Magma properties at deep earth's conditions from electronic structure of silica measured using X-ray Raman Spectroscopy

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Melt properties at high pressure are crucial to model the evolution of the deep part of the Earth formation and evolution. SiO₂ is the main component of silicate melts in the Earth's deep mantle and controls their network structure and physical properties with pressure, e.g. density, viscosity. Knowledge of the short-range atomic and electronic structure in melts brings important constraints about their compressibility and viscosity at depth. We measured the O K-edge and the Si L_{2,3}-edge in silica up to 110 GPa using X-ray Raman scattering spectroscopy, with a striking match to calculated spectra of the quenched high-pressure melt based on structures from molecular dynamics simulations [1]. Our data show two major discontinuities at high pressure that are related to coordination changes. Between 20 and 27 GPa, at the transition zone (660 km), ^[4]Si species are converted into a mixture of ^[5]Si and [6]Si species. Between 60 and 70 GPa, in the lower mantle, a further transition marks the decrease of ^[5]Si species with ^[6]Si becoming dominant above 70 GPa without crossing-over the 6-fold references stishovite and CaCl₂ phases up to at least 110 GPa. These two discontinuities are found at the same pressure of change in compressibility and density measured on the same SiO₂ glass using the X-ray absorption method [2]. The changes of coordination and density measured on SiO₂ may have direct influence on the properties of silicate melts at depth with changes in viscosity and partitioning of elements at such pressures. Higher coordination than 6 only takes place beyond 140 GPa corroborating brillouin scattering measurements in agreement with our results with a further increase in density at such pressure. Silicate melts containing network modifiers elements may potentially densify at a lower pressure making magmas neutrally buoyant at the depth of the core-mantle boundary.

References

[1] - S. Petitgirard *et al.* Magma properties at deep Earth's conditions from electronic structure of silica. *Geochem. Persp. Let.* **9**, 32-37 (2019).

[2] - S. Petitgirard et al., SiO₂ glass density to lower-mantle pressures. Phys. Rev. Lett. 119, 215701 (2017).