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Glass transition and viscosity of simple glasses and liquids[1]
TAKESHI EGAMI, University of Tennessee, S. JOSEPH POON, University of Virginia, VALENTIN LEVASHOV, University of Tennessee, RACHEL AGA, JAMES MORRIS, Oak Ridge National Laboratory — The theoretical understanding of liquids and glasses at an atomistic level lags well behind that of crystalline materials, even though they are important in many fields including biology and the medical sciences. We present a simple microscopic model for the glass transition based on topological fluctuations in the bonding network. The model makes predictions for important parameters of the glassy state, such as the glass transition temperature, T_g, and the liquid fragility coefficient, m, based on microscopic variables. Excellent agreement with a number of experimental observations from metallic glasses is demonstrated. A key to this success is to focus on the dependence on Poisson's ratio, following the work of Novikov and Sokolov,[1] that characterizes the interaction between local density and shear fluctuations. To our knowledge, this is the first model to predict T_g and m quantitatively from microscopic variables. It presents a simple conceptual framework that should provide the basis for a more general microscopic understanding of liquids and glasses, including molecular systems.
1. V. N. Novikov and A. P. Sokolov, *Nature*, **431**, 961-963 (2004).

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