Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Atomic-scale reversibility in sheared glasses MENG FAN, MINGLEI WANG, YANHUI LIU, JAN SCHROERS, Department of Mechanical Engineering and Materials Science, Yale University, MARK SHATTUCK, Department of Physics and Benjamin Levich Institute, The City College of the City University of New York, New York, COREY O'HERN, Department of Mechanical Engineering and Materials Science, Yale University — Systems become irreversible on a macroscopic scale when they are sheared beyond the yield strain and begin flowing. Using computer simulations of oscillatory shear, we investigate atomic scale reversibility. We employ molecular dynamics simulations to cool binary Lennard-Jones liquids to zero temperature over a wide range of cooling rates. We then apply oscillatory quasistatic shear at constant pressure to the zero-temperature glasses and identify neighbor-switching atomic rearrangement events. We determine the critical strain γ^*, beyond which atoms in the system do not return to their original positions upon reversing the strain. We show that for more slowly cooled glasses, the average potential energy is lower and the typical size of atomic rearrangements is smaller, which correlates with larger γ^*. Finally, we connect atomic- and macro-scale reversibility by determining the number of and correlations between the atomic rearrangements that occur as the system reaches the yield strain.

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Date submitted: 05 Nov 2015 Electronic form version 1.4