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Strain-rate and temperature dependence of yield stress of amorphous solids via a self-learning metabasin escape algorithm

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ABSTRACT

A general self-learning metabasin escape (SLME) algorithm (Cao et al., 2012) is coupled in this work with continuous shear deformations to probe the yield stress as a function of strain rate and temperature for a binary Lennard-Jones (LJ) amorphous solid. The approach is shown to match the results of classical molecular dynamics (MD) at high strain rates where the MD results are valid, but, importantly, is able to access experimental strain rates that are about ten orders of magnitude slower than MD. In doing so, we find in agreement with previous experimental studies that a substantial decrease in yield stress is observed with a decreasing strain rate. At room temperature and laboratory strain rates, the activation volume associated with yield is found to contain about 10 LJ particles, while the yield stress is as sensitive to a $1.5\%T_g$ increase in temperature as it is to a one order of magnitude decrease in the strain rate. Moreover, our SLME results suggest that the SLME and extrapolated results from MD simulations follow distinctly different energetic pathways during the applied shear deformation at low temperatures and experimental strain rates, which implies that extrapolation of the governing deformation mechanisms from MD strain rates to experimental may not be valid.

1. Introduction

The plasticity of amorphous solids such as metallic glasses has been extensively studied in recent years (Schuh et al., 2007). A key parameter that must be accurately predicted in this regard is the yield stress, because amorphous solids typically fail catastrophically immediately following yield via shearbanding (Cheng and Ma, 2011a) due to their lack of strain hardening. However, a definitive link between the effects of temperature and experimentally relevant strain rates on the yield stress has not been established to-date.

There has recently been significant effort in studying the inelastic deformation of amorphous solids using atomistic simulation techniques such as classical molecular dynamics (MD) (Falk and Langer, 1998; Cao et al., 2009; Zink et al., 2006; Shimizu et al., 2006; Cheng and Ma, 2011b; Shi and Falk, 2007; Murali et al., 2011). However, MD simulations suffer from well-known issues related to strain rates that are about 10 orders of magnitude larger than the experimentally accessible

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ones. Other researchers have attempted to avoid the time scale and strain rate issues that are inherent to MD by utilizing athermal, quasistatic shear (AQS) of amorphous solids to study the mechanisms leading to strain localization (Tsamados et al., 2009; Maloney and Lemaitre, 2006; Tanguy et al., 2006; Karmakar et al., 2010; Dasgupta et al., 2012). Because there is no thermal energy in the system as would be the case in real experiments, the energetic barriers that are crossed on the potential energy surface (PES) are artificially low, and thus the system does not explore all possible configurations (i.e. deformation mechanisms) that it would experimentally. A more recent approach to avoiding the limitations of MD to study the yielding and plasticity of amorphous solids is so-called PES exploration techniques (Rodney and Schuh, 2009a,b; Delogu, 2008; Mayr, 2006). These methods have had some success in calculating the activation energy and volumes of shear transformation zones (STZs) (Delogu, 2008; Mayr, 2006). However, none of these studies has been able to explore a sufficiently large portion of the PES to make definitive statements about the strain rate and temperature-dependence of the yield stress for amorphous solids, particularly at laboratory strain rates.

The above discussion makes clear that there is a pressing need for advanced atomistic simulation techniques that are able to access experimental strain rates, and thus give new insights into the mechanical behavior and properties of amorphous solids at these slower strain rates. Therefore, there are two key objectives of this work. The first is to introduce a new approach to studying the mechanics of amorphous solids at strain rates ranging from experimental to those seen in MD simulations. We accomplish this by presenting a new computational technique that couples the recently developed self-learning metabasin escape (SLME) algorithm for PES exploration (Cao et al., 2012; Cao et al., 2013) with shear deformation and the standard Monte Carlo approach. As a first step, we verify the ability of the SLME approach to reproduce benchmark classical MD simulation results at high strain rates. The second objective of this work is to determine the effects of strain rate and temperature on the yield stress of amorphous solids, with an emphasis on studying these quantities using the SLME method at experimentally relevant strain rates that MD cannot access. The findings have implications for the validity of interpreting recently developed universal scaling laws for amorphous solids (Johnson and Samwer, 2005) within the context of extrapolating the results of high strain rate MD simulations to experimental strain rates, as has recently been proposed (Cheng and Ma, 2011b), and also for the universality of the yield mechanism (Johnson and Samwer, 2005) for amorphous solids for all strain rates and temperatures. We also establish the strain rate equivalent of temperature on the yield stress at experimentally accessible strain rates.

2. Simulation details

2.1. Binary Lennard-Jones model

A binary Lennard-Jones (bLJ) potential (Kob and Andersen, 1995) is used in our simulations with periodic boundary conditions in all three directions. This bLJ potential is widely utilized for atomistic studies of amorphous solids because its ground state is not crystalline. The system contained $N=1000$ particles of the same unit mass, with an A:B particle ratio of 4:1. Standard parameters are used as follows: $\epsilon_{AA}=1.0$, $\epsilon_{AB}=1.5$, $\epsilon_{BB}=0.5$, $\sigma_{AA}=1.0$, $\sigma_{AB}=0.8$, and $\sigma_{BB}=0.88$, while the cutoff distances are set to $2.5\sigma_{AA}$. Supercooled liquids were prepared by equilibrating the system at temperature $T=2.0$ followed by slow quenching to $T=1.0$ using the *NVT* ensemble at a constant particle density of 1.2. These supercooled liquids were then further quenched at constant *NPT* to obtain stress-free glassy structures at different target temperatures, $T=0.05$, 0.1, 0.15, 0.2, 0.3 and 0.4 near and below the glass transition temperature $T_g=0.37$ (Kushima et al., 2009a), where all cooling was done at a constant rate of 4×10^{-6} (Sastry et al., 1998). All units in this section, as well as the rest of the paper, are given in reduced (dimensionless) LJ form.

2.2. Self-learning metabasin escape algorithm

We now overview the computational technique, the self-learning metabasin escape (SLME) algorithm that we use to explore the PES for each state of strain for a given strain rate. As illustrated in Fig. 1, Kushima et al. (2009a) recently developed the autonomous basin climbing (ABC) algorithm to explore the PES for a given atomistic system. The ABC method works in a very intuitive manner. Starting from any local energy minimum, penalty functions $\phi_i(\mathbf{r})$ are successively applied in order to climb out of the current local minima well and explore other, neighboring energy wells. Mathematically, this is written as

$$\Psi(\mathbf{r})=E(\mathbf{r})+\sum_{i=1}^{p}\phi_i(\mathbf{r}), \tag{1}$$

where $\Psi(\mathbf{r})$ is the augmented potential energy due to the addition of the penalty functions, $E(\mathbf{r})$ is the original potential energy function, i.e. the bLJ potential in the present case, and p is the total number of penalty functions. Although in principle any type of localized functions (i.e. Gaussians, Laio and Parrinello, 2002; Kushima et al., 2009a,b) can be used in Eq. (1), we chose quartic penalty functions in this work due to their desirable property of naturally vanishing energy and forces at the penalized subspace boundaries (Cao et al., 2012).

As can be inferred from Eq. (1), many small penalty functions are needed in order to push the system out of a given energy basin. However, all of these penalty functions must be kept such that the system does not fall back into an energy basin that has already been explored. Clearly, the requirement to store all previous penalty functions becomes expensive as