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# Strengthening mechanisms in nanoporous metallic glasses

Xiaoling Zhou[a,*], Longqi Wang[b], C.Q. Chen[c,*]

[a] Shanghai Institute of Aerospace System Engineering, Shanghai 201109, China
[b] School of Civil & Environmental Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore
[c] Department of Engineering Mechanics, CNMM & AML, Tsinghua University, Beijing 100084, China

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ABSTRACT

It has been shown that metallic glasses (MGs) can have enhanced ductility by properly introduced pores. However, the pore effects on the yield strength and the underlying mechanisms have yet to be fully clarified. In this paper, nanoporous MGs with regularly distributed elliptical pores are investigated by large scale molecular dynamics simulations. Obtained results show that, when increasing the semi-axis $a$ in the loading direction and fixing the other semi-axis $b$ of the pores, the strength of the nanoporous MGs increase firstly to reach a maximum value and then decreases. It is found that the porosity and pore shape are the main factors affecting the strength. For a given porosity, the yield strength increases first and then approaches an asymptotic value with increasing $a$. The underlying mechanism is that the shear bands transit from localization to spreading. For a given pore shape, the yield stress decrease with increasing $a$. And this is because the increase of porosity leads to reduction in strength. Due to the above mechanisms, there exists a maximum strength at a critical size where the shear band evolution transition occurs. A model for the critical size of $a_{cri}$ is proposed to predict the maximum strength.

## 1. Introduction

Metallic glass (MG) is a promising engineering material due to its excellent mechanical properties, such as high strength, high hardness and good abrasion resistance [1–3]. However, the contradiction in strength and tensile ductility limits the application of MGs [4]. Numerous methods, e.g., crystalline or fiber reinforced amorphous composites [5–7], MG nanowires [8,9] and heterogeneous MGs [10,11] have been proposed to improve the plasticity of MGs. Recently, it has been reported that good plasticity can be obtained by introducing pores into MGs [12–14]. Because porous MGs have an additional advantage of lightweight, they attracts a lot of interest in both scientific and engineering fields.

In 2003, Schroers et al. [15] first obtained $Pd_{43}Ni_{10}Cu_{27}P_{20}$ MG foam with the pore size of 0.2–1 μm. Wada et al. [16] synthesized porous MGs with different porosity and pore geometries. They found that the compressive strains are highly affected by the pore geometry which can change the stress concentration around pores. Xie et al. [17] utilized the spark plasma sintering process to fabricate MG foams and reported that the MG foams have better plasticity than the corresponding bulk MG. Pauly [18] and Lee et al. [19] reported micro-lattice MGs fabricated by the 3D printing method. Lee et al. [19] found that, by reducing the ligament size, porous MGs show a brittle to ductile transition in compression deformation. In the above studies, much attention was paid to the synthesis and compressive behaviors of MG porous foams. For bulk MGs, it is important to improve their tensile ductility without sacrifice in strength.

Sarac and Schroers [13] used Si mould and thermoplastic forming to fabricate 2D porous MGs with a honeycomb-like structure and good tensile ductility was achieved. They found that the size, arrangement and ligament of pores have important effects on the plasticity and toughness. In their experiments, it is shown that the mechanical properties of the porous MGs are governed by the shear bands evolutions and crack growth behaviors. The thermoplastic forming method provides a good way to obtain porous MGs with different types of pores. Gao et al. [14] reported that 2D porous MG with circular pores have apparent tensile ductility. They claimed that the pores change the stress field and hinder brittle fracture. From the above experiments, it can be concluded that proper introduction of pores into MGs is an effective way to improve their tensile ductility. Note that recent advances in manufacturing technology make it possible to control the geometry of the pores in 2D honeycomb-like MGs. Liu et al. [20] combined the thermoplastic forming based patterning and a parallel joining technique to fabricate 3D honeycomb-like MGs and they showed that the porosity have a great influence on the energy absorbing ability. Chen et al. [21] investigated the energy absorbing behaviors of porous MGs with

* Corresponding authors.
*E-mail addresses:* zhouxiaoling87@163.com (X. Zhou), chencq@tsinghua.edu.cn (C.Q. Chen).

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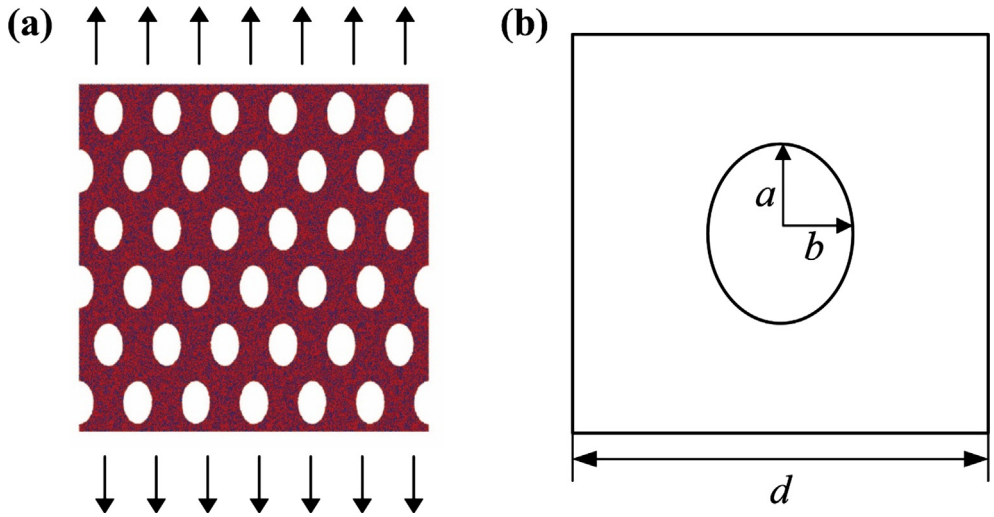


