

第 5 回極限物質科学研究会
The 5th Workshop for Extreme Materials Science
“Silicate Melts and Glasses”

Date: 14:00-17:00 Oct. 6th (Fri), 2017.

2017年10月6日(金) 14:00-17:10

Place: Small Meeting Room 1(west), Welfare and Conference Bldg. (C61), Riken, Wako.
理研和光 統合支援施設小会議室1(西)建物番号C61

http://www.riken.jp/en/access/wako-map/#campus_map

Organizer: Toshiaki Iitaka (tiitaka@riken.jp)

Participation: Free

Sponsor: **Post-K Computer Challenging Problems, “Challenge of Basic Science”**,
Subproject C “Structure and Properties of Materials in deep Earth and Planets”

ポスト「京」萌芽的課題「基礎科学の挑戦」

サブ課題C「地球惑星深部物質の構造と物性」

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Scope

Silicate melt is one of the most important materials for understanding the formation and dynamics of the Earth and earth-like planets and also for industrial applications. In this meeting four young distinguished researchers will talk about their recent experimental and theoretical study on silicate melt and glass.

Program

14:00-14:10 Toshiaki IITAKA: Opening

14:10-14:50 Kyusei TSUNO 津野究成 (Rice Univ.) 【INVITED】

The effect of sulfur on carbon solubility and partitioning in the alloy-silicate systems: Implications for core-mantle fractionation of carbon and sulfur during accretion of Earth

<https://scholar.google.co.jp/citations?user=2Kgz3mEAAAAJ>

<http://dasgupta.rice.edu/expert/people.html>

14:50-15:30 Akihiro YAMADA 山田明寛 (Univ. Shiga Prefect.)

High-pressure XRD investigation on the structure of feldspar melts

https://www.researchgate.net/profile/Akihiro_Yamada2

(Break)

15:50-16:30 Fumiya NORITAKE 則竹史哉 (Yamanashi Univ.)

Ionic-Network Liquid transformation in sodium-silicate liquids

<http://fnoritake.futene.net/papers.html>

16:30-17:10 Tomonori OHASHI 大橋智典 (Tohoku Univ.)

Structure measurements of basaltic glass at high pressure using X-ray and neutron diffraction techniques

<http://www.es.tohoku.ac.jp/JP/groups/group10/index.html>

http://epms.es.tohoku.ac.jp/seminar/history/2017_abstract/20170511_Ohashi.pdf

Closing

The effect of sulfur on carbon solubility and partitioning in the alloy-silicate systems: Implications for core-mantle fractionation of carbon and sulfur during accretion of Earth

Kyusei Tsuno

Department of Earth, Environmental and Planetary Sciences, Rice University, Houston, TX 77005, USA

Constraining the carbon (C) fractionation between the silicate magma ocean and core-forming alloy liquid during early differentiation of Earth and terrestrial planets is required to determine the origin and present-day distribution of C between planetary reservoirs such as exosphere, mantle and core [1][1]. Experiments on the metal-silicate partitioning of C have shown that preferential fractionation of C into the alloy liquid would have left the bulk silicate Earth (BSE) devoid of C [2-4][2, 3, 4, 5]. It has been recently proposed that merger of a sulfur (S)-rich differentiated body into the proto-Earth could have supplied almost the entire C budget of the present-day BSE [5][5]. However, systematic experimental data at high pressures on the effect of S on C solubility in alloy liquid and the effect of S on partitioning of C between Fe-rich alloy liquid and silicate melt are not fully known.

We have performed multi-anvil experiments at 6–13 GPa and 1800–2000 °C to examine the effects of S and Ni on the solubility limit of carbon in Fe-rich alloy liquid and simultaneous determination of C and S partitioning between alloy liquid and silicate melt. The composition of alloy liquid, including carbon, was determined using EPMA. Major elements and volatiles (C and H₂O) in the silicate glass were obtained using EPMA and SIMS, respectively. The obtained data were used to quantify the effect of S on the distribution of C between the silicate magma ocean and core-forming alloy liquid of Mars-sized impacting body. A simple two-stage equilibrium core formation model was tested to determine whether the merger of an S-rich impacting body to a volatile-depleted proto-Earth can satisfy C and S contents as well as C/S ratio of the BSE [6].

[1] R. Dasgupta, in *Carbon in Earth*, edited by R. M. Hazen, A. P. Jones, and J. A. Baross (Mineralogical Soc Amer, Chantilly, 2013), pp. 183.

