Molecular Dynamics Simulations of Metallic Nanoglasses

*Sara Adibi^{1,2}, Paulo S. Branicio², Shailendra P. Joshi¹
¹Department of Mechanical Engineering, National University of Singapore, Singapore
²A*STAR, Institute of High Performance Computing, Singapore

*Corresponding author: sara.adibi@nus.edu.sg

Metallic glasses exhibit high strength and high hardness, but severe lack of tensile ductility. In order to improve the plasticity a new type of metallic glass architecture referred to as *nanoglass* has been recently proposed. In this work, we use molecular dynamics simulations to investigate the mechanical behavior of 2D $Cu_{64}Zr_{36}$ films nanoglass over a range of particle sizes. The architectures are generated using Voronoi tessellation in a procedure that qualitatively mimics the real synthesis approach. Results show that films with nanoglass architectures experience a transition from a localized deformation in the form of a single dominant shear band to a near homogeneous plastic deformation with decreasing particle size. This occurs because the interfacial regions act as preferred channels for plasticity, causing the generation of an interconnected motif of shear bands that depends on the microstructure particle size. These results highlight the intriguing effects of nanoglass architectures in amorphous metallic alloys.

Keywords: Metallic Nanoglasses, Plasticity, tensile ductility, Molecular Dynamics.