

Correlating Structural Heterogeneity to Deformation of Metallic Glasses Using 4-D Scanning Nanodiffraction and Mesoscale Simulation

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We present the direct determination of the heterogeneity at the nano to mesoscale structure of metallic glasses (MGs) using 4-dimensional (4-D) nanodiffraction in scanning transmission electron microscopy (STEM). Understanding the heterogeneity is critical because it may be related to the important characteristics of MG deformation, including the initiation and distribution of shear bands that can directly influence the overall plasticity of the material. The 4-D STEM based on the new generation pixelated fast STEM detectors enables the direct characterization of the details of the heterogeneity, including the type, size, distribution, and volume fraction of the medium range atomic ordering that constitutes the heterogeneity. The heterogeneity information determined using 4-D STEM is then incorporated into the heterogeneously randomized mesoscale model to simulate realistic deformation beyond the spatial and temporal limits of the atomistic level simulations. The combined use of 4-D STEM and the state-of-the-art simulation can therefore substantially advance our knowledge on how the change in heterogeneity dictates shear localization and overall ductility of MGs.

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