CROSSOVER IN DYNAMICS OF GRANULAR PACKINGS UNDER CYCLIC SHEAR

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Summary We have performed molecular dynamics simulations of 2D frictionless disk packings under cyclic shear. We present mechanical as well as dynamical properties of these systems as a function of strain. In particular, we find two distinct regimes in the dynamics as a function of reversal amplitude. These regimes appear to correspond to distinct regimes in the mechanics, as characterized by their stress-strain relationships.

INTRODUCTION

A recent experimental study done by our group [1] of a granular packing exposed to repeated loading and unloading via cyclic shear has demonstrated a pronounced crossover in particle dynamics from a sub-diffusive to a diffusive regime. Sub-diffusive motions occur for low reversal amplitudes γ_r, while diffusive motions occur for higher γ_r. While our measurements of the dynamics of all particles in 3D under cyclic shear have revealed that the crossover occurs at a similar strain as a change in the collective dynamics of all particles, our experiments are not able to probe the connection between particle dynamics and the mechanical properties of the packing. In order to connect the dynamics to mechanical properties, and so better understand the origin of this crossover, we have conducted molecular dynamics simulations of simple model granular systems under cyclic shear. Our systems are 50/50 bidisperse frictionless 2D packings of 8000 grains with fixed pressure, comparable to the number of particles investigated in our experiments. Shear strain is applied to a simulation box of size L with Lees-Edwards boundary conditions, and shear rate is exceedingly low (boundaries are moved 10^{-6}L during each integration step) so as to approximate the quasi-static regime. Eight reversal amplitudes (5%-22.5% strain) have been studied for several hundred cycles each.

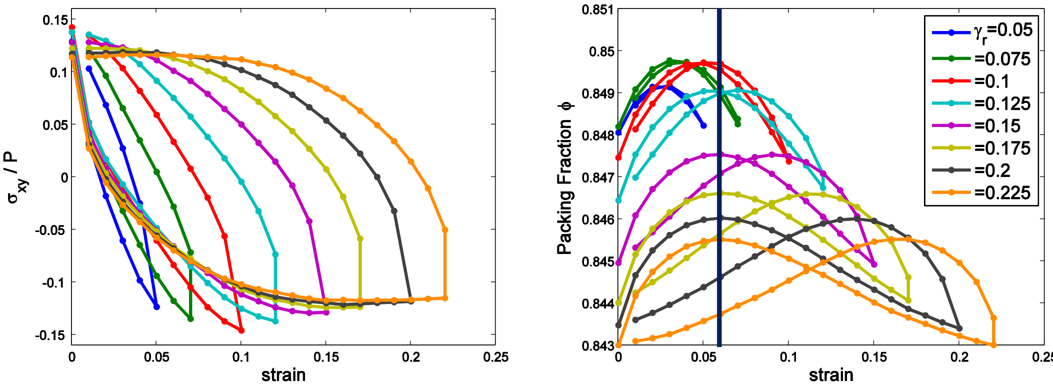

Figure 1: (left) shear stress divided by the (fixed) pressure shown as a function of the strain applied at the boundary, in terms of the linear system size. Curves are mean results averaged over several hundred cycles. (Right) The packing fraction is also reported. For the lowest four reversal amplitudes, the peak compaction appears shift, while the peak compaction for higher amplitudes appears to be independent of the amplitude. A vertical line is drawn through the peaks of the largest amplitudes to guide the eye. Legend applies to all plots.

AMPLITUDE DEPENDENT BULK PROPERTIES

Our main observation is a cycle amplitude dependent, hysteretic stress-strain relationship when averaged over many cycles (Figure 1, left). Furthermore, the peak stress (the off-diagonal component of the total stress tensor) is reached at zero strain. This peak is γ_r dependent, and increases to a maximal value at a strain amplitude of ~10%, then decreases again with increasing strain to a saturation value (what we will refer to as the yield stress) apparent at large γ_r.

The evolution of the packing fraction Φ during the shear cycle (Figure 1, right) also exhibits interesting behavior: We observe a non-monotonic behavior with increasing strain up in a single cycle. The granular ensemble reaches peak compaction at a strain value of about 5% and then dilates with further increase in strain. The strain at which the peak amount of compaction is reached is independent of strain amplitude for large γ_r, but decreases with decreasing strain amplitude below crossover amplitude γ_c . The finding that the strain needed to reach peak compaction depends on strain amplitude in steady state shows a capacity for the packing to be 'trained,' by the prior oscillations, i.e. there are important and not well understood memory effects during the shear trajectory.

