



Full length article

Thermally-activated stress relaxation in a model amorphous solid and the formation of a system-spanning shear event

P.M. Derlet ^{a,*}, R. Maaß ^b^a Condensed Matter Theory Group, Paul Scherrer Institut, CH-5232, Villigen PSI, Switzerland^b Department of Materials Science and Engineering and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana Champaign, 1304 West Green Street, Urbana, IL, 61801, USA

ARTICLE INFO

Article history:

Received 7 July 2017

Received in revised form

13 September 2017

Accepted 6 October 2017

Available online 9 October 2017

Keywords:

Bulk metallic glasses

Amorphous

Plasticity

Structural relaxation

Atomistic simulation

ABSTRACT

Molecular dynamics simulations are performed to investigate the underlying thermally activated processes contributing to stress relaxation in a model binary amorphous system. Amorphous samples are first shear strained at zero kelvin and then the temperature is ramped up to the glass transition regime. Four orders of magnitude in the temperature ramp rate are considered. It is found that depending on the degree to which the amorphous solid is relaxed, significant atomic-scale activity is seen well below the glass transition regime, and that this is largely independent of the external load. The stress relaxation below the glass-transition temperature is mediated by spatially localized and thermally activated structural excitations. Over time, such thermally driven stochastic activity can collectively lead to a global gauge shearing, the location of which correlates with regions of low icosahedral content with lower coordination and higher density.

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1. Introduction

The amorphous solid contains no long-range order and therefore, unlike a crystal with its canonical defect structure, there exists no obvious finite lower bound in the length and energy scale associated with its structural excitations. Because of the disorder, there is a general consensus that such excitations are local in nature, which is also a central assumption of early microscopic models on the thermally activated deformation of metallic glasses [1,2]. The collective activity of such local plastic events are believed to be responsible for bulk emergent plastic behaviour, a picture that has been used by thermally driven coarse grained models [3–8] and supported by stress driven atomistic simulations [9–12] (see also the review article Ref. [13]).

It is however usual to ascribe a defined energy scale to such forms of plasticity, the value of which depends on the length scale one is probing. For example, the typically reported barrier energy for a local atomic jump is approximately $15\text{--}25 k_B T_g$ ($< 1\text{--}2$ eV) and approximately $20\text{--}120 k_B T_g$ ($1\text{--}5$ eV) [14] for a shear-transformation zone, or, if one considers the framework of

relaxations defined via mechanical spectroscopy, values of 5 eV [15], 0.6–1.5 eV [16,17] and 0.2–0.6 eV [18,19] are found for alpha, beta, and gamma relaxations, respectively. These defined barrier energies, or ranges of barrier energies, are somewhat at odds with a general consideration that the disordered material should admit a broad distribution of barrier energies, of which the lower-end tail can be expected to play a dominant role upon loading at finite temperatures. However, it is an experimentally delicate endeavor to determine such a distribution of barrier energies, where most mechanical testing protocols allow only an effective mean barrier energy to be determined that typically falls well into the aforementioned ranges. Such effective barrier energies can, for example, be obtained indirectly with rate-dependent nanoindentation [20], stress-relaxation or creep [21–23], temperature-dependent deformation [24,25], or mechanical spectroscopy [17]. The fact that significant structural modifications can occur in metallic glasses at ambient conditions at stresses below the yield stress [26], and indeed at levels as low as 1% of the yield stress [27], suggests the viewpoint of ample structural activity at virtually any stress and the activation of numerous structural rearrangements with correspondingly small energy barriers [28].

Atomistic simulations are much more suited to obtain a detailed view of the energy scale of structural transitions. Indeed, potential energy landscape explorations of model amorphous materials give

* Corresponding author.

E-mail addresses: peter.derlet@psi.ch (P.M. Derlet), rmaass@illinois.edu (R. Maaß).

direct support of a local structural transition picture at the microscopic level [29–37]. In these simulations, the Activation Relaxation Technique nouveau (ARTn) method [38,39] is used to catalog nearby saddle-point configurations of a zero-force and zero-temperature configuration. The central results of such potential energy landscape exploration are 1) the saddle-point configurations of the model amorphous structures involve atomic displacements which are spatially localized and 2) a distribution of saddle-point energies is observed which, when subtracted from the energy of the starting configuration, gives a positive definite distribution of barrier energies. For a sufficiently relaxed sample, such distributions appear to tend to zero as the barrier energy approaches zero and suggests no obvious finite lower bound for the barrier-energy scale.

If there is no lower bound to the barrier energy scale, thermally-activated structural excitations should exist at all temperatures, a subset of which would be accessible using long-time molecular dynamic (MD) simulations. Such logic has motivated our recent work in which thermally-activated structural transformations are studied using direct molecular dynamics (MD) [40]. In that work, the atomic scale activity of a model Lennard-Jones (LJ) system was studied as a function of increasing temperature. In particular, two 50:50 binary LJ configurations, one more relaxed than the other, were found to admit a significant amount of thermally driven structural activity well below the glass-transition temperature regime, which induced relaxation in the form of a lower cohesive energy and a higher icosahedral fraction. This relaxation was mediated by local structural excitations (LSEs) usually consisting of a chain of central atoms undergoing maximum displacement that is surrounded by a field of smaller displacements. This characteristic was also seen in ARTn investigations of the same system [33,34].

