

Yield point of metallic glass

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Abstract

Shear bands form in most bulk metallic glasses (BMGs) within a narrow range of uniaxial strain $\varepsilon_y \cong 2\%$. We propose this critical condition corresponds to embryonic shear band (ESB) propagation, not its nucleation. To propagate an ESB, the far-field shear stress $\tau_\infty \approx E\varepsilon_y/2$ must exceed the quasi-steady-state glue traction τ_{glue} of shear-alienated glass until the glass transition temperature is approached internally due to frictional heating, at which point ESB matures as a runaway shear crack. The incubation length scale l_{inc} necessary for this maturation is estimated to be $\sim 10^2$ nm for Zr-based BMGs, below which sample size-scale shear localization does not happen. In shear-alienated glass, the last resistance against localized shearing comes from extremely fast downhill dissipative dynamics of timescale comparable to atomic vibrations, allowing molecular dynamics (MD) simulations to capture this recovery process which governs τ_{glue} . We model four metallic glasses: a binary Lennard-Jones system, two binary embedded atom potential systems and a quaternary embedded atom system. Despite vast differences in the structure and interatomic interactions, the four MD calculations give ε_y predictions of 2.4%, 2.1%, 2.6% and 2.9%, respectively.

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1. Shear band model

Bulk metallic glasses (BMGs) are emerging engineering materials [1] with very high yield strength, relatively high fracture toughness, low internal friction and good corrosion resistance. A particular feature of this class of materials is that the plastic yield points of most BMGs fall within a small range around $\varepsilon_y = 2\%$ at room temperature [1,2], beyond which shear bands nucleate and propagate globally [3,4], apparently with little further resistance. The “mature” shear bands amenable to microscopy characterizations are of width $w \sim 10^1$ – 10^2 nm wide [3–5], with offset shear displacement δ of the same scale [4]. Infrared camera videos show that the shear bands are roughly planar and nucleate preferentially from the surface, with intense heating [4] and evidence of melting at the trailing edges [4,6,7].

Despite its relevance, a quantitative description of how a shear band forms in BMGs [8–11], and the stress and temperature fields of this dynamical defect, are lacking. Several questions can be raised. (a) Is the measured ε_y controlled by shear band nucleation or propagation – in what sense precisely, and determined by processes at what time and length scales [8–10]? (b) Is the shear band stress field similar to that of a dislocation or a crack [9,12]? (That is, is shear traction fully restored behind the shear band tip or lost? The former induces an r^{-1} -type while the latter induces an $r^{-1/2}$ -type elastic stress field.) (c) Why is ε_y nearly universal [2]?

A mature shear band (MSB) in a BMG is proposed to be similar to a mode II or III dynamical shear crack [11,13] as illustrated in Fig. 1a, driven by far-field shear stress τ_∞ . The band has four zones. The last zone is liquid or near-liquid, due to friction-induced high temperature $T \sim T_g$ (where T_g is the glass transition temperature), and basically cannot sustain traction since $\tau \propto \eta_{\text{liquid}}$, where

