Final report: Multiscale modeling of shear banding in metallic glasses

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Principal Investigator Information: Prof. Lin Li, Department of Metallurgical and Materials Engineering, The University of Alabama, Tuscaloosa, AL 35406
Email: lin.li@eng.ua.edu; Phone: 205-348-4971
Participating National Laboratories: Lawrence Berkeley National Lab; Oak Ridge National Lab.

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Project Scope:

Metallic glasses (MGs) possess remarkably high strength but suffer from minimal tensile ductility due to the formation of catastrophic shear bands. The goal of this research project is to develop an understanding of the microstructures and deformation mechanisms that control shear banding in MGs, which will enable the development of MGs with enhanced plasticity. Two scientific objectives have been pursued. (1) Understand the underlying mechanisms of shear banding phenomena in presence of nanoscale heterogeneities in MGs. (2) Understand the evolution of MG heterogenous structure upon thermomechanical stimuli for plasticity enhancement through controlling and distributing multiple shear bands.

Accomplishments

Shear banding mechanisms in presence of nanostructural heterogeneity

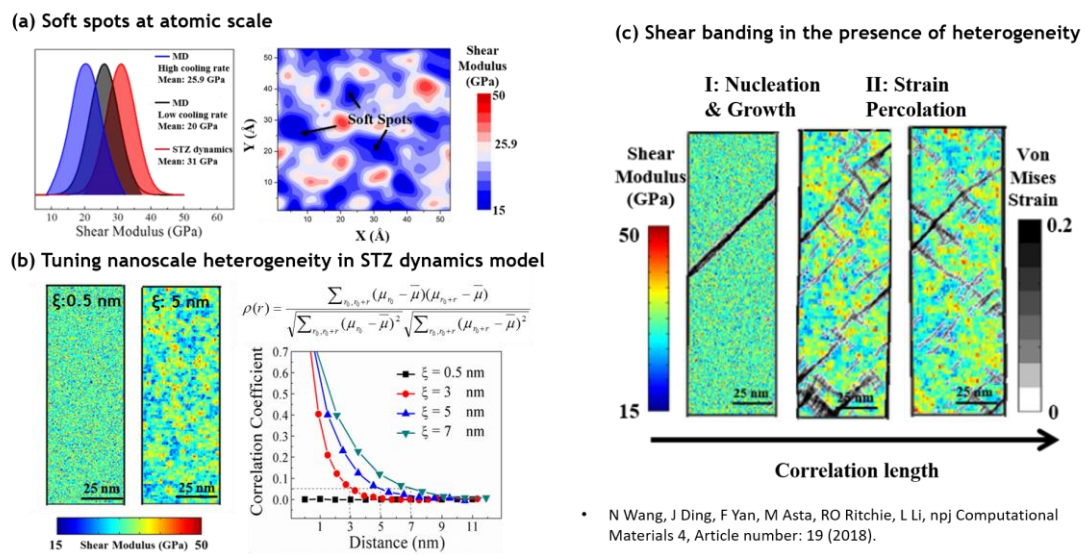

Figure 1: Multiscale model connects intrinsic heterogeneity with shear banding. (from N Wang et al., npj Computational Materials 2018). (a) Local shear moduli of $Cu_{64}Zr_{36}$ MG obtained by molecular dynamics simulations. (b) Tuning the spatial distribution of local shear moduli in the samples of STZ dyanmics simulations. (c) Transition of shear banding mechanisms with nanoscale heterogeneity.

MGs possess amorphous structures with inherent heterogeneity at the nanoscale, which has profound impacts on glass dynamics and mechanical properties. This part of the work employs a multi-scale modeling framework, combining atomistic simulations and mesoscale shear transformation zone (STZ) dynamics simulations, to study the effect of spatial correlation of nanoscale elastic heterogeneity on tuning the shear banding behavior. At the atomic scale, as shown in **Fig. 1a**, a highly heterogeneous, Gaussian-type shear modulus distribution at the nanoscale is revealed by atomistic simulations in $Cu_{64}Zr_{36}$ MGs, in which the soft population of the distribution exhibits a marked propensity to undergo an inelastic shear transformation. By employing a mesoscale shear transformation zone dynamics model, we find that the organization of such nanometer-scale shear transformation events into shear band patterns are dependent on the spatial heterogeneity of the local shear moduli. A critical spatial correlation length of elastic heterogeneity is identified for the simulated MGs to achieve the best tensile ductility, which is associated with a transition of shear-band formation mechanisms: from stress-dictated nucleation and growth to structure-dictated strain percolation, as well as a saturation of elastically soft sites participating in plastic flow, as illustrated in **Fig. 1b-1c**. This discovery is important for the fundamental understanding of the role of spatial heterogeneity in influencing the deformation behavior of MGs. We envision that this can facilitate the design and development of new ductile monolithic MGs by the process of tuning the inherent heterogeneity to achieve enhanced ductility in these high-strength metallic alloys. This work was published in npj Computational Materials [1], and selected as DOE Science Highlights.

