Atomistic simulation of deformation in metallic glasses

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Abstract

We have studied the deformation of an amorphous nano-wire under uniaxial tension using molecular dynamics (MD) simulations. We find that the stress, after increasing in a linear fashion until the elastic limit, drops and then increases in repetitive way. The sharp drops in the stress-strain curve are due to cooperative shear events, which result local structural defects such as shear bands. These local defects have been studied by analyzing the crystallographic orientation compared to the orientation before yielding. However, this kind of simple structural analysis does not work for glasses because there is no well-defined long-range structural order in glasses. In this study, we introduce an improved generic method to capture the local defects, which can be used for both glass and crystalline material. Using this method, we successfully capture the local defects and find that the defects localize as the strain increases. The localization of shear is associated with the absence of strain hardening (work hardening) mechanisms, possible strain softening mechanisms, and thermal softening during adiabatic heating of the material.

Acknowledgments

This work was supported in part by the MRSEC Program of the National Science Foundation under Award Number DMR-0080065.

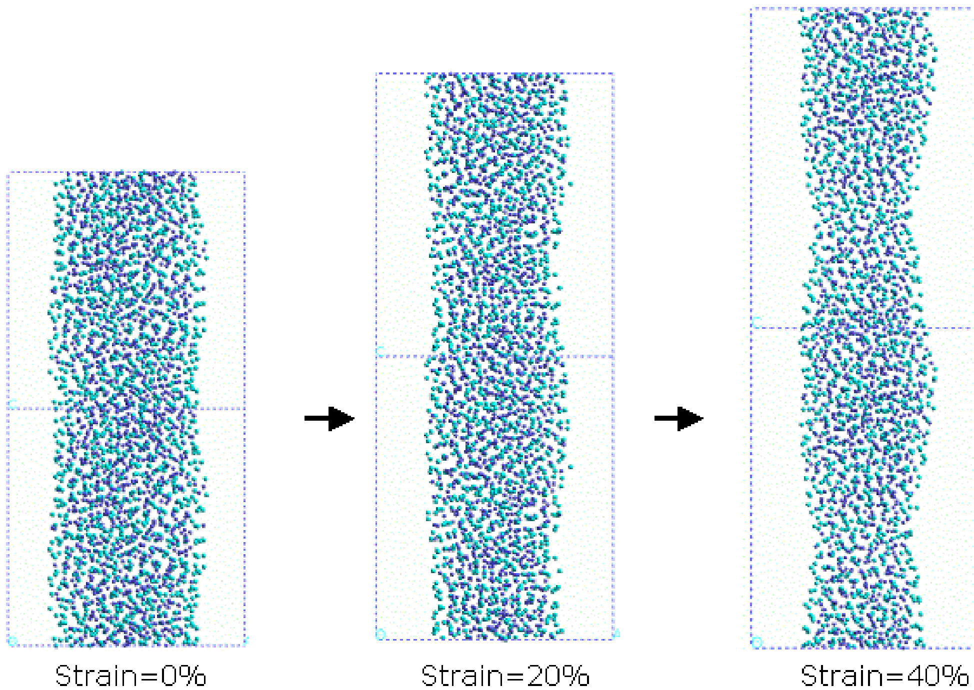

Figure 1. Snapshots of the metallic glass nano-wire at different strains. As the strain increases, plastic deformation such as necking is more fully developed and more localized.

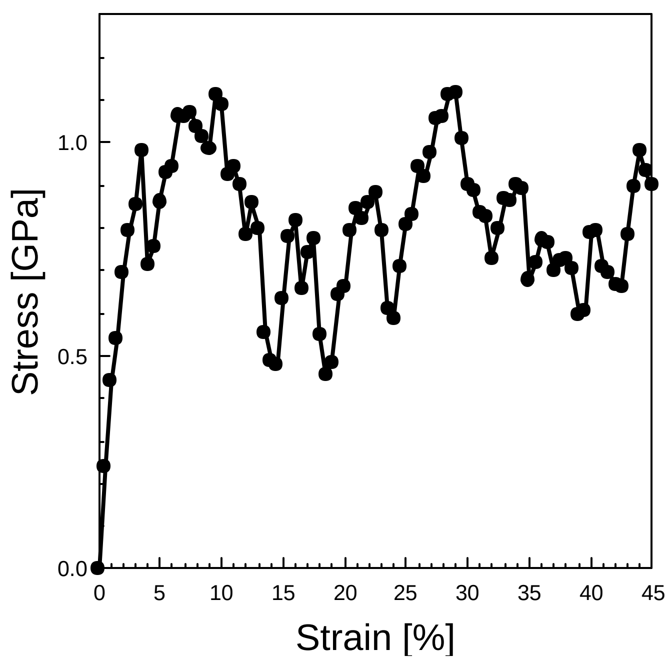

Figure 2. The stress-strain curve of the metallic glass nano-wire loaded in uniaxial tension for stain rate of 0.5%/10ps at 300K. Due to coherent shearing events, the curve shows a serrated yielding.