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Amorphous and ordered states of concentrated hard spheres under oscillatory shear

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ABSTRACT

Hard sphere colloidal particles are a basic model system to study phase transitions, self-assembly and out-of-equilibrium states. Experimentally it has been shown that oscillatory shearing of a monodisperse hard sphere glass, produces two different crystal orientations; a face centered cubic (FCC) crystal with the close packed direction parallel to shear at high strains and an FCC crystal with the close packed direction perpendicular to shear at low strains. Here, using Brownian dynamics simulations of hard sphere particles, we have examined high volume fraction shear-induced crystals under oscillatory shear as well their glass counterparts at the same volume fraction. While particle displacements under shear in the glass are almost isotropic, the sheared FCC crystal structures oriented parallel to shear, are anisotropic due to the cooperative motion of velocity–vorticity layers of particles sliding over each other. These sliding layers generally result in lower stresses and less overall particle displacements. Additionally, from the two crystal types, the perpendicular crystal exhibits less stresses and displacements at smaller strains, however at larger strains, the sliding layers of the parallel crystal are found to be more efficient in minimizing stresses and displacements, while the perpendicular crystal becomes unstable. The findings of this work suggest that the process of shear-induced ordering for a colloidal glass is facilitated by large out of cage displacements, which allow the system to explore the energy landscape and find the minima in energy, stresses and displacements by configuring particles into a crystal oriented parallel to shear.

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1. Introduction

Suspensions of colloidal hard spheres have been used as model systems [1], to offer insights into many fundamental phenomena of condensed matter physics such as equilibrium phase transitions [2], but also out of equilibrium states such as glasses, gels and attractive glass transitions [3,4]. The defining feature of a colloidal glass is low particle mobility within a disordered solid, orders of magnitude smaller than that [5] of a corresponding fluid. Colloids provide a valuable model system for the examination of the glass transition due to the time and length scale accessibility [6]. Thus, considerable insight is gained into features such as motion cooperativity and dynamic heterogeneity [7,8]. Furthermore, due to their large particle size, colloids form soft solids which flow under the

application of shear [9], where non linear rheological properties can be studied.

For hard spheres, there is a single parameter which completely determines the phase behavior at rest, the particle volume fraction ϕ . Hard spheres exhibit a liquid phase at volume fractions beneath 0.494, where the particles are free to diffuse and explore the whole volume available. A liquid-crystal phase coexistence is observed at volume fractions ranging from 0.494 to 0.545 and a fully crystalline structure from 0.545 to about 0.58 [10,11]. The increase of entropy through the increase of average local free volume is the driving forces behind the crystallization of hard sphere colloids. The ordered crystal structure allows each particle a larger volume of motion around their lattice site in comparison to a disordered state of the same volume fraction. Even though the particles are in an ordered state, the increase of entropy due to individual motion and free volume is greater than the reduction of the total configurational entropy [10]. The crystal structures initially assembled to when left at rest are a mixture of face-centred cubic (FCC) and hexagonally close packed (HCP) regions that are randomly oriented [12]. If particles polydispersity increases,

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crystallization dynamics become slower as different particles sizes are not easily accommodated in the crystal lattice. At about 10% polydispersity, the distribution of sizes is too large and crystallization is suppressed [10,13–15].

Further increasing the volume fraction, for φ above 0.58, the particles are unable to move into the entropically favorable crystal positions due to space restrictions and become trapped in a dynamically arrested glass phase [4,16,17]; Molecular dynamics simulations have brought up a discussion on the definition of the glass transition volume fraction and the appearance of crystallization in the glass regime [15]. While highly polydisperse hard sphere systems are unable to crystallize, the arrested glassy state at high φ remains unchanged. Above the glass transition, although long-range diffusion is essentially frozen [18,19], dynamic heterogeneities may allow slow non-diffusive relaxations related with activated hopping mechanisms [7,20]. By observing the positions of the fastest and slowest particles [8] it was found that just below the glass transition the motions of the fast-moving particles were strongly correlated spatially in clusters. As the glass transition is approached these domains grow in size, although when entering the glass phase, the average size of these clusters is reduced, providing a dynamic signature of the glass transition [21,22]. The dynamic heterogeneities near and above the glass transition have also been discussed [23] and shown to relate with large distance spatial correlations of a few particle diameters which increase with φ , although showing no divergent behavior near or above the glass transition.

