

described above.

We complement this analysis with preliminary results from dissipative molecular-dynamics simulations that access strain-rates above the quasistatic regime. This allows us to assess the importance of dynamic effects in limiting access to certain regions of the landscape. Indeed, the results at larger strain rate are system size independent, and reveal a surprising growth of the strength of the heterogeneities with increasing packing fraction away from ϕ_c .

2 Simulations

Our system consists of N soft spherical particles with harmonic contact interactions

$$E(r) = k(r - r_c)^2. \quad (1)$$

Two particles, having radii r_i and r_j , only interact, when they are “in contact”, i.e. when their distance r is less than the interaction diameter $r_c = r_i + r_j$. This system has been studied in several contexts, for example in.^{16,26,32} The mixture consists of two types of particles (50 : 50) with radii $r_1 = 0.5d$ and $r_2 = 0.7d$ in two-dimensions. Three different system-sizes have been simulated with $N = 900$, 1600 and 2500 particles, respectively. The unit of length is the diameter, d , of the smaller particle, the unit of energy is kd^2 , where k is the spring constant of the interaction potential. We use quasistatic shear simulation, and compare some of the results with those obtained from dissipative molecular-dynamics simulations at zero temperature.

Quasistatic simulations consists of successively applying small steps of shear followed by a minimization of the total potential energy. The shear is implemented with Lee-Edwards boundary conditions with an elementary strain step of $\Delta\gamma = 5 \cdot 10^{-5}$. After each change in boundary conditions the particles are moved affinely to define the starting configuration for the minimization, which is performed using conjugate gradient techniques.³³ The minimization is stopped when the nearest energy minimum is found. Thus, as the energy landscape evolves under shear the system always remains at a local energy minimum, characterized by a potential energy, a pressure p and a shear stress σ .

The molecular dynamics simulations were performed by integrating Newton’s equations of motion with elastic forces as deduced from Eq. (1) and dissipative forces

$$\vec{F}_{ij} = -b[(\vec{v}_i - \vec{v}_j) \cdot \hat{r}_{ij}] \hat{r}_{ij}, \quad (2)$$

proportional to the velocity differences along the direction \hat{r}_{ij} that connects the particle pair. The damping coefficient is chosen to be $b = 1$. Rough boundaries are used during the shear, the boundaries being built by freezing some particles at the extreme ends in the y -direction, from a quenched liquid configuration at a given ϕ . The system is sheared by driving one of the walls at a fixed velocity in the x direction, using periodic boundary conditions in this direction.

For all system sizes, the distance between the top and bottom boundaries is $52.8d$ and each of the boundaries has a thickness of $4.2d$. The system size is changed by modifying the length of the box in the x -direction.

3 Results

3.1 Quasistatic simulations

As is readily apparent from Fig. 1, a typical feature of quasistatic stress-strain relations is the interplay of “elastic branches” and “plastic events”. During elastic branches stress grows linearly with strain and the response is reversible. In plastic events the stress drops rapidly and energy is dissipated.

In setting the elementary strain step, $\Delta\gamma$, care must be taken to properly resolve these events. Too large strain steps would make the simulations miss certain relaxation events. We chose a strain step small enough, such that most minimization steps do not involve any plastic relaxations. In consequence, the elastic branches are well resolved, each consisting of many individual strain steps.

The succession of elastic and plastic events defines the flow of the material just above its yield-stress $\sigma_y(\phi)$. The value of the yield-stress depends on volume-fraction and nominally vanishes at ϕ_c (see Fig. 2). For finite systems, however, finite-size effects dominate close to ϕ_c such that one cannot observe a clear vanishing of σ_y . Rather, as Fig. 1 shows, one enters an intermittent regime, i.e. a finite interval in volume-fraction in which the stress-