

Effective particle size as a control parameter for rough hard-particle fluids

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We numerically investigate how particle surface roughness affects the static and dynamic properties of a hard-particle fluid across a wide range of densities, ρ . These simulations of a simple model of granular systems reveal that, although the amplitude and coverage of surface corrugation significantly influence the ρ dependence of system properties, the qualitative behavior of this dependence remains unchanged. These findings can be described quantitatively by introducing an effective particle size, which enables a direct mapping of the rough particle systems to equivalent hard-disk systems. Analytical calculations provide an explicit form of this mapping and allow us to predict the static and dynamic properties of rough particles using standard liquid-state theories for hard disks.

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I. INTRODUCTION

Granular systems are ubiquitous in nature and technological applications since they are closely related to phenomena like landslides, avalanches, or food and powder processing [1–5]. These materials are inherently athermal, frictional, and dissipative, so they can have highly complex structures and relaxation dynamics, making them paradigmatic examples that allow us to explore nonequilibrium physics [6–10].

Recent studies have advanced our understanding regarding the influence of friction on the static properties of the packs, notably the phenomenon of jamming and the details of the local packing geometry [11–16]. However, its effect on dynamic quantities is still an open problem since the induced coupling between the translational degrees of freedom and the orientational ones renders the particle motion highly complex [17–20]. Also surface roughness is an important feature of granular systems since it has been shown to affect the static and dynamical properties of the system in a similar manner as friction [21–26]. However, their origin is fundamentally different: Friction is due to the tangential resistive force at contacts, influencing sliding and rolling [14,27], whereas geometric roughness introduces steric constraints and modifies the excluded volume even in the absence of tangential forces [28]. So far, insight into the connection between surface

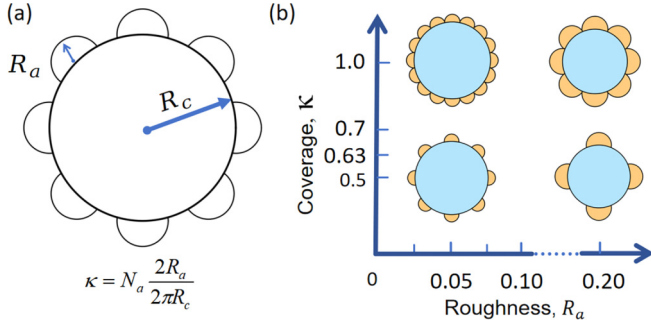
roughness and friction is still missing since theory struggles to describe the properties of rough particles, while in experiments it is difficult to vary the roughness in a systematic manner, although recent advances in three-dimensional (3D) printing techniques have allowed to address this problem [29–32].

Simple models that allow to tune the roughness show that the jamming density and coordination number decrease with roughness and converge to the behavior of the frictional case [29], but the important case of densities beyond this point has so far remained unexplored. Previous computational studies examined the jamming of various types of frictionless nonspherical smooth particles and showed that the packs can remain mechanically stable even if the average contact number is less to the number of degrees of freedom, thus demonstrating that a nontrivial particle shape can strongly influence the properties of the pack [33–35]. Rheological experiments demonstrate that rough particles exhibit more pronounced discontinuous shear thickening and an earlier onset of dilatancy compared to their smooth counterparts, emphasizing the importance of asperity-induced solid-solid contacts [25,26,29,36–41]. While these findings demonstrate the importance of roughness for the macroscopic behavior of the system, we lack at present a theoretical framework that allows to describe such systems in a wider range of densities, which also hinders to establish the connection between friction and surface roughness in these systems.

Here, we present the results of large-scale computer simulations of systems of rough particles. We find that in a wide range of densities, their structural and dynamic properties can be mapped onto a hard-disk fluid with an effective particle size that can be predicted analytically, thus allowing well-known liquid-state theory approaches to describe these complex systems.

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II. MODEL

To probe how the properties of a fluid depend on particle roughness, we consider a two-dimensional (2D) model of disks that are decorated by asperities [27]. Using the diameter, $2R_c$, of the central particle as unit length, the relevant parameters characterizing a mesoparticle (MP) are the radius of the asperities, R_a , and the fraction of the perimeter of the central particle that is covered by the latter, κ (see Fig. 1). We consider $0 \leq R_a \leq 0.2$ and for κ the values 1.0, 0.7, 0.63, and 0.5. MPs interact with each other by means of a Hertzian central force [27], i.e., $F_{\text{HZ}} = [R_i R_j / (R_i + R_j)]^{1/2} k_n \delta^{3/2}$, where δ is the overlap between disks i and j , whose radii satisfy $R_i, R_j \in \{R_c, R_a\}$ and $k_n = 2 \times 10^8$, a value that is sufficiently large to ensure that the MPs are very similar to hard bodies. The total number of MPs was 10^4 , large enough to avoid significant finite size effects but small enough that Mermin-Wagner fluctuations do not significantly affect the system properties on the length scales and timescales considered here [42]. More details on the simulations are given in the Appendix.

