Strain rate and temperature effect on $Zr_{50}Cu_{50}$ metallic glass under pure shear

IOP Conf. Series: Journal of Physics: Conf. Series **1043** (2018) 012040 doi:10.1088/1742-6596/1043/1/012040

Strain rate and temperature effect on $Zr_{50}Cu_{50}$ metallic glass under pure shear

M. Sepulveda–Macias[1], G. Gutierrez[1] and F. Lund[2]

[1] Grupo de NanoMateriales, Departamento de Física, Facultad de Ciencias, Universidad de Chile, casilla 653, Santiago, Chile.
[2] Departamento de Física, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Santiago, Chile.

E-mail: msepmacias@gmail.com

Abstract. We present a molecular dynamics study of the mechanical properties of $Zr_{50}Cu_{50}$ glass under pure shear. The samples have 145.200 atoms with dimensions of $40 \times 20 \times 2$ nm in the x, y and z directions, respectively. After quenching, we obtain 3 different systems at temperatures of 10, 50, 300 K. All systems were then subjected to dynamic pure shear at constant shear rates of $2.5{\times}10^8$ s^{-1}, $5{\times}10^8$ s^{-1} and $2.5{\times}10^9$ s^{-1}. We investigate the changes of mechanical properties as a function of temperature and shear rate, and find that the shear modulus is not sensitive to the changes of the shear rate, but decreases as the temperature rises. Ultimate strength is enhanced at higher shear rates and decreases with temperature. A study of the atomic structure reveals that the low values of ultimate strength are associated with high values of local atomic shear strain. These results are reminiscent of what happens at the jamming transition.

1. Introduction

Metallic glasses (MGs) are noncrystalline solids obtained by continuous cooling from the liquid state. They are much stronger than most metals and alloys, and have high hardness and elastic limit [1–3]. These properties make MGs attractive for structural applications [4]. However, they have limited ductility and suffer catastrophic failure without noticeable plastic deformation at room temperature. It has been hypothesized that this behavior can be explained by means of localization of structural and dynamical heterogeneities called shear transformation zones (STZs) [5]. They lead to the generation of free volume and the nucleation of shear bands (SBs), leading the MG to a fragile fracture. Despite this explanation, the microscopic understanding of the transition from elastic to plastic behavior, and the formation and evolution of shear bands submitted to external forces is an open research area.

To explore this area, molecular dynamics simulations are an excellent tool widely used in recent years. This technique allows us to track the position of atoms and calculate their mechanical properties avoiding the experimental limitations. Salient are the works presented by Dasgupta *et al* . [6] and Albaret *et al* . [7] who have studied the role played by the non-affine atomic displacement field, particularly "plastic events", as described by Eshelby inclusions [8, 9] on Lennard-Jones glasses [6] and amorphous silicon [7]. The present work shows results of a preliminary study on the relation between microscopic structure and macroscopic plastic behavior for $Zr_{50}Cu_{50}$ metallic glass.

We study the evolution of the atomic structure of a $Cu_{50}Zr_{50}$ metallic glass system using molecular dynamics simulation at three temperatures according to the applied shear via a dynamical shearing test, where the local structure of atoms is analysed using the local atomic shear strain.

2. Methodology

In our molecular dynamics (MD) simulations, we adopt the embedded–atom method (EAM) potential proposed by Mendelev *et al* . for ZrCu systems [10] as implemented in LAMMPS code [11]. The EAM gives the total energy of an atomic system in the form

$$E_i = F_\alpha \left(\sum_{j \neq i} \rho_\beta(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij}) \, , \tag{1}$$

where F is the embedding energy which is a function of the atomic electron density ρ. In the second term, ϕ is a pair potential interaction and α and β are the element types of atoms i and j.

