

実験報告書様式(一般利用課題・成果公開利用)

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課題番号 Project No. 2017A0012 実験課題名 Title of experiment Neutron diffraction structure determination of hydrous silicate glasses under high pressure conditions: Implications for deep dense hydrous magma in the interior of the Earth 実験責任者名 Name of principal investigator Tatsuya Sakamaki 所属 Affiliation Tohoku University	装置責任者 Name of Instrument scientist Takanori Hattori 装置名 Name of Instrument/(BL No.) BL11 PLANET 実施日 Date of Experiment Oct 29 2017-Nov 4 2017

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。(適宜、図表添付のこと)  
 Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.
<p>The sample is synthesized basaltic glass by quenching molten mixture of several oxides and carbonates. The basaltic composition is universal igneous rock, and glass is an analog of magma in the interior of the Earth.</p>

2. 実験方法及び結果（実験がうまくいかなかった場合、その理由を記述してください。）

Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.

The structure of basaltic glass under pressure was determined using time-flight neutron diffraction technique. Paris-Edinburgh press was used as a high-pressure apparatus. The neutron diffraction experiments were performed at different pressure conditions (P: 1 atm ~ 18.0 GPa). Figure 1 shows the structure factor,  $S(Q)$ , of basaltic glass. In order to understand the structural evolution of the glass, we focused on a change in the first sharp diffraction peak (FSDP) in  $S(Q)$  with pressure. Since the FSDP reflects the intermediate-range order (IRO) of silicate network, the pressure dependence of the FSDP is a good indicator of pressure-induced structural changes of the glass. Enlarged  $S(Q)$  is shown in Figure 2. This clearly demonstrates the shift of the FSDP to higher-Q with pressure, which indicates the shrinkage of IRO structure with increasing pressure. This figure also exhibits that second peak on the right of the FSDP changes drastically with pressure. The peak is called the second sharp diffraction peak, SSDP, and reflects shorter-range ordering.

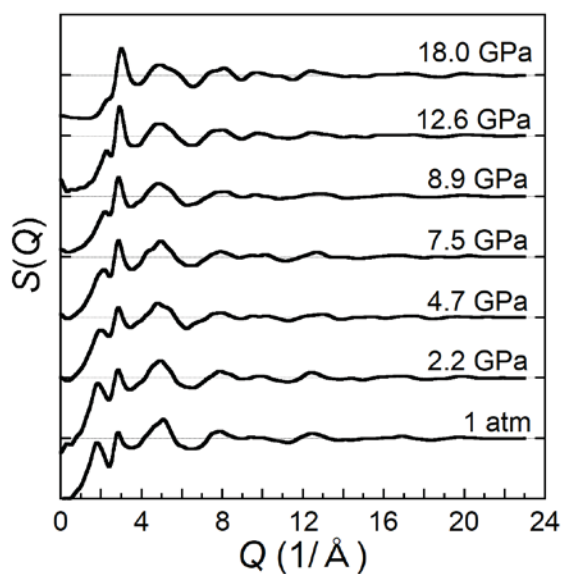


Figure 1  
Structure factor,  $S(Q)$ , of basaltic glass at different pressure.

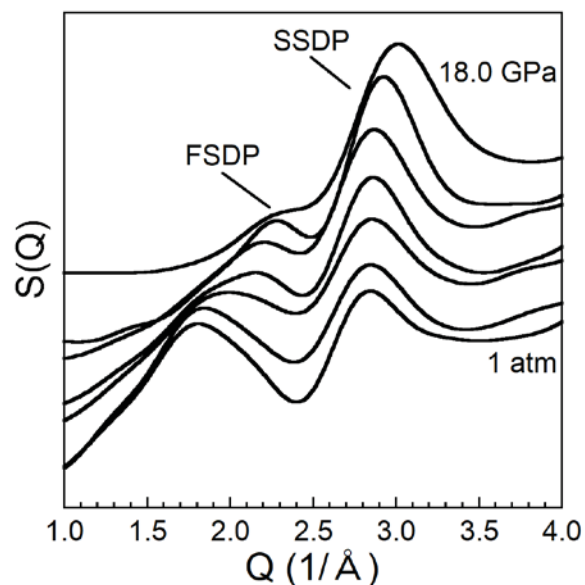


Figure 2  
Pressure-induced change of the FSDP and the SSDP.

