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A Maxwell-extreme constitutive model of Zr-based bulk metallic glass in supercooled liquid region

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ABSTRACT

The uniaxial compression tests were performed to research the deformation behavior of $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ (Vit1) bulk metallic glass (BMG) in a wide range of strain-rates and temperatures. The true stress-strain curves in the supercooled liquid region (SLR) fitted by Maxwell-pulse constitutive model have been compared with the experimental data. It was found that there were larger deviation between the true stress-strain curves obtained from compression tests and Maxwell-pulse model. In order to describe the whole flow process more accurately, the influences of ambient temperature and strain rate on viscous flow and stress overshoot related to structural relaxation, which were ignored in Maxwell-pulse model, were introduced to construct a new constitutive relationship of Vit1 alloy in SLR. The constitutive models before and after modified were then written into the finite element (FE) simulation software, respectively. It was provided that the fitting results simulated by the new constitutive model were in better agreement with the uniaxial compression test data than those of Maxwell-pulse.

1. Introduction

In the past decades, Zr-based bulk metallic glasses (BMGs) have been considered as a kind of promising structural and functional materials due to their unique physical properties and mechanical properties, such as superior specific strength, high hardness, large elastic limit, excellent corrosion resistance and high wear resistance [1–6]. Among these Zr-based BMGs, $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ alloy (Vit1) has attracted growing attention owing to its high glass forming ability -a typical characteristic of fully amorphous structure can be possessed under the cooling rates as low as 1–10 K/s [7]. Vit1 alloy shows a broad temperature range in the region of the glass transition, indicating a larger resistance of crystallization during hot working. It is expected to serve as an important material in micro-electromechanical systems manufacturing field because of its better plasticity and high structural stability under high temperatures [8]. Furthermore, the high fluidity and the wide supercooled liquid region (SLR) [9] also mean that Vit1 alloy can be formed with many processing technologies in a wide temperature range, for instance, imprinting, forging, consolidation, blowing and extrusion [10–12].

In order to simulate and predict the forming processes of BMG components, it is necessary to establish a constitutive model which can describe the deformation behavior of BMGs and construct a finite element (FE) simulation. Recently, the related researches have been performed and some constitutive models in terms of quantitative or qualitative description have also been proposed to describe the flow behavior of BMGs in SLR [13–24]. Besides, some constitutive models based on free volume theory can express the flow behavior of BMGs at temperatures in SLR and below the SLR [25,26]. In particular, Thamburaja et al. [27,28] have proposed the excellent coupled thermo-mechanical model to describe the deformation process of BMGs quantitatively, such as elastic behavior, stress overshoot, the transition of flow mode and even the multi-axial deformation behavior. Although a lot of investigations have been achieved and some results have been reported [29–32]. These models mentioned above either cannot quantitatively demonstrate the constitutive relationship of BMGs in SLR including Newton and non-Newton flow behaviors or be applied as a result of their complex processes. For solving these problems, Wang [33] et al. have presented the Maxwell-pulse model on the basis of the fictive stress model and pulse model. This constitutive model, which can fit both steady state flow and stress overshoot of Vit1 alloy, consists of Maxwell model and pulse model. The Maxwell model contains two parts: a Hooke spring reflects elastic deformation, and a Newtonian dashpot describes plastic deformation. In order to describe the structural relaxation process with energy dissipation, a strain related double exponential pulse function, which expresses the variation of the stress peak, can be used to characterize the overshoot stress for its higher magnitude and wider range. But there are larger deviations between the stress-strain curves calculated and experimental data.

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In this paper, the Maxwell-pulse constitutive model, which is employed to express the thermoplastic deformation behavior of Vit1 alloy in SLR, has been derived from the results of uniaxial compression tests. The extreme function, which refers to the temperature and strain rate dependences of deformation behavior, is proposed to modify the Maxwell-pulse model constitutive model according to viscosity theory and fictive stress model. Afterwards, the presented constitutive models will be input into the finite element software Deform3D to predict the distribution of effective strain and true stress-strain curves of uniaxial compression tests for the micro cylindrical specimens.

2. Materials and methods

The alloy ingots with nominal composition $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ (at.%) were prepared by arc melting of high purity metals. All master alloy ingots were remelted and inverted at least three times under a Ti-gettered argon atmosphere for ensuring their chemical homogeneity, and then suck-cast into a copper mold to produce the 50 mm long amorphous alloy cylindrical rods with a diameter of 10 mm. The microstructures of these alloy cylindrical rods were examined using X-ray diffraction (XRD, Philipus X'Pert) with Cu-Kα radiation and their thermal properties were studied by differential scanning calorimetry (DSC, Perkin Elmer Pyris DSC 1) at the continuous heating rates of 20 K/min under a flow of high purity argon. The results indicates that Vit1 alloy has a typical characteristic of a fully amorphous structure and the glass transition temperature T_g, the onset crystallization temperature T_x, and the temperature range corresponding to SLR ΔT_x ($\Delta T_x = T_x - T_g$) of Vit1 alloy are 630 K, 712 K and 82 K, respectively.

