Strain Localization in Metallic Glasses: Role of Mechanical Heterogeneity

PAVAN VALAVALA, Department of Materials Science and Engineering, Johns Hopkins University, MICHAEL FALK, Departments of Materials Science and Engineering, Mechanical Engineering, Physics and Astronomy, Johns Hopkins University — Metallic glasses are a technologically interesting material in large part because their flow behavior near the glass transition temperature makes them optimal for complex manufacturing processes. At lower temperatures, however, these materials tend to accommodate strain in “shear bands” resulting in macroscopically brittle behavior undesirable for load bearing applications. In order to better characterize the plastic processes that govern flow in these materials, we analyze spatial changes in local elastic response during molecular dynamics simulations of strain localization in a binary Lennard-Jones (LJ) glass. Isothermal elastic stiffnesses are evaluated at different length scales from equilibrium stress and strain fluctuations for the glass and a LJ crystal. The differences in convergence and variations in the elastic properties measured using stress and strain fluctuation methods are compared for the ordered and disordered systems. The average elastic properties are verified against direct measurements on the atomistic models. Finally, the consequences of mechanical heterogeneity on plastic response and strain localization in the glass will be discussed.