
Densification mechanisms of amorphous silicates at high pressure and temperature

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Abstract

The interconnected network of SiO₄ tetrahedra is the main structural feature of silicate glasses and liquids at pressures up to 15 GPa. Polymerized silicate glasses (SiO₂-MgSiO₃ binary) exhibit unusual volumetric and elastic properties at high pressure and room temperature, including the observation that compressibility increases or is weakly pressure dependent on compression. The anomalous behavior of polymerized silicate glasses is consistent with densification being controlled by network flexibility, rather than the compression of interatomic distances as exhibited in their crystalline counterparts. Moreover, depolymerized compositions (MgSiO₃ – Mg₂SiO₄ binary) have anomalously high proportions of interconnected SiO₄ tetrahedra compared to the predictions based on stoichiometry, suggesting that network flexibility may play an important role in the high pressure properties of depolymerized amorphous silicates as well. To determine the P-T-X range over which network flexibility controls densification, we measure combined *in situ* X-ray diffraction and microtomography datasets at elevated pressure and temperature in the Rotational Tomography Paris-Edinburgh Cell at the SOLEIL synchrotron for a suite of silicate glasses spanning the SiO₂-MgSiO₄ binary. Simultaneous acquisition of X-ray diffraction on a large Q-range (up to 160 nm⁻¹) and 3D tomography were performed under extreme conditions, permitting direct comparison of density from volumetric measurements with changes in atomic structure. We use these results to investigate the role of network flexibility and polyamorphism in the anomalous high pressure behavior.

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