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By invitation only: overview article

Deformation of metallic glasses: Recent developments in theory, simulations, and experiments

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ABSTRACT

We review recent research into elastic and plastic deformation of metallic glasses, with an emphasis on making connections between developments in theory and simulation (largely from the physics community) and experimental results (largely from the metallurgy community). Topics covered include strain measurement via scattering techniques, non-affine atomic displacements during elastic deformation, shear transformations, constitutive equations, shear bands, and strain hardening. Where possible we connect the observed behavior and properties to the structure of the glass on the atomic- and nano-scales.

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1. Introduction

Over the more than fifty years since their discovery [1] there has been extensive research into the structure and properties of metallic glasses. The earliest metallic glasses required rapid solidification and could therefore be produced only in limited forms. The development of bulk glass-forming alloys [2–4] not only provided samples suitable for traditional mechanical testing techniques but also raised the possibility that amorphous alloys might be employed in structural applications.

In 2007, two of us were co-authors on a review article summarizing the state of understanding of mechanical behavior of metallic glasses and proposing directions for future research [5]. Since then interest in the mechanical behavior of metallic glasses has remained intense and an updated review seems timely. In this article we review several areas where significant progress has been made and develop a few new ideas, particularly with regard to insights from theoretical and computational investigations of mechanical response of amorphous alloys (and disordered materials more generally). For a more comprehensive discussion we refer the reader to the earlier review [5] or to several other reviews of mechanical behavior of metallic glasses that have been published since 2007 [6–11].

The central paradigm of materials science states that the structure, properties, and processing of materials are interrelated. The periodicity of crystalline materials facilitates connections between their mechanical response and their atomic-scale structure, both experimentally (for example, by making dislocations visible in transmission electron microscopy) and theoretically. Such connections are much more challenging in metallic glasses, which lack long-range order and therefore are not as amenable to detailed characterization by traditional diffraction-based techniques. Nevertheless, experimental investigations using nanoscale probes now complement a rich set of computer simulations and theoretical analyses [12,13] to provide an emerging consensus of the phenomenology of the structural origin of mechanical response in these materials.

Connections between structure and properties, therefore, provide a unifying theme for the topics discussed in this review. After a brief review of our current understanding of the structure of metallic glasses, we begin our discussion of mechanical behavior at the atomic- and nano-scale by considering the use of scattering techniques for measuring elastic strain in metallic glasses, and the implications and limitations of this new technique. This leads into a

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discussion of non-affine atomic displacements during elastic deformation and the connection of these features to plastic deformation through shear transformations. We next consider how the structure of metallic glasses evolves under load and recent attempts to capture this evolution in the form of constitutive relations that could be useful for modeling of mechanical behavior. Moving to larger length scales, we examine localized plastic flow in shear bands with an emphasis on recent studies of their structure and dynamics. This introduces the topic of strain hardening in metallic glasses, through two recently-reported mechanisms: Exhaustion hardening and inherent hardening by relaxation. As in our original review [5], the last section points out important and promising directions for future research.

2. Structure of metallic glasses

The salient feature of the structure of metallic glasses is that they are disordered—a statement that is not as much of a truism as it may appear. The possible structural states of matter occupy a continuum from the perfect regularity and homogeneity of defect-free crystals to the utter disorder of ideal gases. Liquids and glasses are undoubtedly among the more disordered forms of condensed matter, but exactly how much structural order exists, what form it takes, and the length scale over which it extends are difficult questions that are the subject of ongoing research. The literature on this subject is extensive, but fortunately a comprehensive review of the structure of metallic glasses has recently been provided by Cheng and Ma [8], along with a more recent brief review by Ma [14]. In this section we highlight several key results that are important for understanding what follows; the interested reader is referred to those papers for a more complete discussion.