[2] R. Dasgupta *et al.*, *Geochim. Cosmochim. Acta* **102**, 191 (2013).

<http://dx.doi.org/10.1016/j.gca.2012.10.011>

[3] H. Chi *et al.*, *Geochim. Cosmochim. Acta* **139**, 447 (2014).

<http://dx.doi.org/10.1016/j.gca.2014.04.046>

[4] Y. Li, R. Dasgupta, and K. Tsuno, *Earth Planet Sc Lett* **415**, 54 (2015).

<http://dx.doi.org/10.1016/j.epsl.2015.01.017>

[5] Y. Li *et al.*, *Nature Geoscience* **9**, 781 (2016).

<http://dx.doi.org/10.1038/ngeo2801>

[6] M. M. Hirschmann, *Am Mineral* **101**, 540 (2016).

<http://dx.doi.org/10.2138/am-2016-5452>

High-pressure XRD investigation on the structure of hydrous and anhydrous feldspar melts

Akihiro Yamada

Center for Glass Science and Technology, School of Engineering, The University of Shiga Prefecture, 2500 Hassaka, Hikone, 5220533, Japan

Feldspar is the major rock-forming mineral in Earth's shallow part such as crust, which have relatively low melting temperature due to containing alkaline elements. Similarly, water, which is commonly thought to be provided to the Earth's interior via subducting slab, enhances the magma genesis and changes the properties drastically. Although magma is not major component in the current Earth's interior, the high mobility and activity should influence significantly surrounding materials. In particular, pressure dependence on the properties (e.g., viscosity: e.g., [1] and density) of melt including Al, which acts as "network former" or "network modifier" in melt, has been reported not to be simple due to the coordination transformation in AlOn polyhedra. To infer the Al coordination at high pressure, spectroscopic approaches on aluminosilicate glasses recovered from high pressure have been performed and found some evidences for highly coordinated Al in densified glass structure (e.g., NMR: [2]). However, since melted silicates at high pressure are typical "unquenchable" phase, it is necessary to investigate in situ for the better understanding of the properties at high pressures.

High-pressure and -temperature X-ray diffraction technique has been applied for the structural analysis of albite ($\text{NaAlSi}_3\text{O}_8$) and orthoclase (KAlSi_3O_8) melts, using synchrotron X-ray radiation plus multi-anvil apparatus at NE5C, KEK. In the presentation, the detail of the experiment and results including Radial Distribution Functions of the melts, which show the pressure-induced modification AlOn polyhedra and the effect of water, will be introduced.

[1] Suzuki et al., Phys. Chem. Minerals, 29, 159-165 (2002)

<https://doi.org/10.1007/s00269-001-0216-4>

[2] Allwardt et. al., Am. Mine, 90, 1218-1222 (2005)

<https://doi.org/10.2138/am.2005.1836>

Ionic-Network Liquid transformation in sodium-silicate liquids

Fumiya Noritake

The anomalous behavior displayed by silicate liquid/glass is a long-standing issue in physics, earth sciences, and glass technology. One such well-known unusual behavior is the contrary pressure dependence of silica-rich liquids on transport coefficients in comparison to other liquids [1,2,3]. Recently, our previous work proposed that the structural transformation from an ionic to network liquid is the origin of contrary pressure dependence [4]. To investigate the origin of this anomalous behavior of silicate liquids, several analyses are newly developed and applied to molecular dynamics simulations of sodium silicate liquids. For instance, the cluster analysis performed on a Si–O network and simplex sphere reveals obvious structural changes arising as a function of pressure and composition. At lower pressure and/or low silica content, all simplex oxygen spheres containing the modifier cations are connected together, and multiple Si–O networks exist in the liquid structure. In contrast, at high pressure and/or high silica content, all SiO₄ tetrahedra belong to a single cluster, and the cluster of simplex oxygen spheres containing the modifier cations is split into multiple clusters. The cluster analysis and other analyses reveal the pressure- and composition-dependent changes in the dominant network in silicate liquids. When the network of corner-sharing SiO₄ tetrahedra is the dominant species in silicate liquids, the Si–O bonds become weaker as a result of the Si–O–Si angle bending, and the shear viscosity decreases with increasing pressure. In contrast, the transport coefficients show normal pressure dependence when the cation domain is fully connected in silicate liquids [5].

[1] I. Kushiro (1976), *J. Geophys. Res.*, 81, 1955.

