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A systematic study of the effects of volatile species on the structure and physical properties of amorphous SiO_2

LINDSAY M. HARRISON[1], ADAM R. SARAFIAN[2], CRAIG D. NIE[2], GALAN G. MOORE[2], JAMES E. TINGLEY[2], RANDALL E. YOUNGMAN[2], MATTHEW E. MCKENZIE[2], NICOLE E. HALL[2], LISA A. MOORE[2] AND ALISHA N. CLARK[1]

[1]University of Colorado Boulder

[2]Corning Incorporated

Presenting Author: lindsay.harrison@colorado.edu

Volatile species play an important role in planetary evolution by lowering the melting temperatures of rock, stabilizing silicate melt phases over a larger pressure range. Understanding their influence on the physical properties of silicate melts is important for modeling differentiation processes in planetary interiors, as well as interpreting geophysical observations for the present-day Earth. We use resonance ultrasound spectroscopy and measure density to obtain the elastic moduli—Young's modulus, shear modulus, Poisson's ratio, and bulk modulus—of amorphous silicas doped with anions with -1 valence states: fluorine, chlorine, and hydroxyl. Our data show that increasing volatile content systematically decreases Young's modulus, bulk modulus, and density for all compositions. However, shear moduli and Poisson's ratio yield contrasting trends for OH^{-1} relative to F^{-1} and Cl^{-1}. For example, increasing F^{-1} and Cl^{-1} contents lead to increasing Poisson's ratios with increasing dopant concentration, whereas increasing hydroxyl content silicas strongly decreases Poisson's ratio. To understand the atomistic mechanisms which underlie differences in the elastic properties for these volatiles, we present results from Raman spectroscopy, Fourier transform infrared (FTIR) spectroscopy, nuclear magnetic resonance-magic angle spinning (NMR-MAS) spectroscopy, and molecular dynamics (MD) simulations. Raman spectroscopy measurements for F- and Cl-doped silicas show decreasing intensities in the R-band, which is attributed to the abundances of 5- or higher-membered rings, with increasing halogen content. This indicates that, as the content of F^{-1} and Cl^{-1} increases, the number of large (5+ silica tetrahedra) rings decreases. The MD results show that increasing OH^{-1} content yields increased average ring size and inter-tetrahedral angle distribution, whereas increasing F^{-1} and Cl^{-1} content yields decreased average ring size and inter-tetrahedral angle distribution. Determining the incorporation mechanisms of these volatiles in amorphous SiO_2 and how they affect physical properties, such as elastic moduli, can provide insight into how volatile accretion in the solar system might affect differentiation processes in terrestrial planets.