A multi-faceted experimental study on the dynamic behavior of MgSiO$_3$ glass in the Earth’s deep interior

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**ABSTRACT**

Pressure-induced structural modifications in silicate melts play a crucial role in controlling dynamic processes in the deep interiors of the Earth and other planets. The correlation between structural and macroscopic properties of silicate liquids (densification, viscosity, chemical differentiation, etc.), however, remains poorly understood. Here we report the evolution of structural modifications and elastic properties of MgSiO$_3$ glass to pressures up to ~70 GPa using a combination of experimental techniques, including micro-confocal Raman spectroscopy, angle-dispersive X-ray scattering, and Brillouin spectroscopy in the diamond-anvil cell. Our combined data set provides consistent and complementary evidence of a series of pressure-induced structural modifications in MgSiO$_3$ glass at ~2, ~8, ~20, and ~40 GPa. Based on these results, a structural evolution model for MgSiO$_3$ glass is proposed. We also discuss the role of Mg-O component in MgSiO$_3$ and Mg$_2$SiO$_4$ glasses in controlling pressure-induced structural modifications and mechanical responses in these supercooled liquids.

**Keywords:** MgSiO$_3$ glass, high pressure, structural modification, Raman spectroscopy, Brillouin spectroscopy, X-ray scattering

**INTRODUCTION**

The present day Earth possesses a crust composed of low-density minerals enriched in incompatible lithophile elements and a high-density metallic core beneath the rocky mantle, indicating that our planet is a well-differentiated body. Chemical differentiation of the mantle is generally attributed to melting and subsequent crystallization in the early Earth. It is believed that the mantle underwent large-scale melting after the Moon-forming giant impact event (Agee and Walker 1988; Ohtani 1988). Materials with different chemical compositions were produced through melting, with incompatible elements partitioning preferentially into the melts, which were then separated by gravitational effects, forming the crust. High $^{142}$Nd/$^{144}$Nd ratios in terrestrial samples relative to chondritic meteorites suggest an early enriched reservoir in the deep mantle (Boyet and Carlson 2005). Such a magma ocean scenario, in turn, plays an important role in understanding the formation process (Badro et al. 2015; Li and Agee 1996). Deep mantle melting has been used to explain the wide range of seismic and geochemical observations. One example is the proposal that the ultralow-velocity zone (ULVZ) in the D$^\theta$ layer may represent a melt layer at the core-mantle boundary (Labrosse et al. 2007). Structural and physical properties of silicate melts under deep mantle conditions are required to understand the physics of deep melts and verify these hypotheses.

Experimental information on the structure, density, and compressibility of silicate liquids and glasses (super-cooled liquids) at high pressure (HP) and high temperature (HT) is vital in the evaluation of the deep magma ocean hypothesis and the related interpretations of geophysical observations. Considerable progress has been made over the past few decades in establishing the correlation between structure and properties (such as density and elasticity) of silicate liquids, at pressure up to ~5 or ~6 GPa. Recent molecular dynamics (MD) simulations have shown that the dominant effects of increasing density and bulk modulus are the closure of voids space in the structure at low-pressure regime and the rearrangement of cation-oxygen bond length and angles, as well as changes in coordination environment at high pressures (Karki 2010; Kubicki and Lasaga 1988). Experimental studies on both silicate liquids and glasses show that, upon compression, the atomic arrangements become much more efficiently packed by increasing cation-oxygen coordination numbers (CN), resulting in a significant density increase (McMillan 1984; Meade and Jeanloz 1988; Prescher et al. 2017).

MgSiO$_3$ is a major component in the Earth’s upper mantle and the dominant constituent of the lower mantle. No direct information on MgSiO$_3$ liquid has been obtained experimentally under lower mantle conditions, because simultaneous HP and HT conditions impose severe technical challenges in the collection of structural and property data. Instead, MgSiO$_3$ glass, the supercooled liquid, is studied, in terms of the structure, density, and elasticity (Cormier and Cuello 2011; Kono et al. 2018;