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Nontrivial correlation length distinguishes melt from glass in a large-scale atomistic non-equilibrium simulation of a glass transition[1]
KRANTHI MANDADAPU, Lawrence Berkeley National Laboratory, ALEXANDER HUDSON, DAVID CHANDLER, University of California Berkeley — Dynamical facilitation theory [1,2] predicts the emergence of a non-trivial correlation length from the cooling process that transforms the reversible melt to the irreversible glass [3]. A decrease in cooling rate produces an increase in correlation length, and an increase in correlation length coincides with an increase in stability and aging rate of the glass. Here, we present results from a large-scale non-equilibrium numerical simulation that provide the first demonstration of the emergent nonequilbrium correlation length for an atomistic model. The study also tests the ability of the theory to predict the value of the nonequilibrium length and its corresponding glass transition temperature in terms of material properties and cooling protocols.

1. J. P. Garrahan & D. Chandler, PNAS 100, 9710 (2003)

2. A. S. Keys et al. Phys. Rev. X 1, 021013 (2011)

3. A. S. Keys, J. P. Garrahan & D. Chandler, PNAS 110, 4482 (2013)

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