Evolution of the MG heterogenous structure during thermomechanical processing

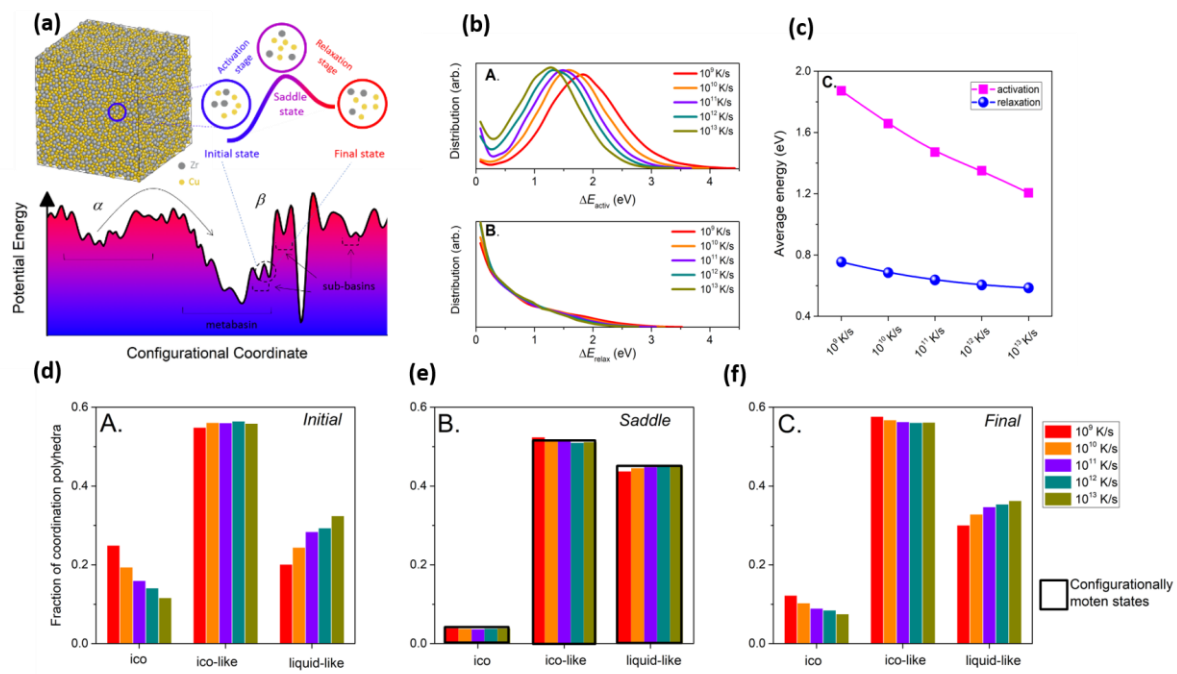

Figure 2: (a) Schematic description of potential energy landscape for MGs. (b) Activation and relaxation energy spectra of elementary thermally-activated events in $Cu_{64}Zr_{36}$ MGs. (c) The variation of activation and relaxation energies vs. thermal history. (d)-(f) The short-range atomic structural evolution in the thermally-activated process from activation to relaxation.