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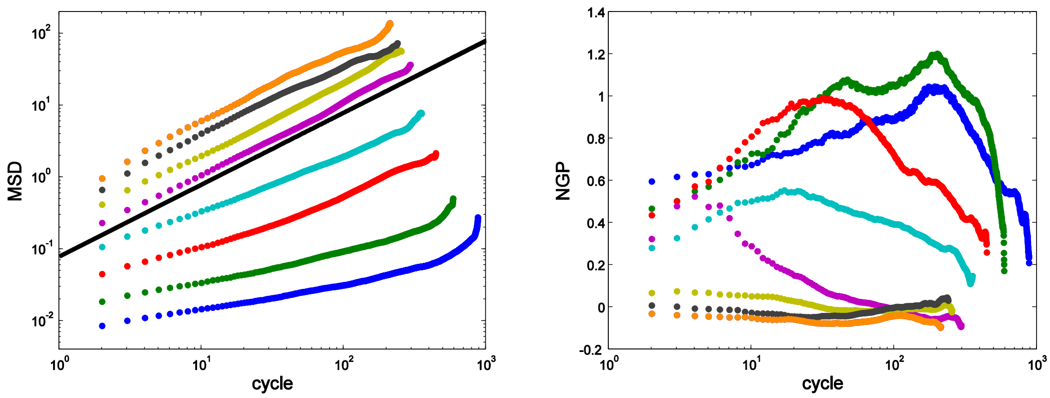

Figure 2: (left) the mean-squared displacements for different reversal amplitudes. The black line has a slope 1. The upturned tail at large cycle number is the result of systematic decrease of particle displacements. (Right) the non-gaussian parameter (NGP) exhibits a characteristic peak which shifts to zero as reversal amplitude increases.

PARTICLE DYNAMICS AND CORRELATED MOTION

The particle distributions of displacements also show interesting γ_r dependencies. In particular, the mean-squared displacements (MSD) exhibit a crossover from sub-diffusion to diffusion (Figure 2, left), where cycle number is the time variable, and the location of this crossover again corresponds with γ_c. In addition, we measure the non-Gaussian parameter (NGP), a quantity which reflects the degree to which distributions of displacements are not consistent with a simple random process. The NGP exhibits a novel time scale associated with the peak of the deviation from gaussian in the displacement distributions (Figure 2, right). The time scale that emerges decreases to zero with increasing strain amplitude and reaches zero at the amplitude corresponding to γ_c. The NGP has been used in the past to estimate time scales associated with long-time rearrangements in granular systems [2]. We do observe a decrease at long times in the overall particle displacements at low γ_r , and so time averaging the MSD's with increasing time origins leads to spurious results at large times (cycle numbers), as can be seen in the MSD tails in Figure 2. However, the slopes of the MSD curves as well as the peaks of the NGP are not sensitive to this long time overall decrease in particle displacements.
Finally, we consider the dynamical (or four point) susceptibility, which measures fluctuations in a space and time dependent order parameter. In our case, we use the 'Q' parameter, which takes the value of 1 or 0 depending on whether or not a particle has returned to within a distance 'a' of its original location after a time 't'[3]. In this sense, Q=Q(a,t). One extracts a dynamical time scale from the value of t at which the four-point susceptibility peaks, and a length scale from the value of this peak [4]. In our simulations we find that the time scale extracted in this way appears to be approximately the same as the timescale at which the largest amount of non-Gaussianity is observed, and that the length scale is constant as a function of reversal amplitude (about 8 grain diameters in size, or about 3% of the system size). This is in agreement with experiments of cyclically sheared steel cylinders of a similar system size [4]. We believe our investigation is the first systematic study of the γ_r dependence of these scales.

CONCLUSIONS

We present novel results from simulations of a simple model granular system under cyclic shear with strain amplitude γ_r. We find a γ_r dependence on shear stress as well as packing fraction, and interesting memory effects. The first evidence of a crossover between two regimes is seen in the mechanical properties, where a above a strain amplitude of γ_c a yield stress emerges. This γ_c also corresponds to a crossover from sub-diffusive to diffusive dynamics as seen in the MSD and also seen in the decreasing time scale of the NGP that eventually vanishes at γ_c. These observations suggest a connection between particle dynamics and mechanical properties of the packing under cyclic shear. These observations lead us to expect a structural relaxation during shear reversal, which is able to reorganize so as to resist shear in the opposite direction, but only after enough strain is applied. The crossover amplitude $\gamma_{c,}$ then, is likely associated with the minimal strain needed to erase and completely reorganize the structure of the packing.

References

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