Rheologically, hard sphere glasses are an interesting system, exhibiting solid like response at rest, while showing complex features under non-linear shear. Earlier work [24] studied the linear elasticity of hard sphere dispersions near and above the glass transition, concerning the amorphous and shear induced ordered states, finding a power law increase of elasticity as a function of the distance from maximum packing, while additionally successfully applying the Mode Coupling Theory for the frequency dependence of the moduli. Creep and recovery experiments [25] as well as some oscillatory shear measurements coupled with DLS echo [9,26] were used to examine the nonlinear properties of a polydisperse hard sphere glass and concluded that it can tolerate a high amount of strain (10–15%) before yielding irreversibly as related to breaking of the hard sphere entropic cages. Moreover, a recent study presented an overview of the various rheological properties of concentrated hard sphere suspensions in comparison to their softer counterparts [27], covering linear viscoelasticity and non-linear steady and oscillatory measurements, as well as providing an experimental rheological signature of the glass transition.

There has also been recent scientific activity in the experimental determination of the microscopic properties of concentrated hard sphere glasses under shear. With the use of confocal microscopy coupled with steady shear, a sub linear power law dependence for the shear induced diffusion coefficient with increasing shear rate is found [28], whereas the terminal relaxation frequency as measured by orthogonal superposition rheometry exhibits a linear increase with shear rate [29]. Moreover, recent work [30] relates the shear banding instability in high concentration glasses to shear concentration coupling, while mapping the occurrence of banding with applied rate and volume fraction. Through microscopy and steady shear, localized irreversible shear transformation zones were identified and their formation energy and topology were determined [31], while other work [32] related the microscopic motions of the particles under shear to a modified Stokes–Einstein relation which replaces the thermal energy with shear energy. Additionally, the dynamic heterogeneities under steady shear have been analyzed for a super-cooled liquid [33], while also recently studied in terms of creep flow [34], showing an increase of the heterogeneous regions as a function of strain.

The source of the transient overshoot for steady rate start-up has been associated with structural changes of the glassy cage [35–37], while a secondary yield strain was found in simple hard sphere glasses [38], explained through distinct yielding mechanisms at different time scales. In a collaborative effort on glasses under shear, the relaxation of stresses after the application of flow was examined with theory, simulations and various experiments [39], showing that finite residual stresses are governed by the preshear rate through long-lived memory effects.

In a monodisperse system of hard spheres, the addition of shear has been found to induce ordering. While crystallization in quiescent hard sphere systems occurs within hours or days as randomly oriented crystallites, under oscillatory shear, crystallization may occur within a few minutes and is oriented with the flow [40]. Depending on the studied volume fraction, the created crystal under shear may be transient ($\varphi < 0.454$), partial ($0.454 < \varphi < 0.545$) or monocrystalline ($\varphi > 0.545$) [41], while it flows in complicated fashion with crystal layers sliding one over the other [42]. It has been found for dense suspensions of hard spheres ($\varphi > 0.545$) under oscillatory strain that two different orientations of crystals arise depending on the strain of oscillation; while high strains ($\gamma_0 > 50\%$) produce a monocrystal with the closed packed direction parallel to shear, while low strains ($\gamma_0 < 50\%$) produce a distribution of crystallites with orientations around a crystal with the closed packed direction perpendicular to shear [40,41,43].

At low strains, the crystal has been found to have some sort of polycrystallinity as the sample would not be fully oriented in the perpendicular direction, but would have grains which had a preferred direction which was perpendicular to the shear direction [41]. At high strains the sample would reorient parallel to shear and the polycrystallinity would disappear. In the case of the cone and plate geometries, crystallization manifested only as a crystal with the closed packed direction parallel to shear, possibly due to spatial constrictions for the perpendicular crystal in a rotational configuration [24]. In [44] there is a discussion on the physical interpretation of the change of orientation from perpendicular at low strains to parallel to shear at high strains.

Static light scattering in addition to oscillatory shear was used to examine the time dependent growth of a crystal under shear, while exploring the parameters for optimum crystallization [45]. Light scattering echo and optical microscopy were used to examine hard sphere glasses under oscillatory shear strain [43], finding the crystal growth time scales for high φ glass. Two dimensional simulations of repulsive and attractive systems under shear revealed an optimal shear rate where crystallization speed is enhanced over the one at rest [46]. Brownian dynamics simulations were carried out on crystal nucleation with the application of steady shear and an umbrella sampling technique, which found that shear suppresses nucleation and leads to a larger critical nucleus, which promotes crystallization [47,48]. Other work [49] has examined the shear induced ordering in an attractive gel with microscopy and light scattering echo and proposed a model for particle escape time and crystallization. Through simulations and confocal microscopy, investigations of the real-space structure revealed four distinct oscillatory shear-induced phases in hard-sphere fluids [50]. Furthermore, a range of different simulation techniques to examine the mechanism of shear induced ordering on jammed systems deduced that ordering occurs as shear pushes the system to lower energy minima [51].

Other colloidal systems such as charged stabilized spheres [52–54], latex particles [55] and microgels [56] also exhibit ordering when submitted to steady and oscillatory shear. There is an interesting general review on colloidal shear induced ordering [57], while a more recent review of nucleation in 2D and 3D crystals at rest and under external fields [58] has also been published.

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