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COUPLED THERMO- MECHANICAL ANALYSIS OF SHEAR LOCALIZATION IN BULK METALLIC GLASSES

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ABSTRACT

A Coupled-thermo-mechanical, finite deformation based constitutive model to describe the deformation behavior of bulk metallic glasses was recently developed by Thamburaja and Ekambaram [1] and implemented in ABAQUS/Explicit (2007) finite-element program by writing a user material sub-routine. In this work, the effectiveness of this temperature-displacement model, particularly while simulating the localizing behavior of metallic glasses which are deformed within the super-cooled liquid region is comprehensively analyzed.

Numerical simulations were performed using the set of constitutive equations and list of material parameters from Thamburaja and Ekambaram [1] for Vitreloy-1 metallic glass. Coupled-temperature-displacement simulations were performed under specified deformation rates to study the shear localization phenomena for temperatures around and above the glass transition temperature. These deformation rates were obtained from the experimentally determined localization mapping from Lu, J. et. al. [2] for Vitreloy-1. The results from our finite element simulations could distinctively delineate the incidence of shear bands for strain rates well within the experimentally obtained range for localization, for ambient temperatures near the glass transition region.

KEY WORDS

Metallic glass; Constitutive modelling; Viscoplasticity; Finite-elements.

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INTRODUCTION

Amorphous alloy also widely known as Metallic Glass was first invented in the year 1960 and since then has continually been an active subject of research in the field of materials science globally. These metallic glasses are produced by rapid quenching of molten alloys to avoid nucleation and growth of crystals. To date there are few hundreds of types of metallic glasses available based on a variety of metals including rare-earths. These can be produced into amorphous structure, with sizes varying from ribbon forms of few microns to bulk forms of few centimeters in thickness, the later ones are generally termed as *Bulk Metallic Glass*. Due to the unique mechanical and physical properties of these materials including high yield strength, high elastic strain limit, excellent wear resistance, bio-medical compatibility, excellent formability characteristics, these are being used as structural materials, sporting goods, defense applications, aerospace applications, in the field of MEMS, bio-medical equipments, fine jewelry, etc. The widely used bulk metallic glass for most of the applications mentioned above is the Zirconium based $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ alloy, which is also commercially known as Vitreloy-1.

A typical metal forming operation requires the material to flow easily under an applied stress field; hence these materials are heated up to temperatures around the glass transition region before deforming them into required shapes. Even though these materials flow easily and attain high strain levels at temperatures within the super-cooled liquid region, they tend to fracture or fail spontaneously forming thin bands of local deformation called shear bands once the deformation rate is higher than a critical rate for that given temperature. Hence it becomes imperative for a constitutive model to accurately predict this critical localization strain rate causing failure, for its efficient applicability.

The main focus of this work is to make use of the constitutive equations and the corresponding set of material parameters from Thamburaja and Ekambaram [1] for Vitreloy-1 to simulate shear localization at temperatures around the glass transition temperature and compare the results with the experimental data available from the work of Lu, J. et. al. [2].

NUMERICAL ANALYSIS

The numerical simulations in this work are conducted using ABAQUS/Explicit (2007) finite element program. All the material parameters for Vitreloy-1 were obtained from the work of Thamburaja and Ekambaram [1]. To study the shear localization problem we have modeled a two-dimensional mesh having an initial dimension of 3.7mm by 7.4mm. All the simulations are performed using an initial mesh with 800 continuum plane-strain elements as shown in Fig. 2. A very slight taper along the axial length, between the top and bottom surfaces is introduced as a means of geometrical imperfection to the specimen in order to suppress formation of multiple shear bands across one another. The top and bottom surfaces are maintained at the ambient temperature throughout the simulation to imitate the effect of compression platens during real experiments. Required velocity profiles are applied to the top node set along compressive direction to simulate the required strain rate.

The boundary between the two modes of deformation namely homogeneous and in-homogeneous deformations for a range of strain-rates and temperatures are experimentally determined and graphically depicted by Lu et. al. [2], as shown in Fig. 1. Our aim is to perform numerical simulation and predict the shear localization using our constitutive model for those strain rates along the boundary between homogeneous and in-homogeneous deformations for different ambient temperatures near the glass transition region.

