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Property optimization of porous metallic glasses via structural design

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ABSTRACT

Systematization of material parameters is essential for property optimization. In this work, a gradient-extended continuum mechanical model implemented into a finite element code is utilized to analyze the influence of pore hierarchy on the overall mechanical response of porous metallic glasses. A spectrum of samples with randomized (stochastic) pore designs is comparatively studied with their periodic counterparts. It is shown that the pore design as well as the volume fraction has a strong effect on the mechanical response of the porous metallic glass structures. The results underline design aspects for certain applications.

1. Introduction

Metallic glasses constitute an important research focus due to their unique mechanical properties. To exemplify, very high yield strength close to the theoretical limit and large elastic strain at room temperature are typical properties of these advanced alloys. However, limited plasticity due to their amorphous nature creates a serious bottleneck for the applicability of monolithic metallic glasses. To overcome this drawback, several approaches to create metallic glass foams have been pursued. The foams can remarkably toughen the glass by forming localized shear bands through energy dissipation within the matrix [1–3]. Sarac et al. [4,5] address the influence of pores on the mechanical properties of bulk metallic glasses by a novel microstructure design strategy experimentally and numerically. In these studies, samples of various pore sizes, spacings, configurations and porosities were examined under uniaxial compression or tension, where periodic pore design facilitated for quantitative analyses.

The design criterion of advanced structures depends on customers' needs and application field, which is strongly correlated with optimization of one or several material parameters. Particularly for the optimization of mechanical properties, one must always consider the tradeoffs which significantly alter the performance of the final product. For example, it has recently been shown that high elastic energy storage during in-plane compression is observed by a geometric effect through pore configuration [6,7]. To improve the overall plasticity and toughness, a more effective stress transfer method during deformation is generated by the reconfiguration of microstructure. For example, nature-inspired metallic glass structures such as three dimensional scaffolds with random packing of foams [8] and two-dimensional cellular structures with stochastic patterns [9] revealed the high resistance of porous structures against localized deformation and fracture with relatively minor sacrifice on the yield strength.

Despite the high reliability of experimental data, time and financial investments to optimize the technical performance of advanced materials steer material's community towards numerical simulations [5]. Within this work, the model of Bargmann et al. [10] is used to investigate the effect of damage tolerance on the deformation characteristics of $Zr_{35}Ti_{30}Cu_{7.5}Be_{27.5}$ metallic glass under uniaxial in-plane compression for a range of stochastic micropore designs of different porosities. Furthermore, performance evaluation of these structures is comparatively conducted with the structures containing periodic pores.

2. Mathematical modeling and implementation

The rate-dependent, gradient-extended model is formulated thermodynamically consistently in the framework of continuum mechanics, and is based on the Helmholtz free energy and dissipation potential provided in [10,11]. Our model accounts for free volume generation and plastic slip and, thereby, maps size effects, shear localization and tension–compression asymmetry (for a model with similar characteristics see also [12]). The highly nonlinear and strongly coupled governing equations are solved by a dual mixed finite element algorithm [13]. Displacement controlled

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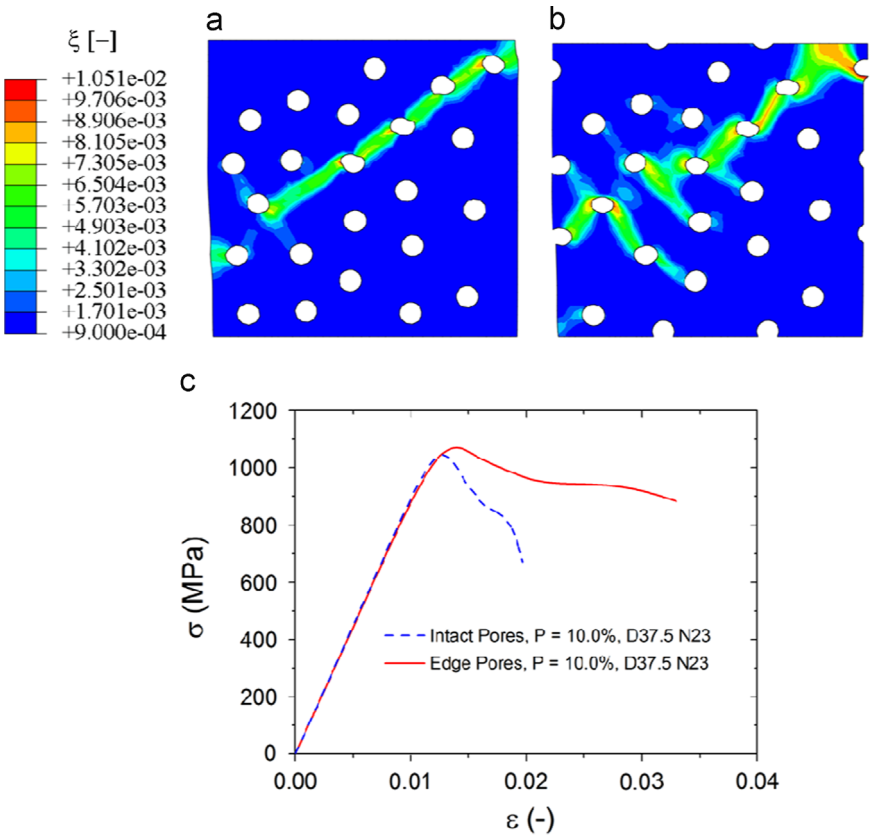