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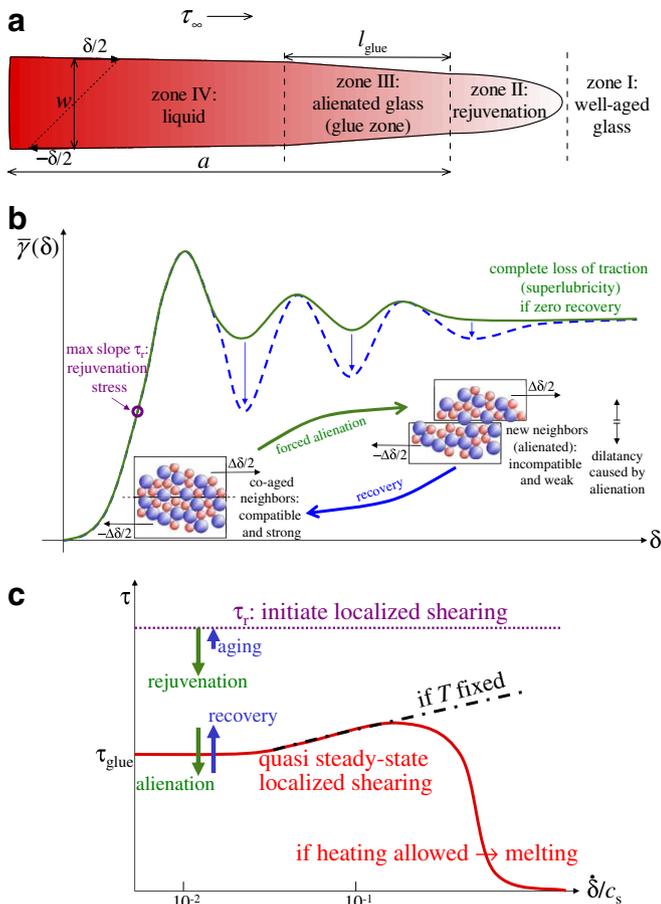


Fig. 1. (a) Aged-rejuvenation-glass-liquid (ARGL) model of shear band in BMGs. The shading represents temperature. (b) GSF $\bar{\gamma}(\delta)$ of a glass as a function of a sharp displacement discontinuity δ . The solid curve illustrates the behavior without any recovery process. The dashed curve shows that, as time increases, recovery occurs and the energy traps get deeper. (c) Shear traction of glass as a function of local sliding speed, evaluated at a fixed observation time t_{eval} .

η_{liquid} is the viscosity and $\dot{\gamma}$ the strain rate. η_{liquid} is many orders of magnitude smaller than η_{glass} , so the traction offered by the liquid is negligibly small compared to that of the glass. Zone III is the “glue” region: its temperature is below T_g and consists of shear-rejuvenated [14] and subsequently shear-alienated glass. The traction it offers, τ_{glue} , over a length l_{glue} , provides the main resistance against shear band propagation. (τ_{glue} is conceptually similar to the drag of a stacking fault behind a Shockley partial dislocation: only when $\tau_{\infty} > \tau_{\text{glue}}$ can one move the shear singularity.) Zone I consists of well-aged glass [15] not yet processed by the shear front and thus deforms elastically. Zone II at the “crack tip” is the rejuvenation region, where the glass undergoes transition from well-aged to rejuvenated state [14], under a locally very high shear stress $\tau > \tau_r$, where τ_r is the rejuvenation stress, an intrinsic property of well-aged glass (Fig. 1b).

The idea of softened materials inside the shear band follows common views [8–11]. The question relevant for understanding the near-universal ε_y is what the leading physical cause of softening is: heating [11], free-volume

aggregation, or some other effects; the time sequence of the softening effects; and if we can quantify them atomistically.

2. Alienation-induced softening

Here we introduce the conceptual aid of generalized stacking fault energy (GSF) $\bar{\gamma}(\delta)$ [16,17] to disordered systems. Imagine we take a well-aged glass, draw a horizon line that separates the atoms into two halves and slide the upper half against the lower half in the x -direction by δ . To prevent atom impingement, we allow all atoms to relax freely in y and z , but their x are constrained. We take a large enough sampling area S_0 and define GSF by the average energy increase per area: $\bar{\gamma}(\delta) \equiv \Delta E(\delta)/S_0$. The derivative $\bar{\gamma}'(\delta)$ is the resistance traction against highly localized shearing. $\max_{\delta} \bar{\gamma}'(\delta)$ is then analogous to the athermal nucleation strength [18], or rejuvenation stress τ_r of the glass, when constrained by this highly localized deformation mode. For crystals, the above procedure yields an identical result if S_0 is taken to be that of a unit cell. For disordered systems, a much larger sampling area $S_0 \sim 100b^2$ needs to be taken for good statistics, where $b \equiv (\Omega/N)^{1/3}$ is the mean atomic spacing. In crystals, $\bar{\gamma}(\delta)$ is a periodic function of δ with degenerate minima at integer multiples of the Burgers vector. In amorphous materials this is not so. And here lies a softening mechanism distinct from heating or free-volume aggregation which we call alienation (Figs. 1b and 3b). Alienation is a special form of rejuvenation [14] (the reverse of aging [15]) in the limit of intense localized shearing at extremely fast rates.

