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Insight into plasticity mechanisms in metallic glasses by means of a Brazilian test and numerical simulation

J.S. Brest [a,b], V. Keryvin [a,*], P. Longère [b], Y. Yokoyama [c]

[a] Université Européenne de Bretagne, Université de Bretagne-Sud, LIMATB EA 4250, Campus de Saint Maudé, BP 92116, 56321 Lorient Cedex, France
[b] Université de Toulouse, Institut Supérieur de l'Aéronautique et de l'Espace, ICA EA 814, 10 av. E. Belin, BP 54032, 31055 Toulouse Cedex 4, France
[c] Tohoku University, Laboratory for Advanced Materials, IMR, Katahira 2-1-1, Aoba-ku Sendai City, Miyagi Prefecture 980-8577, Japan

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ABSTRACT

Multiaxial and heterogeneous mechanical experiments, by means of the diametral compression test (Brazilian test), were carried out on Zr-based Bulk Metallic Glass. Attention was notably focused on obtaining the displacement field in the area of interest (large strains) employing a Digital Image Correlation device, in addition to the measurement of the usual global load–displacement curve. In order to reproduce the behaviour of the BMG at stake, several constitutive equations were considered with growing complexity: von Mises, Drucker–Prager (pressure dependence), free volume based model as well as a viscoplastic Coulomb–Mohr type model. The two latter were implemented as user-material in a Finite Element computation code. The results of these investigations including experiments and computational simulations are discussed.

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1. Introduction

Bulk metallic glasses (BMGs) are a quite recent class of materials that exhibit exceptional mechanical properties including strength, resilience, hardness or fracture toughness as well as large yield strains [1–3]. The mechanisms of deformation, damage and failure of these materials must be fully identified for designing compositions of metallic glasses even more resistant and ductile. The numerical prediction of the mechanical resistance for these new materials requires an advanced modelling of their behaviour. A better understanding of the plastic deformation (in terms of localised thin shear bands), the consideration of temperature, viscosity and pressure effects are necessary parameters.

Obtained *via* a rapid solidification from the liquid state, BMG belong to the class of amorphous alloys characterised by the absence of structural long range ordering. Their macroscopic mechanisms of plasticity mainly proceed from the propagation and interaction of very thin shear bands. From the microscopic viewpoint, BMG plasticity does not result from the accumulation and motion of dislocations, as it is the case for crystalline alloys, but may be depicted, depending on the authors, by the theories of shear transformation zones (STZ) [4] or free volume (FV) [5]. Starting from the aforementioned models (STZ and FV), several authors have tried to describe the macroscopic response of BMG to various loading cases, see e.g. Schuh et al. [1] and Gao [6] (FV model), respectively. Following another way, Anand and Su (AS model) [7] developed a Coulomb–Mohr type constitutive theory to reproduce the elastic-viscoplastic behaviour of BMG.

The present work aims at investigating in a first step the mechanical behaviour on Zr-based BMG by means of a multiaxial and heterogeneous test. BMG exhibiting an apparent brittle behaviour in tension as well as in compression at room temperature, the information, namely plasticity, provided by the usual tension or compression tests on these materials are *de facto* far from being suitable. To get some insight on plasticity mechanisms, the indentation test is commonly carried out [8–11], so are bending [12] or constrained tests [13]. There exist other tests, though being less known for this type of material, which may also be of particular interest. Among them is the diametral compression test [14], also called Brazilian test, which is extensively used on brittle materials like concrete. It allows one to generate a tensile loading in the sample section transversally to the compression axis; it also generates heterogeneous mechanical fields in the sample, some parts of the sample remaining almost free of loading. The present approach differs from previous indentation studies since it allows to record extensive plastic fields during the test in addition to the mean response (the load–displacement curve) and it creates multiaxial stress states different from those underneath an indenter. For the indentation test, they are highly compressive and localised underneath the indenter tip, while for the Brazilian test, they are

* Corresponding author at: Université Européenne de Bretagne, LIMATB EA 4250, Campus de Saint Maudé, BP 92116, 56321 Lorient Cedex, France.
E-mail address: vincent.keryvin@univ-ubs.fr (V. Keryvin).

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compressive close to the loading conditions, tensile close to the free boundaries and close to pure shear at the centre.

In a second step, computational simulations employing the engineering Finite Element computation code Abaqus are conducted, involving configurations with different BMG constitutive models. The models which do not belong to the standard model library of the computation code were implemented as user materials. The numerical results are commented and compared to experimental ones.

The material and experimental procedures are displayed in Section 2 with the corresponding results. The constitutive models and the numerical procedures are presented in Section 3. The given results are then compared to experiments in Section 4.

2. Materials and experiments

2.1. Materials and samples

The $Zr_{55}Cu_{30}Al_{10}Ni_5$ (at.%) BMG is studied in this paper. By a very careful tilt-casting process and with highly purified (50 ppm of oxygen) iodine refining processed Zr, specimens with less than 300 ppm of oxygen and no micrometric crystalline defects are prepared (see [15] for details). The material is supplied in the form of 60 mm long and 8 mm diameter rods. The samples used are cut and polished to obtain 6 or 15 mm long cylinders.

Experiments were carried out at room temperature and atmospheric pressure employing a hydraulic tension–compression machine (INSTRON 8803) equipped with a 500 kN capacity load cell with a 8 N resolution. A 0.8 μm resolution mechanical extensometer was used to measure the global displacement between the compression anvils, and two cameras were installed to monitor the displacement (with a 0.25 mm resolution) of a cloud of dots sprayed on a side of the sample (see Fig. 1), and further derived the related strain field using a Digital Image Correlation (DIC) software [16] (Aramis). The tests were carried out at a displacement rate of 0.05 mm min^{-1}. For questions of reproducibility, the same test was made on four different samples times from the same batch. The load–displacement curves were the same within less than 5%.

