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Structural signature of a sheared granular flow

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ABSTRACT

Various types of mesoscopic structures form in jammed granular materials due to the self-organization of their constituent particles. Internal structural degrees of freedom are introduced in addition to the translational degree of freedom, and both impact the intrinsic properties of granular materials from its constituent ordinary objects. In this study, we perform numerical simulations of plane shear granular flows confined with a constant pressure. Using the radical tessellation method, we investigate the temporal and spatial evolutions of granular structures. The simulation results show that the degree of local fivefold symmetry (LFFS) is a unique structural indicator due to its significant spatial heterogeneity and dramatic variance with shearing. In the steady state, regions with small LFFS possess large linear velocity gradients, large angular velocities, and consequently large fluctuations in kinetic energy and elastic energy. Thus, LFFS may link the internal structures and dynamic properties of granular materials. Inspired by this spatial distribution scenario consisting of LFFS and energy, we propose a structural unit composed of a strong force network (SFN) and a weak force network (WFN). The SFN has a high shear resistance that acts as the elastic backbone that supports the entire matrix of a granular assembly, whereas the WFN with high energy dissipation consists of embedded "inclusions" among the SFN. This structural analysis aids the understanding of the complex phenomena of granular materials and provides insight into the mechanisms.

1. Introduction

Some particles self-organize into various types of coherent structures, such as vortices and force networks, due to their discrete and dissipative nature, which indicates that such particles have a pronounced short-range order but no long-range structural order [1]. Such mesoscopic structures create the unique properties of granular materials not present in other materials, and are dependent on the extent of mechanical loading (e.g., shear rate or confining pressure as indicated by jamming phase diagrams [2], [3]). Examples include elasto-plastic granular solids, Herschel–Bulkley type granular flows, or combinations of the two. When in a solid state, each particle of a granular assembly stays in a mechanical balance with its local neighbors [4]. However, the packing of cohesionless spheres with a finite value of surface friction μ is hyper-static except at the isostatic limits when $\mu = 0$ or $\mu \to \infty$. This means that, for a single granular packing, many different sets of force networks exist that satisfy the force balance on each particle. Thus, the force network ensemble (FNE) has proven to be a useful tool for studying the stress states of static granular packings [5], [6]. Under loading, particles are propelled to move, which causes consequent dramatic evolutions of internal structures and leads to the sticks and slips observed in stress and nonaffine deformations due to particle rearrangements [7], [8]. One major challenge is how to effectively characterize the internal structures and extract the key structural features relevant to the fundamentals of granular properties. Moreover, understanding the evolution of structures would certainly be of considerable help when describing and predicting natural geophysical hazards [9], particularly the frequent granular-type debris flows that occur in the mountainous areas of Southwestern China.

Extensive numerical and theoretical efforts have been devoted to studying granular structures. Under external loading, forces are transmitted from one particle to the next via particle contact [10], which forms an inhomogeneous contact network [11]. Sanfratello et al. [12] developed a magnetic resonance elastography (MRE) technique to experimentally investigate the force chain structure within a densely packed 3D granular assembly. The force network was postulated to play a key role in controlling the mechanical responses of the granular system [13]. There have also been numerous attempts to characterize such a contact network [10], [14]. Instabilities emerge at multiple length scales in a deformed granular material and the buckling of force chains is a prevalent source of instability, for which a structural mechanical model was developed by Tordesillas et al. [15], [16].

There are a few parameters that are often used to measure the structural features in granular matter. The pair distribution function (PDF) is a pair correlation representing the probability of finding a particle as a function of distance r from an average center particle, where the structural information is embedded in the peak position, peak width, and relative intensity. Conventionally, the configuration of the nearest-neighbor shell, which contributes to the first peak in the PDF, constitutes the short-range order, whereas the structural

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features beyond the first peak to a distance of up to several radii, are referred to as the medium-range order. At larger r, the PDF gradually converges to unity, which means that no long-range order/correlation exists [17], [3]. One can perform Fourier transformations to obtain the PDF in real space, with the structure factor measured in an X-ray or neutron experiment [18]. The weakness of PDF is that the detailed three-dimensional information is lost as a result of statistical averages and it does not provide much information about the topology of the local structures in the particle-size scale [19]. As the long-range order rapidly decreases in a random packing, the local structures near each particle are probably the most effective mesoscopic characterization of the packing. The coordination number (CN) is the number of particles that contact a given center particle. A low CN value is common for loose packing, while a high CN is expected for dense packing [20], [21]. However, CN only considers the cluster of contacting particles and does not reflect any topological information of granular materials. The Voronoi tessellation is a scheme to divide a 3-D space into cells centered by each particle. It is well established that the structure of a packing can be quantified in terms of the metric and topological properties of such a tessellation. This type of analysis can provide much more detailed information than the one-dimensional PDF and CN analyses [22]. However, Voronoi tessellation is not adequate for polydispersed particles because it may cut the larger spheres; moreover, touching large spheres are not always neighbors. An alternative approach is radical tessellation in which the bisecting plane is replaced by the radical plane (i.e. all of the points in the radical plane have the same tangent length), which has been easily implemented with polydispersed granular systems [23], [24]. Moreover, the topological graph theory has been used to explore the order structures of granular materials [25].The analysis of the channel size distribution, based on the local neighbor correlation of four particle positions, is shown to be useful in distinguishing states of hard sphere systems [19].

