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The anomalous yield behavior of fused silica glass

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ABSTRACT

We develop a critical-state model of fused silica plasticity on the basis of data mined from molecular dynamics (MD) calculations. The MD data is suggestive of an irreversible densification transition in volumetric compression resulting in permanent, or plastic, densification upon unloading. The MD data also reveals an evolution towards a critical state of constant volume under pressure-shear deformation. The trend towards constant volume is from above, when the glass is overconsolidated, or from below, when it is underconsolidated. We show that these characteristic behaviors are well-captured by a critical state model of plasticity, where the densification law for glass takes the place of the classical consolidation law of granular media and the locus of constant-volume states defines the critical-state line. A salient feature of the critical-state line of fused silica, as identified from the MD data, that renders its yield behavior anomalous is that it is strongly non-convex, owing to the existence of two well-differentiated phases at low and high pressures. We argue that this strong non-convexity of yield explains the patterning that is observed in molecular dynamics calculations of amorphous solids deforming in shear. We employ an explicit and exact rank-2 envelope construction to upscale the microscopic critical-state model to the macroscale. Remarkably, owing to the equilibrium constraint the resulting effective macroscopic behavior is still characterized by a non-convex critical-state line. Despite this lack of convexity, the effective macroscopic model is stable against microstructure formation and defines well-posed boundary-value problems.

1. Introduction

The anomalous shear modulus behavior of silica glass has been a long-standing topic of investigation. For instance, Kondo et al. (1981) and references therein examined the non-monotonic dependence of the elastic moduli on pressure for fused quartz, cf. Fig. 1(a). Notably, between 0 and 2.5 GPa, the shear modulus and bulk modulus decreases. Likewise, the anomalous pressure dependence of the strength of amorphous silica has also received considerable attention. For instance, Meade and Jeanloz (1988) made measurements of the yield strength at pressures up to 81 GPa at room temperature and showed that the strength of amorphous silica decreases significantly as it is compressed to denser structures with higher coordination, Fig. 1(b). Clifton et al. (1998), Abou-Sayed and Clifton (1976), Sundaram and Clifton (1998) and Simha and Gupta (2004) investigated the effect of pressure on failure waves in silica and soda-lime glass through angled flyer plate impact experiments and observed a loss of shear strength as the failure wave traversed the glass at pressures of 4–6 GPa.

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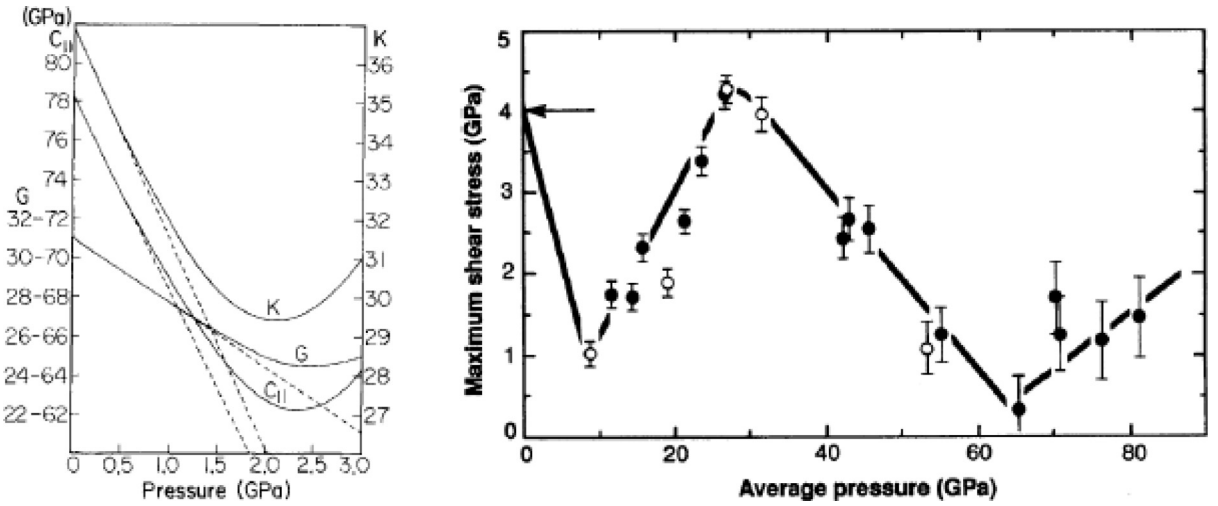

Fig. 1. (a) Elastic moduli *vs.* pressure as measured by Kondo et al. (1981); (b) Measurements of the yield strength of SiO_2 glass at pressures as high as 81 GPa at room temperature showing the variation of the strength of amorphous silica as it is compressed to denser structures with higher coordination (Meade and Jeanloz, 1988).

