

Abstract Submitted
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Microsecond molecular dynamics simulations of stress relaxation and slow quench in silica melts and glasses J. MATTHEW D. LANE, Sandia National Laboratories — Quench rates and stress relaxation in molecular dynamics simulations of glasses are usually studied on time-scales which are many orders of magnitude faster than those in experiment. We present results from relaxation of hydrostatic compressive stress in silica glass using classical molecular dynamics simulations. Structural variation will be discussed as a function of quench rate for glasses quenched 2 to 3 orders of magnitude slower than previously reported. Stress relaxation curves plotted in $\log t$ show time-temperature superposition holds over a wide-range of temperatures for 3% initial volume compression. Silica melts and glasses were modeled with the BKS interatomic potential and were produced through a melt-quench process. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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