Just like the pair distribution function, $\bar{\gamma}(\delta)$ is not featureless in amorphous materials. It has a steep first slope (Fig. 1b), because atomic neighbors in a well-aged glass are derived from very long (compared to the vibrational timescale $t_v \sim 1$ ps) quenching processes, which include thermally activated diffusion (uphill in the potential energy landscape) as well as steepest descent-like downhill relaxations. However, as δ is constrained to increase, these co-aged neighbors are forced to separate (atoms are alienated), and new atomic neighbors move in across the horizontal line. In other words, short-range order (SRO) is disrupted. These new neighbors, because they were originally far from the atom in question and had co-aged with some other atoms, are less geometrically compatible [19]. This results in weaker and weaker oscillation in $\bar{\gamma}(\delta)$ as δ increases. Indeed, when $\delta \gg b$, $\bar{\gamma}(\delta)$ becomes flat, meaning the interface loses shear traction completely. This “superlubricity” [20] has been experimentally observed between incommensurate interfaces, such as between two misoriented graphene sheets. Superlubricity happens because simultaneously the same number of bonds is being broken as being formed, and there is a complete cancellation of potential energy oscillation. In the case of amorphous–amorphous interfaces, one may also say that at large δ , if without any recovery process (similar to aging [15], but diffusionless, and in the limit of localized shear at extremely

fast rates), the interface would become so alienated that $\delta + \Delta\delta$ would not make any difference. Note the dilation illustrated in Fig. 1b; this free volume increase is, however, a mechanical side effect (not the cause) of shear and shear-induced alienation.

It thus seems reasonable to postulate that ε_y is controlled by τ_r . Specifically $\varepsilon_y = 2\tau_r/E$, where E is Young's modulus and 2 the Schmid factor, beyond which shear bands nucleate like dislocations in a pristine crystal when the ideal shear strength is reached [18]. However, this criterion does not work. Our finite- T molecular dynamics (MD) simulations (Table 1 and also Fig. 2) show that ε_y values estimated from $2\tau_r/E$ show too much dependence on the condition by which the glass was made (quenching rate in MD simulations) and the rate of shearing [21]. Furthermore, the values are too large, often by a factor of two. Thus, nucleation of embryonic shear bands (ESBs) does not control ε_y .

3. Localization length scale

An alternative criterion is $\tau_\infty = E\varepsilon_y/2 > \tau_{\text{glue}}$, where τ_{glue} is the stress required to maintain quasi-steady-state propagation of an ESB. The distinction between MSBs and ESBs is that an ESB has no liquid zone, $a \approx l_{\text{glue}}$, because the internal temperature has not risen high enough yet. Propagation of an ESB can only be quasi-steady-state, because it is the nature of the heat diffusion equation [7] that materials at the center will eventually melt, no matter how small the frictional heat generation rate $h \equiv \tau_{\text{glue}}\dot{\delta}$ is. Scaling analysis shows that the width of the heated zone is proportional to $\sqrt{\alpha t}$, where α is the thermal diffusivity. However, heat ht is dumped at the center, so it only takes time $t_{\text{inc}} \propto \alpha c_v^2 (T_g - T_{\text{env}})^2 / h^2$ to reach T_g at the center, where T_{env} is the ambient temperature and c_v is the volumetric specific heat. Substituting the experimental α , c_v values for Zr-based BMGs, and taking τ_{glue} to be of the order

Table 1
Properties of metallic glasses calculated by finite- T molecular dynamics