## 2. 実験方法及び結果(つづき) Experimental method and results (continued)

Radial distribution function,  $G(r)$ , which is obtained by Fourier transformation of  $S(Q)$ , provides us an information about glass structure of real space. Figure 3 exhibits the  $G(r)$  at different experimental conditions. The peak around 1.6 Å indicates the bond length between tetrahedral cation (T) and oxygen (O), and the length is less sensitive to pressure. On the other hand, O-O bond length is shown around 2.6 Å and the bond length became shorter with pressure.

We can find clear difference between neutron and X-ray diffraction of basaltic glass. Figure 4 and Figure 5 indicate the comparison of  $S(Q)$  and  $G(r)$  between neutron (red) and X-ray (black) diffraction, respectively. In the case of neutron diffraction, scattering intensity from oxygen is larger than X-ray. Therefore, results of neutron diffraction enable us to better understand the change in  $\text{TO}_4$  tetrahedra under pressure. Combining both neutron and X-ray diffraction, we can reveal the magma behavior at the depth of the Earth.

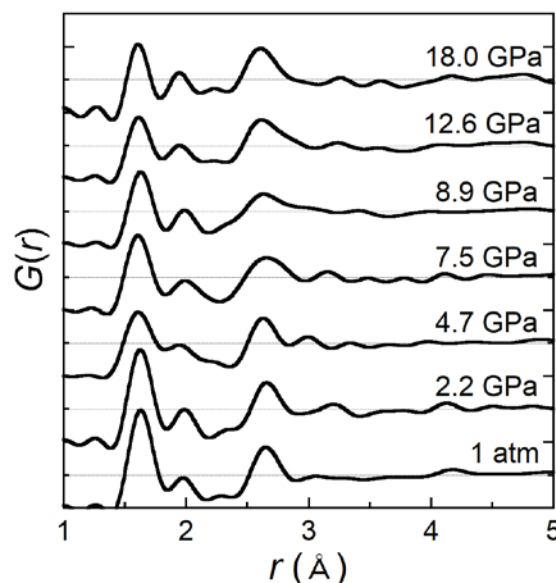


Figure 3  
Radial distribution function,  $G(r)$  of basaltic glass at different pressure.

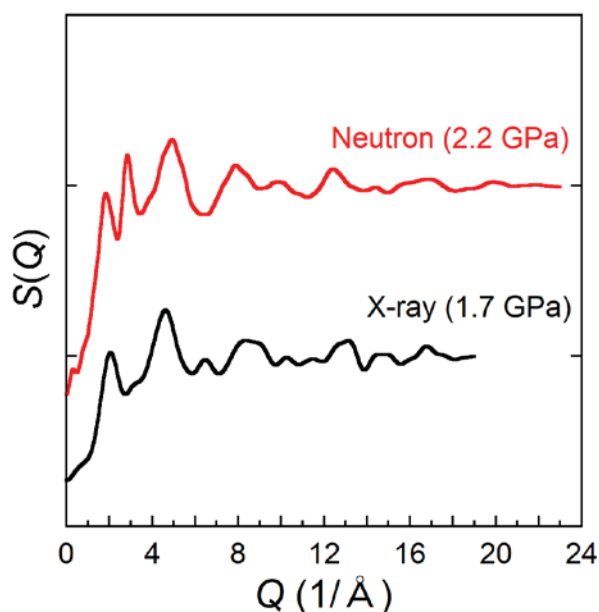


Figure 4  
Comparison of  $S(Q)$  between neutron and X-ray diffraction.

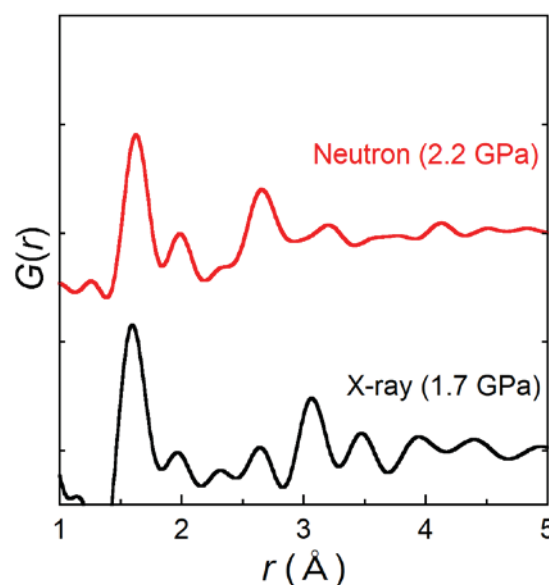


Figure 5  
Comparison of  $G(r)$  between neutron and X-ray diffraction.