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Constitutive model for high temperature deformation behavior of Ti–Zr–Ni–Be bulk metallic glass in supercooled liquid region

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ABSTRACT

A constitutive equation based on a free volume model, that describes the strain rate dependent deformation behavior of bulk metallic glasses (BMGs) within the supercooled liquid region, has been modified in this paper in order to reproduce the stress increment that occurs due to crystalline phase formation during lengthy exposure to high temperature in compression deformation. A comparison of the simulated results obtained from finite element analyzes with the compression test results for Ti–Zr–Ni–Be BMG alloy has been conducted to determine the validity of the proposed model. Plastic deformation modes such as Newtonian and non-Newtonian viscous flows of this BMG alloy were found to be reproduced well by the finite element method simulations combined with the free volume based constitutive relations and to show a phenomenon of stress increment deviated from the steady state. Therefore, the constitutive relations introduced here are expected to allow accurate reproduction of the high temperature behavior and better estimation of the formability of BMG alloys.

1. Introduction

The deformation behavior of bulk metallic glass (BMG) alloys can be classified into two modes according to macroplasticity, e.g. inhomogeneous and homogeneous. Inhomogeneous deformation behavior of BMG alloys has generally been known to be concentrated in only narrow shear bands and is characterized by brittle fracturing due to rapid propagation of the primary shear band generated at room temperature, and at high strain rates and high temperatures that are below the crystallization onset temperature [1–7]. Homogeneous deformation behavior of BMG alloys has been characterized as exhibiting a uniform deformation throughout the entire specimen, and at the same time has been reported to occur at a low strain rate near the glass transition temperature and to be composed with Newtonian and non-Newtonian viscous flow transposed according to the creation and annihilation ratio of the free volume due to strain rate [8–13]. Newtonian and non-Newtonian viscous flows are observed at low and high strain rates under elevated temperature, respectively, and can be distinguished by the existence of stress overshoot in the stress–strain curve [11,14,15]. Non-Newtonian viscous flow without stress overshoot has, however, been reported in a BMG composite [16].

The Newtonian viscous flow of BMGs exhibiting high strain rate sensitivity ($m \approx 1$) is considered to be a very important characteristic in various thermoplastic forming (TPF) processes performed within the supercooled liquid region (SLR) because it allows superplastic-like deformation behavior. Since the introduction of TPF by Patterson and Jones [17], various TPF processes have been developed for BMGs, such as a powder extrusion approach reported by Kawamura et al. [18], bulk extrusion by Lee and Chang [19], microforming pioneered by Saotome et al. [20], nano-imprinting by Kumar et al. [21], and boss forming by Jun et al. [22]. One of the advantages of these TPF processes is that they restrict the formation and growth of crystalline phases due to having a much shorter forming time than the slower casting processes generally required for a good cast quality [23–25]. If forming takes longer than the crystallization onset time, crystalline phases formed during deformation have been known to induce an embrittlement of BMGs, and the formability of BMG alloys then becomes poor due to the rapid increase of viscosity after the volume fraction of the crystalline phases increases over a critical value that affects stress [16,26]. Stress deviation from the steady state of a Newtonian viscous flow can also be increased due to crystalline phases [27]. The stress increase phenomenon was reproduced through a constitutive model introducing the back stress by Bletry et al. [9]. This model is, however, estimated to have insufficient physical meaning because it did not account for increments in viscosity and decrements in free volume.

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This study, therefore, focuses on the accurate reproduction of high temperature deformation behavior through modification of the model corrected by Jun et al. [28] from the original model of Anand and Su [29] based on the free volume mechanism [30].

2. Modified constitutive model based on free volume mechanism

The constitutive model for BMG alloys used in this work originated from the study of Anand and Su [29] and is applied here to experimental data obtained from compression tests of a Pd–Ni–P alloy [31] at the temperatures between 0.7 T_g (glass transition temperature) and T_g. The original model has been modified to extend the temperature regime in our previous work because the studies related to both the high temperature deformation behavior and forming process of BMG alloys are concerned with the SLR, viz. between T_g and the crystallization onset temperature $\mathbf{T}_x^0$, and those studies checked the validity of the modified model through reproduction of compression data from Vitreloy1 [28]. The modified model has, however, the disadvantage that the phenomenon of stress increase after the steady state of Newtonian viscous flow due to crystallization during deformation at high temperature cannot be reproduced. Additional modification of the model has been performed for accurate estimation of deformation behavior and formability of BMG alloys, and the changes to the model are as follows.

