Correlation range in a supercooled liquid via Green-Kubo expression for viscosity, local atomic stresses, and MD simulations VALENTIN A. LEVASHOV, TAKESHI EGAMI, JAMES R. MORRIS, University of Tennessee and Oak Ridge National Laboratory — We present a new approach to the issue of correlation range in supercooled liquids based on Green-Kubo expression for viscosity. The integrand of this expression is the average stress-stress autocorrelation function. This correlation function could be rewritten in terms of correlations among local atomic stresses at different times and distances. The features of the autocorrelation function decay with time depend on temperature and correlation range. Through this approach we can study the development of spatial correlation with time, thus directly addressing the question of dynamic heterogeneity. We performed MD simulations on a single component system of particles interacting through short range pair potential. Our results indicate that even above the crossover temperature correlations extend well beyond the nearest neighbors. Surprisingly we found that the system size effects exist even on relatively large systems. We also address the role of diffusion in decay of stress-stress correlation function.

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