

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Tunable structures and properties in vitreous silica¹ LIPING HUANG, North Carolina State University, JOHN KIEFFER, University of Michigan — We studied the structures and properties of vitreous silica samples prepared by specific high pressure processing routes, using molecular dynamics simulations based on a charge-transfer three-body potential. Our study shows that the ability of the glass to undergo irreversible densification is inherently connected to its anomalous thermo-mechanical properties, such as the minimum in the bulk modulus at ~ 2 -3 GPa and the negative thermal expansion while under pressure. These behaviors can be tuned by controlling the pressure under which the initial glass was quenched. By preparing silica glass in ways that eliminates anomalous thermo-mechanical behaviors, e.g., by quenching a melt under pressure, the propensity of the glass to undergo irreversible densification can be eradicated. Such “pressure-treated” silica glass is less susceptible to radiation damage and can potentially increase the lifetime of many optical components.

¹NSF-DMR 0230662

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Date submitted: 20 Nov 2006

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