III. STATIC PROPERTIES

The structural order of a fluid is usually characterized by means of the radial distribution function $g(r)$ [43] (see Fig. S1 in the Supplemental Material [44]). However, the nature of the local order can be studied better by means of a three-point correlation function, such as the bond-orientational order $\bar{\psi}_6$ [45], which is the system average of the local sixfold bond-orientational order parameter $\psi_6(k)$, defined for particle k as

$$\psi_6(k) = \left| \frac{1}{N_k} \sum_{j=1}^{N_k} \exp[i6\theta_{kj}] \right|, \quad (1)$$

where the sum runs over the N_k Voronoi neighbors of particle k , and θ_{kj} is the angle between the bond vector $\mathbf{r}_{kj}$ and a fixed reference axis.

Figure 2(a) shows the ρ dependence of $\bar{\psi}_6$ (see Figs. S2 and S3 in the Supplemental Material [44] for the probability distribution function (PDF) of ψ_6). At low densities, $\bar{\psi}_6$ is small, but increases quickly at intermediate densities, reflecting the formation of a local order, before it saturates at high ρ due to the formation of intermediate-range order in the form

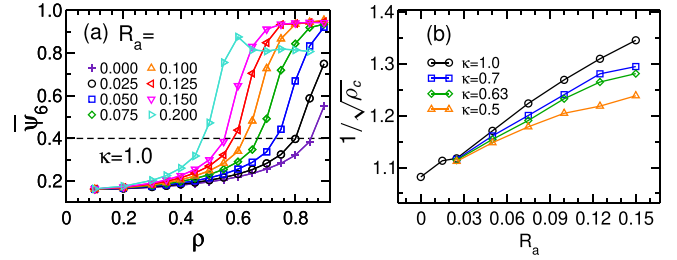


FIG. 2. (a) Bond-orientational order parameter $\bar{\psi}_6$ as a function of number density ρ for $\kappa = 1.0$ and different asperity radii R_a . The horizontal dashed line shows $\bar{\psi}_6(\rho_c) = 0.4$ and serves to define ρ_c presented in panel (b). (b) $1/\sqrt{\rho_c}$ as a function of R_a for different values of κ .

of polycrystals. The shape of the curves for the different R_a is independent of R_a , and only the density at which $\bar{\psi}_6$ shoots up depends on R_a . This suggests that systems with different R_a can be mapped onto each other and this conclusion holds also for other values of coverage κ or local structural observables (see the Supplemental Material [44]).

For this mapping, we introduce an effective radius R_{eff} :

$$R_{\text{eff}}(R_a, \kappa) = R_c(1 + B(\kappa)R_a/R_c). \quad (2)$$

Here, $B(\kappa)$ is a fit parameter that depends on κ and determines the effective size of a mesoparticle. The effective packing fraction is then given by

$$\phi_{\text{eff}} = \rho \pi R_{\text{eff}}^2. \quad (3)$$

To obtain B , we determine for a given R_a the density ρ_c at which $\bar{\psi}_6$ takes the value 0.4 [horizontal dashed line in Fig. 2(a)]. (The exact value of this threshold is not important.) Assuming that ρ_c corresponds to a fixed ϕ_{eff} , one obtains from Eq. (3) that $1/\sqrt{\rho_c} \propto R_{\text{eff}}$. Figure 2(b) shows that $1/\sqrt{\rho_c}$ is indeed a linear function of R_a if R_a/R_c is small, i.e., weak roughness, with the slope of the curves giving $B(\kappa)$.

Figures 3(a)–3(c) present $\bar{\psi}_6$ as a function of ϕ_{eff} and one sees that the different datasets fall perfectly on a master curve, demonstrating that one can indeed map the properties of systems with different R_a onto each other by means of Eq. (2). The figure hints that the master curves are basically independent of the coverage κ . That this is indeed the case is demonstrated in Fig. 3(d) where we superimpose the data for the different values of κ . From this plot, one thus concludes that the ρ , R_a , and κ dependence of the local structure, as characterized by $\bar{\psi}_6$, can be obtained from a single function that depends only on ϕ_{eff} . In the Supplemental Material [44], we show that this conclusion holds not only for $\bar{\psi}_6$ but for other observables as well, such as the bond-angle distribution or the local order parameter T_6 [46].