The $Zr_{50}Cu_{50}$ metallic glasses are prepared as follows: First, a crystalline Cu system is created and then 50% of Cu atoms are randomly chosen and replaced by zirconium, thus obtaining a system composed by 145.200 atoms with dimensions of $40 \times 20 \times 2$ nm in the x, y and z directions, respectively. Free boundary conditions are applied along the x and y direction and periodic boundary conditions along z. As an example we describe in detail the procedure to obtain the system at 10 K. In this case the temperature and pressure are set at 2200 K and 0 GPa respectively, allowing the system to relax for 200 ps using NPT ensemble to ensure a well–equilibrated sample. The integration timestep is set at 1 fs. Then, the system is cooled down to the final temperature during 1370 ps, using the Berendsen thermostat [12]. This new configuration is allowed to relax during 100 ps, at 10 K, to ensure a well–equilibrated metallic glass. After quenching, we obtain 3 different systems at temperatures of 10, 50, 300 K, each one with a cooling rate of 2.19, 3 and 1 K/ps, respectively. All systems were then subjected to dynamic pure shear in the axial direction at constant shear rates of $2.5{\times}10^9$ s^{-1}, 5×10^8 s^{-1} and 2.5×10^8 s^{-1} in the NVE ensemble. For that purpose we fix the boundaries of the material, and assign to them a fixed velocity in the axial direction to obtain the pure shear. All the MD simulations are carried out using the classical molecular dynamics code LAMMPS [11].

We have investigated the change of the mechanical properties as a function of temperature and shear rate. To this end, stress–strain curves have been measured, using the (xy) component of the stress and strain tensors. To quantify the microstructural changes of the sample we use the local atomic shear strain η^{Mises} [13]. This parameter requires two atomic configurations, the current and reference one, defined as

$$\eta_i^{\text{Mises}} = \sqrt{\eta_{yz}^2 + \eta_{xz}^2 + \eta_{xy}^2 + \frac{(\eta_{yy} - \eta_{zz})^2 + (\eta_{xx} - \eta_{zz})^2 + (\eta_{xx} - \eta_{yy})^2}{6}}, \tag{2}$$

where $\eta_{\alpha\beta}$ are the components of the strain tensor of atom i. We visualize η_i^{Mises} using the software OVITO [14].

3. Results and Discussion

The stress–strain curves for the three temperatures and strain rates under study are presented in Figure 1. As a function of strain γ, all curves present an elastic behavior up to a strain of 4%, reach a maximum between 4% and 6%, and slowly but steadily decrease beyond 6% up to the maximum strain used in the simulation, 25%. The shear modulus G and ultimate shear stress σ_{u} (obtained as the maximum stress value at the stress–strain curve) of each curve are

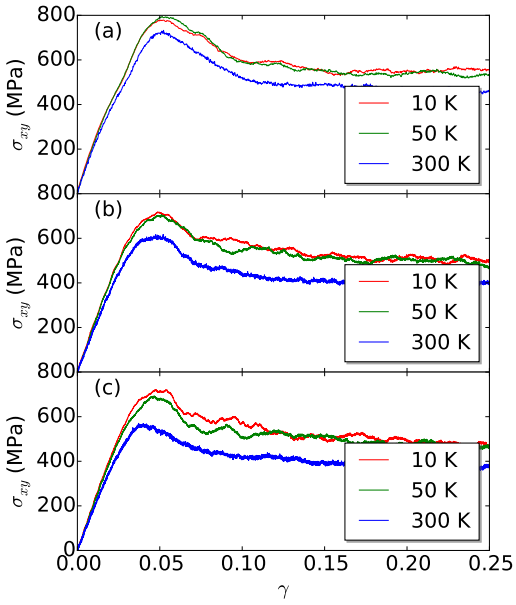

Figure 1. Calculated stress–strain curves for quasi–twodimensional $Zr_{50}Cu_{50}$ metallic glasses under the effect of pure shear at different shear rates. In (a) we present the case of $2.5 \times 10^9\,s^{-1}$, (b) $5 \times 10^8\,s^{-1}$ and (c) for $2.5 \times 10^8\,s^{-1}$.

summarized in Table 1. From Table 1 we observe that for a given temperature, T, there is no significant change in G as a function of the shear rate. For a given shear rate however, G is a decreasing function of T, as expected. Concerning σ_u, at fixed temperature it increases by 15–30% with increasing shear rate, with higher increases at higher T.

