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Heterogeneity of particle assemblies and discrete element simulation on its mechanical behaviors

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ABSTRACT

Based on the configuration of hexagonal packing of identical particles, the radial and the circumferential heterogeneous degrees for granular materials are defined. The relationship between original heterogeneous degrees and strain distribution are concerned. The consistency of strain distribution and heterogeneity is verified. Both configurations and force chains in specimens are analyzed to explore different deformation modes. In the loading process, the first peak stress is defined; the linear relationship between average heterogeneous degrees and first peak stress is clarified. According to the tensor theory, some quadratic invariants of the couple stress tensor are investigated to study the scope of the couple stress effect. Analyses of the volume average of the invariants are carried out to determine the effective range of the couple stress, namely the characterization size of the couple stress.

1. Introduction

The mechanical properties of granular materials are not only connected with relevant material parameters but also with configuration of particle assembly [1–3]. Heterogeneity is an indispensable part in discussing particle configuration. In the process of loading and deformation, it's very significant to understand the correlation between heterogeneity and macro-mesoscopic mechanical properties such as strain distribution, microstructure evolution, internal stress state etc. [4–5].

As one of the important experimental design methods, Uniform Design (UD) was firstly put forward in 1978 by Hua and Yuan [6] and Fang [7] which has been widely used in many fields now. Through decades of research, many methods were come up with to effectively evaluate the homogeneity of granular materials. Based on a large number of experiments, in order to gain the distribution uniformity, Comparison Method analyzes the standard deviation variance and segregation degree of particle specimens [8]. Although Scanning Electron Microscopy can be used to observe samples directly and conveniently, constrained by the selection of observation points the representation of this method is not satisfactory. In addition, it is hard to describe the homogeneity of granular materials quantitatively [9]. Variation coefficient is used to describe the uniformity in the Mass Composition Method, which is only suitable for the separation of mixture particles [10]. The Fractal Dimension Method used particle size distribution to analyze the uniformity [11–12]. But the calculation methods have certain limitations that the fractal dimension value of particle size distribution may appear negative which is not in accordance with physical facts. Dividing specimens by pixel grid according to different grey levels, Pixel Grid Analysis Method compares specimen images through computer analysis. Sampling problem can be avoided in this visual, simple method which is also easy to operate. However, limited by the scope of images, sometimes the representation is not good enough. In addition, this method can gain good results only on condition that grey levels of particles differ a lot from each other [13–14]. Researches show that there are three kinds of measurement methods of uniformity [15–16]: the first class is based on the concept of distance, the second class is derived from the optimal design, and the third class is based on the deviation. In all of these measurement methods, some methods are too complicated to gain useful results, some methods are constrained by application fields, and others are only used under rigorous conditions such as the special place of the coordinate's origin [17].

In this paper, combined with characteristics of granular materials, considering both distance and deviation, based on the configuration of hexagonal packing of particles, a quantitative measurement method of heterogeneity for granular material is proposed. The influences of heterogeneity on the macro and micro mechanical properties of granular materials are discussed. The distribution of heterogeneous degrees, generation and growth of shear bands, evolution of microstructure, relation between average heterogeneous degrees and first peak stress have been

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discussed in turn. In the end, the characterization size of the couple stress effect is suggested by analyzing the change of the invariant volume average of the couple stress tensor.

2. Definition of heterogeneous degrees

Analyzing the configuration of hexagonal packing of identical particles as shown in Fig. 1(a), there are 6 particles A_i ($i = 1 \sim 6$) distributed around the central particle O. The distance between particle O and particle A_i is r_i; the included angle between two adjacent particles and the central particle is θ_i. Calculating the degree of deviation from the mean value of radial distance r_i and tangential angle θ_i, the definition of heterogeneous degrees is as follows:

$$H = \sum_{i=1}^{n} \sqrt{\left(\frac{x_i - \overline{x}}{\overline{x}}\right)^2} \quad (1)$$

where $i = 1 \sim 6$, $\overline{x}$ refers to mean value of x, H contains two targets: h_r and h_t, where $x = r$ and $x = \theta$ respectively.

