



Strain-induced deformation of the porous structure in binary glasses under tensile loading

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ABSTRACT

The evolution of porous structure and mechanical properties of binary glasses under tensile loading were examined using molecular dynamics simulations. We consider vitreous systems obtained in the process of phase separation taking place after a rapid isochoric quench of a glass-forming liquid to temperatures below the glass transition point. The porous structure in undeformed samples varies from a connected porous network to a random distribution of isolated pores with increasing average density. We find that the elastic modulus follows a power-law dependence on the average glass density and the pore size distribution at small strain remains nearly the same as in quiescent samples. Upon further loading, the pores become significantly deformed and coalesce into larger voids that leads to formation of system-spanning empty regions associated with failure of the material.

1. Introduction

Recent progress in the development of porous structural materials with applications ranging from biomedicine to energy conversion and storage as well as civil infrastructure, requires a thorough understanding of their microstructure-property relationships [1,5,3,4,2]. An accurate pore characterization in microporous materials, which involves numerical analysis of the probe-accessible and -occupiable pore volume, allows determination of their permeability to guest molecules as well as internal void volume and surface area [6]. The results of experimental and computational studies have shown that mechanical properties of bulk metallic glasses with periodic arrays of pores are governed by shear localization between adjacent pores in a regime of plastic deformation [7–9]. Similar to ductile metallic alloys, it was found that in highly strained nanoporous silica glasses, multiple cracks are initiated at void surfaces, which leads to void coalescence and intervoid ligament failure [10]. It was further shown that mechanical properties of porous silica glasses are improved in samples with channel pore morphology rather than isolated pore configurations [11]. Despite extensive efforts, the precise connection between individual pore morphologies and elastic, shear and bulk moduli has not yet been determined.

During the last decade, the mechanical properties of metallic glass nanowires subjected to uniaxial tension have been extensively

investigated using molecular dynamics simulations [12–16] and experimental measurements [17–20]. It was found that, when the size of metallic glass samples is reduced down to the nanoscale, the deformation mode changes from brittle to ductile [15–20]. The difference in the deformation behavior can be visually detected by direct observation of either shear localization along a plane, called a shear band, or the formation of extended necking along the loading direction [12,18]. A subsequent analysis of irradiated samples that were emulated in MD simulations by randomly removing a small fraction of atoms, has shown an enhanced tensile ductility; while this effect is reduced if only the outer shell of a nanowire is rejuvenated [15]. In Ref. [14], it was shown that brittle-to-ductile transition dependence on size in nanoscale metallic glasses is defined by a fundamental characteristic size effect in the failure mode under tensile loading. It was argued that nanosized specimens with surface roughness exhibit a clear transition from shear banding to necking instability, when roughness exceeds some threshold value of the surface roughness to the sample diameter ratio [14]. Furthermore, it was also demonstrated that a homogeneous bulk metallic glass under uniaxial tension exhibits only one dominant shear band, whereas multiple shear bands are initiated at interfaces between grains in a nanoglass [21]. Moreover, it was found that the shear-band orientation with respect to the loading direction is different in the cases of uniaxial compression and extension of two-dimensional athermal amorphous solids [22]. However, the combination of several

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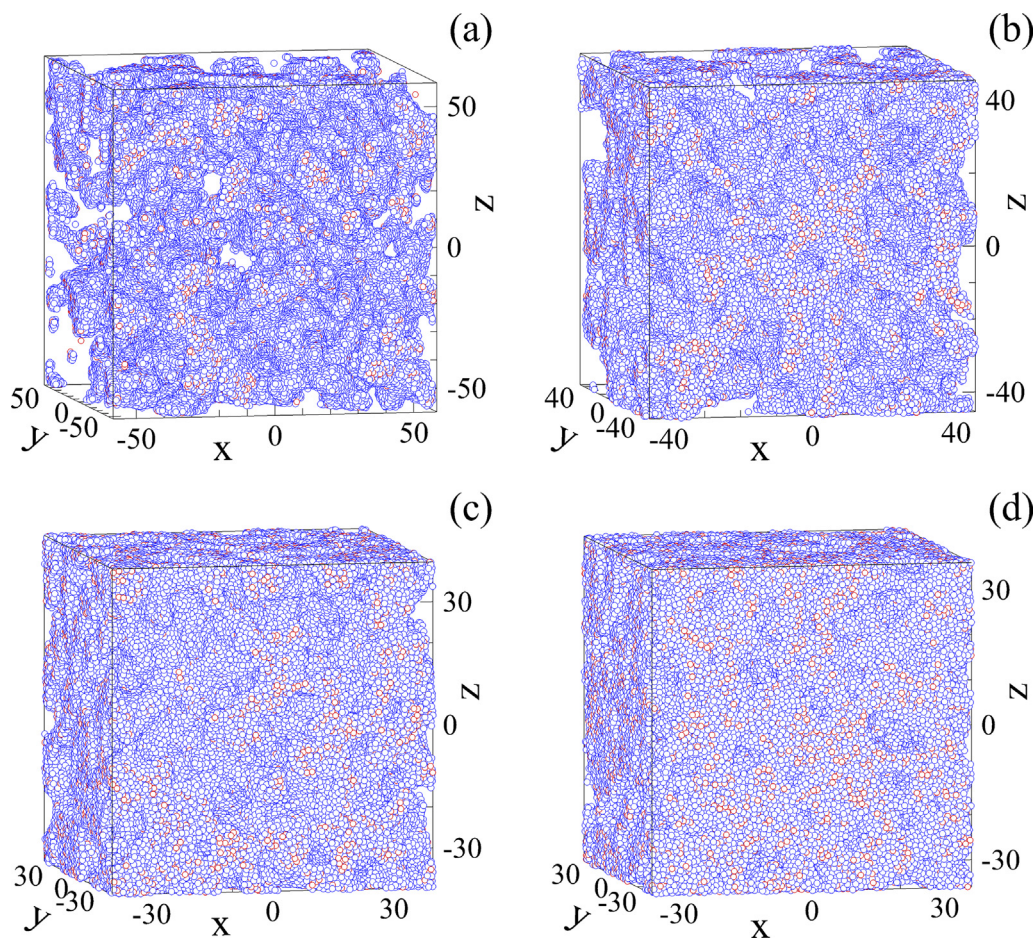


