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ELF を利用した機能性高充填密度ガラスの融液物性計測と機能発現メカニズムの解明

Physical property measurements of functional densely packed oxide glass melts by using ELF for understanding the atomistic origin of the functionality

増野敦信
Atsunobu MASUNO
京都大学大学院工学研究科，Graduate School of Engineering, Kyoto University

1. Introduction

Oxide glasses are generally considered to be substances in which network former oxides such as SiO_2, B_2O_3, and P_2O_5 are the main components. The three-dimensional network is formed by random corner-sharing connections between MO_4 tetrahedra consisting of the cation M^{n+} and oxide ion O^{2-}. On the other hand, we have recently succeeded in synthesizing a large number of unconventional glasses without any network formation of the network former oxides by using a levitation technique (Figure 1)[1,2]. It was found that these glasses exhibited outstanding physical properties such as a high refractive index, strong luminescence, high elastic modulus, large crack resistance, high dielectric constant, and large magneto-optic effect. These features are derived from the high packing density caused by no network formation, however, the correlation between the functionality and the atomic arrangement of the glasses is still unexplored. Furthermore, the elucidation of the structural origin for glass formation without network formation is one of the greatest challenges in glass science because breaking the random corner-sharing networks should inevitably decrease glass forming ability. Understanding glass formation process during cooling from a melt at an atomic or electronic level will provide critical information to investigate the origin of the functionality and glass formation.

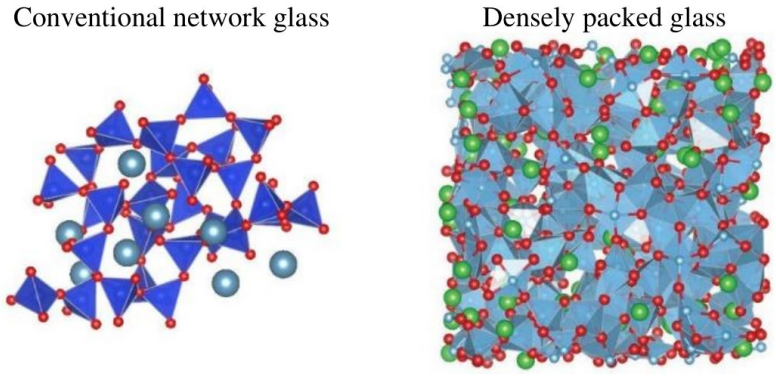

Figure 1. Structural models of conventional network glass and densely packed glass.

2. Purpose of the project

The purpose of the project is to elucidate the structural and electronical mechanism for the functionality and glass formation of unconventional densely packed oxide glasses. Two approaches are planned to achieve the purpose. One is to obtain thermophysical properties of a melt and supercooled liquid. The temperature dependence of density and viscosity is required to evaluate glass formation and glass forming ability. The use of the electrostatic levitation furnace (ELF) on the ISS Kibo is essential to accurately measure the density and viscosity from above the melting point to lower temperatures with large supercooling[3,4]. This is because an electrostatic levitation furnace on the ground, which requires a high vacuum to prevent electrical discharges, cannot provide accurate data due to the loss of oxygen from the oxide melt. The ELF, which can levitate the melt in air, are the most suitable for the purpose of this project. The target compositions of the melts are aluminosilicate, rare-earth borate, rare-earth molybdate, aluminatantalate, and rare-earth silicate. These were selected among many candidates of unconventional glasses prepared by a levitation technique because the glasses exhibit large crack-resistance, IR transparency, low thermal expansion, high elastic modulus, and high hardness. The data obtained will be compared with those of the melts that will become glass and those that will not, in order to quantify the glass-forming ability of the melts. Second approach is to perform structural analysis of the melt. Raman scattering spectroscopy and X-ray and neutron diffraction experiments will be done on the ground. Structural model that reproduces the experimental data will be prepared by molecular dynamics simulation. The reliability of the structural model can be greatly improved by using the densities obtained from space experiments. The structural model is analyzed using various geometrical methods to extract characteristic atomic arrangements that are responsible for the functionality[5,6]. Combination of thermophysical data and structural information of the unconventional oxide glass melts will provide important clues on the issues of the atomistic origin of the functionality and glass formation. The results of this project will not only advance glass science, but also lead to the synthesis of new highly functional glasses by optimizing the composition design and synthesis conditions in the future.

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