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Molecular simulation of elementary shear banding in model metallic glasses.

*** Craig E. Maloney[1,2] and Mark O. Robbins[2]**

[1] CMU Dept. of Civil and Environmental Engineering
5000 Forbes Ave. Pittsburgh, PA 15213
craigmaloney@cmu.edu

[2] Johns Hopkins; Dept. of Physics and Astronomy
3400 N Charles. Baltimore, MD, 21218
mr@pha.jhu.edu

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ABSTRACT

Authors: C. E. Maloney and M. O. Robbins

Title: Molecular simulation of elementary shear banding in model metallic glasses.

Abstract: Metallic glasses are an attractive engineering material owing to their simultaneous high formability and strength. The observation of shear localization in these materials is universal, yet despite several decades of work, there is still much debate surrounding the elementary mechanisms which govern it.

We present results on an extensive set of computer simulations on simple model atomistic amorphous solids in 2D. The deformation which results is shown to consist of avalanches of plastic activity which localize onto elementary shear bands, similar to those observed in analog macroscopic laboratory models such as bubble rafts and foams. These *elementary* shear bands have widths on the order of atomic dimensions and their role in the formation of the much larger-scale shear bands which are observed experimentally is currently a crucial open question.

An analysis of the plastic avalanches leads to the identification of a quantum of slip which can be viewed as a rough analog of a Burger's vector. The spatial structure of the elementary bands is shown to be fractal with no identifiable characteristic length. The nature of this fractal structure is novel with a strong anisotropy in the scaling exponents which characterize the fractal geometry. The particular form of this anisotropy can be understood qualitatively in terms of the pressure sensitivity of the local yielding behavior. We also discuss the nature of the spatio-temporal correlations of the elementary shear bands as further understanding of them will be crucial in making connections between atomic lengthscales and the micron-scale bands observed in laboratory samples.