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Simulations of shear banding in metallic glasses[1]

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Metallic glasses represent a promising high strength material, but their use is limited by the onset of a shear banding instability when their material strength is exceeded. Recent simulation studies of the initiation and development of localized deformation in molecular dynamics simulations of a number of amorphous systems reveal the structural changes that accompany plastic deformation and localization involve a decrease in the local short range ordering. We have simulated both two-dimensional and three-dimensional systems in nanoindentation [1,2], uniaxial tension [3] and compression [4] in plane strain. The degree of strain localization depends sensitively on the quench rate during sample preparation, with localization only arising in more gradually quenched samples. A systematic analysis of simulated systems in simple shear geometries [5] reveals that a Boltzmann-like relationship between strain rate and structure holds over large variations in both the applied strain rate and the initial structural state of the glass. Scaling is observed over eight orders of magnitude in strain rate. The consequences of this scaling for constitutive models of glass plasticity will be discussed.

[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, "The structural origin of shear band formation in metallic glass studied via simulated nanoindentation," Acta Materialia , Vol. 55, pp. 4317 (2007).
[3] Y. Shi and M.L. Falk, "Strain localization and percolation of stable structure in amorphous solids," Physical Review Letters, Vol. 95, pp. 095502 (2005).
[4] Y. Shi and M.L. Falk, "Atomic-scale simulations of strain localization in three-dimensional model amorphous solids," Physical Review B, Vol. 73, pp. 214201 (2006).
[5] Y. Shi, M.B. Katz, H. Li and M.L. Falk, "Evaluation of the 'disorder temperature' and 'free volume' formalisms via simulations of shear banding in amorphous solids," Physical Review Letters, Vol. 98, 185505 (2007).

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