The evolution rates of slip resistance ($\dot{h}$) and free volume ($\dot{\beta}$) in Anand's original model are expressed in a coupled form of a dynamic production and a static recovery term as

$$\begin{cases} \dot{s} = h\dot{\gamma} - r_s \\ \dot{\eta} = \beta\dot{\gamma} - r_\eta \end{cases}, \qquad (1)$$

with

$$\left\{ \begin{array}{l} \dot{h} = h_0(s_* - s)\nu, \\ \dot{\beta} = g_0\left(1 - \frac{\eta}{\eta_*}\right)\nu \end{array} \right\}, \qquad (2)$$

where the work hardening parameter h characterizes slip resistance during plastic flow to describe a hardening and a softening with $h > 0$ (i.e. $s^* > s$) and with $h < 0$, respectively. The critical value s^* then controls the transition between the hardening and softening and was assumed to depend on the current values of plastic strain rate, temperature, and free volume. The critical free volume η_* should also depend on the strain rate and temperature, which represents the dilation and contraction of materials when $\beta > 0$ *viz.* $\eta < \eta^*$ and $\eta > \eta^*$, respectively. The static thermal recovery terms r_s and r_η in Eq. (1) represent the recovery rate of slip resistance s and the free volume η at a given temperature, respectively, entirely due to the thermal effect alone, *viz.* when $\dot{\gamma} = 0$. The subscript o used in Eq. (2) represents an initial value of corresponding parameters.

Crystalline phases formed due to crystallization can be estimated to cause an increment in slip resistance and a decrement in free volume. Eq. (2) can, therefore, be transformed as

$$\begin{array}{ll} \left\{ \begin{array}{l} \dot{h} = h_0(s_* - s)\nu, \\ \dot{\beta} = g_0\left(1 - \frac{\eta}{\eta_*}\right)\nu \end{array} \right\} & (t_{\mathrm{cry}} < t_{\mathrm{def}}), \\ \left\{ \begin{array}{l} \dot{h} = c\exp[h_0(s_* - s)\nu], \\ \dot{\beta} = g_0\log\left(1 - \frac{\eta}{\eta_*}\right)\nu \end{array} \right\} & (t_{\mathrm{cry}} > t_{\mathrm{def}}) \end{array} \qquad (3)$$

where t_{def} and t_{cry} are the time taken for deformation and the crystalline onset time of the specimen, respectively. c and g_0 are material parameters. Eq. (3) indicates that the slip resistance and free volume are varied by the modified models after crystallization. The evolution of free volume will be shown in the next chapter.

A new constitutive model has been developed in this study by modifying the previous constitutive model [28] to reproduce the stress increase phenomenon that occurs due to crystallization within the SLR. This modified model was used to generate compressive stress *vs.* strain curves through the finite element method (FEM) simulations using DEFORM-2D software [32], and the results were compared with experimental results previously obtained from compression tests and formability assessment of Ti–Zr–Ni–Be BMG alloy [33] within the SLR, as given in Fig. 1.

3. Estimation of material parameters for Ti–Zr–Ni–Be

The material parameters of the $Ti_{43.3}Zr_{21.7}Ni_{7.5}Be_{27.5}$ (at.%) used in this study have not yet been reported, and thus they were analogized from parameters of Vitreloy-1, Zr-based bulk metallic glass, which have been used for most of the studies involving

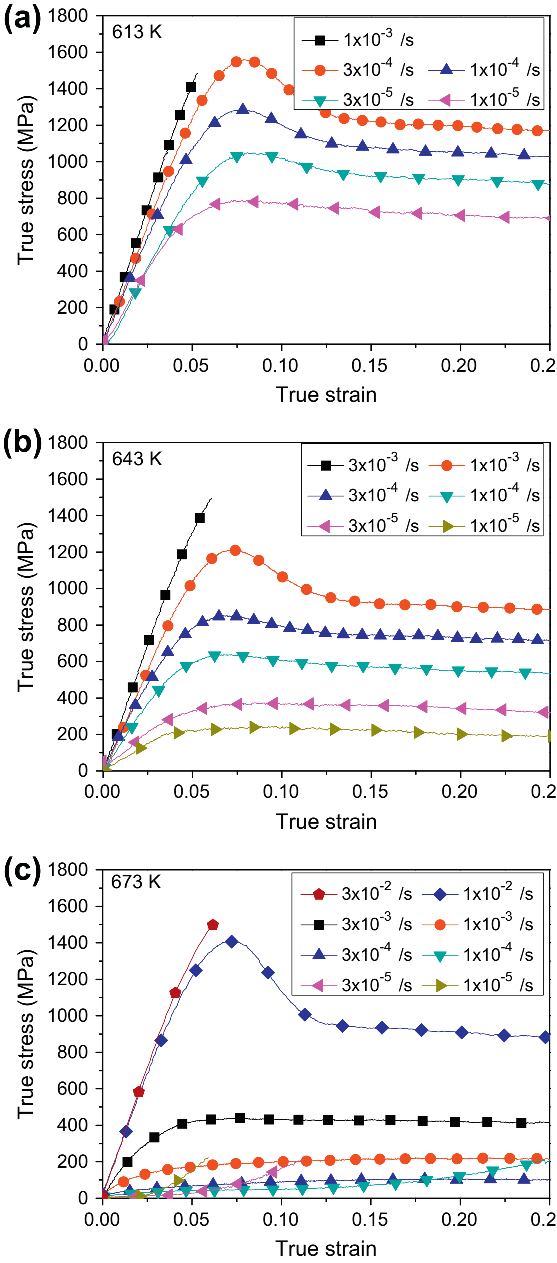

Fig. 1. Representative true stress–strain curves of Ti–Zr–Ni–Be BMG alloy obtained previously under various strain rates at temperatures within the SLR [33].