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A microscopic continuum model for defect dynamics in metallic glasses

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ABSTRACT

Motivated by results of the topological theory of glasses accounting for geometric frustration, we develop the simplest possible continuum mechanical model of defect dynamics in metallic glasses that accounts for topological, energetic, and kinetic ideas. A geometrical description of ingredients of the structure of metallic glasses using the concept of local order based on Frank–Kasper phases and the notion of disclinations as topological defects in these structures is proposed. This novel kinematics is incorporated in a continuum mechanical framework capable of describing the interactions of disclinations and also of dislocations (interpreted as pairs of opposite disclinations). The model is aimed towards the development of a microscopic understanding of the plasticity of such materials. We discuss the expected predictive capabilities of the model vis-a-vis some observed physical behaviors of metallic glasses.

1. Introduction

Despite their technological relevance, there does not exist a fundamental characterization of the process of plastic deformation in a metallic glass, relating its structure and ‘defects’ to deformation (Greer et al., 2013; Schuh et al., 2007); indeed, whether any structural defect in a glass can be characterized at all seems to be an open question. In many ways this is surprising as there exists a beautiful body of work in the physics literature based on topological ideas related to geometric frustration and the so-called polytope model of glass that does rationalize defects in glass structure that are linked to atomic configurations (of at least mono-atomic materials interacting by pair potentials). Glasses have also been vigorously studied from the mechanics of materials and materials science perspectives, but without making connection to the physics literature related to geometric frustration. Gilman (1973) did propose a model of plasticity in glasses based on dislocation motion, and an attempt to observe glass-dislocations in an atomistic model was made in Chaudhari et al. (1979), but these ideas have not lead to widespread adoption in the community of metallic glass researchers. Currently, there is no theory available to study the far-from-equilibrium mechanical response of bulk metallic glasses that gives equal importance to topological, energetic, and kinetic ideas. As mentioned, a primary hindrance has been the unequivocal identification of a structural defect as the essential carrier of inelastic deformation in metallic glasses (Srolovitz et al., 1981). The concept of a shear transformation zone originated by Argon (1979) and developed by Falk and Langer (1998) comes close, but it is not identifiable as a rigorous structural state variable from atomic configurations of glass-forming alloys. The work of Spaepen (1977) related

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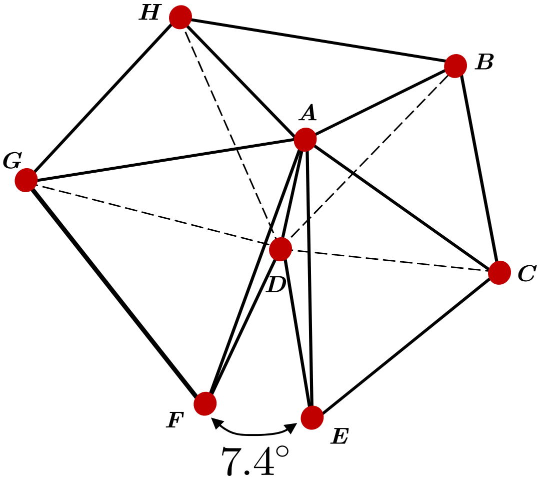

Fig. 1. Schematic of geometric frustration arising from tiling space with regular tetrahedra.

to free-volume is the other advance in the direction of characterizing a structural state variable for glasses. Quite surprisingly, the ideas of Nelson (1983), making a direct connection between 'glass dislocations' consisting of disclination-dipoles and atomic configurations, have not been considered in the vast literature on attempts to understand structure-deformation connections in metallic glasses (Anand and Su, 2005; Falk and Langer, 1998; Greer et al., 2013; Schuh et al., 2007; Takeuchi and Edagawa, 2011). Our goal in this paper is to address this gap with the hope that it may lend complementary insight into the modeling of the mechanical behavior of metallic glasses and amorphous materials.

Specifically, we will model the metallic glass as a sea of geometrically frustrated regular tetrahedra arranged predominantly in clusters of five around static backbones of 5-fold disclination lines. This sea is thought of as punctuated by mobile 4 and 6-fold disclination dipole lines that can be interpreted as dislocation lines (with spread out cores) in the medium, following the topological theory of defects (Nelson, 1983). There appears to be evidence that regions of non-pentagonal packing seem to suffer the most plasticity for amorphous materials (Ding et al., 2014; Takeuchi and Edagawa, 2011). We combine these insights based essentially on homotopy theory describing possible lowest-energy static states of the glass with a partial differential equation based model of dislocation dynamics. The result is a model for dissipative defect dynamics in metallic glasses and similar amorphous materials. With no further assumptions beyond this rigorous kinematics and the simplest linear kinetic assumptions arising from enforcing the second law of thermodynamics, we show that the proposed model provides plausible explanations for

- the origin of a stochastic, observed internal stress field
- dilatancy in observed plastic flow of metallic glasses
- pressure dependence of observed plastic flow
- threshold behavior in the motion of these glass dislocations in response to stress
- structure and dynamics of deformation localization in the form of shear bands; in particular their longitudinal propagation taking full account of the effects of material inertia.

The outline of the paper is as follows: in Section 2 we briefly review a few elements of the vast literature on the physics and engineering of amorphous solids, including a summary of Nelson's proposal (Nelson, 1983) for modeling the kinematics of glasses. Section 3 describes the adaptation of Nelson's idea to a flat, 3-d space treatment, showing how, in the first approximation, 'glass-dislocations' may be rationalized. We substantiate these ideas with quantum mechanical electronic structure calculations showing these defects. With this kinematic basis, in Section 4 we adapt a continuum model for dislocation dynamics (Acharya, 2001, 2010; Zhang et al., 2015), but now involving disclinations as well for goals particular to this application, and show some of its implications related to the 'predictions' mentioned above.

2. Brief review of the literature

The fundamental idea in understanding the mechanics of glasses is geometric frustration (Kleman and Friedel, 2008). This refers to the fact that *regular* tetrahedra, all with equal edge-lengths, cannot tile space. The easiest way to see this is to visualize a set of five regular tetrahedra sharing a common edge as in Fig. 1. The dihedral gap-angle is calculated based on the geometry of a regular tetrahedron shown in Fig. 2. One considers tetrahedra as the basic structural building block since it is easy to see (Nelson, 1983) that for atoms interacting by pair potentials, a regular tetrahedron of four atoms has to be a ground state. Putting five such tetrahedra without a gap as in Fig. 1 necessarily means an atomic assembly under stress.