Journal of Alloys and Compounds xxx (2016) 1–6

Contents lists available at ScienceDirect

Journal of Alloys and Compounds

journal homepage: http://www.elsevier.com/locate/jalcom

Plastic deformation induced anisotropy in metallic glasses: A molecular dynamics study

J. Enrique Velasco [a], Amadeu Concustell [b], Eloi Pineda [a], Daniel Crespo [a, *]

[a] Dept. Física, Universitat Politècnica Catalunya - BarcelonaTech, 08860 Castelldefels, Catalonia, Spain
[b] Department of Materials Science and Metallurgical Engineering, University of Barcelona, Spain

ARTICLE INFO

Article history:
Received 31 July 2016
Received in revised form
16 December 2016
Accepted 18 December 2016
Available online xxx

Keywords:
Amorphous alloys
Aging and rejuvenation
Anisotropy
Mechanical deformation

ABSTRACT

The atomic structure of a $Cu_{13}Ni_{34}Pd_{53}$ metallic glass was studied by molecular dynamics simulation at different temperatures along a shear deformation cycle. A simulation box of 1 million atoms was deformed in the x axis and then the original orthogonal shape was recovered. Directional pair distribution functions were computed in the coordinate planes and some significant directions along the shear deformation cycle. No anisotropy was found in the initial state, while post-deformation anisotropy was revealed by significant differences of the partial pair distribution functions. The analysis of atomic environments concluded that the remnant anisotropy remains constrained into the shear plane. Low temperature samples showed remnant anisotropy after the full shear sample, while close to the glass transition the anisotropy induced by the initial shear process is removed by the subsequent recovery process.

1. Introduction

Unlike crystalline alloys, metallic glasses are amorphous metallic materials with short and medium range order but lacking the crystalline structure, this generates different mechanical properties than those observed in crystalline alloys with same composition. Metallic glasses exhibit some unique mechanical properties suitable for a variety of engineering applications [1].

Metallic glasses are produced by rapid quenching from the melt, the critical cooling rate to avoid crystallization is on the order of 10^6 K s^{-1} for conventional binary metallic glasses (MGs) and 10^2 K s^{-1} for bulk metallic glasses (BMGs) [2]. Indeed, glasses quenched at different rates are in different isoconfigurational states, characterized by its fictive temperature T_f, and their mechanical behavior is largely dependent on T_f [3,4]. MGs, ideally isotropic, can be anisotropic due to the solidification process [5], elastic and anelastic deformation [6,7], creep [8] and plastic inhomogeneous deformation [9]. While the atomistic origin of anelastic induced anisotropy has been attributed to bond-orientation anisotropy [8,10], the origin of flow induced anisotropy has not been unveiled yet. In fact, preliminary diffraction analyses suggest that flow induced anisotropy, if existent, should be very low. But, in a recent work [11], the anisotropy of metallic glasses induced during the Non-Newtonian homogenous deformation regime was explored in La, Pd and Ce based metallic glasses. In this deformation regime, at temperatures close to the glass transition T_g, the remanence of anisotropy after tensile or compressive deformations was observed for Weissenberg numbers (Wi) higher than 1–10.

In this work we show the results of numerical simulations on a $Cu_{13}Ni_{34}Pd_{53}$ metallic glass under shear homogeneous deformation at a very high Wi number. This composition was chosen to approach a Pd-based metallic glass, given that some of the few available experimental results have been obtained in one of these alloys [12]. It is well known that the accuracy of an atomistic simulation depends on the potential function. Many studies of MGs have adopted pairwise potentials such as the Lennard-Jones potential [13]. However, it has been reported that pairwise potentials are unable to accurately describe the properties of metals such as the Cauchy discrepancy of elastic constants, vacancy formation energies, stacking fault energies, surface structure, and relaxation behavior [14,15]. Unfortunately, no potential is available for Pd-(Ni-Cu)-P alloys, in particular for Phosphorus, but Pd, Ni and Cu are common elements of many metallic glasses. The simulated composition shows glass formation without structural signatures of crystalline order after the applied quenching rates and we expect it will capture the essential features of the shearing process in this family of

* Corresponding author.
E-mail addresses: velasco85@gmail.com (J.E. Velasco), aconcustell@cptub.eu (A. Concustell), eloi.pineda@upc.edu (E. Pineda), daniel.crespo@upc.edu (D. Crespo).

http://dx.doi.org/10.1016/j.jallcom.2016.12.233
0925-8388/

metallic glasses. Due to the high value of *Wi* number, the shearing numerical experiment is expected to induce a high degree of anisotropy in the metallic glass sample, this allowing us to characterize the distinctive structural features of this anisotropy.

2. Materials and methods

In this study, we adopted the EAM potential to describe interatomic interactions in the simulation model. The potential consists of a simple additive potential function and an embedded function given by:

$$U = \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}\phi_{ij}(r_{ij}) + \sum_{i=1}^{N}F_i(\rho_i) \quad (1)$$

where $\phi_{ij}(r_{ij})$ is the short-range pair potential and r_{ij} is the distance between atoms i and j, ρ_i is the total density and $F_i(\rho_i)$ is the embedded atom function depending on the local electronic density. The MD (Molecular dynamics) simulations were carried out using the LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) simulation package [16]. The potentials used are given in Ref. [17]. The sample $Cu_{13}Ni_{34}Pd_{53}$ with a total number of 1 million atoms was prepared in multiple steps, always using the NPT ensemble. A simple cubic lattice was generated by putting the atomic species in random lattice sites. This structure was subsequently melted by heating it up to 2000 K and the liquid was equilibrated for 2 ns. The liquid character of the alloy was checked by visual inspection and by computation of the pair distribution function. Subsequently, the sample was quenched to 800 K, 780 K, 740 K, 720 K, 700 K, 680 K, 650 K, 300 K and 0 K at a cooling rate of 10^{13} K s^{-1}. Then, the samples were equilibrated at these temperatures for 2 ns. The time step was 1 fs and the glass transition at this cooling rate, detected as the change of slope in the volume vs temperature evolution, was found at 715 K.