In addition to these regular structural parameters, many indicators related to the mechanical properties of metallic glasses (MG) have been proposed, such as the shear transformation zone [26], [27], free volume, and local potential energy [28]. Atomic symmetry is a general concept found with glass-forming alloys in which both local five-fold and translational symmetries are present [29]. Nuclear magnetic resonance (NMR) experiments have shown that local cluster symmetry plays an important role in the glass-forming ability of MGs [30]. Molecular dynamics studies have also identified the unique behavior for the Voronoi pentagons during the quenching process [28]. Peng et al. indicated that the degree of local fivefold symmetry (LFFS) was crucial for understanding the structural relaxation and mechanical properties of MGs [31]. These studies on the structure of metallic glasses indeed shed insight into discovering the key features of short-to-medium range order, and help to identify the underlying physical principles that constitute the structural basis of granular properties [17].

In this work, we investigate the statistical information of granular structures, and quantify the temporal and spatial evolutions of the structures using radical tessellation. The focus of this work is the role of local fivefold symmetry. In the next section, we describe the numerical model used for our simulations. Section 3 shows the temporal and spatial evolutions of the structural parameters such as the topological properties and the metric properties. Section 4 primarily discusses the LFFS and its connection to other kinetic parameters, and in Section 5 we propose a new structural unit in terms of the LFFS and energy distributions.

2. Numerical model

Here, plane shear is modeled in its simplest flow configuration, which consists of spherical grains sheared between two rough plates composed of glued spheres [9], illustrated in the left figure of Fig. 2. The confining pressure P remains constant by employing a servo mechanism, i.e. a vertical motion of the upper wall at speed $v_w = \min(v_{\max}, (P - P_w)\eta)$, where $v_{\max}$ is the prescribed maximum velocity, η is a viscous damping parameter, and P_w is the normal stress exerted by the grains on the moving wall. The steady state corresponds to $\langle P_w \rangle = P$, and periodic boundaries are applied in the x and y directions. In this work, the gravity is ignored in comparison with the confining pressure. We move the top wall in the y direction at a constant velocity v_{y0}, while the lower wall is fixed. The contact model we used follows the Hertz–Mindlin theory [32]. We also adopt Coulomb sliding friction and damping components related to the coefficient of restitution, as first developed by Tsuji et al. [33] and recently used by Hill and Tan [34].

$$F_n = -k_n \delta_n^{3/2} - \eta_n \delta_n^{1/4} \dot{\delta}_n \tag{1}$$

$$F_s = \min\left(-k_t \delta_n^{1/2} \delta_t - \eta_t \delta_n^{1/4} \dot{\delta}_t, \mu F_n\right) \tag{2}$$

where F_n and F_s are the contact forces in the normal and tangential directions, respectively, to the contact plane between two contacting particles, and δ_n and δ_t are the corresponding deformations. The coefficients in the force model are related to the material properties of the two contacting particles, as listed in Table 1. As mentioned above, we used the function presented in Ref. [32] to determine the damping coefficient,

$$\alpha(\varepsilon) = \frac{-\sqrt{5}\ln\varepsilon}{\sqrt{\ln^2\varepsilon + \pi^2}} \tag{3}$$

where ε is the restitution coefficient. In this study, the density of particles was $\rho = 1000$ kg/m^3, the value of inter-particle friction was $\mu = 0.5$, the shear velocity was $v_{y0} = 1$ m/s, the maximum velocity applied along the z-axis was $v_{\max} = 0.1$ m/s, and the viscous damping parameter used in the formula determining the vertical speed of the upper wall was $\eta = 0.1$. The normal and tangential restitution coefficients were $\varepsilon_n = \varepsilon_t = 0.9$, Poisson's ratio was $\nu = 0.15$, and Young's modulus was $E = 100$ MPa. Nearly 17,000 spheres with a mean particle diameter $d = 0.007$ m were initially generated with a seed number of 1 in the region of $0.2 \times 0.2 \times 0.51$ m^3. Then, the height of the sample would be contracted to 0.2 m after applying the pressure, $P = 10$ kPa, and the volume fraction would appropriately achieve 0.57. Note that bi-dispersed particles with a radius ratio of 1:1.3 and a number ratio of 1:1 were used to prevent crystallization [2]. Therefore, in Table 1, only the radii and the masses of the contacting particles may be different and other parameters, such as Young's moduli and Poisson's ratios, were identical for contacting particles. Radical tessellation was adopted to divide the 3-D space into cells rather than Voronoi tessellation. In radical tessellation, the bisecting plane is replaced by the radical plane, with all of the points having the same tangency length for the two spheres [23]. As shown in Fig. 1, in the 2-dimensional case, O_1 and O_2 are the center points of the sphere 1 and 2 respectively. Points A and C are the tangential points. If B

Table 1
Formulas for calculating stiffness and damping coefficients in Eqs. (1) and (2). Subscripts 1 and 2 refer to the species of the two particles in contact. E_i, ν_i, m_i and R_i are the Young's modulus, Poisson's ratio, mass and radius respectively of particle i. Damping coefficient α can be calculated by Eq. (3).

Variable	Formula
k_n	$4\sqrt{R_{eff}}E_{eff}/3$
k_t	$8\sqrt{R_{eff}}G_{eff}$
η_n	$\alpha\sqrt{m_{eff}k_n}$
η_t	$\alpha\sqrt{m_{eff}k_t}$
R_{eff}	$(1/R_1 + 1/R_2)^{-1}$
E_{eff}	$[(1-\nu_1^2)/E_1 + (1-\nu_2^2)/E_2]^{-1}$
G_{eff}	$[2(1+\nu_1)(2-\nu_1)/E_1 + 2(1+\nu_2)(2-\nu_2)/E_2]^{-1}$
m_{eff}	$(1/m_1 + 1/m_2)^{-1}$