American Minerlogist, Volume 109, pages 1045–1053, 2024

Different structural behavior of $MgSiO_3$ and $CaSiO_3$ glasses at high pressures

Nozomi M. Kondo[1,2,*], Yoshio Kono[1,6], Itaru Ohira[3], Rostislav Hrubiak[4], Koji Ohara[5], Kiyofumi Nitta[5], and Oki Sekizawa[5]

[1]Geodynamics Research Center, Ehime University, 2-5 Bunkyo-cho, Matsuyama, Ehime 790-0826, Japan
[2]Present address: Institute for Planetary Materials, Okayama University, 827 Yamada, Misasa, Tottori 682-0193, Japan
[3]Department of Chemistry, Gakushuin University, Mejiro, Toshima-ku, Tokyo 171-8588, Japan
[4]High Pressure Collaborative Access Team, X-ray Science Division, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, Illinois 60439, U.S.A.
[5]SPring-8 Synchrotron Facility, Japan Synchrotron Radiation Research Institute, 1-1-1 Kouto, Sayo-cho, Sayo-gun, Hyogo 679-5198, Japan
[6]Present address: Department of Physics and Astronomy, Kwansei Gakuin University, 1 Gakuen-Uegahara, Sanda, 669-1330 Japan

Abstract

Knowledge of the structural behavior of silicate melts and/or glasses at high pressures provides fundamental information for discussing the nature and properties of silicate magmas in the Earth's interior. The behavior of Si-O structures under high-pressure conditions has been widely studied, while the effect of cation atoms on the high-pressure structural behavior of silicate melts or glasses has not been well investigated. In this study, we investigated the structures of $MgSiO_3$ and $CaSiO_3$ glasses up to 5.4 GPa by in situ X-ray pair distribution function measurements to understand the effect of different cations (Mg^{2+} and Ca^{2+}) on high-pressure structural behavior of silicate glasses. We found that the structural behavior of $MgSiO_3$ and $CaSiO_3$ glasses are different at high pressures. The structure of $MgSiO_3$ glass changes by shrinking of Si-O-Si angle with increasing pressures, which is consistent with previous studies for SiO_2 and $MgSiO_3$ glasses. On the other hand, $CaSiO_3$ glass shows almost no change in Si-Si distance at high pressures, while the intensities of two peaks at ~3.0 and ~3.5 Å change with increasing pressure. The structural change in $CaSiO_3$ glass at high pressure is interpreted as the change in the fraction of the edge-shared and corner-shared CaO_6-SiO_4 structures. The different high-pressure structural behavior observed in $MgSiO_3$ and $CaSiO_3$ glasses may be the origin of differences in properties, such as viscosity between $MgSiO_3$ and $CaSiO_3$ melts at high pressures. This signifies the importance of different structural behaviors due to different cations in investigations of the nature and properties of silicate magmas in Earth's interior.

Keywords: Glass structure, $MgSiO_3$, $CaSiO_3$, pair distribution function, high pressure