For investigating the deformation behavior of Vit1 alloy in SLR, the uniaxial compression tests were performed using a electromechanical Instron 8810 testing machine which equipped with a heating furnace in the temperature range from 633 K to 673 K with various strain rates of 2×10^{-4} s^{-1}, 5×10^{-4} s^{-1}, 1×10^{-3} s^{-1}, 2×10^{-3} s^{-1}, 5×10^{-3} s^{-1}, 1×10^{-2} s^{-1} and 2×10^{-2} s^{-1}. The *as*-cast rods were cut into short cylinders with the size of $\Phi 2 \times 3$ mm for compression tests. Both ends of these specimens were polished to make them parallel to each other before tests. The indenters were preheated to the setting temperature with heating furnace. Afterwards, the specimens were placed into the heating furnace and held for 240 s to stabilize the temperature before compression tests began.

Compression specimens for FE simulations were built with dimensions of $\Phi 2 \times 3$ mm and divided into 50,000 mesh elements. The deformation processes were performed at 653 K with the compression rate of 0.003 mm/s and 0.03 mm/s. The simulations based on different constitutive models were achieved to 80 steps and completed at the stroke of 2 mm (the true strain is approximately 110%). Then the compressed specimens were sliced along the *z*-axis to obtain the distribution of effective strain.

3. Results

Fig. 1a shows an example of the true stress-strain curves obtained at strain rate of 5×10^{-3} s^{-1} in the temperature range of 633–673 K. The initial slopes of the stress-strain curves exhibit an obvious increase as the temperature decreased. At lower temperatures (ranging from 633 K to 653 K), there are stress overshoot phenomena existing in the early stage of deformation process. When the experimental temperature increases over 663 K, the stress overshoot peaks disappear and the flow stress increases monotonically as the strain increased until it reaches a certain value and subsequently keep steady with the strain increasing further. In addition to the strong temperature dependence of the deformation behaviors for Vit1 alloy, the effect of strain rate on the true stress-strain curves have also been investigated. Fig. 1b shows a series of typical true stress-strain curves of Vit1 alloy we have prepared, it can be seen that the stress overshoot and the steady-state flow stress gradually decrease with decreasing strain rate at 633 K. When the strain rate decreases to 2×10^{-4} s^{-1}, the Vit1 alloy is in Newtonian viscous flow region, and stress overshoot phenomenon cannot be observed on the true stress-strain curves. It suggests that decrease of strain rate results in a transition from non-Newtonian flow to Newtonian flow, and the stress overshoot phenomenon is also controlled by the deformation modes [34]. The peak stress is a main parameter which characterizes the strength of the BMGs under a certain experiment condition. Fig. 2 plots the peak stress of Vit1 alloy as a function of strain rate and experimental temperature. The experimental data reveals that there is an approximately linear correlation between the peak stress and log $\dot{\varepsilon}$ and a remarkable drop in peak stress occurs as the temperature increases and strain rate decreases. It is clear that at the strain rate of 1×10^{-3} s^{-1}, the peak stress drops from 569 MPa at 633 K to about 45 MPa at 673 K, by a factor of 12.5 for a change in temperature of only 40 K. Compared with the traditional crystalline metallic materials, Vit1 alloy possesses larger temperature sensitivity because the steady-state flow stress decreases by about 550 MPa as the temperature increases by 50 K. Different from the influence of temperature, the peak stress increases with strain rate increasing. That means the deformation behaviors of Vit1 alloy at lower temperatures is analogous to that at higher strain rates, which follows the time-temperature correspondence principle [35]. All these results indicate that Vit1 alloy will not be employed as a structural material which subject to high temperature environment, but lower flow stress under high temperature means that it can be processed into forming easily.

4. Discussion and modeling

The free volume is considered as excess volume in the metastable non-equilibrium structures of BMGs [36], and atoms with the smaller volumes can move to these positions without energy change [37]. If

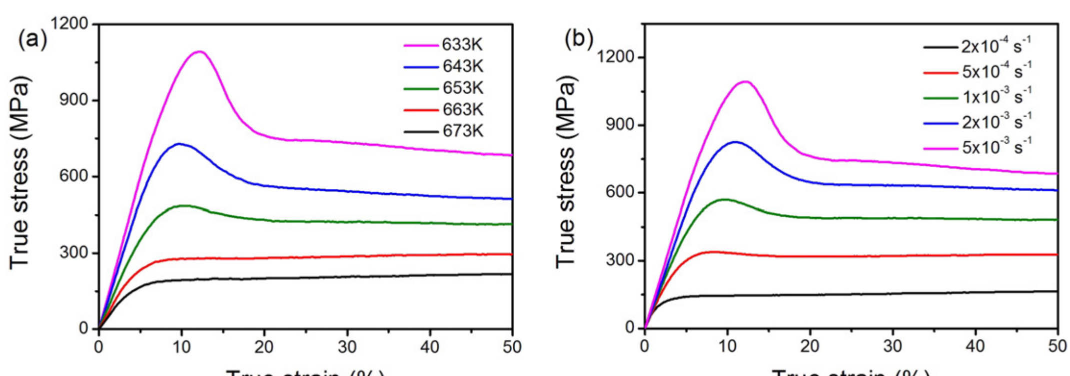

Fig. 1. Engineering stress-strain curves of Vit1 alloy in SLR: (a) 5×10^{-3} s^{-1} at different temperatures, and (b) 633 K with different strain rates.