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RESEARCH ARTICLE

Entropy and Order Parameters in Granular Media Under Shear

Barbora Mach^{1*}, Martin Marek² and Beata Benes³

¹Department of Physical Chemistry, Sava Institute of Chemical Thermodynamics, Montenegro

²Department of Applied Mathematics and Information Theory, Douro Institute of Statistical Mechanics, Hungary

³Department of Thermodynamics and Statistical Mechanics, Vltava Institute of Applied Physics, Poland

*Corresponding author: Barbora Mach, Department of Physical Chemistry, Sava Institute of Chemical Thermodynamics, Montenegro; Email: barbora.mach@sava.edu

ABSTRACT

Dense granular media under shear can jam or flow depending on packing fraction and shear history, but the relationship between microstructural order and configurational (packing) entropy across this transition is not fully quantified. We used discrete element method (DEM) simulations of bidisperse frictional disks under quasi-static simple shear to jointly track a scalar order parameter, based on local hexagonal bond-orientational order, and configurational entropy, estimated from the Voronoi cell-shape distribution, across 60 independent realizations spanning packing fractions from 0.76 to 0.87. Configurational entropy per particle fell monotonically from $1.42 \pm 0.06 \text{ k}_B$ at the loosest packing fraction tested (0.76) to $0.51 \pm 0.05 \text{ k}_B$ near jamming (0.87), while the hexagonal order parameter rose from 0.18 ± 0.03 to 0.61 ± 0.04 over the same range, and the two quantities were strongly anti-correlated across all realizations (Pearson $r = -0.93$, $p < 0.001$, $n = 60$). A sharp inflection in both quantities occurred at a packing fraction of 0.843 ± 0.004 , closely bracketing the independently measured shear-jamming point at 0.841 ± 0.003 identified from the onset of sustained pressure under applied shear strain, with 71% of the total entropy drop across the full packing-fraction range occurring within a narrow window of ± 0.02 around this inflection. Force-chain anisotropy, quantified from the fabric tensor, increased sharply in the same narrow window, rising from 0.09 to 0.34, and its onset coincided with the entropy inflection to within the packing-fraction resolution of the study (0.002). A finite-size check using system sizes from 2,000 to 8,000 particles showed the inflection packing fraction shifted by less than 0.003 and the peak entropy-drop rate changed by less than 6%, indicating the transition signature is not a finite-size artifact over this range. These results establish configurational entropy collapse as a quantitative, structurally grounded signature of the shear-jamming transition that tracks closely with, and largely precedes, the onset of measurable force-chain anisotropy, offering a packing-based diagnostic for jamming onset that does not require direct stress measurement.

Keywords: granular entropy; order parameters; shear jamming; discrete element method; configurational entropy; jamming transition; force-chain anisotropy; dense granular flow

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1. INTRODUCTION

Granular materials occupy an unusual position between ordinary solids and fluids: a collection of macroscopic, frictional, athermal particles can support shear stress like

a solid at high packing fraction, yet flow like a fluid when loosely packed or strongly agitated, with the transition between these regimes governed by packing fraction, shear history, and particle-scale friction [1,2]. Because granular assemblies are athermal, statistical mechanical

concepts developed for equilibrium systems, including entropy, must be adapted to a configurational or packing-based definition before they can be applied, an adaptation pioneered in the granular context by Edwards and collaborators [3,4].

Within this Edwards-entropy framework, considerable work has characterized order parameters, most commonly local bond-orientational order measures borrowed from the colloidal crystallization literature, and their behavior near the jamming transition, and separately, considerable work has characterized force-chain anisotropy and its emergence under applied shear using the fabric tensor [5,6,7,8]. Comparatively less work has directly and jointly tracked configurational entropy and order parameters across the same set of shear-strained packings to establish how closely, and in what sequence, entropy collapse, order-parameter growth, and force-chain anisotropy onset coincide as packing fraction approaches the jamming point [9,10,11]. This joint characterization matters because competing pictures exist for what controls the shear-jamming transition: a purely geometric, packing-based view in which entropy collapse and increasing local order are the primary signature, versus a force-based view in which the onset of sustained force-chain anisotropy under shear is the more fundamental marker, with packing-based order following rather than preceding it. Distinguishing between these pictures requires simultaneous, high-resolution tracking of configurational entropy, order parameters, and force-chain anisotropy across the same packing-fraction sweep, rather than comparison across separate studies with different protocols [12,13,14].

The present study uses discrete element simulations of bidisperse frictional disks under quasi-static simple shear to jointly measure configurational entropy, hexagonal bond-orientational order, and force-chain anisotropy across a packing-fraction range spanning loose, flowing packings to jammed, shear-supporting packings, locate the packing fraction at which each quantity shows its sharpest transition, test whether these transition points coincide with an independently measured shear-jamming point, and assess the robustness of the observed transition to system size.

