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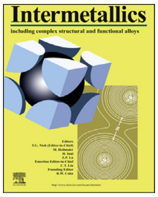

On the applicability of a mesoscopic interface sliding controlled model for understanding superplastic flow in bulk metallic glasses

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ABSTRACT

It is demonstrated that a mesoscopic interface sliding controlled flow model, which has already been shown to account for superplastic deformation in different types of crystalline materials, is also capable of describing superplastic flow in bulk metallic glasses. The only difference is that the random high-angle grain boundaries in crystalline materials along which deformation is concentrated, have to be replaced by the transient interfaces which are formed by interconnecting shear transformation zones in the region of homogeneous flow in bulk metallic glasses. Comparison with experimental results concerning superplastic flow in eight bulk metallic glasses shows that the numerical solutions obtained in the paper for the transcendental stress–strain rate equation of superplastic deformation lead to accurate predictions.

1. Introduction

Deformation of metallic glasses, including that of bulk metallic glasses, has been studied and reviewed extensively [1–19]. Inhomogeneous deformation, characterized by the formation of localized shear bands, their rapid propagation and sudden fracture, is present at low, e.g., ambient, temperatures. Homogeneous deformation of bulk metallic glasses (BMGs) takes place at temperatures near and above the glass transition temperature. Deformation behavior in this domain depends on the strain rate. At low strain rates, Newtonian behavior is seen (strain rate sensitivity index, $m = 1.00$). But, at higher strain rates non-Newtonian response is encountered. In the latter range in some systems crystallization is reported [16] to occur as a consequence of the shear, i.e. crystallization of the deformed samples was observed after holding the specimens at certain temperatures for defined durations where without shear crystallization was not observed. In other systems no such observation has been made. This communication is concerned with the homogeneous deformation region in which in quite a few bulk metallic glasses superplasticity is present. Recently [20], a mesoscopic grain boundary/interface sliding controlled flow model [21–33] was shown to be capable of accounting for superplastic flow in different classes of materials, viz., pseudo-single phase and microduplex metallic materials of grain size in the micrometer-range, sub-micron grained dispersion strengthened alloys, ceramics, metal-matrix and ceramic-matrix composites, intermetallics, a material containing quasi-crystalline particles and nanostructured materials. That continuum model is based on the activation of mesoscopic regions that accommodate/carry forward the shear stress by local yielding. Since this concept bears similarities with the picture of shear transformation zones that underlie the deformation of metallic glasses, it has been extended in this work to encompass also the description of superplastic deformation of metallic glasses near and above their glass transition temperature (but below the crystallization temperature). It is demonstrated here that this model is useful in understanding superplastic flow in bulk metallic glasses also, without invoking the additional concept of crystallization in the supercooled liquid region, as done in some analyses, to account for the non-linear stress–strain rate response in the higher strain rate range. The present method, which applies to the overall steady state

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response of a bulk metallic glass, will remain substantially the same even when crystallization is present, with appropriate values for the free energy of activation, the threshold stress needed for the onset of mesoscopic interface sliding and the excess volume fraction present in the basic unit of interface sliding. This is because the model assumes that the rate controlling processes are confined to boundary/interface regions only and the basic units of boundary/interface sliding are similar for all systems, except for the nature and strength of the interatomic forces and the excess volume fraction present in the relevant atomic ensemble.

2. The model

Concerning the model description of superplastic deformation of metallic glasses near their glass transition temperature and in the super-cooled region, a simplified picture is assumed that is based on the presence of individual regions in the material, the so-called shear transformation zones (STZs), that have a higher susceptibility for yielding in an external stress field due to the excess free volume fraction being greater than in the rest of the regions. For mathematical development of the ideas, the STZs are assumed to have equal size throughout the material and it is also assumed that they are present throughout the bulk in ample amount. According to the description by Falk and Langer [34], these STZs are described as two-level systems that accommodate the local shear stress by atomic rearrangements within the STZs that consist of several tens atoms. Macroscopic shear thus requires an overlap of the stress fields of the individual STZs, which, at low homologous temperatures, results in the formation of shear bands. These latter defects are extended, plate-like defects with typical widths of not more than 5–10 nm [35]. At higher homologous temperatures, as considered in this work, the glasses deform homogeneously at sufficiently low strain rates without the formation of permanent shear bands. However, since recent work has indicated a direct coupling between the relaxation dynamics of glasses and the presence of STZs and since the relaxation dynamics of glasses is continuous up to the glass transition temperature, T_g, and also at temperatures above T_g, we assume that the units of shear, the STZs, are equally responsible for the deformation of metallic glasses in this temperature region. This is consistent with the mode coupling theory, which predicts a dynamic phase transition at a critical temperature Tc far above the glass transition temperature [36]. Recent results on diffusion in bulk metallic glasses show that the mechanism of diffusion changes from viscoelastic flow above Tc to a cage-like motion below [37]. No change of the mechanism is detectable at Tg. Following this result it would appear that the basic mechanism of deformation is the same above and below Tg. A note, however, is due here: while at low homologous temperatures the activation of STZs leads to the formation of shear bands with widths that are much larger than the diameter of the STZs, this is unlikely to be the case for shear deformation near T_g. Due to the enhanced diffusivity of the constituent atoms near the glass transition, local stresses can more easily be accommodated and macroscopic shear can thus be achieved by the “transient formation of interconnecting STZs” that are thus treated in this model as effective “interfaces” – see Fig. 1. Compared with the typical STZ size at low homologous temperatures, where shear band formation is prominent during shear deformation, the size of the STZs near T_g is expected to be markedly smaller, due to the more readily available excess volume at higher temperatures that allows for faster and energetically less costly atomic rearrangements.

