Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Deformation in Metallic Glass: Connecting Atoms to Continua[1]
ADAM R. HINKLE[2], MICHAEL L. FALK, Johns Hopkins University, CHRIS H. RYCROFT, Harvard University, MICHAEL D. SHIELDS, Johns Hopkins University — Metallic glasses like other amorphous solids experience strain localization as the primary mode of failure. However, the development of continuum constitutive laws which provide a quantitative description of disorder and mechanical deformation remains an open challenge. Recent progress has shown the necessity of accurately capturing fluctuations in material structure, in particular the statistical changes in potential energy of the atomic constituents during the non-equilibrium process of applied shear. Here we directly cross-compare molecular dynamics shear simulations of a ZrCu glass with continuum shear transformation zone (STZ) theory representations. We present preliminary results for a methodology to coarse-grain detailed molecular dynamics data with the goal of initializing a continuum representation in the STZ theory.

[1]NSF Grants Awards 1107838, 1408685, and 0801471
[2]NSF IGERT Fellowship Award Number 0801471

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Date submitted: 06 Nov 2015 Electronic form version 1.4