<http://onlinelibrary.wiley.com/doi/10.1029/JB081i035p06347/abstract>

[2] I. Kushiro: *In High-Pressure Research: Application in Geophysics.*, ed., M. H. Manghnani, S. Akimot (Academic Press, New York, 1977), 25.

[3] C. M. Scarfe et al., (1979), *Carnegie Inst. Wash. Yearb.*, 78, 574.

[4] F. Noritake, K. Kawamura (2016), *J. Non-Cryst. Sol.*, 447, 141.

<https://doi.org/10.1016/j.jnoncrysol.2016.08.013>

[5] F. Noritake (2017), *J. Non-Cryst. Sol.*, 473, 102.

<http://dx.doi.org/10.1016/j.jnoncrysol.2017.08.004>

Structure measurements of basaltic glass at high pressure using X-ray and neutron diffraction techniques

Tomonori Ohashi¹, Tatsuya Sakamaki¹, Takanori Hattori², Asami Sano-Furukawa², Ken-ichi Funakoshi³, Akio Suzuki¹

- 1 Department of Earth and Planetary Materials Science, Tohoku University, Aoba, Sendai 980-8578, Japan.
- 2 Nuclear Science Research Institute, Japan Atomic Energy Agency (JAEA), Tokai, Ibaraki 319-1195, Japan.
- 3 Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society (CROSS-Tokai), Tokai, Ibaraki 319-1106, Japan.

Magmas have been suspected to exist discretely in the interior of the Earth according to geophysical observations. This implies that these magmas are gravitationally stable in the interior of the Earth due to the larger density than surrounding mantle rocks. Understanding the deep magmas, the densification mechanism needs to be investigated. Since the density of magmas is closely related to their microscopic structure and silicate glasses are known to be good analogues for magmas, we studied the structure of basaltic glass using both of X-ray diffraction (XRD) and neutron diffraction techniques.

Energy-dispersive X-ray diffraction experiment was conducted at NE5C beamline in Photon Factory Advanced Ring (PF-AR). The starting material is synthesized basaltic glass, and it was compressed by MAX80 up to 6 GPa. The significant oscillation in $S(Q)$ was found up to at least 18 \AA^{-1} . This means that the resolution in the pair distribution function (PDF) is $r = 0.33 \text{ \AA}$. On the other hand, a time-of-flight neutron diffraction was performed at PLANET beamline in Japan Photon Accelerator Research Complex (J-PARC). We conducted the high-pressure experiment using Paris-Edinburgh press up to 7 GPa. The resolution in the PDF is $r = 0.27 \text{ \AA}$.

Firstly, structure factor, $S(Q)$ obtained by in-situ X-ray and neutron diffractions for basaltic glass at high pressure suggests that the position of first sharp diffraction peak (FSDP) shifts to higher- Q with increasing pressure up to 6-7 GPa, which indicates the contraction of its intermediate-range ordered (IRO) structure. Additionally, $S(Q)$ obtained from the neutron diffraction shows the pressure-induced attenuation of FSDP. This implies the special repeat disordering of the IRO, represented by T-T [1, 2]. Here, T is a tetrahedrally coordinated cation such as Si^{4+} and Al^{3+} . On the other hand, the second peak, which is usually called principal peak [3] or second sharp diffraction peak (SSDP) [4], shows the opposite behavior: the intensification of SSDP with increasing pressure. This result suggests the collapse of short-range order, and these may relate to an increase in coordination number of T-O bond [1].

Secondly, from each data-set of $S(Q)$, we derived pair distribution functions (PDFs), and it shows that the shrinkage of average T-T length as pressure increases, but indicates no detectable change of the average T-O length. This result implies that the positional shift of FSDP is attributed to the decrease in the average T-O-T angle with the concomitant shortening of the T-T length, and consequently, the density of basaltic glass rapidly increases by compression of IRO structure. Other corresponding behavior is also found in PDFs. We will show a detailed discussion about the pressure dependence of short- and intermediate-range ordered structure of basaltic glass.

- [1] Yamada *et al.*, High Press. Res., **28**, 255 (2008).
<http://www.tandfonline.com/doi/full/10.1080/08957950802261042>
- [2] Sakamaki *et al.*, Earth Planet. Sci. Lett., **391**, 288 (2014).
<https://doi.org/10.1016/j.epsl.2014.02.008>
- [3] Salmon *et al.*, Nature, **435**, 75 (2005).
<https://doi.org/10.1038/nature03475>
- [4] Elliott, Phys. Rev. B, **51**, 8599 (1995).
<https://doi.org/10.1103/PhysRevB.51.8599>