An equivalent shear strain used in this paper is defined as:

$$\varepsilon^{eq} = \sqrt{\frac{2}{3}\underset{\sim}{e} : \underset{\sim}{e}} \tag{1}$$

where $\underset{\sim}{e}$ is the deviatoric part of the strain tensor $\underset{\sim}{\varepsilon}$ and ":" denotes the double contracted product.

2.2. Experimental results

The load–displacement (P–u) curve is presented in Fig. 2. The carried out test is a sequence of two successive loadings: the first one on a 15 mm sample, and the second one on the same sample cut to 6 mm long, after unloading of the former, to be able to reach fracture without damaging the compression anvils (100 kN limit load). Therefore P stands for a load per unit length. On Fig. 2 one can clearly distinguish two distinctive steps during the deformation process, a stiff part followed by a more compliant one. The numerical results presented in Section 4 provide an explanation to this phenomenon. A higher magnification of the last part of the plot displays the presence of regularly spaced serrations, already reported elsewhere for different tests [13,17]. They are assumed to be the consequences of the sequential formation and emergence of shear bands inside and at the surface of the sample.

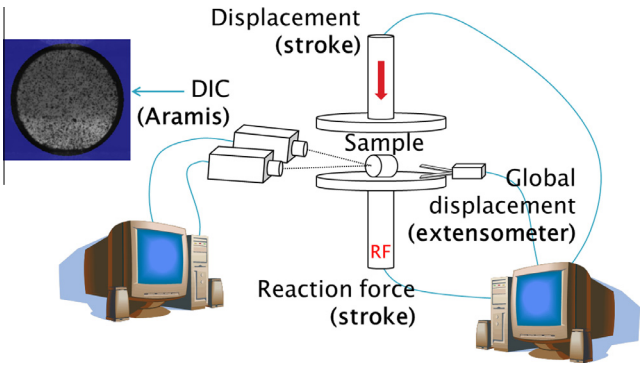

Fig. 1. Schematics of the experimental set-up and its instrumentation.

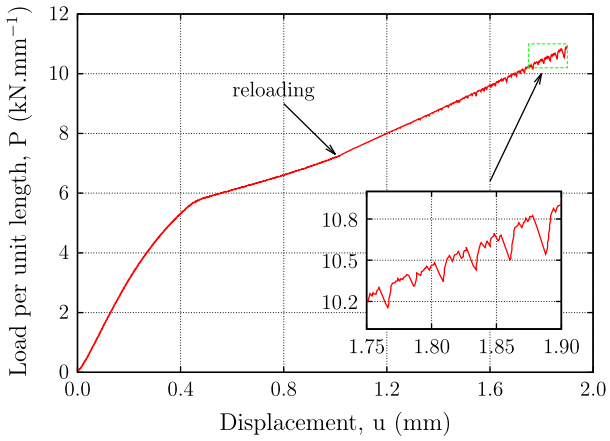

Fig. 2. Diametral compression results – plot of load per unit length vs displacement – magnification of the serrations at the end of the curve.

DIC allows one to capture the deformation pattern of the sample (see Fig. 3). During the first part of the loading (below ~11 kN/mm) it concentrates in a column underneath the load with a maximum equivalent strain of ~0.2 close to the anvil (indentation-like feature) and at the centre of the sample (Brazilian-like feature). At the end of the second loading, before fracture, most of the deformation fields are localised in a cross with a maximum intensity reached in its centre. The equivalent strain in this cross is more than 0.3, while in the centre the deformation is higher than 0.6. These strains are average values since the shear bands thickness is 10–100 nm [18] while the DIC's resolution is 0.25 mm. Much larger strains are expected inside the shear bands.

3. Constitutive modelling and numerical simulations

3.1. Principles of the different approaches

Metallic glasses are often compared to polycrystalline metallic alloys for their chemical composition and atomic bonds, with poly-

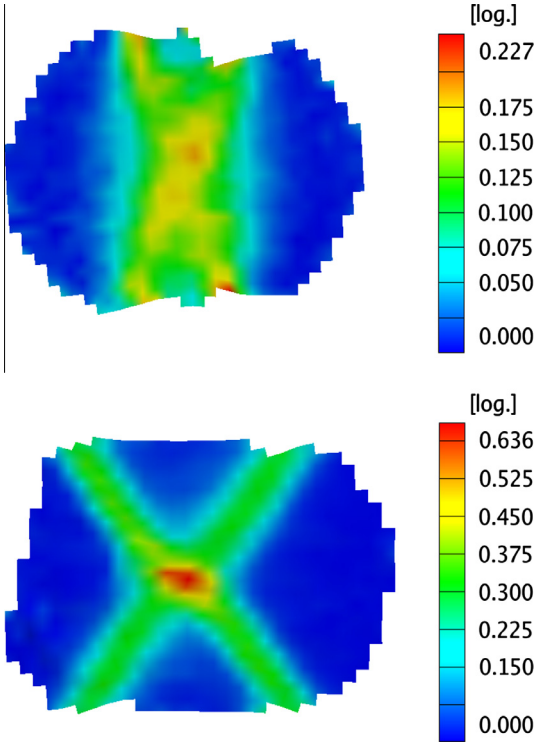

Fig. 3. Map of equivalent strain (logarithmic measure $\log(1+\varepsilon^{eq})$) obtained by DIC; at the end of the first loading (~11 kN mm^{-1}, top) and at the end of the second loading up to fracture (bottom, strain reinitialised to zero).

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