The understanding of structural evolution in response to external forces in amorphous materials remains incomplete due to the complexity of their structure. As such, various complex phenomena in amorphous materials have been interpreted using the concept of the potential energy landscape, as shown in **Fig. 2a**. In this work, the evolution of atomic configuration in an elementary thermally-activated deformation process is investigated using atomistic simulations in several model MG systems with different cooling histories spanning five orders of magnitude. By probing the reconfiguration of the short-range order clusters at key states on the potential energy landscape, a universal short-range order state is found at the saddle states, which is invariant with cooling history and composition (ref. to **Fig. 2d-2f**). Furthermore, such a universal short-range order state manifests a special form of melts, referred to as a configurationally molten state with the effective temperature hundreds of degrees above the glass transition temperature. The short-lived melting at the saddle states is responsible for wiping out the prior thermal history, explaining the decoupling of the activation and relaxation stages of the elementary β process in MGs. The findings highlight the importance of understanding the nature of the saddle states in elucidating the MG system dynamics and provide a complementary view of the current understanding of the potential energy landscape. It could greatly simplify the dynamics of glass inherent structure evolution, and apply to postulates of the glass rejuvenation route via thermomechanical protocols. A manuscript describing our findings has been submitted and is currently under review [2].

Automating parallelized computations to study the evolution of materials

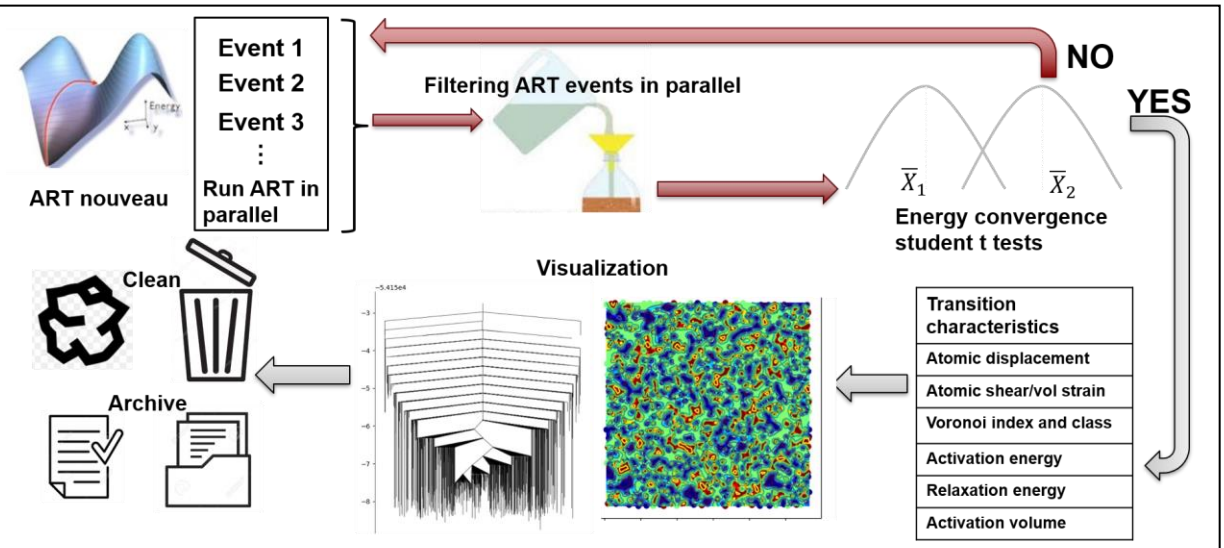

Figure 3: The pipeline software architecture of this ART_data_analyzer package allows user customization in running various module tasks in a standard workflow. (from Tian L, et al., Software X 2019).

The kinetics and dynamic evolution of material structures need a comprehensive understanding of the potential energy landscape, which can be probed by a powerful atomistic simulation tool, Activation–Relaxation Technique nouveau (ARTn). However, the ARTn software has not implemented the parallelization of each ARTn simulation, which implies that the user needs to spend considerable efforts in manually handling large amount of ART events data. Therefore, we have developed this ART_data_analyzer computational software to allow users to automate the generation and manipulation of a large amount of events data in parallel, the pipeline of which is

shown in **Fig. 3**. This convergence of sampled events data can be verified by the implemented student t statistical convergence test. The automation of various post-processing tasks in this ART_data_analyzer package includes filtering events, calculating, visualizing, correlating various physical quantities, and/or their changes. The main advantage of this ART_data_analyzer software is to reach the necessary user-friendliness through automation while still maintaining the essential physics workflow for a user to understand various task processes they are performing. In addition, this ART_data_analyzer software is also very robust to any interruption during calculation due to either machine failure or human intervention by providing various well-documented and simple-to-use command options. This ART_data_analyzer also has the benefits of convenient data management by archiving most necessary data files or deleting unused data files to consolidate data for saving disk space, which will promote the accessibility of research data between research teams. The significance and impact of this software lie in its ability to study the kinetics and dynamic evolution for a broad range of material classes, such as crystalline materials and their defects (e.g., grain boundaries and interfaces) and amorphous materials. This ART_data_analyzer software was published in the journal Software X [3].

