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ScienceDirect

Acta Materialia 77 (2014) 411–422

Acta MATERIALIA

www.elsevier.com/locate/actamat

Materials by design: An experimental and computational investigation on the microanatomy arrangement of porous metallic glasses

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Received 15 May 2014; accepted 26 May 2014
Available online 12 July 2014

Abstract

The correlation of a material's structure with its properties is one of the important unresolved issues in materials science research. This paper discusses a novel experimental and computational approach by which the influence of the pores on the mechanical properties of bulk metallic glasses (BMGs) can be systematically and quantitatively analyzed. The experimental stage involves the fabrication of a template whose pore configurations are pre-determined by computer-aided design tools, and replication of the designed patterns with BMGs. Quasi-static mechanical characterization of these complex microstructures is conducted under uniaxial tension and in-plane compression. For the numerical simulations, a non-local gradient-enhanced continuum mechanical model is established, using thermodynamic principles and periodic boundary conditions. The combination of the experimental and numerical results has identified the importance of the pore configuration, overall porosity and diameter to the spacing ratio of the pores to attain optimized material properties.

Keywords: Bulk metallic glass; Porous material; Finite element modeling; Mechanical testing; Continuum mechanics

1. Introduction

Advanced microstructures with desirable properties have long been of interest to materials scientists for investigating the relationship between a material's internal structure and its physical properties, such as strength, flexibility and durability. This holds true for various materials. This contribution focuses on metallic glass—an amorphous solid that is stronger than its crystalline counterpart, but usually also brittle. One important task is to design metallic glasses optimized for tensile ductility.

Today's state-of-the-art is not fulfilling the needs of current technology to decipher microstructural complexity, owing to the multi-scale nature of advanced alloy systems determined by undercooling [1,2]. An important barrier is imposed by fabrication techniques, where the strong network between different second-phase parameters (i.e. density, size, shape, dispersion of second phases, and residual stress distribution over the sample) does not permit the construction of a targeted microstructure to thereby achieve the desired material properties.

Bulk metallic glasses (BMGs) possess an exclusive combination of very high fracture strength and strain as well as extensive elasticity [3–7], along with thermoplastic processability [8,9]. These favorable material characteristics emerge from the absence of grain boundaries and dislocations in the glassy state, which permits deformation to evolve isotropically. Furthermore, it has been suggested previously through experiments and observations that

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http://dx.doi.org/10.1016/j.actamat.2014.05.053
1359-6454/

shear band localization in BMG heterostructures alters the mode of deformation and enables controlled shear development as long as the spacing between the second-phase features is equal to or smaller than the critical crack length of the sample [10–12]. This effect is more pronounced under uniaxial compressive deformation, where multiple shear band activation between the second-phase particles remarkably enhances the mechanical response [13–16]. Yet, essentially missing in this puzzle is the quantitative assessment of the influence of each second-phase feature on mechanical behavior. A novel study has addressed this drawback by arranging the microanatomy of engineering materials using a two-step fabrication technique and analyzing heterostructures (systems with more than one phase, i.e. pores as second phase) described in Refs. [17–19], where the influence of parameters on structural properties can be individually traced.

Computational methods such as molecular dynamics simulations [20–26], jammed granular matter [27,28], Bernal's hard sphere model [29,30] or colloidal systems [31–34] have been employed to analyze the atomic packing and free volume creation, which is particularly useful for analyzing the deformation mechanism at the nano-scale. However, the findings based on the atomic–colloidal interactions and the other methods pursued impose a challenge when the entire sample size is orders of magnitude bigger than the characteristic feature size. This limitation is accounted for by the representative volume element selected or inaccurate representation of kinetics in computational systems, which limits the applicability of this technique on wider length scales. However, classical continuum mechanics approaches have been introduced to study the size dependence of metallic glasses using finite element methods [35–39], where they provide significant advantages in terms of simulation time and system size compared with the corresponding experimental methods. Nevertheless, these material models are either not considering non-local stress distributions or showing deviations from the actual response at large deformations owing to local truncation errors of the numerical approximation.

Thamburaja [38] presented one of the first approaches in which an explicit model is implemented to capture the deformation behavior of nanometric sized samples. In recent works by our group [40,41], size effects in metallic glasses have been investigated based on a gradient-enhanced, energy-based mathematical model. The model is formulated as thermodynamically consistent, and captures important physical aspects such as free volume generation, shear localization and fracture mechanism in small-sized metallic glasses. Moreover, the finite-deformation-based theories can be used to monitor the influence of intrinsic material length scale on feature sizes through shear band development and arrest in multi-phase systems.

A critical limitation for an experimental study occurs when the thickness of the sample is one order of magnitude smaller than the other dimensions, which is imposed mainly by the maximum depth of the silicon templates achievable with the anisotropic etching through conventional lithography, as well as the flow kinematics of the viscous metallic glass in its supercooled region. This limitation is also reflected on in-plane compression tests with circular pores, where samples with low porosity (e.g. $P \leqslant 30\%$) are challenged by out-of-plane deformation caused by the Euler buckling instability, which prevails before the structures reach their yield strength [19]. To this extent, numerical analysis of the metallic glass heterostructure under plane-strain conditions brings an advantage and accuracy over the previously pursued experimental study by eliminating the out-of-plane buckling problem.

This work benefits from the aforementioned non-local energy-based mathematical model to investigate the size effect in metallic glasses under in-plane compression. A variety of metallic glass heterostructures with different porosities and pore configurations are numerically analyzed within a finite element framework. In addition, the numerical results are integrated with the experimental studies of these periodic heterostructures, on which quantitative parameter investigations are simultaneously conducted.

2. Experimental background

This paper uses $Zr_{35}Ti_{30}Cu_{7.5}Be_{27.5}$ BMG alloy, which possesses high strength of 1430 MPa under compression, comparable density with light metals, and entensive processing window of ~160 K [43]. The considered attributes confer excellent thermoplastic processability to the selected alloy, which allows for precise micro-replication of highly complicated shapes [43,44]. Second-phase features with significantly smaller radius of curvature (e.g. oval pores or pores with sharp edges) are found to be causing deterioration to the mechanical properties because the stress concentration generally accumulates at the sharp tips, causing the material to break along a single shear band (as previously discussed in Refs. [19,45]). For this reason, the shape of the pores is selected to be circular in both experimental and numerical studies, which provides the most uniform stress distribution throughout the sample.

A selection of experimental specimens for uniaxial tension and in-plane compression are fabricated using a two-step production method, where the templates out of a silicon wafer are created by conventional lithography. The templates are subsequently imprinted onto the metallic glass using the concept of thermoplastic forming (Fig. 1a). The prepressed $Zr_{35}Ti_{30}Cu_{7.5}Be_{27.5}$ BMG disc, with a thickness of ~1 mm was filled into the template at 700 K for 1 min under an applied pressure of 50 MPa. The low viscosity at this processing temperature ($\eta = 10^6$ Pa s) with a calculated lateral flow stress of ~0.3 MPa (assuming Newtonian flow behavior $\sigma = 3\eta\dot{\varepsilon}$ and quasi-static conditions ($\dot{\varepsilon} = 10^{-1}s^{-1}$) accommodates template replication with convenience and precision. The surfaces of replicated samples are at first ground and polished to establish a fine surface smoothness. The samples are then taken out of the mold by chemical etching, using a diluted KOH (35%