

# Bridging from Atoms to Continua in the Plastic Localization of Amorphous Solids

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## ABSTRACT

The primary mode of failure in disordered solids results from the formation and persistence of highly localized regions of large plastic strains known as shear bands. Continuum-level field theories capable of predicting this mechanical response rely significantly upon an accurate representation of the both the initial and evolving states of the amorphous structure which can be characterized by the local potential energy and an effective temperature. We perform molecular dynamics simulations of a metallic glass under shear in the athermal limit, [1] and present a methodology where a single, weighting parameter defines the system's coarse-grained atomic energies and strains. A criterion connecting the imposed shear deformation to the bi-modal energy statistics is established to distinguish the coarse-grained degrees-of-freedom inside the emerging shear band from those of the surrounding material. We use the resulting coarse-grained representation to provide the initial condition to a two-dimensional, numerical implementation of the shear transformation zone (STZ) theory. [2] Direct comparisons of the evolving amorphous structure and the macroscopic response of the atomistic data and the continuum model implemented by a novel finite differencing technique [3] are made. [4]

## REFERENCES

- [1] M.L. Falk and C.E. Maloney, "Simulating the mechanical response of amorphous solids using atomistic methods," *European Physics Journal B*, **75**, 405-413 (2010).
- [2] M.L. Falk and J.S. Langer, "Deformation and Failure of Amorphous Solidlike Materials," *Annual Review of Condensed Matter Physics*, **2**, 353-373 (2011).
- [3] C. Rycroft, Y. Sui, and E. Bouchbinder, "An Eulerian projection method for quasi-static elastoplasticity," *Journal of Computational Physics*, **300**, 136-166 (2015).
- [4] A.R. Hinkle, C.H. Rycroft, M.D. Shields, M.L. Falk, "Coarse-graining atomistic simulations of plastically deforming amorphous solids," under review.