These phenomena appear to be intimately linked to structural rearrangements occurring at the atomic level. Sato and Funamori (2008, 2010) performed structural measurements of SiO_2 glass Si-O bond length and coordination number at pressures from 20 to 100 GPa using a diamond anvil cell and x-ray diffraction. They observed a transition from four-fold to six-fold coordinated structure that comes to completion at around 45 GPa. Wakabayashi et al. (2011) studied the densification behavior again using a diamond anvil cell experimental setup and concluded that permanent densification occurs for pressures between 9 and 13 GPa. Vandembroucq et al. (2008) observed pressure-induced reorganizations of the amorphous network allowing a more efficient packing of tetrahedra that remain linked at their vertices only. Inamura et al. (2004) studied transformations at pressures of up to about 20 GPa and temperatures of up to about 700 C. Their results are indicative of the existence of a high pressure variant of silica glass. However, a sharp phase transformation was not observed, which is suggestive of a volumetric plastic hardening mechanism. Luo et al. (2004) reported a novel dense silica polymorph retrieved from shock-wave and diamond-anvil cell experiments. The polymorph is composed of face-sharing polyhedra and it has a density similar to stishovite. Sterical constraints on the bond angles induce an intrinsic disorder in the Si positions and the resulting Si-coordination is transitional between four and sixfold.

Beyond the specific instance of fused silica, there exists an extensive literature on the microstructural mechanisms that mediate plastic deformation in amorphous solids. Demkowicz and Argon (2005) observed that in amorphous silicon plastic deformation is mediated by autocatalytic *avalanches* of unit inelastic shearing events. They performed a bond-angle analysis in order to correlate changes in the average bond angle to discrete relaxation events. Falk and Langer (1998) and Langer (2001) formulated a theory of *shear transformation zones* (STZ) to describe viscoplastic deformation in amorphous solids. Langer's theory accounts for the formation of deformation patterns such as shear banding in metallic glasses. An alternative theory of structural rearrangement in bulk metallic solids is based on *free-volume* kinetics. Chen and Goldstein (1972) observed that the flow in metallic glasses is strongly inhomogeneous at high stresses and low temperatures, and attributed the patterning to local reductions in flow strength. Polk and Turnbull (1972) and Spaepen (1977) argued that these reductions are due to the formation of free volume, and that the attendant inhomogeneous flow is controlled by the competition between the stress-driven creation and diffusional annihilation of free volume. This hypothesis was later verified experimentally by Argon (1979).

There have also been extensive molecular dynamics studies of the densification behavior and plastic deformations of amorphous silica. Pilla et al. (2003), Lacks (1998), Wu et al. (2012) and Huang and Kieffer (2004a, 2004b) computed pressure-density relationships over a broad range of pressures and temperatures. The attendant mechanisms of deformation entail transitions from four-fold to six-fold coordination. In particular, Wu et al. (2012) argued that the four-fold to six-fold transition is not direct but involves the formation of an intermediate five-fold coordinated structures at $\sim$12 GPa and is only complete at $\sim$60 GPa. Liang et al. (2007) noted anomalous behavior in the form of a minimum shear strength occurring at $\sim$10 GPa and proposed a mechanism involving unquenchable 5-fold defects. Mantisi et al. (2012) utilized an NVE ensemble along with monoclinic change in the simulation box orientation to study combined pressure-shear loading. They observed steps, or *jerking*, in the shear stress *vs.* shear strain response, which they attribute to either finite size effects or localized dissipative rearrangements. Several authors (Lemaître and Caroli, 2009; Maloney and Robbins, 2008) have performed molecular dynamics calculations on amorphous solids deforming under shear and found that the resulting deformation field forms distinctive patterns to accommodate permanent deformations, Fig. 2.

This past work strongly suggests that the plastic deformation of amorphous solids and, in particular, fused silica glass, is mediated by localized atomic-level instabilities that promote deformation patterning, Fig. 2. Such fine-scale pattern forma-