Modeling and Simulation of Homogenous and Inhomogeneous Deformation Behavior of Metallic Glasses

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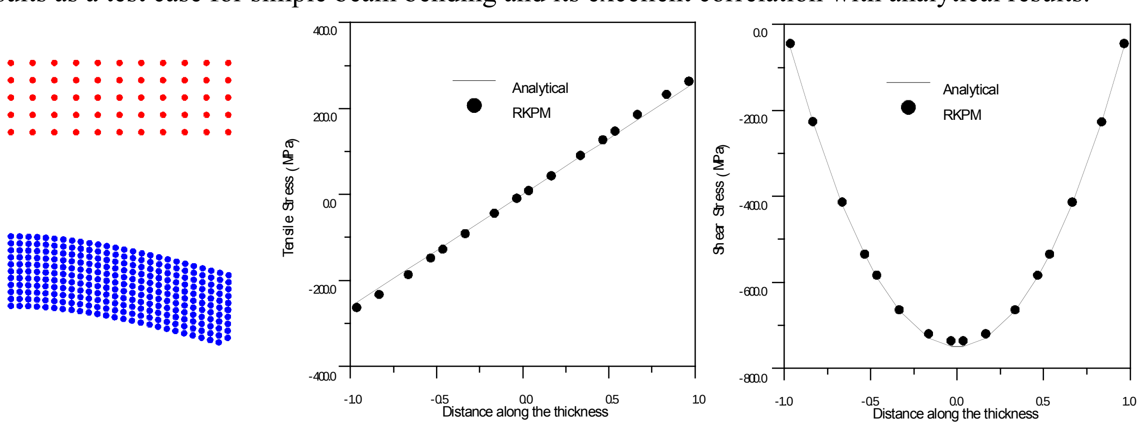
Abstract:

The deformation behavior of metallic glasses (MGs) can be classified by either inhomogeneous (non-Newtonian) or homogeneous (Newtonian) deformation depending upon the temperature and the loading rate. Inhomogeneous deformation is characterized by the formation of adiabatic intense shear bands, followed by unstable fracture. In this deformation mode MGs usually exhibit very limited ductility and fracture toughness. Despite the limited macroscopic plasticity, in such a deformation mode, local strains in the shear bands can be quite significant (as high as 30-50%). These bands are typically 50-100nm in width. Homogenous deformation takes place at temperatures greater than half of the glass transition temperature and MGs exhibit significant plasticity without the occurrence of the intense shear bands. The transition temperature between inhomogenous and homogenous modes of deformation is strongly controlled by the rate of the deformation. The objectives of this study are to better understand, through modeling and simulation, the underlying mechanisms that are responsible for these deformation modes and resulting microstructural evolution in MGs.

Recent Results:

The main research tool for our investigations will be computational simulations. These simulations will be concerned with the mechanisms associated with the deformation kinetics of metallic glasses and will be supplemented with the experimental observations. It is now well documented that classical Finite Element Analysis (FEM) is not suitable for analysis of shear localization that is approaching microscopic length scales due to so-called mesh-alignment sensitivity (i.e., FEM is unable to resolve localized shearing at angles oblique to the element boundaries). Therefore, our simulations will utilize the mesh/element-free Reproducing Kernel Particle Method (RKPM). In this technique the approximated function is constructed from a set points that defines the geometry and the boundary. The RKPM was developed very recently and has not yet reached the same maturity of common numerical techniques that are currently used in continuum mechanics. Although its derivation is available, many salient details necessary for computer implementation are not discussed in the open literature, in contrast to elements in classical finite element method. The figure shown below shows our linear elastic RPKM code results as a test case for simple beam bending and its excellent correlation with analytical results.



Significance:

One other advantage of the numerical approach developed in this study is adaptive refinement of the solution due to multi-scaling of the shear banding. The simulations will provide us the length and time scales of the energy landscape (both thermal and strain energy) of the shear bands in metallic glasses. By utilizing this information, the microstructural evolution within the shear-bands and the corresponding equilibrium morphologies due to the elastic misfit between the parent and evolving phases will be examined. Therefore, our ultimate aim will be to couple the RKPM continuum deformation code with nano-scale phase evolution models.

Future Work:

We are currently implementing the coupled thermoelastic behavior to our linear elastic code. Subsequently, we will introduce time-dependent visco-elastic material constitutive behavior to elucidate the evolution of large inelastic strains within the adiabatic shear bands. One of the main objectives of these simulations is to determine the magnitude of temperature evolution within the shear bands and assess whether local temperature increases are sufficient for devitrification or even local melting during deformation, as has been speculated in the literature. This work will also elucidate for a given deformation rate and temperature how the geometry and loading modes influence the morphology of the shear-bands and spatial-temporal temperature evolution during the course of deformation.

Interactions:

Although RKPM is very accurate for simulation of evolution of shear bands, due to the nature of the algorithm definition of natural boundaries are difficult and computationally every intensive. Therefore, we are also exploring the viability of other meshless methods such as Boundary Element Method in collaboration with Prof. A.K. Mitra (ISU).

Correlation of simulation results with experimental studies, carefully designed mechanical testing studies will be conducted in collaborations with Drs. D.J. Sordelet and S. Chumbly.