	ρ (g/cm ³)	E (GPa)	B (GPa)	μ (GPa)	ν	$2\tau_r/E$ (%)	$2\tau_{\text{glue}}/E$ (%)
Binary LJ system ^a [22]	1.2 ^a	39 ^a	60 ^a	15 ^a	0.36	~4.5	2.4
Cu ₄₀ Ag ₆₀ ^b [23]	9.6	39	85	12	0.44	~3.3	2.1
Cu ₄₆ Zr ₅₄ ^b [24]	6.9	38	89	12	0.44	~3.9	2.6
Zr _{52.5} Cu _{17.9} Ni _{14.6} Al ₁₀ Ti ₅ ^b [25]	7.0	71	153	27	0.42	~5.2	2.9

^a $T = 0.2$ (all numbers in this row are in reduced unit).

^b $T = 300$ K.

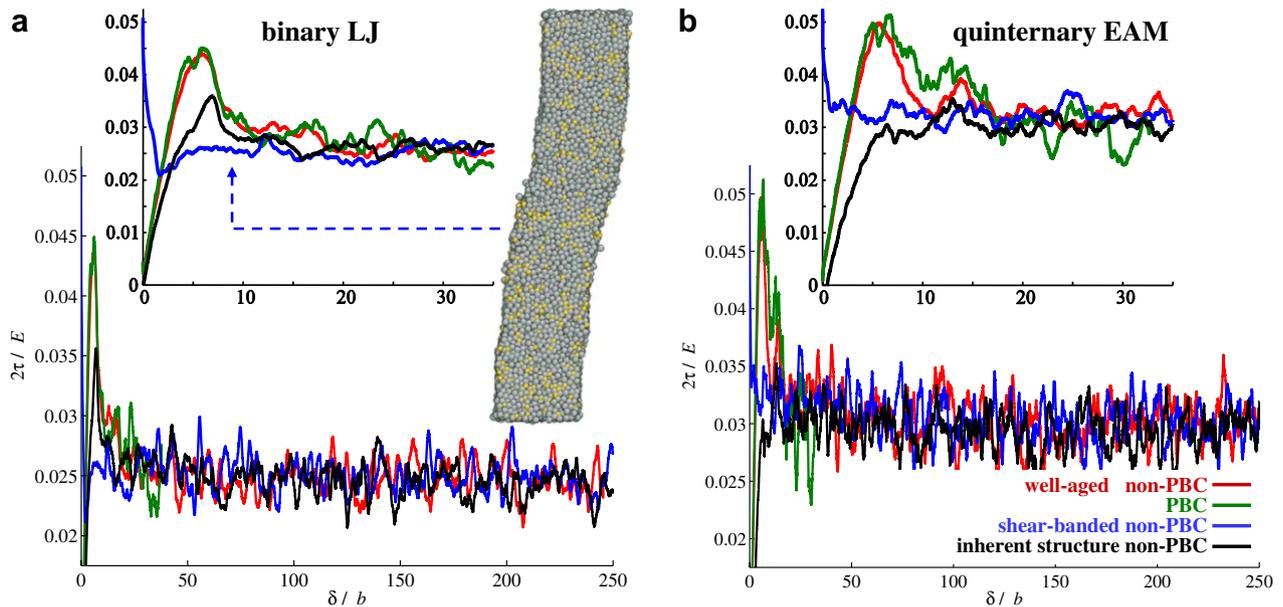


Fig. 2. Shear stress–strain in MD simulations of (a) binary LJ system (20,000 atoms, $T=0.2$ reduced unit, $\dot{\delta} = 0.02c_s$) [22] and (b) Zr_{52.5}Cu_{17.9}Ni_{14.6}Al₁₀Ti₅ (20,000 atoms, $T = 300$ K, $\dot{\delta} = 0.0087c_s$) [25]. Red and green curves are well-aged glasses produced by slow quench from the liquid, deformed by moving grip (non-PBC) and supercell tilting (PBC) methods, respectively. Blue curves are well-aged glasses with a pre-existing shear band, created artificially by an imposed initial sharp displacement field. Black curves are not from glasses at all, but the inherent structures [28] of liquids produced by steepest-descent freezing.