**Fig. 1.** Schematic illustration of a porous MG model. (a) The atomic configuration of porous $Mg_{80}Al_{20}$ model subject to uniaxial tensile loading, and (b) its unit cell.

quadrangle pores. It is found that struts bending and crack blunting in the materials contribute to the good energy absorbing ability. Chen et al. [22] studied the compressive properties of porous MGs with hexagonal pores and found that the defect structures have significant effects on the plasticity and failure mode. Zhao et al. [23] found that the compressive plasticity of MGs can be improved by two symmetrical semi-circular notches because of the large-scale stress gradient around the notches. It is now clear that the pores have great effects on the mechanical properties of the porous MGs. However, the relationship between the pores and the mechanical properties of the porous MGs has yet to be elucidated.

For MGs, the deformation mechanisms are different from the crystalline metals due to the lack of microstructures like lattice structures, grain boundaries, twin boundaries and so on. Shear transformation zone (STZ) [24] and shear band [4,25] are important to investigate the mechanical properties of MGs. To reveal the influences of microstructures on the mechanical properties of MGs, large scale molecular dynamics (MD) simulation is an effective method because the STZ and shear band can be captured easily [26,27]. For example, large scale MD simulations are used to reveal the relationships between mechanical properties and the microstructures in MG composites [28,29], heterogeneous MGs [30,31] and MG nanowires [32,33]. Sha et al. [34] conducted MD simulations to study the strengthening mechanisms caused by notches in MGs. Lei et al. [35] used MD simulations to explain the observed notch strengthening in MGs. Wang et al. [36] studied the effects of nano-pores on the strength and plasticity of MGs under compression and nanoindentation. In their MD simulations, it is found that pores cause strain concentration and promote multiple shear bands. Sopu et al. [37] studied the structure-property relationships in nanoporous MGs by both MD simulations and the finite element method (FEM). The effects of pore density, distribution, size and number on the mechanical properties of porous MGs are discussed. Zhang et al. [38] revealed the compressive deformation behaviors and failure mechanisms of nanoscale cellular MGs with hexagonal pores. Sarac et al. [39] performed FEM simulations to show the effects of pore distribution and volume fraction on the mechanical properties of porous MGs. However, they did not give the dependence of strength on the pores. In micro and nano scales, the strength of MGs could be affected by the size of ligaments [8,9,32,40] and hence the pores may have a great influence on the strength. Large scale MD simulations are needed to elucidate the strengthening mechanism of porous MGs.

In this paper, the tensile behaviors of the honeycomb-like MGs with elliptical pores are studied by MD simulations. The shear band evolutions and their influences on the yield strengths are discussed. The paper is organized as follows. The simulation method and the honeycomb-like MG models are given in Section 2. In Section 3, the yield strength and the plastic deformation behaviors of the porous MGs are investigated. Section 4 shows the results of the influences of the porosity and the pore shape on the yield strength. The shear band evolution governed strengthening in nanoporous MGs are also discussed. A theoretical model of the critical pore size at which the strength is maximum is proposed. The paper is concluded in Section 5.

## 2. Atomistic simulations

### 2.1. Method and models

Large scale MD simulations are conducted to study the tensile deformation of the nanoporous $Mg_{80}Al_{20}$ MGs using LAMMPS [41]. The interatomic interaction between the atoms is described by the embedded atom method (EAM) potential [42]. The melting and cooling method is used to obtain the amorphous structure of the $Mg_{80}Al_{20}$ [26,29]. First, a crystalline $Mg_{80}Al_{20}$ is melt at 2500 K for 100 ps and then cooled down to 1 K in 400 ps. The effective cooling rate is about 6 K/ps. Secondly, the $Mg_{80}Al_{20}$ MG is relaxed at 1 K for an additional 100 ps. Finally, the atoms within the regions of pores are removed from the obtained bulk MG to form nanoporous MGs models.

Fig. 1 shows a developed atomistic MG model with elliptical pores distributed in a triangular honeycomb manner. The semi-axises of the elliptical pores are $a$ and $b$, respectively. The size of the unit cell shown in Fig. 1(b) is $d$. In all the simulations, the out-of-plane thickness of the models is 5 nm. The porous MG models comprises $6 \times 6$ unit cells in the in-plane directions to form a honeycomb-like structure as shown in Fig. 1(a). Periodic boundary conditions are imposed in all three directions. Before stretching, the porous MG model is relaxed at 300 K for 100 ps to reach the equilibrium state. To eliminate the temperature effect, the porous MGs are then cooled down to 1 K and then the model is stretched in the vertical direction at a strain rate of $5 \times 10^8\,s^{-1}$. During the tensile loading, the pressure in other directions keep at 0 bar using NPT ensemble. In all the following simulations, the size of the unit cell is $d = 4b$ unless stated otherwise. Two types of nanoporous MG models with the corresponding semi-axis $b = 5$ nm and $b = 2.5$ nm are investigated. The aspect ratio $a/b$ will be varied from 0.5 to 2. By doing so, the effects of both porosity ($f = \pi ab/d^2$) and void shape can be explored.

### 2.2. Stress calculation

In this paper, the stress of the porous MG models is calculated as the average value of the atomic stress. In MD simulations, the atomic stress