MAR06-2005-000717

Abstract for an Invited Paper
for the MAR06 Meeting of
the American Physical Society

**Simulations of Nano-indentation and Shear Banding in Amorphous Solids**

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Molecular dynamics simulations of a number of amorphous systems reveal the structural changes that accompany plastic localization. We have simulated both two-dimensional and three-dimensional systems in nanoindentation[1], uniaxial tension[2] and compression in plane strain[3]. The degree of strain localization depends sensitively on the quench rate during sample preparation, with localization only arising in more gradually quenched samples. Careful analysis of the strain rate dependence of the localization allows us to extrapolate to the low strain rate limit. This analysis reveals a transition from localized flow to homogeneous flow at a critical value of the potential energy per atom prior to testing. This transition occurs in both two- and three- dimensional systems. The transition appears to be associated with the k-core percolation of short range order (SRO) in the two-dimensional system[2]. We have used a generalization of the Frank-Kasper criterion to identify SRO in the three-dimensional systems. Only in certain systems does this method predict a percolation transition corresponding to the transition in mechanical behavior. We discuss the non-uniqueness of this measure of SRO, and consider whether a more rigorous definition could be derived which applies to systems far from the hard-sphere limit.

[1]Y. Shi and M.L. Falk, "Structural transformation and localization during simulated nanoindentation of a non-crystalline metal film," Applied Physics Letters, Vol. 86, pp. 011914 (2005).
[2]Y. Shi and M.L. Falk, "Strain localization and percolation of stable structure in amorphous solids," Physical Review Letters, Vol. 95, pp. 095502 (2005).
[3]Y. Shi and M.L. Falk, "Does metallic glass have a backbone? The role of percolating short range order in strength and failure," Scripta Materialia, Vol. 54, pp. 381 (2005).