It can be seen from Eq. (1) that for hexagonal packing of particles $h_r = h_t = 0$, which means the specimen is uniform. As shown in Fig. 1(b) for random heterogeneous particles, considering target h_r, the greater difference between distances r_i is, the more scattered particle distribution is, and the value of h_r is greater as well; considering target h_t, the difference between θ_i is greater means that particles aggregate in one certain direction while in other directions particles are loose, and that the value of h_t is greater. Namely the greater H value is, the more heterogeneous the specimen is. Using all values gained on every single particle, we can calculate averages respectively to characterize the heterogeneous degree of the whole specimen $\overline{H}$. Similarly, the value of $\overline{H}$ approaches to zero means that the specimen is nearly uniform, conversely the greater the value of $\overline{H}$ is, the more heterogeneous the specimen is.

3. Strain distribution and microstructure evolution

In order to explore the relationship between heterogeneity and strain distribution in the loading process, biaxial compressions are carried out. The specimen size, calculation parameters and average heterogeneous degrees $\overline{h}_r$ and $\overline{h}_t$ are all shown in Table 1 where r refers to the radius of particles using in all simulations, kn and ks refer to the contact stiffness in normal and tangential direction respectively, μ refers to the friction coefficient All specimens are generated by random packing using random numbers. At first a loose packing is created. When generating the assembly, a random location within the specified region is chosen. If the particle does not fit (i.e., it would overlap an existing particle), another location is chosen at random. Then radii may be increased in order to reduce the porosity and bring the assembly to mechanical equilibrium under low friction. In the biaxial compression, the confining stress is imposed to the specimen by moving the left and right walls to an appropriate position. Confining stress of all simulations in our paper is set as 300 kPa which can be seen in Table 1. During the simulation process, the velocities are given to the upper and lower walls to compress the assemblies. The imposed velocities were determined by the strain when loading complete. The contact forces are calculated using the Hertzian contact model [18–20] with the equations below.

$$\boldsymbol{F}_{hz} = \sqrt{\delta}\sqrt{\frac{\boldsymbol{r}_i \boldsymbol{r}_j}{\boldsymbol{r}_i + \boldsymbol{r}_j}}(\boldsymbol{k}_n \delta \boldsymbol{n}_{ij} - \boldsymbol{k}_s \Delta S_t) \quad (2)$$

where, r = particle radius, delta = overlap distance of 2 particles, Delta St = tangential displacement vector between 2 spherical particles, n_{ij} = unit vector along the line connecting the centers of the 2 particles.

Take specimen A for example, the distribution of the radial heterogeneous degree $h_r$and the circumferential heterogeneous degree h_t are shown in Fig. 2. Consistency of the two targets, as mentioned in the previous chapter, is verified again.

The continuum theory is used for reference for the definition of nominal strain for granular material [21–22]. Fig. 3 shows the position change of particle A and one of its neighboring particles B. In the global

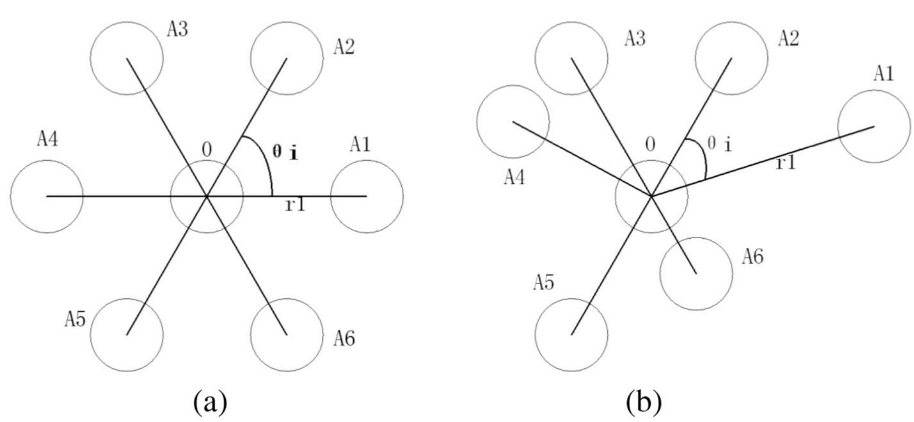

Fig. 1. Particle distribution diagram (a) uniform (b) nonuniform.

Table 1
Calculation parameters and the heterogeneous degrees.

Specimen size/m	r/m	kn/(N/m)	ks/(N/m)	μ	Confining pressure/kPa	Sample no.	$\overline{h_r}$	$\overline{h_t}$
1.0 * 0.67	0.005	5e9	5e8	0.3	300	A	0.22510518	0.31067755
						B	0.23304784	0.32227214
						C	0.26198517	0.36048369
						D	0.26646056	0.36594698

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