of $0.01E$, we find that at sliding speed $\dot{\delta} \sim c_s \equiv \sqrt{\mu/\rho}$, the shear wave speed, it takes only $t_{\text{inc}} \sim 10^2$ ps for the glue zone to approach T_g . (This also means whatever microscopic recovery process that resists the shearing and counterbalances the alienation in zone III needs to be faster than 10^2 ps, which excludes diffusional relaxations because they are thermally activated uphill events that require long waiting times.) Also, when the trailing edge starts to melt, the glue zone is $l_{\text{inc}} \equiv l_{\text{glue}}^{\text{max}} = \dot{\delta} t_{\text{inc}} \sim 100$ nm long. Since $t_{\text{inc}} \propto \dot{\delta}^{-2}$, $l_{\text{inc}} \propto \dot{\delta}^{-1}$, if then for instance $\dot{\delta} \sim 0.1c_s$, the incubation time t_{inc} would be ~ 10 ns and the incubation length $l_{\text{inc}} \sim 1$ μm .

Based on an analysis of our atomistic calculations to be detailed next, τ_{glue} reflects the rate of recovery. Specifically, it depends on the extremely fast, non-diffusive, downhill relaxation dynamics occurring inside the alienated layer, most of which happen at $10^1 t_v$ – $10^2 t_v$ timescales. If there were no recovery, τ_{glue} would vanish as illustrated in Fig. 1b. Even with recovery, due to the lack of long-time diffusive reorganizations at these fast sliding speeds, τ_{glue} is always smaller than τ_r . However, when $\tau_r > \tau_\infty = E\varepsilon_y/2 > \tau_{\text{glue}}$, an ESB is a potentially unstable defect. This is because from elementary elasticity solution, the local shear stress at zone II is amplified as $\tau \propto (\tau_\infty - \tau_{\text{glue}})\sqrt{a/w}$, where the shear band width w is used as an approximate of the front's local curvature. This means that as long as the embryo has a large aspect ratio, τ_r can always be exceeded in zone II. As pointed out earlier [10,26], there are pre-existing flaws in cast BMGs, especially near the surface [4]. Environmental attacks can also create chemically rejuvenated zones near the surface. These nuclei do not have to be very big: a few nanometers and an aspect ratio ~ 5 would suffice to get the shear band going at $\tau_\infty = \tau_{\text{glue}}$ in our direct MD simulations [21,25]. Therefore, nucleating ESB is not a strong condition of instability and can be easily met. Propagation of ESB, on the other hand, is a sufficiently strong condition, because a minimum incubation length scale $l_{\text{inc}} \sim 100$ nm is involved, over which the condition $\tau_\infty > \tau_{\text{glue}}$ must hold true.

This incubation length l_{inc} over which $\tau_\infty > \tau_{\text{glue}}$ can be regarded as a critical “runway” length necessary for a cold ESB to launch and subsequently mature into a hot, bona fide shear crack. If the sample dimension L or the $\tau_\infty > \tau_{\text{glue}}$ region size L' (as might be the case under a nano-indenter [27]) is somehow smaller than l_{inc} , then ESBs cannot mature. This would then remove the means for any ESB to distinguish itself dramatically from all the other ESBs and shear transformation zones (STZs) [9] in the same sample in terms of plastic compliance or softness. And then massive load shedding and global shear localization cannot happen. Thus, l_{inc} is a critical “plastic localization” length scale in BMGs. Only samples with L and L' greater than l_{inc} can develop mature shear bands with macroscopic length, monopolistic softening and sharp global load drops. Specimens smaller than l_{inc} would have many STZs and ESBs (essentially STZs with longer aspect ratio), but no major shear band, and thus would appear to deform

homogeneously at the sample scale. Recent experiments by Cynthia Volkert et al. (private communications) on compressing focused ion beam-carved nanopillars appear to corroborate this theoretical prediction, that there is an intrinsic length scale in BMGs of the order of 10^2 nm, below which sample-scale shear localization does not happen (unless the sample sustains extremely high strain rates $> 10^8/\text{s}$, as in many direct MD simulations [21]).

