JASMAC
Conference of the Japan Society of Microgravity Application

OS4-5

宇宙実験・量子ビーム実験・コンピュータシミュレーションによる $MgO–SiO_2$ 系ガラス・液体の構造物性研究

Structural properties of $MgO-SiO_2$ glasses and liquids by thermophysical properties/quantum beam measurements and computer simulation.

手跡雄太 [1], 金子智昭 [1], 袖山慶太郎 [1], 小野寺陽平 [2], 小山千尋 [3], 増野敦信 [4], 志賀元紀 [5], 岡田純平 [5], 水野章敏 [6], 渡邊勇基 [7], 仲田結衣 [7], 尾原幸治 [8], 織田裕久 [3], 石川毅彦 [3], 小原真司 [1]
Yuta SHUSEKI[1], Tomoaki KANEKO[1], Keitaro SODEYAMA[1], Yohei ONODERA[2], Chihiro KOYAMA[3], Atsunobu MASUNO[4], Motoki SHIGA[5], Junpei T. OKADA[5], Akitoshi MIZUNO[6], Yuki WATANABE[7], Yui NAKATA[7], Koji OHARA[8], Hirohisa ODA[3], Takehiko ISHIKAWA[3] and Shinji KOHARA[1]
[1] 国立研究開発法人 物質・材料研究機構，National institute for materials science,
[2] 京都大学，Kyoto university,
[3] 国立研究開発法人 宇宙航空研究開発機構，Japan aerospace exploration agency,
[4] 弘前大学，Hirosaki university,
[5] 東北大学，Tohoku university,
[6] 函館工業高等専門学校，National institute of Technology, hakodate college,
[7] 株式会社エイ・イー・エス，Advanced engineering services,
[8] 公益財団法人 高輝度光科学研究センター，Japan synchrotron radiation research institute,

1. Introduction

The $MgO–SiO_2$ system is important in both glass science and geo science, because $MgO–SiO_2$ glass is a binary silicate glass system and enstatite (crystalline (*c*-) $MgSiO_3$) and forsterite (*c*-Mg_2SiO_4) are main components of mantle of the earth. Understanding of the structure of both glass and high temperature liquid of $MgSiO_3$ (high glass forming ability (GFA)) and Mg_2SiO_4 (low GFA) makes it possible to understand the origin of glass formation and magma ocean solidification. In this study, we have performed density measurement on electrostatic levitation furnace (ELF) of the international space station (ISS)[1)] and X-ray/neutron diffraction on the liquids. Moreover, we have performed DF−MD simulation to understand structure of glasses and liquids at both atomistic and electronic levels.

2. Experimental methods

The density measurements of high-temperature liquid Mg_2SiO_4 (*l*-Mg_2SiO_4) were carried out with ELF at the ISS. The X-ray diffraction measurements of *g*, *l*-$MgSiO_3$ and *g*, *l*-Mg_2SiO_4 were performed at the BL04B2 beamline of the SPring-8 and the neutron diffraction measurements were carried out at the NOMAD diffractometer at SNS of Oak Ridge National Laboratory in USA. In addition, DF−MD simulations were were perfomed for *g*, *l*-$MgSiO_3$ and *g*.*l*-Mg_2SiO_4.

3. Result and discussion

Figure 1. compares the X-ray and neutron total structure factors, *S*(*Q*), of *g*, *l*-$MgSiO_3$ and Mg_2SiO_4, [2,3]. It is confirmed that the *S*(*Q*) of DF−MD models reproduce experimental diffraction data. Both the glass and liquid *S*(*Q*) of $MgSiO_3$ and Mg_2SiO_4 has a first sharp diffraction peak (FSDP) around Q ~ 2.0 and 2.2 Å^{-1}. These peaks are broad and the position shifts to higher *Q* than those of *g*, *l*-SiO_2 (Q ~ 1.5 Å^{-1}), because the addition of MgO break down the network which is comprised by corner sharing of SiO_4 tetrahedra associated with the reduction of the cavity volume.

The status of density/viscosity measurements at the ISS, quantum beam diffraction measurements at SPring-8 and ORNL will be reported and results of DF-MD simulations will be discussed.

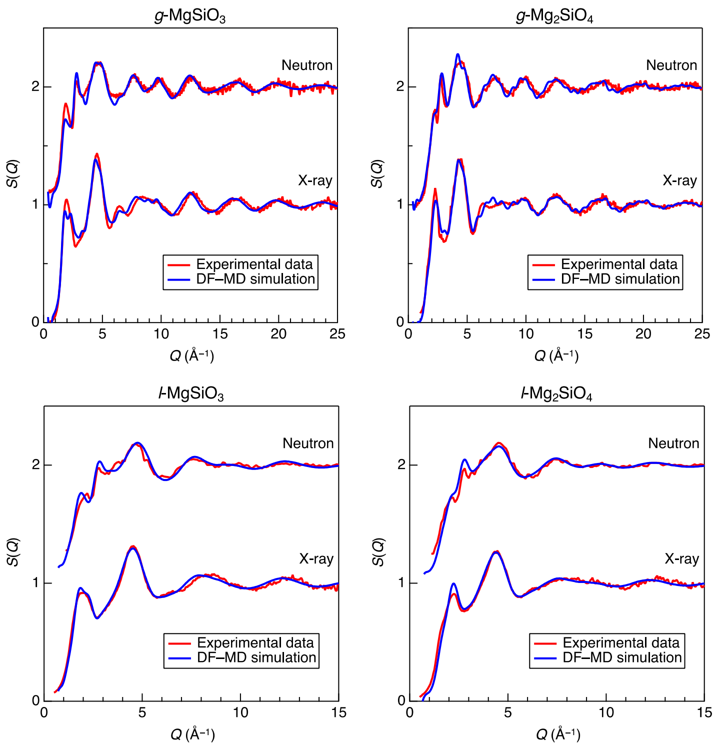

Figure 1. X-ray and Neutron total structure factors *S*(*Q*) of *g*, *l*-$MgSiO_3$ and Mg_2SiO_4.
Red curve: experimental data, blue curve: DF−MD simulation.

References

1) H. Tamaru, C. Koyama, H. Saruwatari, Y. Nakamura, T. Ishikawa and T. Takada: Status of the electrostatic levitation furnace (ELF) in the ISS-KIBO. Microgravity science and technology, **30** (2018) 643, DOI: 10.1007/s12217-018-9631-8.
2) S. Kohara, J. Akola, H. Morita and C. J. Benmore: Relationship between topological order and glass forming ability in densely packed enstatite and forsterite composition glasses. Proceedings of the national academy sciences, **108** (2011) 14780, DOI: 10.1073/pnas.1104692108.
3) S. Kohara, K. Suzuya, K. Takeuchi, C. K. Loong, M. Grimsditch, J. K. R. Weber, J. A. Tangeman and T. S. Key: Glass formation at the limit of insufficient network formers. Science, **303** (2004) 1649, DOI: 10.1126/science.1095047.