In our earlier MD work [40], the central atomic displacements of the LSEs were observed to be less than that of the mean atomic distance for low temperatures, however, as the temperature approached the glass transition regime, these displacements typically approached the magnitude of a bond length. The central atoms of such thermally activated LSEs were found to originate in regions characterized by low coordination, high density and low icosahedral content, and usually involve the smaller atomic species [40]. These simulations were performed under zero load and clearly indicate a lack of a non-negligible finite lower-bound in both length and energy scales.

The present work extends such temperature ramping simulations to the case in which the initial zero-temperature configuration carries an elastic shear load. We find that upon increasing the temperature, thermally-activated structural excitations are again increasingly seen which are no different from the zero-load LSEs observed in Ref. [40]. As the temperature rises, the imposed shear stress reduces. Four orders of temperature ramp rate are considered and it is seen that, for the slower rates, the shear stress undergoes significant reduction at temperatures well below the glass transition regime in parallel with structural relaxation. Indeed for the slowest rate, the shear stress has almost reduced to zero as the glass-transition temperature is reached. For the more relaxed sample, some correlated thermally-activated events are observed resulting in a localized plasticity which spans the entire gauge of the sample. Thus significant thermally-activated plasticity has occurred without rejuvenation. The work concludes with a discussion of the relationship between stress reduction and structural relaxation, and the implication of these results in terms of microscopic shear-band formation.

2. Simulation methods

Model computer generated amorphous structures are produced

for a 50:50 binary system using the Wahnström parametrized Lennard-Jones pair potential [41]. For this potential, the parameter ϵ sets the energy scale and the parameter σ_{11} sets the length scale. The time scale is set by the quantity $\sigma_{11}\sqrt{m_1/\epsilon}$ where m_1 and m_2 are the masses of the two atom types. For the present simulations the masses of two atom types are arbitrarily chosen to be $m_1 = 2$ and $m_2 = 1$ atomic masses. The absolute temperature, T , is expressed as an energy, $k_B T$, using $k_B = 8.617 \times 10^{-5}\epsilon$. The NVT ensemble is used and the LAMMPS software [42] is employed to perform the molecular dynamics simulations. To calculate the icosahedral percentage a Voronoi analysis is done using the OVITO visualization software [43].

For the current simulations, a simulation cell containing 25600 atoms with an aspect ratio 1:1:12.5 is used (corresponding to the x-y-z axes). Three-dimensional periodic boundary conditions are used. Whilst a small material volume to study bulk macroscopic plasticity, it is of a sufficient size to study the thermally-activated LSEs which will mediate the observed stress relaxation. The large aspect ratio is chosen to increase the likelihood of observing collective stochastic activity across the sample's gauge. This later aspect will be discussed in more detail in the proceeding sections.

The quenched sample is prepared by first equilibrating a liquid at a temperature of $k_B T = 0.86\epsilon$. Subsequently, the sample is linearly quenched at a rate of $Q^{\text{LQ}} = -6 \times 10^{-4} \epsilon/\tau$, corresponding to a drop in temperature equal to $100k_B = 0.0086\epsilon$ every 10000 molecular dynamics iterations. This quenching is continued until the temperature approaches 0 K, at which point, a conjugate gradient method is used to relax the structure to a local potential-energy minimum. This configuration is referred to as the quenched sample. Inspection of the potential energy per atom as a function of temperature during the quench reveals a change in slope at , which $k_B T_G \approx 0.55\epsilon$ defines a fictive glass-transition temperature. A second, more relaxed, sample is produced by halting the quench at $0.95T_G$ and performing a long-time ($\approx 23 \times 10^6$ MD steps) constant temperature relaxation at this fixed temperature, after which the sample is linearly quenched to 0 K in the same manner as the previously introduced quenched sample. This sample has an energy per atom which is 0.05ϵ lower, and an icosahedral percentage that is 5.5 (in percentage value) higher than the quenched sample. This sample is therefore more relaxed, and the final 0 K configuration is referred to as the quench-relaxed sample. For more details of this type of preparation procedure see Ref. [40], which also contains an analysis of the structural difference between similarly quenched and quench-relaxed samples.

The presently used Lennard-Jones potential does not allow for a direct quantitative comparison with an experimentally realizable binary bulk metallic glass. The Lennard-Jones potential has however been extensively used for the study of model binary amorphous structures [9,13], giving fundamental insight in to the general properties of glassy structures. Indeed, the potential gives qualitatively similar results as that of the many-body potentials based on, for example, the Embedded Atom Model (EAM) which phenomenologically models the unsaturated nature of the metallic bond [44]. This similarity is due to a number of reasons: 1) both pair potentials and EAM potentials do not contain explicit angular terms, 2) bulk glasses do not contain strong variations in electron density and therefore the embedding term can be well represented by a first order Taylor expansion which results in an effective pair potential, and 3) because of strong non-affine elastic deformation in a structural glass, a pair potential can also induce a breakdown in the Cauchy relation giving ratios of bulk to shear modulus that are comparable with experiment. For a more detailed discussion see Ref. [40].

Finally, the choice of an NVT over an NPT ensemble is motivated

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