To begin with, for an ambient temperature of 623K, experiments suggest that, Vitreloy-1 samples deformed at compressive strain rates in the range of 0.003/s to 0.01/s with a median strain rate of 0.0065/s, results in in-homogeneous deformations also known as strain localization. In order to reproduce this characteristic phenomenon using our constitutive model and material parameters, we perform coupled-temperature-displacement analysis on the initial mesh shown in Fig. 2 at a compressive strain rate of 0.002/s (lower than the minimal required deformation rate for in-homogeneity). Results from the simulation show that the specimen deformes homogeneously and there are no signs of any form of in-homogeneity across the specimen even after total strain of 20%. Hence, this result concludes that our constitutive model is in par with the experimental observation indicating homogeneous deformation for strain rates lower than 0.003/s. Our next task is to predict the experimentally observed shear localization phenomenon for the same ambient temperature of 623K, when the compressive deformed rate was increased to a strain rate within the experimental range for shear localization, i.e., between 0.003 and 0.01/s. Hence, using the same initial mesh and boundary conditions shown in Fig. 2, we perform a numerical simulation under coupled-temperature-displacement setup for a strain rate of 0.003/s (the minimal required deformation rate based on experiment for in-homogeneity) in compression. We assume that, one order increase in plastic strain rate between different regions across the specimen as a rule of thumb required for intense localized deformation that would result in failure of the specimen. It is identified from our simulation that the deformation was no longer homogeneous when the strain rate is increase from 0.002/s to 0.003/s. Moreover, at an instance when the total strain is about 10.4%, the ratio between the plastic strain rates within the core of shear localization region and the regions away from this inhomogeneous region was calculated to be about 27. This being higher than our required ratio of 10 would ultimately result in a localized deformation leading to fracture of the specimen. Hence, the result from our numerical simulation clearly predicts the formation of shear bands as experimentally observed. Based on the above two simulation results performed at strain rates of 0.002/s and 0.003/s, we have actually validated our constitutive model and its material parameters for its applicability in predicting the shear localizing characteristics of Vitreloy-1 bulk metallic glass at an ambient temperature of 623K.

Further, our next task is to extend the validity of our model through other temperatures above the glass transition region. We obtained the extrapolated value of approximate critical strain rate for localization from Fig. 1 at an ambient temperature of 633K; it was found to be 0.016/s. Hence, we performed simulations under deformation rates around 0.016/s to determine whether the critical strain rate from our simulations is comparable with this experimental deformation rate. Results from our simulations show that inhomogeneous deformation does occur when the specimen was deformed at a strain rate of 0.02/s, but no localized deformation ensue when the strain rate was 0.009/s and lower than this. This verifies the fact that the critical rate for localization lies in between 0.009/s and 0.02/s, which precisely agrees with the extrapolated value of 0.016/s for localization from the experiments. Based on this result our constitutive model and material parameters are now validated for another ambient temperature of 633K, consequently the model is also applicable for predicting the shear localization for temperatures in the range from 623K to 633K.

A similar procedure mentioned above was followed for other ambient temperatures, which includes 643K, 653K and 663K to identify the range of strain rates within which the critical localization rate occurs and compared with the experimentally obtained values from Lu et. al. [2]. It was determined that for all these temperatures, the numerical simulations using our constitutive model and material parameters could distinctively delineate the incidence of shear bands at strain rates well within the experimentally obtained range for localization. A chart comparing the experimental range of strain rate for inhomogeneous deformations and the deformation rates exhibiting homogeneous and inhomogeneous deformations obtained by means of numerical simulations based on our constitutive model for different ambient temperatures are shown in Table.1. Also included in Fig. 1 for various temperatures as circular symbols, are those strain rates which resulted in shear localization based on numerical analysis. Here, it must be emphasized that for all the temperatures the strain rates from simulations are within the experimentally obtained range for localization.

CONCLUSION

The thermo-mechanical based constitutive model developed by Thamburaja and Ekambaram [1], has been successfully verified by performing numerical simulations to predict the shear localization in par with the experiments for Viterloy-1 metallic glass. The model could accurately predict the exact deformation rate for inhomogeneous deformations, when the specimen is deformed at any ambient temperature in the range from 623K to 663K which being around and above the super-cooled liquid region.

