

The effect of coordination changes on the bulk moduli of amorphous silicates: The SiO₂-TiO₂ system as a test case

QUENTIN WILLIAMS^{1,*}, MURLI H. MANGHNANI², AND TERUYUKI MATSUI³

¹Department of Earth and Planetary Sciences, University of California, Santa Cruz, California 95064, U.S.A. Orcid 0000-0002-4798-5578

²Hawaii Institute of Geophysics & Planetology, University of Hawaii, Honolulu, Hawaii 96822, U.S.A.

³Knowledge Outsourcing Co., Inc, Nagoya, Japan

ABSTRACT

The elasticity of a sequence of SiO₂-TiO₂ glasses is examined at high pressures and temperatures. A primary goal is to determine how the previously proposed substitution of fivefold-coordinated Ti at low concentrations of Ti and fourfold-coordinated Ti at higher concentrations affects the elastic properties of these glasses. The effect of changing Ti content on the bulk moduli of these glasses is monotonic, and no systematic effect of possible coordination changes is observed. In contrast, there is an apparent decrease in the pressure derivative of the bulk modulus above ~3 wt% TiO₂. This change occurs at a similar composition to that at which a transition from predominantly fivefold to fourfold of Ti has been proposed to occur in these glasses. Hence, this shift in the pressure derivative of the bulk modulus is attributed to a stiffening of the equation of state of these glasses generated by the substitution of fivefold Ti species relative to TiO₄ units. Our results provide rationales for the onset of coordination changes producing a minimal change in the equation of state of silicate melts/glasses, and for bulk moduli determined at ambient pressure producing relatively accurate silicate melt volumes even within liquids that have begun to undergo coordination changes. Thus, our results support the general validity of single equation of state formulations that describe the densities of silicate melts through the transition zone and shallow lower mantle.

Keywords: Glasses, elasticity, ultrasonics, coordination changes, polymerized silicates