Pressure-driven changes in XRS spectra of compressed amorphous $MgSiO_3$ glass

G. Spiekermann[1], S. Petitgirard[2], C. Albers[3], K. Gilmore[4], Ch. J. Sahle[5], C. Weis[3], M. Harder[6], C. Sternemann[3], M. Wilke[1]

[1]Institut für Geowissenschaften, Universität Potsdam, 14476 Potsdam, Germany; [2]Institut für Geochemie and Petrologie, ETH Zürich, 8092 Zürich, Switzerland; [3]Fakultät Physik/DELTA, Technische Universität Dortmund, 44227 Dortmund, Germany; [4]Department of Condensed Matter Physics and Material Science, NBL, Brookhaven, NY, USA; [5]European Synchrotron Radiation Facility, 38000 Grenoble, France; [6]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany; **geospiek@uni-potsdam.de**

The atomic structure of silicate melts at high pressures is intimately linked to macroscopic properties such as density and viscosity [1]. $MgSiO_3$ end-member composition is a key to understand the properties of mafic melts in Earth's deep mantle, and $MgSiO_3$ glass is considered as a good analog of the melt due to the structural similarity.

Experimental structural changes in $MgSiO_3$ glass at high pressures have been investigated using X-ray diffraction (e.g. [2]) and X-ray Raman scattering spectroscopy (XRS) [3,4]. While XRS is the only technique to access the electronic structure of the light elements O, Si and Mg in a confined environment like a diamond anvil cell (DAC), the hitherto recorded spectral quality demands improvement in signal-to-noise ratio and energy resolution because of the high absorption of the diamonds. Further development for XRS high pressure are thus needed to investigate amorphous material.

We present XRS spectra of the oxygen K-edge, the silicon $L_{2,3}$-edge and the magnesium $L_{2,3}$-edge of compressed amorphous $MgSiO_3$ up to 60 GPa. Owing to the strongly reduced absorption by using miniature diamonds [5] an improved signal-to-noise ratio by about a factor of 10 compared to commonly sized diamonds was obtained and the experiment was conducted at lower photon energies resulting in a higher energy resolution below 1 eV. Additionally, the imaging properties at beamline ID20 at the ESRF allow for selective evaluation of the sample signal and thereby further increase the spectral quality.

Bethe-Salpeter spectral calculations [7] of silicate minerals with different coordinations for magnesium allow us to interpret the observed changes in the Mg $L_{2,3}$-edge.

References

[1] - Y. Kono and C. Sanloup (eds.): "Magmas under Pressure - Advances in High-Pressure Experiments on Structure and Properties of Melts", Elsevier Amsterdam (2018).

[2] - Y. Kono, Y. Shibazaki, C. Kenney-Benson, Y. Wang and G. Shen: "Pressure-induced structural change in $MgSiO_3$ glass at pressures near the Earth's core-mantle boundary", Proceedings of the National Academy of Sciences, 115(8), pp. 1742-1747 (2018).

[3] - H. Fukui and N. Hirakoa: "Electronic and local atomistic structure of $MgSiO_3$ glass under pressure: A study of X-ray Raman scattering at the silicon and magnesium L-edges", Physics and Chemistry of Minerals (2017).

[4] - S.K. Lee et al.: "X-ray Raman scattering study of $MgSiO_3$ glass at high pressure: Implication for triclustered $MgSiO_3$ melt in Earth's mantle", Proceedings of the National Academy of Sciences, 105(23), pp. 7925-7929 (2008).

[5] S. Petitgirard et al.: "Miniature diamond anvils for X-ray Raman scattering spectroscopy experiments at high pressure", Journal of Synchrotron Radiation, 24, pp. 276-282 (2017).

[6] Ch.J. Sahle et al.: "Direct tomography imaging for inelastic X-ray scattering experiments at high pressure", Journal of Synchrotron Radiation, 24, pp. 269-275 (2017).

[7] - K. Gilmore et al.: "Efficient implementation of core-excitation Bethe-Salpeter equation calculations", Computer Physics Communications, 197, pp. 109 (2015).