Table 1. Shear modulus G and ultimate shear stress σ_u, of the $Cu_{50}Zr_{50}$ metallic glasses under the effect of pure shear at three different temperatures and shear rates.

		$2.5 \times 10^9\,s^{-1}$	$5 \times 10^8\,s^{-1}$	$2.5 \times 10^8\,s^{-1}$
Property	Temperature (K)	(GPa)	(GPa)	(GPa)
G				
	10	24.51	24.80	24.01
	50	20.96	21.05	20.88
	300	17.19	17.33	19.24
σ_u				
	10	8.07	7.38	7.22
	50	7.95	7.04	6.93
	300	7.35	6.12	5.60

In order to shed light on the behavior of σ_u as a function of shear rate, we have computed the local atomic shear strain η_i^{Mises} at a strain of 6% namely, immediately after the ultimate shear stress σ_u is reached, for the three temperatures and three shear rates studied. The result is shown in Figure 2. The reason to choose a strain of 6% to sample the microstructure is that this point is well within the region of plastic behavior, and σ_u is still a useful tool for qualitative analysis. At higher strains, certainly beyond 8%, the different regions become blurred due to the formation of shear bands. To calculate the η^{Mises} showed in Figure 2 we use, as a reference configuration, the initial condition. The current configuration is the one at 6% of strain. The salient feature that is observed is that the lower the shear rate and, hence, the lower the ultimate

shear stress, the greater the local atomic shear strain. This relation between a macroscopic mechanical property with the microscopic structure of the metallic glass is reminiscent of what happens near the jamming transition [15] where, at a slow shear rate, the system has enough time to explore the phase space, and facilitate the movement of the particles, resulting in a larger plastic deformation. In contrast, for the case of a rapid shear rate, the atoms have no time to explore their vicinity, get stuck, and a higher stress is needed to unlock them.

Another feature that can be gleaned from Figure 2 is that atoms with smaller local atomic shear strain (dark blue) get clustered in regions of a few nm, and are surrounded by atoms with larger local shear strain (light blue) that are spatially connected. This feature becomes more marked at higher temperatures and lower shear rates. A similar behavior has been observed by Feng *et al* . [16] in a compression test, using molecular dynamics simulation, of $Cu_{64}Zr_{36}$.