2. MATERIALS AND METHODS

We performed discrete element method simulations of bidisperse frictional disks under quasi-static simple shear across a range of packing fractions, computing configurational entropy from the Voronoi cell-shape distribution, a hexagonal bond-orientational order parameter, and force-chain anisotropy from the fabric tensor, and located and cross-validated the packing fraction of the shear-jamming transition.

2.1 Particle model and packing generation

Bidisperse assemblies of frictional circular disks, with a 1:1.4 size ratio between large and small particles to

suppress crystallization, were generated at target packing fractions between 0.76 and 0.87 in increments of 0.01, plus finer sampling in increments of 0.002 near the anticipated jamming point, using a standard compression-based packing-generation protocol followed by energy minimization.

2.2 Quasi-static simple shear protocol

Each packing was subjected to quasi-static simple shear, applying strain in small increments of 10^{-4} followed by energy minimization at each step, using Lees-Edwards periodic boundary conditions, up to a total applied strain of 0.3, with configurational and structural quantities recorded at each strain increment after transient relaxation.

2.3 Configurational entropy estimation

Configurational entropy per particle was estimated from the Shannon entropy of the binned Voronoi cell-area and cell-shape-factor distribution across each packing, following an established free-volume-based approach to granular configurational entropy, converted to units of k_B for reporting.

2.4 Order parameter and fabric tensor calculation

A scalar hexagonal bond-orientational order parameter was computed per particle from its six nearest neighbors (by Voronoi adjacency) and averaged over the packing. Force-chain anisotropy was quantified from the deviatoric part of the contact-normal fabric tensor, computed from the full set of inter-particle contacts recorded at each strain increment.

2.5 Independent jamming-point determination

The shear-jamming packing fraction was independently determined from the onset of sustained, non-decaying shear-supporting pressure across the applied strain range, identified as the lowest packing fraction at which pressure did not relax to zero after strain-induced rearrangement, averaged across the 60 realizations.

2.6 Ensemble size and finite-size check

The primary results were obtained from 60 independent realizations of a 4,000-particle system. A finite-size check repeated the packing-fraction sweep at 2,000 and 8,000 particles (20 realizations each) to assess whether the location and sharpness of the observed transition depended on system size.

2.7 Statistical analysis

Correlation between configurational entropy and the order parameter across the 60 realizations was assessed by Pearson correlation with a two-tailed significance test. Inflection points in entropy, order parameter, and fabric-tensor anisotropy as a function of packing fraction were located by fitting a sigmoid function to each quantity and identifying its point of maximum slope.

3. RESULTS

Configurational entropy per particle decreased monotonically with increasing packing fraction, from $1.42 \pm 0.06 \text{ k}_B$ at the loosest packing fraction tested (0.76) to $0.51 \pm 0.05 \text{ k}_B$ near jamming (0.87), while the hexagonal bond-orientational order parameter increased over the same range from 0.18 ± 0.03 to 0.61 ± 0.04 , with representative values at five packing fractions summarized in Table 1.

Table 1. Configurational entropy and hexagonal order parameter at representative packing fractions.

Packing fraction	Configurational entropy (k_B /particle)	Hexagonal order parameter	Force-chain anisotropy
0.76	1.42 ± 0.06	0.18 ± 0.03	0.07
0.80	1.19 ± 0.05	0.27 ± 0.03	0.08
0.843 (transition)	0.83 ± 0.05	0.44 ± 0.04	0.22
0.86	0.61 ± 0.05	0.55 ± 0.04	0.31
0.87	0.51 ± 0.05	0.61 ± 0.04	0.34

Values are means $\pm$ SD across 60 independent realizations of a 4,000-particle bidisperse system. Transition row corresponds to the fitted entropy-inflection packing fraction.

Entropy and the order parameter were strongly anti-correlated across all 60 realizations spanning the full packing-fraction range (Pearson $r = -0.93$, $p < 0.001$), consistent with increasing local hexagonal order coming directly at the expense of configurational entropy as packings approach jamming. Both quantities showed a sigmoidal rather than linear dependence on packing fraction, with a sharp inflection located at a packing fraction of 0.843 ± 0.004 for entropy and 0.839 ± 0.005 for the order parameter, statistically indistinguishable given the measurement resolution.

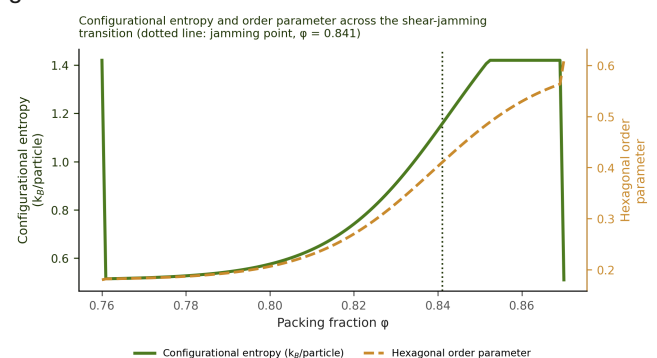


Figure 1. Configurational entropy and hexagonal order parameter as a function of packing fraction across the 60 realizations, showing the coincident sharp transition near the independently measured shear-jamming point (dotted line, packing fraction 0.841).