To recapitulate, as long as there exists an incubation volume in a BMG of size l_{inc} with critical stress $\tau_\infty > \tau_{\text{glue}}$ stored inside, an ESB can run to maturity within it. Once T_g is approached in the trailing edge of the shear band, with associated shear traction loss, the MSB becomes unstoppable and is likely to shear through the whole sample. A continuous cycle of recruiting well-aged materials in front, rejuvenating them by brute-force shear, subsequent alienation, heating, and casting behind as liquid becomes self-perpetuating, because a stopped MSB would have projected in front an amplified shear stress $\sim \tau_\infty \sqrt{a/w}$ that can rejuvenate and alienate any material. The actual MSB is a dynamical defect, moving with speed close to c_s .

We note that once melting occurs, there will be a tremendous drop in the frictional heat generation rate $h \equiv \tau\dot{\delta}$ compared to when it was still cold glue at $T < T_g$, so the temperature would be effectively pinned at T_g . Thus we predict an extended region in zone IV with temperature very close to T_g . That is probably also the reason why although an ESB initially grows in width w rapidly, as seen in the MD simulations, the eventual width is limited to $\sim 10^1$ – 10^2 nm [3–5].

4. Atomistic calculation results

We propose above that the macroscopic ε_y is not controlled by ESB nucleation, which is highly sample- and surface-dependent, but by the minimum requirement for realizing ESB-to-MSB transition, i.e. the value of the quasi-steady-state shear traction τ_{glue} offered by the glue material, when it is already alienated and shearing at high rates. It remains to be seen whether atomistic calculations can give the correct τ_{glue} value or not, compared to experimental ε_y . For this reason, we always convert the atomistically computed shear traction τ to dimensionless uniaxial strain equivalent, $2\tau/E$, assuming an ideal Schmid factor of 2.

We performed three-dimensional finite-temperature MD and zero-temperature GSF calculations for four metallic glass systems, a binary Lennard-Jones (LJ) system [22], $\text{Cu}_{40}\text{Ag}_{60}$ [23], $\text{Cu}_{46}\text{Zr}_{54}$ [24] and $\text{Zr}_{52.5}\text{Cu}_{17.9}\text{Ni}_{14.6}\text{Al}_{10}\text{Ti}_5$ [25], by embedded atom (EAM) potentials. The first three amorphous systems were carefully characterized in the original papers, and we follow the same sample preparation scheme and have verified that we obtain identical results for T_g , pair distribution functions, etc. For the quinary system we adopt the potential of Cleri and Rosato [29] and take algebraic or geometric means for the cross-interaction parameters, but enhance an attractive cross-interaction

uniformly by a single factor λ until the glass is fully miscible (no glass–glass phase separation) and best matches the experimental elastic constants. This should only be considered as a model system.

In Fig. 2, we show the shear stress–strain responses of the LJ and quaternary EAM systems. It is clear that the large- δ plateau of $\tau(\delta)$ is independent of how the shear band was formed initially, whether nucleated spontaneously (red, green) [21] or artificially created (blue), and we identify the plateau value as τ_{glue} . (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.) We find from MD calculations that τ_{glue} is not sensitive to the sliding speed $\dot{\delta}$ in a regime below $10^{-2}c_s$, and in dimensionless form not very sensitive to the glass composition and interatomic potentials. τ_{glue} is not even affected whether or not only the glass is sheared. We take the inherent structure

[28] of a $T \gg T_g$ liquid (black), produced by immediate steepest-descent freezing of this liquid, instead of traditional slow quench with MD. Upon shearing, a localized glue layer forms spontaneously [21], which gives the same τ_{glue} value as that of the slowly quenched glass, even though the initial rejuvenation stress τ_r differs greatly (see Fig. 2 insets). Clearly, the glue material in zone III is neither conventional liquid nor solid nor even conventional glass, but a highly driven, non-equilibrium material that can only exist transiently. Nonetheless, its intrinsic property τ_{glue} controls the structural integrity of the whole sample made of well-aged glass. Like liquid [2], the glue’s memory is short: this is not because of high temperature, but extreme rates of shearing, sustained over $>10^2$ ps until it truly melts.

