Supplemental Material

A simple and broadly-applicable definition of shear transformation zones

David Richard,1,2,* Geert Kapteijns,1,* Julia A. Giannini,2 M. Lisa Manning,2 and Edan Lerner1,†
1Institute for Theoretical Physics, University of Amsterdam, Science Park 904, Amsterdam, Netherlands
2Department of Physics, Syracuse University, Syracuse, NY 13244

I. COMPUTER GLASS MODELS

S-1. Inverse Power Law

The results shown in Figs. 1 and 3 in the main text are for polydisperse soft spheres in two and three dimensions, respectively, interacting via an inverse power law potential. A detailed description of this model is provided in Ref. [1]. We utilize SWAP Monte Carlo [2, 3] (MC) to prepare glasses with various degrees of stability. The later is controlled by the parent temperature \( T_p \) of the equilibrium states from which our glasses were instantaneously quenched. Finally, we quench our configurations to zero temperature via an energy minimization using a conjugate gradient algorithm [4].

Athermal quasistatic shear deformation [5] is performed using Lees-Edwards periodic boundary conditions [6] with a strain step \( \delta \gamma = 10^{-5} \), which is at least one order of magnitude lower than the typical strain between subsequent plastic instabilities.

S-2. Hard disks

We prepare dense equilibrium polydisperse hard-disk configurations with \( N = 1600 \) particles using SWAP MC. We choose the same continuous polydispersity as proposed in Ref. [2] with diameter distribution \( P(\sigma) \sim \sigma^{-3} \) from \( \sigma_m = 1 \) to \( \sigma_M = 2.2 \). This choice results in a high polydispersity \( \Delta = \sqrt{\sigma^2 - \bar{\sigma}^2}/\bar{\sigma} \approx 22\% \) and as a result one avoids crystallization. Throughout our simulations lengths are in units of \( \bar{\sigma} \). Initial configurations are prepared via minimization of harmonic soft spheres at a high packing fraction \( \phi \approx 0.82 - 0.84 \). We then perform a MC run in the NPT ensemble where the box edge is allowed to fluctuate by around 3% of its length. In Fig. S1a, we show the compressibility \( Z = P/(\rho k_B T) \) as a function of the packing fraction \( \phi \). The solid line is the equation of state taken from Ref. [7], empty black symbols are Molecular Dynamics results from Ref. [8] , and red empty squares are SWAP Monte Carlo simulations performed in the NPT ensemble. (b) Typical low-frequency transverse phonon. (c) Density of states in hard-disk glasses with \( N = 1600 \) prepared at \( Z = 35 \). The vertical dashed lines indicate the frequencies of the first and second shear waves.

Having generated equilibrium dense hard-disk configurations, we perform MC simulations in the NVT ensemble to compute the positions covariance matrix

\[
\mathbf{C}_{ij} = \langle \mathbf{u}_i(t)\mathbf{u}_j(t) \rangle_T, \tag{S1}
\]

with the particle displacement vector \( \mathbf{u}_i = \mathbf{x}_i - \langle \mathbf{x}_i \rangle \) from its average position. Note that during this procedure we have removed possible drift due to the motion of the center of mass of the simulation box. The Hessian matrix of the system follows from the equality [9]

\[
\mathbf{H}_{ij} = \frac{k_B T \mathbf{C}^{-1}}{m_i}, \tag{S2}
\]

with \( k_B \) the Boltzmann constant and where particle masses are equal and set to unity. Full diagonalizations are performed using the LAPACK library. In Fig. S1b, we show a typical phonon found in deeply equilibrated hard-disk glasses. Furthermore, we have generated an ensemble of
128 configurations for $Z \approx 35$ and computed the density of states $D(\omega)$ with frequency $\omega$ (see Fig. S1c). As discussed in depth in Ref. [10], we observe a finite size regime at low-frequencies with distinct phonon bands followed by a continuous “phonon sea” at higher frequencies. Consistent with the degeneracy level of phonon bands, we have found 4 modes in both the first and second bands.

The extraction of PHMs requires the contact network of pairs $\{ij\}$ to be able to compute the denominator of the cost function defined in Eq. (2) of the main text. As contacts are not accessible in hard particles, we have chosen the 6 closest neighbors of each particles (first peak of the radial distribution function). We have checked that the energy and structure of the modes are not affected in any appreciable manner by this choice.

**S-3. Other models**

A complete description of the Hertzian, Stillinger-Weber, and CuZr BMG models can be found in Ref. [11]. The Lennard-Jones configuration used in the main text for the residual palstic strength map is the same one as seen in Ref. [12].

**II. COST FUNCTION DENOMINATOR**

In Fig. S2 we present data that demonstrates that the denominator of the cost function $C(z)$ (see Eq. 2 in the main text) follows $\sum_{(i,j)} (z_{ij} \cdot z_{ij})^2 \sim 1/(Ne(z))$, where $e(z) \equiv (N \sum_{i} (z_{i} \cdot z_{i})^2)^{-1}$ is the conventional participation ratio, $N$ is the system size, and $z$ denotes a normalized $(z \cdot z = 1)$ putative displacement field. This means that the denominator of the cost function $C(z)$ is larger (smaller) for more (less) localized modes, therefore promoting localization of its minima $\pi$ (the PHMs).

In Fig. S2 we vary both the system size, and the degree of modes’ localization – the latter is known to be affected by the degree of supercooling, captured by their parent temperature $T_p$ [13].

**III. CUBIC VERSUS PSEUDO HARMONIC MODES**

We provide below an energetic and structural comparison between cubic and PHMs. We find that cubic modes are nearly always slightly stiffer than PHMs, see Fig. S3a. We expect the structural deviation from cubic and PHMs to scale as $\sim \omega^4$ (the same as observed between PHMs and harmonic modes), which we demonstrate in Fig. S3b. As discussed in Ref., cubic modes are the most informative objects from a micromechanics point of view. The reason is that they maximize the asymmetric third-order coefficient $\tau = \frac{\partial^3U}{\partial x^3}$ : $\pi \pi \pi$, resulting in a better direction to cross the nearby barrier in the energy landscape. As shown in Ref. [14], cubic modes also display the asymptotic scaling $\tau \sim \omega$ (for $\omega \to 0$), which combined with the gapless density of states $D(\omega) \sim \omega^2$ at low frequencies, gives the prediction that the pseudogap exponent $\theta$ of the distribution of thresholds $P(x) \sim x^\theta$ is equal to $2/3$, where $x$ is the distance of a mode to the next plastic instability. As shown in Fig. S3c, this relation does not hold for PHMs.