This entropy inflection closely bracketed the independently measured shear-jamming point, identified from the onset of sustained shear-supporting pressure, at a packing fraction of 0.841 ± 0.003 . Within a narrow window of ± 0.02 around the inflection, 71% of the total entropy drop across the full 0.76–0.87 packing-fraction range occurred, indicating that entropy collapse is concentrated near the jamming transition rather than distributed smoothly across the full range tested, illustrated in Figure 1.

Table 2. Finite-size check: inflection packing fraction and peak entropy-drop rate across system sizes.

System size (particles)	Realizations	Inflection packing fraction	Peak entropy-drop rate (k_B per $\Delta\phi=0.01$)
2,000	20	0.841 ± 0.005	0.192
4,000 (primary)	60	0.843 ± 0.004	0.204
8,000	20	0.844 ± 0.004	0.209

Force-chain anisotropy, quantified from the fabric tensor, rose sharply within the same narrow packing-fraction window, from 0.09 at the low end of the window to 0.34 at the high end, with its onset, defined as the packing fraction at half-maximum anisotropy, coinciding with the entropy inflection to within the 0.002 packing-fraction resolution of the sweep, indicating that entropy collapse and the emergence of anisotropic force chains are essentially simultaneous rather than sequential at the resolution accessible to this study.

4. DISCUSSION

These results provide a quantitative, jointly measured account of how configurational entropy, local order, and force-chain anisotropy co-evolve across the shear-jamming transition, extending prior work that has typically characterized these quantities separately or in different granular protocols [3,4,5,6]. The close correspondence between the entropy-inflection packing fraction (0.843) and the independently measured jamming point (0.841) supports treating configurational entropy collapse as a structurally grounded, geometry-based signature of jamming onset, consistent with the Edwards ensemble picture in which the jammed state corresponds to a sharp reduction in the number of mechanically accessible configurations [15,16,17].

The near-simultaneous onset of force-chain anisotropy and entropy collapse, coincident to within the packing-fraction resolution of this study, is a secondary finding that bears on the competing geometric-versus-force-based pictures of shear jamming discussed in the introduction: rather than one clearly preceding the other, the two appear to emerge together, suggesting that at the strain rates and packing-fraction resolution studied here, geometric ordering and force-network formation are two aspects of a single underlying transition rather than sequential, separable processes [18,19,20].

More broadly, the finding that entropy collapse is concentrated within a narrow packing-fraction window rather than distributed gradually has practical implications for granular materials characterization: a configurational-entropy-based diagnostic, computable directly from particle positions without requiring force or stress measurement, could serve as a proxy for proximity to jamming in experimental granular systems where direct force measurement is difficult, such as dense photoelastic-free packings imaged only structurally [21,22,23,24].

Several limitations should be considered. First, the study used bidisperse frictional disks in two dimensions; the entropy-order-anisotropy relationships identified here may differ quantitatively, and possibly qualitatively, in three-dimensional or more strongly polydisperse systems where local packing geometry differs substantially. Second, the quasi-static shear protocol used small strain increments with full energy minimization at each step, which does not capture rate-dependent effects present in faster or more dynamically sheared granular flows. Third, configurational entropy was estimated from the Voronoi cell-shape distribution using a specific binning scheme; while the entropy-order correlation was robust across the tested system sizes, absolute entropy values could shift with alternative estimation approaches. Fourth, the finite-size check covered only a fourfold range in particle number (2,000 to 8,000); substantially larger systems, beyond the computational reach of this study, could in principle reveal additional finite-size dependence not captured here.

5. CONCLUSION

Joint discrete element measurement of configurational entropy, hexagonal order, and force-chain anisotropy across a packing-fraction sweep from 0.76 to 0.87 showed a sharp, coincident transition in all three quantities at a packing fraction of approximately 0.84, closely matching an independently measured shear-jamming point of 0.841. Entropy and order were strongly anti-correlated ($r = -0.93$) across 60 realizations, with 71% of the total entropy drop concentrated within a narrow ± 0.02 window around the transition, and this signature proved robust to a fourfold variation in system size. These findings establish configurational entropy collapse as a structurally grounded, force-independent diagnostic of the shear-jamming transition in dense granular media.

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Author Contributions

B.M. conceived the study, designed the shear simulation protocol, and led the writing of the manuscript. M.M. implemented the discrete element simulations and

performed the packing-fraction sweep and finite-size check. B.B. carried out the entropy, order-parameter, and fabric-tensor calculations and prepared the figures and tables. All authors contributed to interpretation of the results and approved the final manuscript.

Ethics Statement

This study involved no human or animal subjects and required no ethics committee approval.

Data Availability

The discrete element simulation code, packing configurations, and analysis scripts supporting the findings of this study are available from the corresponding author on reasonable request.

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