The mapping of the data for a given observable and fixed κ onto a common master curve might *a priori* depend on the observable considered. That this is not the case is shown in Fig. 4, which shows that the κ dependence of B for the different observables is basically independent of the quantity considered. In particular, we present the value of B as obtained from making scaling plots like the ones shown in Fig. 3 for the observables $\bar{\psi}_6$, from the area A under the main peak in the bond-angle distribution function θ_{ijk} between three parti-

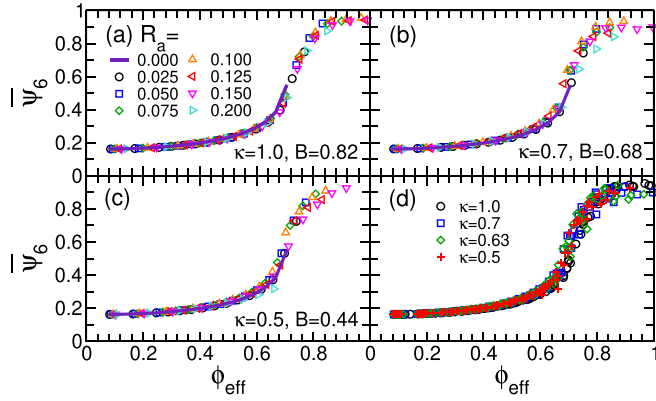


FIG. 3. Bond-orientational order parameter $\bar{\psi}_6$ as a function of the effective packing fraction ϕ_{eff} for different values of the asperity radius R_a . Panels (a)–(c) correspond to $\kappa = 1.0, 0.7$, and 0.5 , respectively, while panel (d) combines the data for all κ ($\kappa = 1.0, 0.7, 0.63$, and 0.5) to illustrate the resulting master-curve collapse. For each κ , the factor B used to make the master curve is indicated in the panel. Note that we show only data points for which the samples have not crystallized.

cles that are mutual nearest neighbors, the local orientational order parameter T_6 , and the size of the cage formed by the nearest neighbors of a particle, i.e., the Lindemann ratio (see the Supplemental Material [44] for a precise definition of these quantities). That $B(\kappa)$ increases monotonically with the coverage is consistent with the expectation that particles with larger κ possess a more complete ring of asperities and thus a stronger excluded-volume effect, i.e., a larger zone in which the repulsive interaction is very large. The independence of B

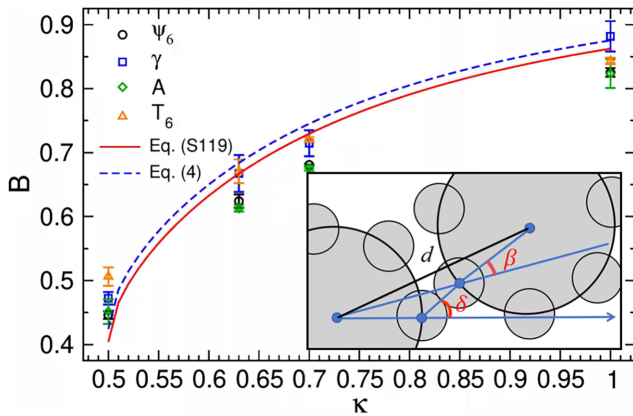


FIG. 4. Scaling factor B as a function of the surface coverage ratio κ , extracted from four different structural quantities: the bond-orientational order parameter $\bar{\psi}_6$, the Lindemann ratio γ , the bond-angle distribution A , and the triplet orientational order parameter T_6 (see the Supplemental Material [44] for definitions). The red solid line shows the result of our analytical calculation [Eq. (S119) in the Supplemental Material [44]], while the blue dashed line corresponds to its first-order approximation [Eq. (4)]. Inset: Illustration of the generic contact geometry between two MPs: The relative rotation of the right particle around the contact point (angles β and δ) yields all configurations needed to calculate the effective distance $\bar{d}$ between the two centers (see the Supplemental Material [44] for details).

from the observable considered leads to the conclusion that the mapping given by Eq. (2) allows to obtain a universal, i.e., observable-independent, master curve, with B being the only unknown (κ -dependent) parameter. In other terms, once one has obtained this master curve, for example, for the case of smooth hard disks, one can predict via Eq. (2) the properties of all the systems with $R_a > 0$ and $\kappa > 0$.

