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P. Thamburaja, U. Ramamurty

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# Plastic Deformation and Failure Mechanisms in Nano-scale Notched Metallic Glass Specimens under Tensile Loading

Tanmay Dutta[a], Ashish Chauniyal[b], I. Singh[c], R. Narasimhan[a,*], P. Thamburaja[d], U. Ramamurty[b]

[a]*Department of Mechanical Engineering, Indian Institute of Science, Bangalore 560012, India*
[b]*Department of Materials Engineering, Indian Institute of Science, Bangalore 560012, India*
[c]*Department of Mechanical Engineering, IIT Indore, Simrol 453552, India*
[d]*Department of Mechanical and Materials Engineering, Universiti Kebangsaan Malaysia (UKM), Bangi 43600, Malaysia*

**Abstract**

In this work, numerical simulations using molecular dynamics and non-local plasticity based finite element analysis are carried out on tensile loading of nano-scale double edge notched metallic glass specimens. The effect of acuteness of notches as well as the metallic glass chemical composition or internal material length scale on the plastic deformation response of the specimens are studied. Both MD and FE simulations, in spite of the fundamental differences in their nature, indicate near-identical deformation features. Results show two distinct transitions in the notch tip deformation behavior as the acuity is increased, first from single shear band dominant plastic flow localization to ligament necking, and then to double shear banding in notches that are very sharp. Specimens with moderately blunt notches and composition showing wider shear bands or higher material length scale characterizing the interaction stress associated with flow defects display profuse plastic deformation and failure by ligament necking. These results are rationalized from the role of the interaction stress and development of the notch root plastic zones.

*Keywords:* Metallic glasses; plastic deformation; failure mechanisms; notched specimens; Molecular dynamics; Finite element analysis.

*Corresponding author. Tel.: +91 80 2293 2959.
*Email address:* narasi@mecheng.iisc.ernet.in. (R. Narasimhan )