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Using particle rearrangement statistics to quantify ductility in amorphous solids MENG FAN, MINGLEI WANG, YANHUI LIU, JAN SCHROERS, Department of Mechanical Engineering and Material Sciences, Yale University, MARK SHATTUCK, Department of Physics and Benjamin Levich Institute, The City College of the City, University of New York, COREY O'HERN, Department of Mechanical Engineering and Material Sciences, Yale University — The response of amorphous solids to applied shear has several distinct regimes: quasi-elastic, yielding, and plastic flow regimes in the absence of fracture. Both non-affine particle motion and particle rearrangement events give rise to the strong nonlinear behavior of the stress versus strain curve. Here, we focus on computational studies of the mechanical behavior of binary Lennard-Jones glasses in three spatial dimensions that are prepared over a wide range of cooling rates. We apply athermal quasistatic pure shear to the glasses and uniquely identify each particle rearrangement event. We then determine the frequency of rearrangements and the energy drop after each event. We also quantify ductility by measuring the critical strain at which the material fractures during tensile tests. We find that more rapidly cooled glasses undergo more frequent particle rearrangements with larger energy drops on average. In contrast, rearrangements are much less frequent and dissipate less energy in more slowly cooled glasses, and thus are more susceptible to fracture than rapidly cooled glasses. In fact, we can predict the ductility of amorphous solids by measuring the total energy loss per strain in the putative linear stress versus strain regime before fracture occurs.

Meng Fan Department of Mechanical Engineering and Material Sciences, Yale University

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