Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Frequency and Wavevector Dependence of the Atomic Level Stress-Stress Correlation Function in a Model Supercooled Liquid[1] VALENTIN A. LEVASHOV, JAMES R. MORRIS, TAKESHI EGAMI, University of Tennesse and Oak Ridge National Laboratory — Temporal and spatial correlations among the local atomic level shear stresses were studied for a model liquid iron by molecular dynamics simulation [PRL 106,115703]. Integration over time and space of the shear stress correlation function $F(r,t)$ yields viscosity via Green-Kubo relation. The stress correlation function in time and space $F(r,t)$ was Fourier transformed to study the dependence on frequency, E, and wave vector, Q. The results, $F(Q,E)$, showed damped shear stress waves propagating in the liquid for small Q at high and low temperatures. We also observed additional diffuse feature that appears as temperature is reduced below crossover temperature of potential energy landscape at relatively low frequencies at small Q. We suggest that this additional feature might be related to dynamic heterogeneity and boson peaks. We also discuss a relation between the time-scale of the stress-stress correlation function and the alpha-relaxation time of the intermediate self-scattering function $S(Q,E)$.

[1]This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering

Valentin A. Levashov
University of Tennesse and Oak Ridge National Laboratory

Date submitted: 11 Nov 2011 Electronic form version 1.4