Scripta Materialia 141 (2017) 115–119

Contents lists available at ScienceDirect

Scripta Materialia

journal homepage: www.elsevier.com/locate/scriptamat

Regular article

Reinforcement of nanoglasses by interface strengthening

Constanze Kalcher*, Omar Adjaoud, Jochen Rohrer, Alexander Stukowski, Karsten Albe

Institute of Materials Science, Technische Universität Darmstadt, Jovanka-Bontschits-Str. 2 Darmstadt D-64287, Germany

ARTICLE INFO

Article history:
Received 19 June 2017
Received in revised form 26 July 2017
Accepted 2 August 2017
Available online xxxx

Keywords:
Metallic glass
Grain interfaces
Tension test
Molecular dynamics
Nanoglass

ABSTRACT

Nanoglasses consist of glassy grains connected by an amorphous interface. While internal interfaces in nanoglasses help to prevent brittle failure, they are usually not beneficial to the glasses overall strength. In this molecular dynamics study, we manipulate the glass–glass interfaces of a Cu–Zr nanoglass, such that they are replaced by stronger crystalline interphases. Analogous to grain boundary strengthening in crystalline materials, we show that it is possible to reinforce the nanoglass without compromising its ductility.

Metallic glasses (MGs) have been continually advertised for their high yield strength and resilience. However, due to their brittle failure mechanism at room temperature structural applications of MGs are rather limited [1,2]. A general strategy for improving the mechanical properties of MGs has been to introduce crystalline secondary phases in the glass that can lead to enhanced plasticity by reducing shear localization [3–7]. These crystalline phases can occur in various topologies ranging from micrometer-sized dendrites [3,4] to spherical nanoprecipitates [7–9] with significant tensile ductility at room temperature. The volume fraction and geometry of the precipitates define, whether the precipitates participate in the deformation [10]. Recently, it has been shown that the strength of MGs can also be increased by realizing an amorphous/crystalline dual-phase nanostructure with nanocrystals embedded in an amorphous matrix [11]. As an alternative approach nanoglass (NG) microstructures have been successfully synthesized [12–15]. They can be seen in analogy to nanocrystalline metals. NGs are typically produced by cold compaction of glassy particles obtained through inert gas condensation [12,16] or by magnetron sputtering [17]. As compared to their homogeneous MG counterparts, plastic deformation is more delocalized in NGs [16]. The degree of delocalization is also dependent on the grain size: In molecular dynamics (MD) simulations it has been shown that the larger the grain size the more inhomogeneous is the plastic deformation [18,19].

In both scenarios, the presence of interfaces, i.e. either glass–crystal or internal glass–glass interfaces, affects the mechanical behavior: Crystal–glass interfaces are typically weak spots in the material [7]. Thin crystalline interlayers in a MG were found to be metastable or even unstable [20,21], but Ritter et al. have shown that glass-glass interfaces in a Cu–Zr NG persist up to the glass transition temperature T_g [22]. These internal glass–glass interfaces inherent to NGs have been characterized as a soft secondary glass-phase promoting the nucleation of STZs [22,23]. In an earlier study, surface segregation effects in the precursor particles used for cold compaction were found to strongly influence glass–glass interfaces present in the resulting NG [16,24]. In addition to a disturbed short range order, glass–glass interfaces in such a “segregated NG” exhibit a different composition and density than the bulk glass [24]. More recently, phase formation at interfaces has been characterized in terms of complexions [25–29]. This concept may well be applied to NGs, where according to the definition of Dillon and Harmer [25], the interface interphase could be treated as a complexion type V: a wetting film, which itself is separated from the abutting phases through complexions.

All the above efforts to enhance the mechanical properties of MGs can be summarized as a tradeoff between increasing ductility and decreasing strength. In this work, we focus on the effect of internal interfaces in NGs. Hypothetically, if it were possible to freely manipulate the interface phase in the NG architecture without affecting the glassy grains, a sensible choice would be to turn that phase into a reinforcement. This can be seen in analogy to grain boundary strengthening in crystalline materials. By means of MD simulations, we study the mechanical properties of a generic model

* Corresponding author.
E-mail address: kalcher@mm.tu-darmstadt.de (C. Kalcher).