Fig. 1. Atom positions in the porous binary glass after isochoric quench to the temperature $T = 0.05\epsilon/k_B$ for the average glass densities (a) $\rho\sigma^3 = 0.2$, (b) $\rho\sigma^3 = 0.4$, (c) $\rho\sigma^3 = 0.6$, and (d) $\rho\sigma^3 = 0.8$. The blue and red circles indicate atom types A and B. The total number of atoms is $N = 300,000$. Note that atoms are not drawn to scale and the system sizes are different in all panels. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

factors including the processing routes, system size and aspect ratio as well as surface defects and local microstructure makes it difficult to predict accurately the failure mode in strained glasses.

A few years ago, the liquid-gas phase separation kinetics of a glass-forming system quenched rapidly from a liquid state to a temperature below the glass transition was studied via molecular dynamics simulations [23,24]. As a result of the coarsening process at constant volume, a porous amorphous solid is formed, whose porous structure contains isolated voids at higher average glass densities and complex interconnected void-space topologies at lower glass densities [23,24]. More recently, the distributions of pore sizes and local glass densities were further investigated as a function of temperature and average glass density [25]. In particular, it was found that in systems with high porosity, the pore size distribution functions obey a scaling relation up to intermediate length scales, while in highly dense systems, the distribution is nearly Gaussian [25]. Furthermore, under steady shear deformation, the pores become significantly deformed and, at large strain, they were shown to aggregate into large voids that are comparable with the system size [26,27]. It was also demonstrated that the shear modulus follows a power-law dependence as a function of the average glass density [27]. Nevertheless, the mechanical response of porous glasses to different types of loading conditions and the evolution of porous structure during deformation remain not fully understood yet.

In this paper, molecular dynamics simulations are carried out to investigate the pore size distribution and mechanical properties of a model glass under tensile deformation. The porous glass is prepared via a deep quench of a binary mixture in a liquid state to a very low

temperature at constant volume. It will be shown that under tension, the distribution of pore sizes becomes highly skewed towards larger values, and upon further increasing strain, one large dominant pore is formed in the region where failure occurs. The analysis of local density profiles and visualization of atomic configurations reveals that the location of the failure zone is correlated with the extent of a lower glass density region.

The rest of the paper is structured as follows. In the next section, we describe the details of molecular dynamics simulations including model parameters as well as the equilibration and deformation protocols. The results for the stress–strain response, evolution of density profiles and pore size distributions are presented in Section 3. A brief summary and outlook are given in the last section.

2. Details of molecular dynamics simulations

The mechanical properties of porous glasses were investigated using the standard Kob-Andersen (KA) binary (80:20) mixture model [28]. In this model, the interaction between any two atoms are described via the Lennard-Jones (LJ) potential:

$$V_{\alpha\beta}(r) = 4\epsilon_{\alpha\beta} \left[\left(\frac{\sigma_{\alpha\beta}}{r} \right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r} \right)^6 \right], \quad (1)$$

where the parameters are set to $\epsilon_{AA} = 1.0$, $\epsilon_{AB} = 1.5$, $\epsilon_{BB} = 0.5$, $\sigma_{AB} = 0.8$, $\sigma_{BB} = 0.88$, and $m_A = m_B$ [28]. For computational efficiency, the LJ forces were only computed at distances smaller than the cutoff radius $r_{c,\alpha\beta} = 2.5\sigma_{\alpha\beta}$. In what follows, the LJ units of length, mass, energy, and

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