are responsible for the different distributions of the T-O-T and O-T-O angles; consequently, their local structures are significantly different at corresponding pressures. The present theoretical study shows that most of the intrinsic properties, such as bulk modulus, sound velocity, density … etc., of the basaltic glass and the melt are broadly similar but not identical. These properties display parallel trends over a broad pressure range, at least up to 80 GPa. Therefore, the basaltic glass is a close analog to its molten counterpart, but notable structural differences must be taken into account. At low pressure, the basaltic glass at 300 K is approximately 5% denser than its molten counterpart at 2500 K, but their difference becomes smaller at high pressures.

References

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5. Schedule and prospect for the future

The goal specified in fiscal 2020 is almost completed. We need to augmented the results by further

calculations of the x-ray and neutron diffraction patterns and compare with experimental results. We will summarized all the results as a manuscript for publication.,

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

## Fiscal Year 2020 List of Publications Resulting from the Use of the supercomputer

### [Paper accepted by a journal]

A. Majumdar, M. Wu, Y. Pan, T. Iitaka, J.S. Tse, Anomaly in the structural dynamics of basaltic melt at mantle conditions: Implications for magma oceans and superplumes, Nat. Comm. 11, 4815 (2020)
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### [Conference Proceedings]

### [Oral presentation]

### [Poster presentation]

### [Others (Book, Press release, etc.)]