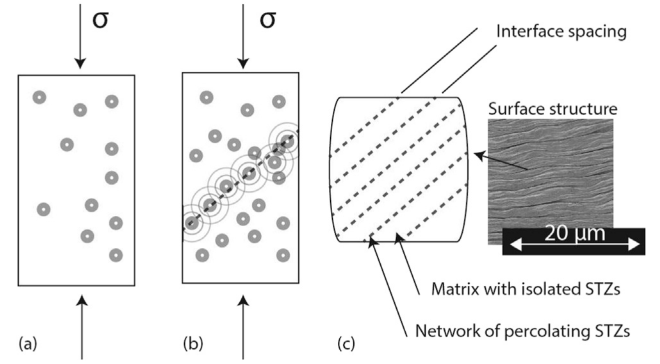

Fig. 1. Evolution of a sample under compressive loading: (a) Once the compression starts, shear transformation zones get activated, (b) Once the concentration of the active STZs is high enough, a network of interconnected STZ forms and creates interfaces for sliding. Due to the fast relaxation time above Tg, these interfaces do not become unstable and shear bands are not formed. (c) The sample consists of a network of percolating STZs and a matrix with only isolated, local STZs. The SEM micrograph of a PdNiP metallic glass sample after compressive deformation shown in Fig. 3 is shown adjacent to (c).

Concerning the continuum model for describing superplastic deformation of metallic glasses near and above their glass transition temperature, only a brief account is presented here, as it is described in detail elsewhere [20–33]. The superplastic material system is assumed to consist of quasi-rigid regions (grains in crystalline or the relatively mostly undeformed matrix in metallic glasses), except for the regions in the vicinity of the transient interfaces, where deformation is present to ensure continuous deformation along these interfaces. The bulk of the deformation is concentrated along these interfaces and the interfaces must percolate for homogeneous, macroscopic shear to occur. Steric hindrance, as e.g., at a triple junction in crystalline materials or by activated STZs that are not aligned in this case, is overcome by plane interface formation (see Fig. 1 of [20]) and this allows boundary sliding on a mesoscopic scale, i.e., over distances of the order of several microns. Superplasticity results when such large scale sliding takes place simultaneously throughout the bulk of the specimen and the plane interfaces thus formed interconnect. In this approach, for crystalline materials, interface sliding is viewed as a two-scale process. At the atomistic level, interface sliding is the result of the consecutive shear of oblate spheroids (an idealized configuration for mathematical development), each of diameter ~5 atomic diameters in the boundary plane and height, on average, of 2.5 atomic diameters (average width of grain boundaries in crystalline materials). A visible interface-sliding offset will result when the deformation proceeds till the end of an interface. The energy associated with the shear and momentary dilatation distortions of the oblate spheroid, as it gets sheared while being embedded inside a solid matrix (going through a saddle point) constitutes the free energy of activation for the rate controlling process. In the present case, the model description follows the same line of thought, with the exception that the oblate spheroids are not localized at pre-existing interfaces (the grain boundaries), but that these regions are distributed throughout the material and form transient interfaces via shear activation. Such an approach makes the present analysis consistent with the description for the formation of shear transformation zones in metallic glasses due to Argon [2], Spaepen [1] and Falk and Langer [34] who also have assumed the size of these zones to be of the order of several tens atoms, which agrees with our assumption for the size of the oblate spheroids that are assumed to extend over ~5 atomic diameters along the shear plane, which is on the lower side of commonly assumed STZ sizes. (The analysis will hardly change if the size of the oblate spheroid is assumed to be somewhat larger.)