http://dx.doi.org/10.1016/j.scriptamat.2017.08.004
1359-6462/

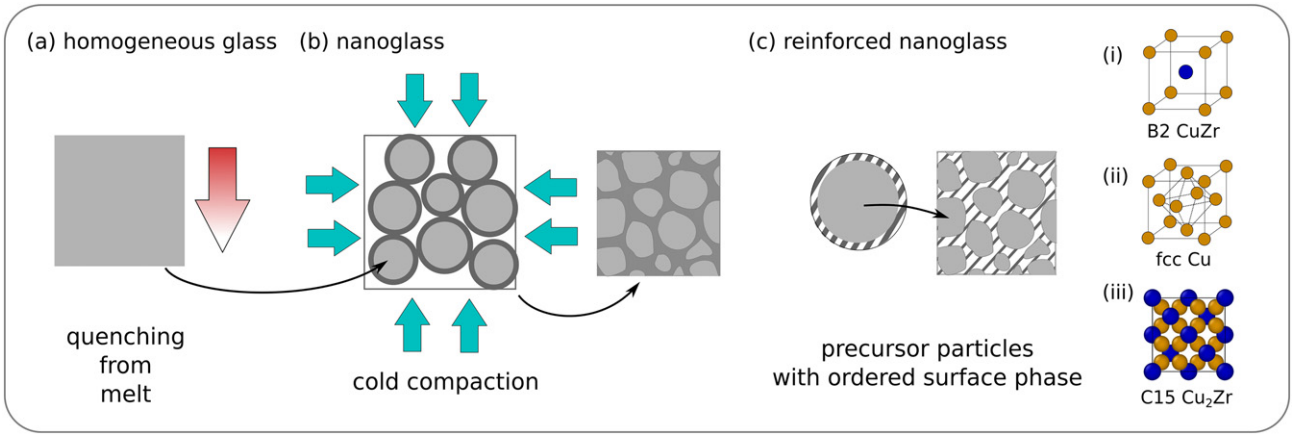

Fig. 1. Overview of the different sample setups. (a) The homogeneous glass is quenched from the melt. (b) Then a conventional NG is produced by cold compaction of surface segregated glassy spheres cut from the bulk sample and subsequently annealed above T_g. (c) To reinforce the conventional NG, the glassy interface interphase is replaced by a crystalline phase. This can be single crystalline (i) B2 CuZr, (ii) fcc Cu or (iii) the C15 Laves phase.

of a Cu–Zr cold-compacted NG and several reinforced NGs. To that end we manipulate the pristine NG by replacing the glass–glass interface with three different crystalline interphases with higher yield strength. The crystalline phases used as grain boundary reinforcement are expected to fail in a brittle manner in their bulk form. However, we will show that on the contrary, the forming interface interphases do not necessarily impair the overall ductility while still being beneficial to the strength of the NG-composite.

The simulation of the NG and reinforced NG composites is realized by using the MD code LAMMPS [30] with an EAM-potential developed by Mendelev et al. [31]. The time step for the integration of the equation of motion is 2 fs in all simulations. For temperature and pressure controls, a Nosé–Hoover thermostat and Parinello–Rahman barostat are used. In all samples, periodic boundary conditions apply in all three dimensions. Tensile tests are simulated with a constant engineering strain rate of $4 \cdot 10^7 s^{-1}$ in z-direction and pressure is controlled in x- and$y$-directions to enable lateral contraction. The strain analysis of the simulation data is performed with the visualization and analysis software OVITO [32]. We evaluate the atomic shear strain [33,34] as a measure for the localized deformation. The cutoff for neighboring atoms that are included in the computation of the strain tensor of a particle is 0.4 nm.

We study three different model types: (a) a homogeneous glass, (b) a conventional nanoglass and (c) nanoglasses reinforced with three different crystalline phases. The different processing routes of the models are shown schematically in Fig. 1: In a first step, a homogeneous Cu–Zr MG is quenched from the melt at ambient pressure with a quenching rate of 0.01 K/ps. The MG has the composition $Cu_{61}Zr_{39}$ and serves as a reference for all other models. For the conventional NG, glassy spheres are cut from a $Cu_{64}Zr_{36}$ homogeneous glass and subsequently annealed above T_g as described in Ref. [24]. In this previous study, it has been shown that during annealing, the glassy spheres get enriched with Cu at the surface layer and depleted of Cu–atoms in the core. The NG model is then produced by simulating cold compaction of these glassy spheres at a compaction pressure of 5 GPa. The surface segregation process causes the surface layer and the core composition to deviate from the nominal composition of $Cu_{64}Zr_{36}$. The glassy spheres then form a $Cu_{72}Zr_{28}$ shell

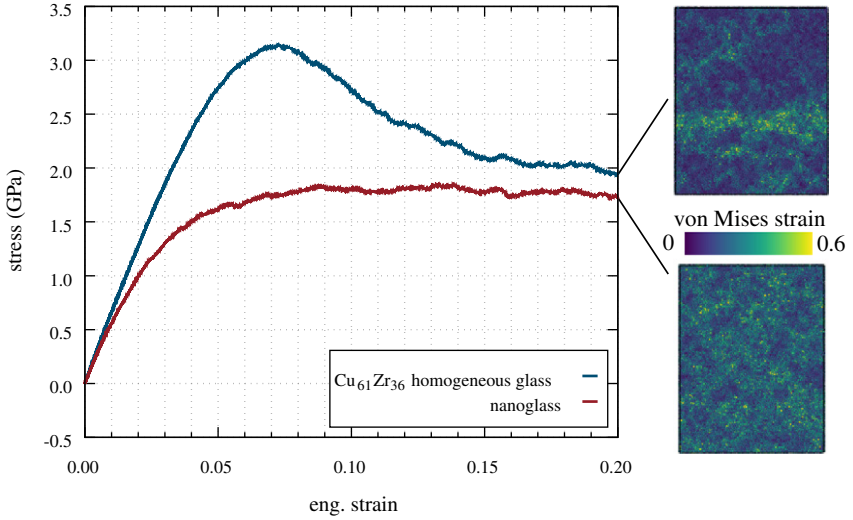

Fig. 2. Tensile tests at 50 K and constant engineering strain rate of a homogeneous MG of composition $Cu_{61}Zr_{39}$ and a segregated NG, where the glassy grains have the same composition as the homogeneous glass. The snapshots of the MG and NG show the local atomic von Mises strain. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)