IV. ANALYTICAL PREDICTION OF THE EFFECTIVE PARTICLE SIZE

The independence of B from the observable considered hints that the static properties of the systems can be obtained from an analytical calculation that takes into account the geometry of the particles. Since this is basically a hard core system, all configurations have the same Boltzmann weight and thus one is faced only with a counting problem to obtain the entropic contribution. For the case of a hard-disk system, this is a formidable problem that is still open, but many excellent approximations exist [47,48]. We now assume that the partition function of our system can be factorized into the one of a hard-disk system and a second factor that depends only on the orientational degrees of freedom. To evaluate this second factor, we consider two MPs that touch each other and calculate their average distance $\bar{d}$ as a function of R_a and κ . Assuming that $\bar{d}$ is a reliable proxy for R_{eff} , this calculation allows us to obtain B from Eq. (2).

For the calculation of $\bar{d}$, one has to take the average over all distances d between the centers of the two touching MPs, which in turn depend on the relative orientations of the MPs, i.e., the angles β and δ defined in the inset of Fig. 4. These calculations are presented in the Supplemental Material [44] and differentiating the resulting $\bar{d}$ with respect to R_a gives B [Eq. (S119) in the Supplemental Material [44]]. By making the approximation that $R_a/R_c \ll 1$, one obtains the expression [see Eq. (S120) in the Supplemental Material [44]],

$$B \approx \frac{1}{4\kappa \arcsin(\frac{1}{2\kappa})} \left(2 - \frac{1}{6\kappa^2} \right) \quad (4)$$

and both results are included in Fig. 4 as well. The good agreement between theory and data from the simulation shows that it is indeed possible to predict the static properties of the systems of MPs if one knows those of a hard-disk system.

V. DYNAMIC PROPERTIES

In disordered systems that relax slowly, the dynamics is closely related to the structure [42], and hence it is of interest to probe whether the effective size R_{eff} of the MPs allows to predict also the relaxation dynamics of the system. To check this, we have determined the mean-squared displacement (MSD) of a tagged particle and, using the Einstein relation, calculated the diffusion constant D . (We recall that in 2D systems the long-time diffusion constant is not well defined because of the long-time tails in the velocity autocorrelation function. However, as it is custom in the field of glass physics, we consider here only MSDs that are much smaller than the size of the system squared; i.e., D is not affected in a noticeable manner by these tails.) Figures 5(a)–5(c) present the density dependence of D for different values of R_a and

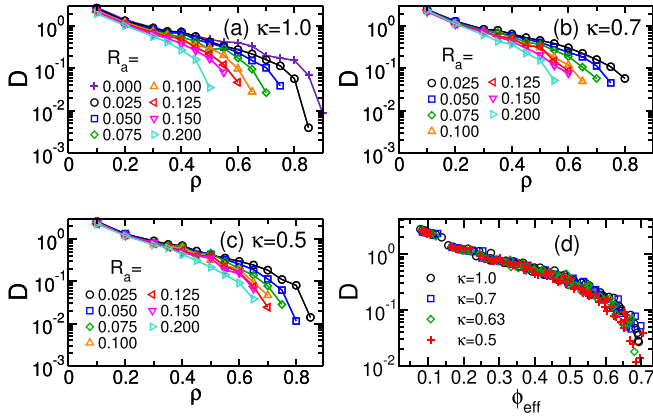


FIG. 5. Diffusion constant D as a function of number density ρ for different asperity radii R_a at fixed κ : (a) $\kappa = 1.0$, (b) $\kappa = 0.7$, and (c) $\kappa = 0.5$. (d) The same data plotted vs the effective packing fraction ϕ_{eff} , showing a collapse onto a master curve.

κ . As expected, and independent of κ , the diffusion coefficient decreases rapidly with increasing density, reflecting the strong dynamical slowing down caused by the buildup of local constraints. We note that also here the overall shape of the curves is independent of R_a , although the density at which the slowdown becomes pronounced changes with κ and R_a . Particles with larger coverage ratios or larger asperities exhibit a reduction in mobility already at lower densities, consistent with the enhanced excluded-volume effects discussed in the structural analysis.