To begin at the shortest length scales, the high density and non-directional bonding of metallic glasses imply a high degree of short-range order based on close-packing of atoms. The basic packing unit is a tetrahedral cluster of four atoms; by allowing each atom to participate in several such clusters it is possible to achieve a high packing density, but because it is impossible to fill space with tetrahedra some degree of geometrical frustration is required (Fig. 1). Different glasses have different structural motifs, or preferred ways of packing tetrahedra (and accommodating the inevitable geometrical frustration). Chen and Ma refer to these different tetrahedral packings as “Z clusters” [8,14] (Fig. 2). One much-discussed Z cluster consists of twelve atoms arranged at the vertices of a icosahedron around a central atom; in such a cluster the central atom plus any three mutually adjacent surface atoms form a tetrahedron (usually distorted). Although “five-fold” bonds—clusters where two adjacent atoms have five neighbors in common—are frequently observed, they should not be taken as indicative of icosahedral clustering which is, in fact, not very common. Rather, the presence of the five-fold bonds reflects dense polytetrahedral packing with a minimum of rotational defects [14,15].

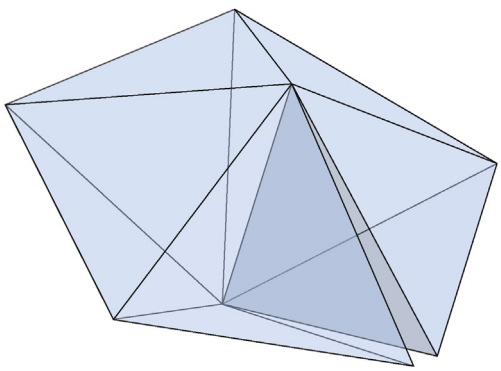

Fig. 1. Space-filling packing of regular tetrahedra is not possible, as illustrated here for the case of five tetrahedra sharing a common edge. (Artwork issued under the terms of the Creative Commons Attribution License and based on an original in Ref. [16].)

An example of the connection of atomic-scale structure to mechanical behavior is provided by atomistic simulations of Cu–Zr alloys. The fraction of Cu-centered icosahedral clusters increases dramatically as the liquid is cooled towards the glass transition, which is correlated with slowing dynamics of the system [15,18,19]. Adding Al to this simulated alloy enhances the development of icosahedral clusters, further slowing the dynamics [20]. The influence of short-range order extends to the glassy state where locally greater icosahedral order correlates with higher stiffness and resistance to yield. Regions of the structure without this favorable short-range order, which have been called “geometrically unfavorable motifs” (GUMs) [14], have lower stiffness and a greater tendency to undergo shear transformations [21,22] as will be discussed in more detail below.

This last observation points out the importance of structural heterogeneity for understanding mechanical behavior of metallic glasses. It is reasonable to suspect that this heterogeneity may reflect the structure of the supercooled liquid from which the glass forms. Because of intense interest in the fundamental nature of the glass transition itself, the structure and dynamics of supercooled liquids near the glass transition have been the subject of extensive research [23] and there is strong evidence of increasing inhomogeneity upon cooling towards the glass transition [24,25].

Beyond the nearest–neighbor interactions some kind of so-called “medium-range” order is required to achieve the high densities observed for metallic glasses. The most developed theory of medium-range order in metallic glasses is the efficient cluster packing model of Miracle and coworkers [26,27]. This model begins with short-range order clusters similar to those discussed above (but centered on solute atoms) and then posits that these clusters are themselves arranged to produce efficient overall packing, for instance into fcc arrays. The structural order is presumed to extend over only a few cluster diameters. The densities predicted on the basis of this model are in reasonable agreement with experiment, and the model has some success in reproducing experimental measurements of the separations of solute atom pairs [27]. As with the nearest–neighbor interactions, it is reasonable to suppose that the structure is heterogeneous on these larger length scales.

3. Elastic deformation

To a metallurgist, elastic deformation of crystals is among the simplest mechanical behaviors to understand. At small strains (<0.2%) deformation is fully reversible and follows Hooke's law (although non-linear and anelastic behavior can also be observed if the crystal has impurities or defects, or at large strains). At low temperatures in simple crystals this elastic response can be calculated as the stress resulting from fully affine deformation of the lattice—that is, a simple rescaling of the lattice parameters commensurate with the imposed loading conditions, accomplished by simply stretching (or compressing) primary atomic bonds.

It has become apparent over the last few years, however, that elastic deformation of metallic glasses is considerably more complex. Unlike crystals, in a disordered material every atom has a unique atomic environment and so the response of every atom to the macroscopic loading conditions can, in principle, be different. This difference leads to a variety of effects, including non-linear behavior, anelasticity, microplasticity at very small strains, and elastic behavior that apparently depends on the length scale of the

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