Structural Mechanisms of Plastic Deformation in Hydrostatically Compressed Calcium Aluminosilicates

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Abstract

From the very first observations of plastic deformation in silicate glasses by Bernhardt and Taylor in the middle of the 19th century, glass scientists have been trying to understand plastic deformation in glasses. Current understanding has disentangled plastic deformation into continuum phenomena: densification and shear and attempted to quantify the relative contributions. In indentation, glasses are identified as anomalous and normal depending on whether they deforming predominantly by densification and shear, respectively. However, despite our definitions of plastic deformation modes on a continuum scale, we still understand little about the atomic mechanisms which constitute each mode and how imposed stresses correlate with each mode. We conducted a series of molecular dynamics simulations in order to better understand the atomic mechanisms of plasticity when glass is subjected to hydrostatic stresses up to 15 GPa. Using a Pedone potential, we simulated calcium aluminosilicate glasses through the range of normal to anomalous glasses. The glasses ranged from 50%-100% SiO2 along the tectosilicate line, which by simple models are expected to contain no NBOs. We show that throughout the composition range there are variations in the deviatoric strain heterogeneity and degree of densification which can be correlated to structural changes such as coordination number, bond angle distribution, ring size distribution, and the degree of ring puckering. With a better understanding of the connection between hydrostatic stress and atomic mechanisms of plasticity, we can begin to understand how glasses deform plastically at the structural level. Since plasticity occurs just before failure, it is important to understand atomic mechanisms of plasticity in complex, real-world stress states.

Keywords: Plasticity Mechanisms, Silicate Glass, Molecular Dynamics, Ring Puckering

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