Identifying flow defects in amorphous alloys using machine learning

Shear transformation zones (STZs) are widely adopted to be the fundamental flow defects that dictate the deformation of amorphous alloys. However, it is difficult to determine the shear transformation zone and their evolutions by experimental methods due to transient nature. In this study, we introduced a method to identify the STZs by outlier detection machine learning algorithms based on the atomistic simulation data. We used this algorithm to identify the size of STZs in a model $Cu_{64}Zr_{36}$ MG. The results are close to the previous physics-based studies on the size of the STZs in CuZr MG systems. When using this algorithm to study the effect of cooling rate on the size of STZs, it is found that the average size of STZs increases slightly with decreasing cooling rate. From the perspective of the data model, the linear random sample consensus (RANSAC) algorithm, as shown in **Fig. 4**, is the most outlier-sensitive algorithm in identifying the STZ atoms. These algorithms are robust to a wide range of training data from atomistic simulations, which can be applied to different systems of amorphous solids in response to various external forces. Additionally, we have implemented the algorithm in our open-source software package ART_data_analyzer for future study. This work was published in Scripta Materialia [4].

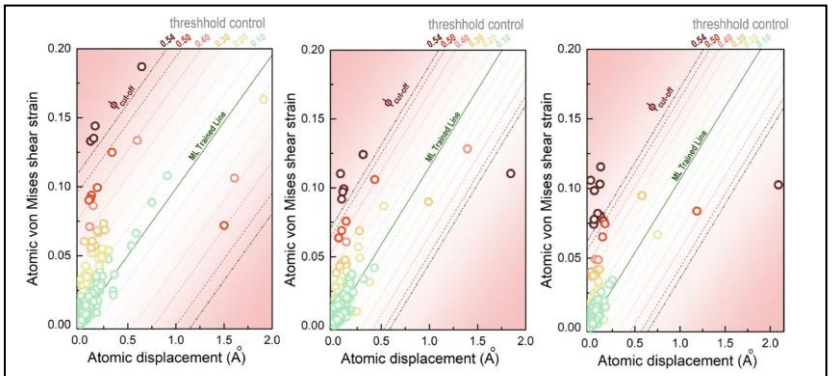

Figure 4: The automation process of the LinearRANSAC machine learning algorithm identifies the outlier atoms of each individual thermally-activated event. (from Tian L, et al., Scripta Materialia 2020)