Fig. 1. Influence of edge pores on the mechanical response. Class I sample with porosity $P=10\%$, diameter of pores $D=37.5$ μm, and number of pores $N=23$. (a) Sample with intact edges. This type of design is affected by shear localization. Shear branching is prevailed by the free volume localization effect particularly caused by the free volume accumulation on the edges. (b) Similar sample of the same porosity and minimum spacing, but with edge pores, showing shear branching throughout the deformation. (c) Samples with edge pores display enhanced overall deformation behavior. Our studies have shown that this behavior also holds for other pore designs with different porosities.

uniaxial compression is applied at the nodal points of the top face at a macroscopic strain rate of 0.005 s^{-1}. The nodal points at the bottom face of the squares are fixed in *x*- and *y*- directions. In addition, micro-free boundary conditions are assumed, i.e., the free volume gradient vanishes in normal direction at all boundaries. The numerical analyses are performed on 2D square specimens (500 μm × 500 μm). Material parameters used for the implementation of the model are adopted from [5]. Samples are discretized into between 2000 and 3000 plane-strain elements depending on the pore design. Mesh-independent deformation behavior is observed due to gradient dependence of the model. Calculations are done in ABAQUS via the UELEMENT interface, and an ABAQUS python script was utilized for post-processing.

3. Micropore design

Previous studies emphasized the importance of using circular pores stacked in AB pattern within the metallic glass matrix, by which the elastic and plastic deformation can be remarkably enhanced [4,5]. Thus, reference samples of different porosities from periodic pattern are generated to compare with samples having stochastic design.

The source code for the generation of stochastic pore design is programmed in C++ and compiled using Visual Studio. For determining the pore positions, a standard pseudo-random number generator is used. A minimum distance between pores is included within the code to prevent overlap and is manually adjusted as a function of radius (or average radii) of the pores depending on the design criteria. The samples generated are periodic at the boundaries to analyze the effect of the exact number of pores and the corresponding porosity on the mechanical behavior. For the sake of simplicity in analysis, a maximum of two different pore sizes is used. For the sets of samples with a single pore size (stochastic class I), a maximum number of pores permitted by the minimum spacing criteria is selected to increase the influence of pores on stress localization. Further, samples with two different pore sizes (stochastic class II) are designed in a way that the total porosity becomes 10.0%, 20.0% or 30.0% (± 0.2% standard deviation), where contributions of pore size and number of pores are investigated in comparison with stochastic class I and periodic class structures with single pore size. Pore diameters of 37.5 μm and 50 μm are chosen for stochastic class II samples to analyze the contribution of a different pore size on the overall response. Each sample set comprises average values of the mechanical properties of three or more samples to increase the accuracy of the data.

An additional constraint of minimum spacing has to be established, if the side pores overlapping with the boundaries are to be eliminated. This arrangement limits the random distribution of pores, which in return alters the deformation behavior (see Fig. 1 and Video 1). Localized shear zones at an angle perpendicular to the loading are generated for a 10.0% porosity sample which decreases the entire performance of the structure (Fig. 1a). Thus, in the following, structures with edge pores are selected due to their higher mechanical properties caused by shear branching (Fig. 1b, and dark yellow squares in Figs. 3–5).

Supplementary data associated with this article can be found in the online version at 10.1016/j.jmps.2010.09.009.