The equilibrated samples were subjected to a shear deformation cycle on axis x. The box was deformed by keeping the lower side fixed and displacing the upper side in the x direction, keeping both sides parallel − shearing process −. After the maximum desired deformation was obtained, the upper side was displaced back to its original position − recovering process −. The deformation cycles were performed with maximum deformations of 10%, 25% and 50% respective to the box length, all starting from the same initial configuration. Both shearing and recovering processes were performed at a deformation rate $\dot{\gamma} = 10^{10}$ s^{-1}.

Shear strain in the samples was computed with ovito [18] following [19,20]. Changes in the atomic distributions were revealed by computing the directional pair distribution function (dPDF) computed in plane sections, defined as

$$g(r) = \frac{1}{N_a}\sum_{i}^{N_a}\frac{1}{N_b}\frac{1}{2\pi r\Delta}\sum_{j}^{N_b}\left(\left\langle\delta\left(\left|\vec{r}_{ij}\right| - r\right)\right\rangle\right) \quad (2)$$

Here, N_a is the number of atoms in the sample, N_b is the number of atoms in a plane section of thickness Δ, and $\vec{r}_{ij}$ is the interatomic distance. By choosing the plane sections with different spatial orientations we can distinguish the different spatial arrangements in different directions, the directional PDF computed in a plane normal to a certain s direction will be noted as s-dPDF. The thickness of the plane sections is taken as Δ = 1.1 Å.

In order to determine if the observed anisotropy is spatially localized, the geometric atomic inertia tensor up to second neighbors was computed, defined as

$$I_{kl}(\vec{r}_i) = \sum_{j}\frac{1}{1+\exp\left(\frac{\left|\vec{r}_{ij}\right|-2\rho_2}{e}\right)}\left(\delta_{kl}\left|\vec{r}_{ij}\right|^2 - r_{ijk}r_{ijl}\right) \quad (3)$$

where k and l are the tensor components and $\vec{r}_{ij}$ is the interatomic distance whose components are r_{ijk}. The diagonal components I_{kk} give a measure of the atomic distribution in the plane orthogonal to the k-axis. The logistic function is inserted as a smooth step function centered in ρ_2, the second maximum of the PDF. Note that only the atomic positions are considered, this is why we refer it as the geometric inertia tensor, as the atomic masses are neglected.

3. Results and discussion

Fig. 1 shows an example of the shear strain distribution of the sample deformed at 300 K after shearing (left) and at the end of the recovery process (right). The atomic shear strain is referred to the initial configuration of neighboring positions until a cutoff distance of 4 Å [19]. Visual inspection shows a heterogeneous distribution of the shear strain but without signature of strain localization in shear bands. The inspection has been performed on multiple planes normal to different directions and for the multiple time steps through the deformation process, thus confirming that no shear bands appear during the shearing at these temperature and deformation rate conditions. This may be due to the high deformation rate, which may be preventing the formation of shear bands. In fact, shear bands were usually found by numerical

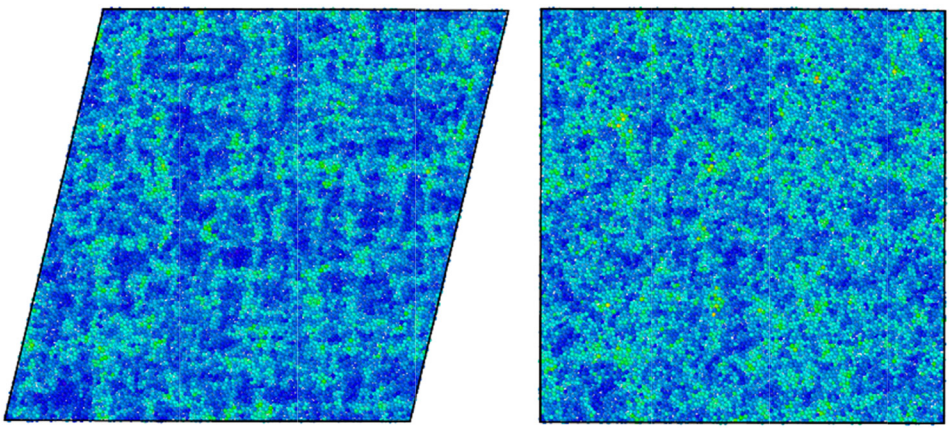

Fig. 1. Shear stress distribution of the sample deformed up to 25% at 300 K in a xy plane, referred to the initial configuration. Left: after shearing. Right: after recovery.

Please cite this article in press as: J.E. Velasco, et al., Plastic deformation induced anisotropy in metallic glasses: A molecular dynamics study, Journal of Alloys and Compounds (2016), http://dx.doi.org/10.1016/j.jallcom.2016.12.233