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Computer Simulations of Non-Equilibrium Dynamics in Silica[1]
CHRISTOPHER H. GORMAN, Wabash College, USA, KATHARINA VOLLMAYR-LEE, Bucknell University, USA, HORACIO E. CASTILLO, Ohio University, USA, AZITA PARSAEIAN, Northwestern University, USA — We present results from molecular dynamics computer simulations of aging silica (modeled by the BKS model). The system is equilibrated at $T_{\rm i} = 5000$ K and quenched instantaneously to $T_{\rm f} = 2500$ K. After a waiting time $t_{\rm w}$ we investigate the dynamics of the Si- and O-atoms as the system evolves over time t. Our simulations run long enough in order to observe the transition from out-of-equilibrium to equilibrium dynamics. We determine for our system the generalized incoherent intermediate scattering function $C(q, t_{\rm w}, t_{\rm w} + t)$ and the dynamic susceptibility $\chi_4(q, t_{\rm w}, t_{\rm w}+t)$ where q corresponds to the wavevector. Curves corresponding to different waiting times $t_{\rm w}$ collapse on the scaling plot $\chi_4(q, t_{\rm w}, t_{\rm w} + t)/\chi_4^{\rm max}(q, t_{\rm w})$ as a function of $(1 - C(q, t_{\rm w}, t_{\rm w} + t))$, which agrees with a prediction from spin glass theory.

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