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Microstructural factors of strain delocalization in model metallic glass matrix composites

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Abstract—Metallic glass matrix (MGM) composites demonstrate impressive plasticity over monolithic metallic glasses due to their ability to delocalize strain and inhibit shear band propagation. This work investigates various microstructural factors (volume fraction, length scale and yield strength) influencing strain delocalization in a model MGM composite. Shear transformation zone dynamics is utilized to model the amorphous phase while a local Taylor dislocation model is used for the crystalline phase. An *N*-factorial experiment examines replicates for various macro- and microscopic measures of strain delocalization and regression analysis is used to identify statistically significant trends in the data. The experiment shows that strain delocalization and the consequent ductility are most strongly influenced by a crystalline phase with a substantially lower yield stress than that of the amorphous matrix. It also shows that increased crystalline volume fraction alone is insufficient to promote strain delocalization in the case of a crystalline phase with high relative yield stress, and that a lower yield stress for the crystalline phase implies lower maximum stresses supported by the composite. Examination of shear band–inclusion interactions indicate that the nucleation and diffuse transmission of numerous shear bands is critical to the strain delocalization. The regression analysis provides continuous functional forms for the various relationships between properties that can be exploited to optimize the microstructure of MGM composites.

Keywords: Metallic glass matrix composite; Micromechanical modeling; Strain delocalization; Shear transformation zone; Shear band

1. Introduction

Metallic glass matrix composites (MGMCs) have demonstrated enormous potential for improved ductility and toughness over traditional bulk metallic glasses (BMGs). Some MGMCs even exhibit toughness comparable to that of aluminum or steel alloys [1,2] while retaining impressive strength and stiffness [3,4]. Of fundamental interest in the design of these MGMCs is the role played by the various microstructural characteristics of the two contributing phases that enable further optimization of these composites.

The crystalline inclusions in MGMCs improve plasticity over that typically exhibited by monolithic metallic glasses (amorphous metals), which exhibit catastrophic failure by shear banding upon yield. This extreme response results from the absence of a crystal lattice, which precludes the plasticity mechanisms found in traditional crystalline materials. Plasticity in amorphous metals occurs by incremental localized shear events called shear transformation zones (STZs) [5]. These zones involve the collective rearrangement of several dozen atoms in response to an applied shear stress. These thermally activated STZs typically have volumes on the order of 10^{-27} m^3 and shear over time scales of 10^{-12} s [6–11]. STZs are energetically much more costly than dislocations or twinning, and differ in that they leave behind local structural changes involving increased free volume [6]. These structural changes and the stress fields in the vicinity of an STZ bias the energy landscape in favor of further STZ activation nearby; consequently, a chain of subsequent STZs activate in this "softer" region, leading to the sudden, catastrophic failure mentioned earlier [12]. As a result of this strain-softening behavior and accompanying catastrophic brittle failure mode, engineering applications that require ductility preclude the use of monolithic metallic glasses and their extraordinarily high strength-to-weight ratio.

The introduction of a second, crystalline phase into the amorphous matrix (to form an MGMC) breaks up shear band events that would otherwise cause failure. This second phase is introduced either in the form of intrinsic crystalline dendrites, which nucleate and grow in certain alloys under specific processing conditions [13,14], or by the addition of extrinsic metal whiskers or particles [15–17].

Recent experimental work has focused on optimizing MGMCs for various loading conditions; behavior under dynamic loading [18,19] and ductility under tensile loading have been of particular interest [3,20–25]. Other experiments have studied how processing – specifically cold rolling – enhances ductility of MGMCs [23,24]. One recent development has demonstrated strain-hardening behavior

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in MGMC alloys with a crystalline phase that exhibits a martensitic transformation [26–29].

Efforts to examine the microstructural factors governing MGMC behavior in a systematic manner have yielded insight towards optimizing such composites [30–34]. After chemistry, the volume fraction of the crystalline phase is the most-examined MGMC design variable [2,35–40]; it seems that increasing the crystalline volume fraction tends to stabilize plasticity and delocalize strain, but decreases the macroscopic strength of the composite. The length scale of the dendritic phase has also been investigated in detail [2,3,14,22,35,39,41] in an effort to find an optimum balance of ductility and strength. Finally, a very few experiments have explicitly examined the effect of ductility or brittleness of the second phase of the MGMC [40]; the effectiveness of the second phase appears to be dependent on the ductility of that phase, and not merely on the inhomogeneity of the composite.