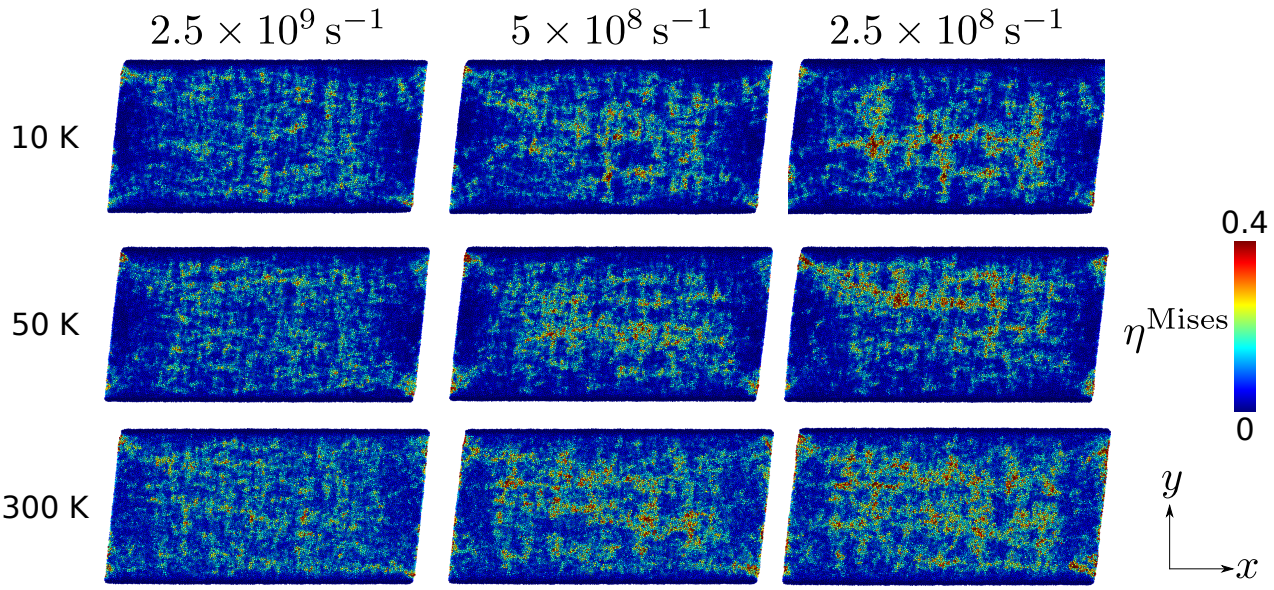

Figure 2. Image of the structure of $Zr_{50}Cu_{50}$ at $\gamma = 0.06$ and for three shear rates under study. Here we present the situation for (a) 10 K, (b) 50 K and (c) 300 K of temperature . Each sample contains 145.200 atoms and are colored according to their local atomic shear strain.

4. Concluding remarks

The changes in mechanical properties and atomic structure for $Zr_{50}Cu_{50}$ metallic glass under the effect of pure shear have been calculated. From the explored range of parameters, preliminary conclusions are that the shear modulus is not sensitive to changes in the shear rate, but is sensitive to changes of temperature. The ultimate strength increases at higher shear rates and decreases at higher temperature. A measurement of the local atomic shear strain reveals that it has higher values at low shear rates, with a geometric distribution similar to the one reported by Feng *et al* . [16] The high values of local atomic shear strain associated with low strain rates are similar to what is observed in the jamming transition [15], where rapid strain rates do not allow atoms to move far apart, thus preventing the appearance of high local shear strain.

Acknowledgments

M.S-M. thanks to CONICyT PhD. fellowship No. 21140904. G.G. thanks PAIFAC-2016, Facultad de Ciencias, Universidad de Chile. F.L. acknowledges to Fondecyt grant 1160823.

References

[1] Telford M 2004 *Materials Today* **7** 36 – 43 ISSN 1369-7021
[2] Wang W, Dong C and Shek C 2004 *Materials Science and Engineering: R: Reports* **44** 45 – 89 ISSN 0927-796X
[3] Ashby M and Greer A 2006 *Scripta Materialia* **54** 321 – 326 ISSN 1359-6462
[4] 2015 *Nat. Mater.* **14** 541–541 ISSN 1476-1122
[5] Falk M L and Langer J S 1998 *Phys. Rev. E* **57**(6) 7192–7205
[6] Dasgupta R, Hentschel H G E and Procaccia I 2012 *Physical Review Letters* **109** 1–4 ISSN 00319007 (*Preprint* 1207.3591)
[7] Albaret T, Tanguy A, Boioli F and Rodney D 2016 *Phys. Rev. E* **93**(5) 053002 URL https://link.aps.org/doi/10.1103/PhysRevE.93.053002
[8] Eshelby J D 1957 *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences* **241** 376–396 ISSN 0080-4630
[9] Eshelby J D 1959 *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences* **252** 561–569 ISSN 0080-4630
[10] Mendelev M I, Kramer M J, Ott R T, Sordelet D J, Yagodin D and Popel P 2009 *Philosophical Magazine* **89** 967–987
[11] Plimpton S 1995 *Journal of Computational Physics* **117** 1 – 19 ISSN 0021-9991
[12] Berendsen H J C, Postma J P M, van Gunsteren W F, DiNola A and Haak J R 1984 *The Journal of Chemical Physics* **81** 3684–3690
[13] Shimizu F, Ogata S and Li J 2007 *Materials Transactions* **48** 2923 – 2927
[14] Stukowski A 2010 *Modelling and Simulation in Materials Science and Engineering* **18** 015012
[15] Biroli G 2007 *Nat Phys* **3** 222–223 ISSN 1745-2473 URL http://dx.doi.org/10.1038/nphys580
[16] Feng S, Qi L, Wang L, Yu P, Zhang S, Ma M, Zhang X, Jing Q, Ngai K, Greer A, Li G and Liu R 2016 *Scripta Materialia* **115** 57 – 61 ISSN 1359-6462