Some details of the LJ system are shown in Fig. 3a. With the localized accumulation of inelastic shear strain [21],

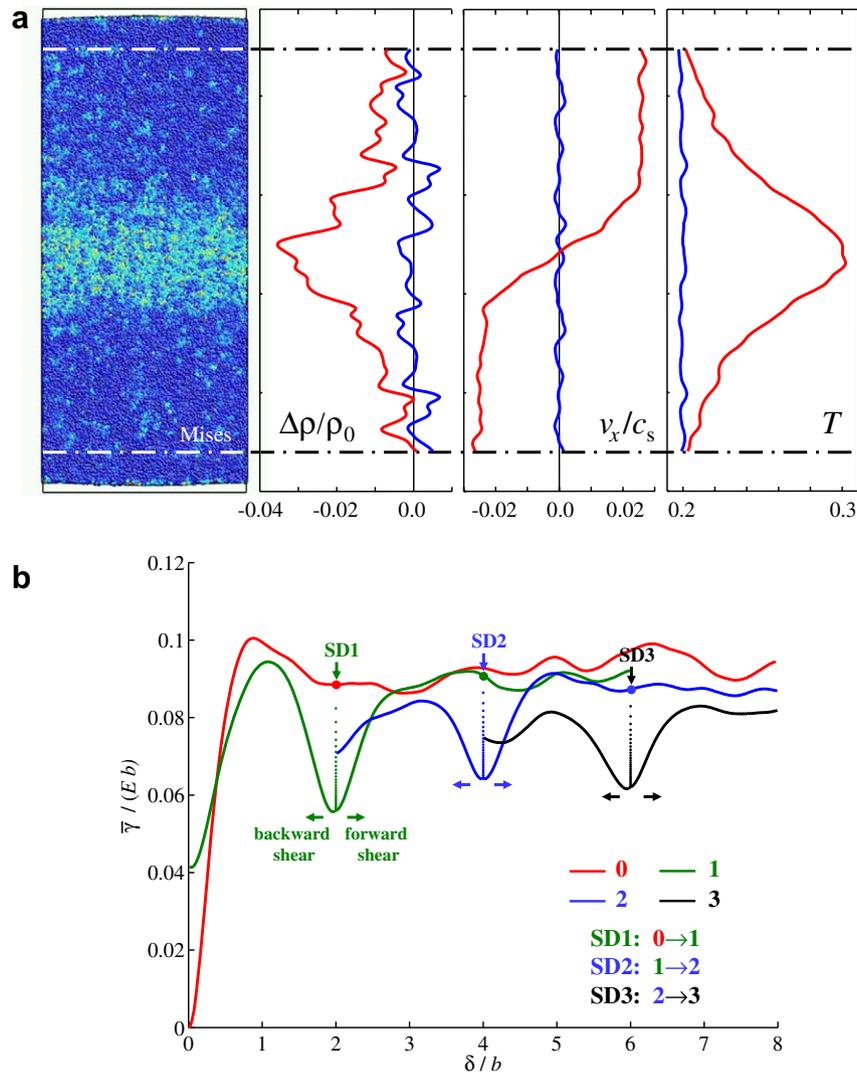


Fig. 3. (a) Snapshot of the atomic configuration and density, velocity and temperature profiles of binary LJ system at $\delta = 26b$. Atoms are colored by their atomic shear strain [21]. Outside of the dotted lines are the grip regions. Unlike in reality, temperature in the grip regions is fixed at 0.2 in reduced unit. Blue curves show profiles of the initial sample. (b) $\bar{\gamma}(\delta)$ calculated for $\text{Cu}_{40}\text{Ag}_{60}$ [23], with sampling area $S_0 = 256b^2$. Red, green, blue and black curves represent four generations of glass configurations, each related to the former by steepest-descent (SD) relaxation at δ values indicated by arrows.

