Shear Banding in Bulk Metallic Glass Matrix Composites with Dendrite Reinforcements

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Abstract. Bulk metallic glass matrix composites (BMGMCs) with metallic dendrite reinforcements combine the excellent strength, hardness, and elastic strain limit of amorphous metallic glass with a ductile crystalline phase to achieve extraordinary toughness with minimal degradation in strength. In order to explore the mechanical interactions between the amorphous and crystalline phases a full-field micromechanical model, which couples a free volume based constitutive model for the matrix with crystal plasticity, has been implemented in an elastic-viscoplastic Fast-Fourier Transform (FFT) solver. The findings indicate that in BMGMCs, local inhomogeneities in the glass phase are less influential on the mechanical performance than the contrast in individual phase properties. Due to the strong contrast in mechanical properties, heterogenous stress fields develop, contributing to regionally confined free volume generation, localized flow and softening in the glass. In these softened regions, plastic flow rapidly localizes into shear bands.

Keywords: Bulk metallic glass · Shear bands · Yield phenomena
Micromechanical simulation

One strategy for mitigating the poor failure resistance in BMGs is to incorporate crystalline phases which dissipate energy and accommodate plastic strain by dislocation slip, effectively blocking long-range shear band propagation. This has led to considerable interest in bulk metallic glass-matrix composites (BMGMCs) with crystalline reinforcements [1]. Computational modeling offers a way to accelerate the design of BMGMCs by exploring the effect of microstructural parameters and individual phase properties on the overall composite mechanical performance. Micromechanical deformation simulations also provide important insight on the nucleation and interaction of shear bands with the crystalline dendrites, as well as how the microstructure and individual phase properties can be tailored to optimize the mechanical performance of the composite.

Prior continuum and atomistic-scale modeling efforts have worked to establish robust constitutive models for BMG and BMGMC deformation, introduce fundamental variables to describe the local state of the material, and develop mathematical frameworks for efficiently simulating the micromechanical deformation associated with shear banding [2, 3]. Here we implement a free volume based constitutive model for the matrix coupled with crystal plasticity within an efficient fast Fourier-transform based

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micromechanical solver [4] for the simulation of quasi-static deformation of BMGMCs, in terms of both the macroscopic mechanical response as well as the local characteristics of shear band operation. We show that in contrast to shear band nucleation in monolithic BMGs, where it is reasonably assumed the nucleation sites arise from chemical and structural fluctuations at the atomic scale, in metallic glass composites, the spatial distribution and contrast in individual phase properties are the dominating factors controlling where, when, and how shear bands are formed. We show that shear bands in metallic glass composites are reproducible in numerical simulations without the introduction of intrinsic flaws or an artificial nucleation sources, provided there exists sufficient contrast in properties between the dendrites and amorphous matrix. We then link experimentally observed oscillatory stress-strain behavior to the concurrent localization of strain in shear bands and the corresponding relaxation of the glass-matrix in the surrounding regions. Results from the simulation showing the development of shear bands along with the result evolution of stress-strain and accumulated strain energy is shown in Fig. 1.

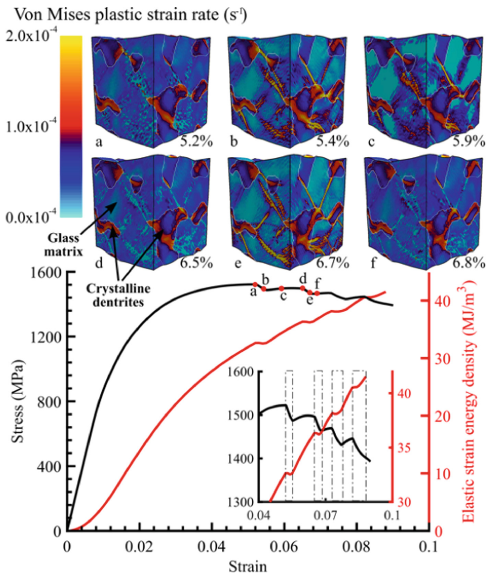

Fig. 1. 3D deformation maps (top) colored by the local plastic strain-rate at overall strain levels corresponding to the marked positions on the stress-strain curve (bottom). The elastic strain energy density highlight its relationship to shear band formation and the associated oscillations in the stress-strain curve.

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