Computational models have also contributed to the understanding of MGMC mechanics [11,42]. At the continuum level, a two-phase finite element model by Qiao [43] quantitatively describes macroscopic MGMC deformation mechanics. The model is based on a five-step deformation regime, which starts with pure elastic deformation, then adds plasticity in the crystalline phase, then goes through three stages where both phases yield, then the crystallites harden, and finally the composite softens and fails. Other finite element approaches have focused on stress heterogeneity and consequent plastic mismatch between the two phases [44], and on the distribution of strain between the two phases at varying degrees of deformation [45].

On much smaller length and time scales, atomistic investigations have resolved many characteristics of STZs and bulk metallic glass behavior [11,46]. Molecular dynamics simulations of MGMCs have yielded insight into shear band behavior around very small crystallites of varying geometry, volume fraction and arrangement [47]. Insight has also been obtained into shear band deflection in amorphous/amorphous composites [48].

Between the continuum and atomistic length and time scales, this paper provides a mesoscale view of the MGMC behavior, which is critical to understanding the role of the various microstructural characteristics. The mesoscale MGMC model builds on the previous STZ dynamics model developed by Homer and Schuh [12,49–51]. An *N*-factorial experiment is designed to examine the effects of the volume fraction, length scale and yield stress of the crystalline phase. The experiment design enables isolation of effects to better understand how the various microstructural variables influence the composite properties. Seven metrics are developed to distill the experimental results, and regression analysis is used to identify statistically significant trends. Different modes of shear band–inclusion interactions and their effect on strain delocalization are also examined. Finally, these trends are discussed in the context of MGMC design. The principles and trends, and particularly the functional forms presented in this work, should enable greater understanding and optimization of MGMCs.

2. Model

In the present model, the behavior of the amorphous matrix is given by the STZ dynamics model, which is based on stochastic activation of coarse-grained STZs [49]. An STZ activation represents an instantaneous, inelastic shearing of a cluster of atoms based on the cluster's local stress state. This is modeled by applying plastic strains to groups of elements in a finite element mesh that represent a potential STZ. After an STZ activates, finite element analysis solves for the resultant stress and strain fields throughout the sample. The resulting stress and strain fields encourage shearing of further STZs (element clusters), and the process repeats. The selection of which STZs to activate is controlled by a modified kinetic Monte Carlo (kMC) algorithm [52], based on the individual activation rates of an ensemble of STZs.

The activation rate $\dot{s}$ of an STZ is given by:

$$\dot{s} = v_0 \exp\left(-\frac{\Delta F - \frac{1}{2}\tau\gamma_0\Omega_0}{kT}\right) \tag{1}$$

where v_0 is the attempt frequency (related to the Debye temperature), ΔF is the intrinsic barrier height of the STZ transition, T is the temperature and k is the Boltzmann constant. The activation rate is biased by the local stress state, τ. Finally, γ_0 and Ω_0 are the increment of shear strain applied to an STZ and the volume of the STZ, respectively. The values for the parameters used in this model are given in Table 1, and a characteristic stress–strain curve for the amorphous phase is shown in Fig. 1.

This paper reports extension of the STZ dynamics model to include a ductile phase, which is used to simulate the crystalline phase of an MGMC. This is accomplished by partitioning the mesh into the two phases and applying the appropriate material or plasticity model to the elements of each phase. The finite element analysis solver evaluates the plastic deformation in the ductile phase in each kMC time step. A maximum time step of 0.01 s is enforced (see Ref. [52] for details).

Following the work of Qiao et al. [43] and Zhang et al. [22], the ductile plastic constitutive law is based on a Taylor dislocation model [53–55]. This is implemented as a UMAT subroutine in ABAQUS. It is worth noting that the simulations in this work use microstructure length scales that are somewhat smaller than those for which the plasticity model has been validated; however, it still captures the requisite ductile behavior exhibited by MGMC microstructures. The plasticity model expresses the tensile stress–strain relation as follows:

$$\sigma = \sigma_{ref}\sqrt{\left(\sigma_y/E + \varepsilon^p\right)^{(2n)} + L\overline{\eta}} \tag{2}$$

where ε^p is plastic strain, E is Young's modulus, σ_y is yield stress, $\sigma_{ref} = E^n/\sigma_y^{n-1}$, n is a hardening coefficient, $L = 180b\left(\frac{a\mu}{\sigma_{ref}}\right)^2$ is an intrinsic material length with μ, b and a being the shear modulus, the Burgers vector length and an empirical constant between 0.1 and 0.5, and $\overline{\eta}$ is the average strain gradient, which is approximated by ε^p/D, where D is a characteristic diameter of the crystalline phase microstructure. The quantities used in this experiment are shown in Table 1 and tensile stress–strain curves are shown in Fig. 1 for two different yield strengths evaluated in this work.

The two models are merged in the finite element model, which is partitioned into amorphous and crystalline elements. The crystalline inclusions are circular and are distributed pseudo-randomly across the sample (their