Chemical variation induced nanoscale heterogeneity in metallic glasses

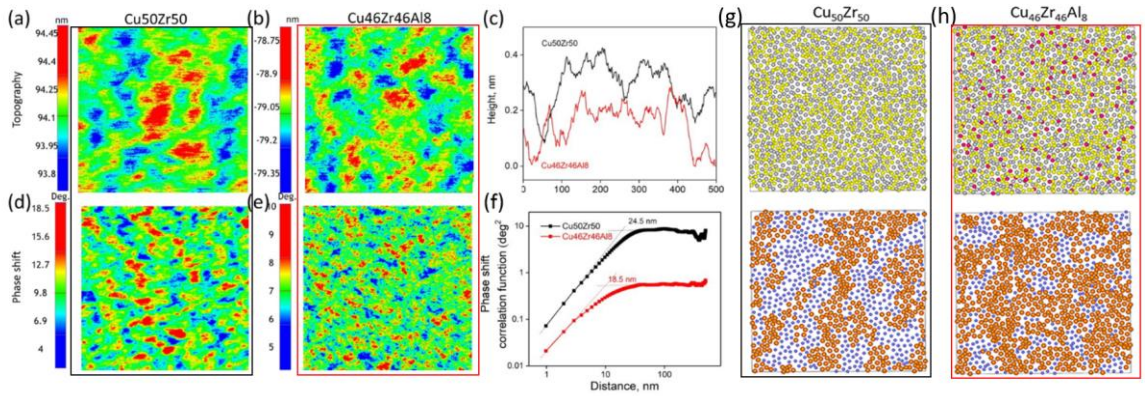

Figure 5: Chemical-modulated nanoscale heterogeneity in $Cu_{50}Zr_{50}$ vs. $Cu_{46}Zr_{46}Al_8$ thin film MGs. AFM results of (a)-(b) the height image with root-mean-square (RMS) roughness less than 1 nm, confirmed by (c) height profile. (d)-(e) the phase shift images, reflecting the variation of nanoscale viscoelastic heterogeneity. (f) The calculated autocorrelation function of phase shifts, quantifying the variation of spatial heterogeneity. (g)-(h) Short-range atomic heterogeneities in model $Cu_{50}Zr_{50}$, $Cu_{46}Zr_{46}Al_8$ MGs, characterized by atomistic simulations. (from Wang N, et al., Materials Research Letter 2018).

Motivated by the impact of the nanoscale feature on the modulating MG flow, we study the chemical effect on tuning the nanoscale mechanical heterogeneity of a representative Cu-Zr-Al MG system using a combined experimental and modeling approach. The amplitude-modulation dynamic atomic force microscopy (AM-AFM) is employed to measure the local mechanical response, revealing a reduction of nanoscale spatial heterogeneity in the local viscoelastic response after introducing Al into the $Cu_{50}Zr_{50}$ MG, as shown in **Fig 5(a)-(f)**. With the assistance of atomistic simulations, the change of such nanoscale heterogeneity is related to the variation of local atomic structures upon Al alloying. The addition of Al increases the population of the short-range ordered icosahedral clusters, enhancing their connection to form a uniform network and thus reducing the structural heterogeneity at the nanoscale. In contrast, the $Cu_{50}Zr_{50}$ MG exhibits less icosahedral clusters, which tend to aggregate and disperse in space, resulting in a larger correlation length of the icosahedral order. This insight provides a fundamental understanding of the role of the nanoscale heterogeneity on the remarkable performance difference in the uniform monolithic MGs. This discovery could further facilitate tailoring the MG properties with selective modulation of chemical composition. This work was published in Materials Research Letter [5].

Publications

[1] Wang N, Ding J, Yan F, Asta M, Ritchie RO, Li L, Spatial correlation of elastic heterogeneity tunes the deformation behaviors of metallic glasses, npj Computational Materials, 19, 2018. (http://dx.doi.org/10.1038/s41524-018-0077-8)

[2] Ding J, Li L, Wang N, Tian L, Asta M, Ritchie RO, Egami TK, "Universal nature of the saddle states of structural excitations in metallic glasses" (submitted).

[3] Tian L, Li L, Ding J, Mousseau N, ART_data_analyzer: a python package that automates parallelized computation in a user workflow for studying the kinetics and dynamic evolution of materials, Software X, 9, 2019, P 238.

(https://doi.org/10.1016/j.softx.2019.03.002)
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(https://doi.org/10.1016/j.scriptamat.2020.05.038)
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(https://doi.org/10.1080/21663831.2018.1532465)
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(http://dx.doi.org/10.1016/j.tsf.2017.02.035)
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Participants involved in this project

PI Lin Li was supported by three-month summer salary from the award. She conducted research, wrote papers, mentored students, and disseminated the results at seminars and conferences.

Graduate students: Neng Wang (100%), Yucong Gu (50%)

Neng Wang performed mesoscale simulations of shear banding behaviors in presence of nanoscale elastic heterogeneity. He defended his thesis and obtained Ph.D. degree in the summer 2018.
Yucong Gu has performed finite element analysis on the nanostructural design for MG plasticity enhancement.

Postdoc: Liang Tian (100%)

Dr. Liang Tian performed atomistic simulations using LAMMPS and activation-relaxation technique. He developed the ART_data_analyzer computational software, automating the generation and manipulation of a large amount of events data in parallel.

National lab patterners

Dr. Jun Ding at Lawrence Berkeley National Lab performed molecular dynamics simulations and guided the graduate students and PostDoc in the atomistic simulations and analysis via emails and phone calls.
Prof. Takishi Egami at Oak Ridge National Lab provided guidance in the potential energy landscape model.

Unexpended funds

The grant is fully expended.