To examine whether also the dynamical properties are governed by the effective size R_{eff} , we plot in Fig. 5(d) the diffusion constant D as a function of the effective packing fraction ϕ_{eff} . Remarkably, the curves for the different R_a and κ collapse onto a single master curve, demonstrating that R_{eff} controls also the translational dynamics.

VI. SUMMARY AND OUTLOOK

The presented results show that the structural and dynamical properties of two-dimensional particles with different surface roughness can be mapped onto a hard-disk system with an effective size R_{eff} and hence an effective packing fraction ϕ_{eff} . This mapping works even for a roughness that is very substantial, i.e., 20%. Our analytical calculation allows to predict with good accuracy this mapping as a function of R_a and κ , thus opening the door to describe the static and dynamic properties of such systems from the knowledge of the well-studied model of hard disks. Hence, we conclude that over a wide range of densities, roughness values, and asperity coverages, (1) geometric roughness primarily renormalizes the excluded volume and thus controls a broad class of structural and transport observables via a single R_{eff} , and (2) the coverage dependence $B(\kappa)$ can be computed from the geometrical properties of the MPs, enabling quantitative predictions from the hard-disk reference system. This insight will allow to make a better connection between the concepts of friction and roughness, a relation that is presently not well understood [26,29].

Whether the proposed approach can be successfully generalized to 3D systems is at present an open question, but the

mean-field nature of the calculation leads to the expectation that this can indeed be done. To what extent this approach is also reliable in the case of sparse asperities' coverage, or if these lockings are strongly orientational, or in the case of multicomponent systems, remains to be tested in the future. A further important question is whether this approach is applicable if the overall shape of the particle is nonspherical (elliptic, kidney-shaped, etc.), i.e., particle geometries that are often found in real granular materials [2]. At high densities, the free energy landscape of such systems can be expected to become significantly more complex than the one of smooth circular objects, with the presence of roughness giving rise to new relaxation channels [21,26,36]. These novel relaxation mechanisms will in turn affect the static and dynamic properties of the system in the jammed and glassy state, i.e., regimes that are so far not well understood. Hence, it will be of interest to probe to what extent the present mean-field-like calculation is able to capture these behaviors.

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Z.Z. and W.K. conceptualized the work; N.X. carried out the simulations and performed the analysis of the data; all authors interpreted the results and wrote the paper.

DATA AVAILABILITY

The data that support the findings of this article are openly available [53].

APPENDIX

1. Model

We consider a one-component granular system composed of MPs, each consisting of a central disk of radius R_c and N_a small disks of radius R_a whose centers are located on the surface of the central disk. The diameter of the central disk will be used as the unit of length. The surface coverage κ quantifies what fraction of the perimeter of the central disk is occupied by these asperities, with $\kappa = 1.0$ corresponding to complete coverage. In the following, we will consider $\kappa = 0.5, 0.63$ (maximal coverage that allows an asperity to contact the central disk), 0.7, and 1.0. The radius R_a of the asperities characterizes the roughness of the mesoparticle [27]. To explore different roughness levels, we vary R_a in the range 0.025–0.2.

The number of asperities is given by

$$N_a = \left\lfloor \frac{2\pi R_c}{2R_a} \kappa \right\rfloor, \quad (\text{A1})$$

where $\lfloor \cdot \rfloor$ denotes the integer floor function. This value of N_a can result in a coverage κ that is slightly smaller than the target value and in that case we have slightly decreased R_a to reach a given κ . These adjustments are typically less than 2% for $\kappa = 1.0$, but can be larger for certain combinations such as $\kappa = 0.5$ and $R_a = 0.15$ (see Tables I and II).

TABLE I. The exact value of R_a used in the simulations to assure a constant value of coverage κ .

	$\kappa = 0.5$	$\kappa = 0.63$	$\kappa = 0.7$	$\kappa = 1.0$
$R_a = 0.025$	0.0245	0.0247	0.0250	0.0250
$R_a = 0.050$	0.0491	0.0495	0.0500	0.0499
$R_a = 0.075$	0.0714	0.0707	0.0733	0.0748
$R_a = 0.100$	0.0982	0.0990	0.1000	0.0982
$R_a = 0.125$	0.1122	0.1237	0.1221	0.1221
$R_a = 0.150$	0.1309	0.1414	0.1374	0.1428
$R_a = 0.200$	0.1964	0.1980	0.1833	0.1964

In order to compare our results with hard-disk-like results, we also simulate a smooth-particle model with $R_a = 0$. To maintain identical simulation protocols (e.g., initialization and temperature control), these particles are implemented by attaching two tiny asperities with $R_a = 10^{-4}$ on opposite sides of the central disk. This minimal perturbation ensures negligible impact on the particle's geometry and dynamics. In all cases, the total mass of each MP is normalized to unity by adjusting the mass density. (The surface of an MP is given in Table III). Denoting by N the number of mesoparticles, the number of interaction sites used in the simulation is given by $N(N_a + 1)$, which ranges between 50 000 and 640 000.

