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Correlation range in a supercooled liquid via Green-Kubo expression for viscosity, local atomic stresses, and MD simulations VALENTIN
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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 vis-
cosity. 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 autocor-
relation 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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