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Table 1. Range of critical deformation rate for various temperatures.

Ambient Temperature [K]	**Experimental Deformation Rate for Localization [/s]**		**Deformation Rate from Numerical Analysis [/s]**	
	Maximum	**Minimum**	**Homogeneous**	**Inhomogeneous**
623	0.01	0.003	0.002	0.003
633	0.016*		0.009	0.02
643	0.1	0.03	0.04	0.06
653	0.16*		0.1	0.3
663	1	0.3	0.5	0.6
* Extrapolated Value for Experimental Critical Strain Rate				

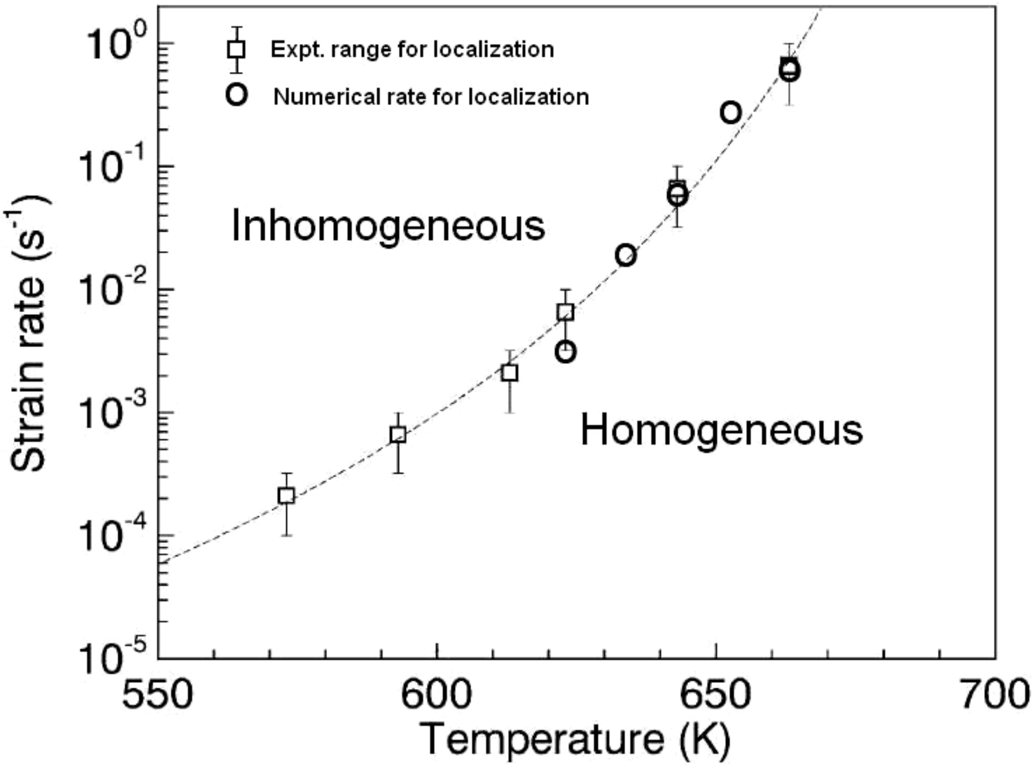

Fig.1. Experimentally obtained deformation mapping (Lu. et. al. [1]).

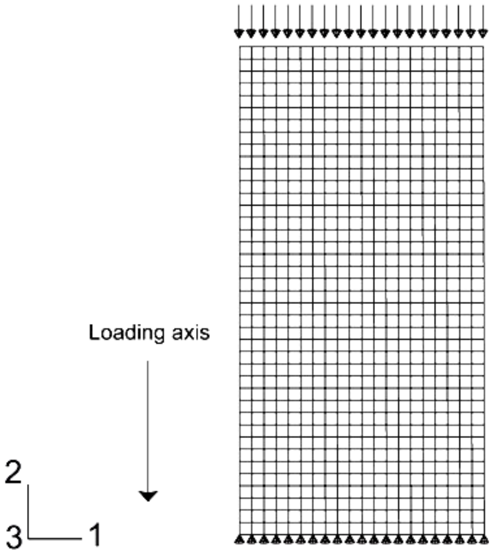

Fig.2. Initial Finite Element Mesh with 800 Plane-strain elements.