2. Interaction potential

The particle interactions in our simulations are given by the Hertzian interaction model; i.e., the interaction force, $\mathbf{F}_{\text{HZ}}$, is given by [54,55]

$$\mathbf{F}_{\text{HZ}} = \sqrt{\frac{R_i R_j}{R_i + R_j}} k_n \delta^{1.5} \mathbf{n}_{ij}. \quad (\text{A2})$$

Here, δ denotes the overlap between two disks i and j , whose radii satisfy $R_i, R_j \in \{R_c, R_a\}$, and $\mathbf{n}_{ij}$ is the unit vector connecting their centers.

We present the results in dimensionless units, with $\sigma = 2R_c$ the unit of length, the mass of an MP as $m = 1.0$, and time in units of $\tau = \sqrt{\frac{m}{k_n \sigma}}$. The parameter k_n is chosen as $k_n =$

TABLE II. The number of asperities for the different simulated systems.

	$\kappa = 0.5$	$\kappa = 0.63$	$\kappa = 0.7$	$\kappa = 1.0$
$R_a = 0.025$	32	40	44	63
$R_a = 0.050$	16	20	22	31
$R_a = 0.075$	11	14	15	21
$R_a = 0.100$	8	10	11	16
$R_a = 0.125$	7	8	10	13
$R_a = 0.150$	6	7	8	11
$R_a = 0.200$	4	5	6	8

TABLE III. The surface area of the complete MP.

	$\kappa = 0.5$	$\kappa = 0.63$	$\kappa = 0.7$	$\kappa = 1.0$
$R_a = 0.025$	0.8153	0.8237	0.8286	0.8475
$R_a = 0.050$	0.8465	0.8633	0.8730	0.9088
$R_a = 0.075$	0.8754	0.8979	0.9154	0.9755
$R_a = 0.100$	0.9107	0.9450	0.9647	1.0373
$R_a = 0.125$	0.9296	0.9870	1.0066	1.0983
$R_a = 0.150$	0.9550	1.0175	1.0359	1.1585
$R_a = 0.200$	1.0468	1.1180	1.1257	1.3094

2×10^8 , a value that ensures that the particles are very similar to frictionless hard core bodies; i.e., the dynamics is strongly dominated by excluded-volume effects and the presence of surface asperities. A similar choice of the parameters has been made in previous studies of sheared granular systems, where they were shown to reproduce realistic relaxation processes while keeping particle overlaps negligible [56,57].

3. Simulation details

Simulations are performed using the large-scale atomic/molecular massively parallel simulator (LAMMPS) [58,59]. Periodic boundary conditions are applied in all three spatial directions, with the z dimension fixed to 0.5 to ensure quasi-two-dimensional confinement. The initial configurations are prepared in a $320 \times 320 \times 0.5$ simulation box by randomly placing $N = 10\,000$ MPs, each one having been assigned a random velocity corresponding to the target temperature of $T = 1.0$. (Since the interaction potential is very stiff, we basically simulate hard disks and hence the value of the temperature is not a relevant quantity.) The box dimensions in the x - y plane are then slowly reduced to achieve the desired number density ρ .

The system is equilibrated in the canonical (NVT) ensemble using a Nosé-Hoover thermostat [60,61] with a target temperature $T = 1.0$ and a thermostat damping time of $\tau_{\text{damp}} = 0.5$. Each simulation consisted of an equilibration stage of 3×10^6 steps, followed by a production run of 7×10^6 steps for data collection. The time step was $\Delta t = 1.0 \times 10^{-4}$, a value that is small because the potential is very stiff. We note that the equilibration time is chosen to be at least one order of magnitude larger than the structural relaxation time at the highest simulated density, thereby ensuring that the system reaches equilibrium before measurements are taken. At the highest densities, the relaxation dynamics of the system becomes very slow due to the formation of a polycrystalline structure. In order to avoid out-of-equilibrium effects, we present only data that are not significantly influenced by these effects.

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