there are significant dilation (negative $\Delta\rho/\rho_0$) and increase of temperature in the shear band. There is no reason to think, however, that this dilation is the cause of shear. The sliding speed is too fast in the MD simulation for free volume to “diffuse” into the shear band, nor is free-volume aggregation absolutely necessary for maintaining or even initiating shear. Rather, as illustrated in Fig. 1b, we think dilation and heating are the mechanical and thermal side effects of localized shearing [17,21,30], caused by brute-force shear stress. One is of course free to choose almost any reaction coordinate or order parameter to describe a reaction or transformation. Multiple choices are all allowed so long as they are not orthogonal to each other. However, for understanding τ_{glue} that governs ESB-to-MSB transition in the present scenario of extreme shear localization, the degree of alienation (DA) seems a more natural order parameter, and causally more direct, than the free volume, because it contains angular and chemical ordering [19] information (see Fig. 1b) beyond local volume expansion. The exact quantification of DA should be based on changes in the species-dependent radial and angular distribution functions inside the glue.

To estimate the kinetic rate of recovery (Fig. 1c), we calculate $\bar{v}(\delta)$ of four generations of $\text{Cu}_{40}\text{Ag}_{60}$ glasses, shown in Fig. 3b. At $\delta = 2b$ of each generation, we remove the x -constraints and perform a steepest-descent relaxation, to create the next generation. The non-dimensionalized hyperspace displacement $\int \sqrt{d\mathbf{x}^{3N} \cdot d\mathbf{x}^{3N}}/S_0$ in each steepest-descent relaxation is no more than 0.15 before convergence is fully reached, yet a large recovery is seen in Fig. 3b. This means only very moderate atomic movements are needed to recover a major piece of the SRO disrupted by shearing. Because the vibrational lifetimes (oscillation damping rates) in these systems are of the order of $10^1 t_v$ – $10^2 t_v$, it means that as long as the sliding speed $\dot{\delta}$ is less than $10^{-2} c_s$, essentially the full benefit of recovery is available to atoms in the shear band, by steepest descent-like downhill dissipative dynamics (DDD). No thermally activated, uphill rare events (compared to vibrational timescale) need to be involved, and they play no role in our τ_{glue} results. Corroborating this interpretation, we indeed find in our MD simulations no appreciable dependence of τ_{glue} on $\dot{\delta}$ over two decades of $\dot{\delta}$, as long as $\dot{\delta} < 0.05 c_s$.

The above results demonstrate somewhat surprisingly that simple MD calculations can capture the essential step that controls τ_{glue} , namely the DDD processes. Imagine a jigsaw puzzle constantly being disrupted by sharp sliding. If the pieces are not allowed to move, the interface would become completely alienated and shear traction would drop to zero. The pieces, however, do have a tendency to reorganize. There is a very slow component (aging [15]) to this reorganization dynamics that involves thermally activated diffusion. A well-aged glass does have higher strength initially, τ_r , but that does not control ε_y because it is not absolutely the last line of defense. Also, at sliding speeds of an appreciable fraction of c_s , diffusive reorganization is not nearly fast enough to balance the rate of alien-

ation. What has been shown in the atomistic calculations is that there is also an exceedingly fast component in the reorganization dynamics, which we call recovery. Recovery and alienation are only defined when there is extreme localized shearing. Recovery is non-diffusive, i.e. driven by damped downhill dynamics on the energy landscape and dissipating energy at $10^1 t_v$ – $10^2 t_v$ timescales; so it is active even at extremely high sliding velocities, and therefore provides truly the last line of defense against localized shearing, which corresponds to the experimentally measured ε_y .

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