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Simulations of the effect of particle size on texture and force transmission in bidisperse granular composites

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Abstract. The objective of this study is to investigate the influence of the particle size ratio on texture and force transmission in two-dimensional cohesionless binary granular composties by using molecular dynamics (MD) simulations. Four numerical composite samples, which differ in terms of the particle size ratios, are used in this study. The samples are composed of two constitutive materials with a stiffness ratio of four between the higher one termed as stiff particle and another termed as soft particle. The samples are subjected to an uniaxial confined vertical compression on the upper wall. The results under static conditions show that the particle size ratio mainly affects the contact sub-networks. The coordination number decreases when the particle size ratios (D_{stiff}/D_{soft} = 1.2 - 3.0) increase, contrary to stiff-any case. Considering the spatial arrangement of contact directions, contacts between stiff particles exhibit an anisotropic distribution. On the contrary, the other contacts, i.e. soft-soft and stiff-soft contacts play a role to support the granular system in equilibrium. It is interesting to note that for all the particle size ratios, an exponential distribution and power-law are observed for the strong and weak network, respectively. Furthermore, almost 60% of the entire contacts transmit the weak forces.

1 Introduction

Granular materials are plentiful around us, which can be encountered in daily life and in many industries. They are constituted from grains with a variety of size, density, rigidity, and other physical properties. Due to a great diversity in grains, the behaviours of granular media are generally complex which cannot distinguish from ordinary matter [1, 2]. No studies really deal with "composite" granular media, i.e. previous studies mainly focused on granular media made of only one type of constitutive material. That is the reason why a few studies on this topic can be found in the literature [3]. This causes a lack of knowledge on mechanics of "composite" granular materials. As a consequence, this study aimed at systematically investigating the influence of the particle size on textural properties and force transmission in two-dimensional bidisperse composite granular materials prepared from two types of disk with different rigidities by means of molecular dynamics simulations.

2 Molecular dynamics simulations

The molecular dynamics (MD) method, which belongs to the discrete element method (DEM) proposed in 1971 by Cundall [4], relies on an explicit algorithm. The particles in this method are taken into account as rigid bodies with non-conforming surfaces [5]. Newton's equations of motion, which govern the motions of each particle with respect to time, are numerically integrated by means of a predictor-corrector scheme with Gear's set of corrector coefficients [6].

2.1 Contact force model

The interaction force between two dry particles is divided into a normal force and a tangential force. In the MD method, the local deformation occurred when two solid bodies are in contact can be simply modelled by a virtual overlap δ at the contact (no change in the particle shape). The normal force model used in this study is a simple model so-called the "linear spring-dashpot" [7], which is given by

$$F_n = k_{eff}\delta + \alpha_n v_n \quad (1)$$

where k_{eff} is the effective contact stiffness, α_n is a normal damping coefficient, and v_n is the normal velocity (time derivative of the virtual overlap).

In the case of the tangential force, a "regularized" form of the exact Coulomb's law of friction [7] is adopted in this study to calculate the tangential force between two contacting particles. This model can be written by

$$F_t = \min\left\{\left|\gamma_s v_s\right|, \mu F_n\right\} \cdot \text{sign}\left(v_s\right) \quad (2)$$

where γ_s is the tangential viscosity coefficient and μ the coefficient of friction. Note that the rotational motion

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due to the tangential force is permitted to be free in this study.

2.2 Performing the simulations

The 2D numerical composite granular sample under study was prepared from two different base materials with differ in rigidities: one is referred to as a "stiff" particle and another to a "soft" particle. The contact stiffness ratio between them is four. The bidisperse sample, which was comprised of 4000 disks, was established by randomly depositing both stiff and soft particles inside a square box consisting of four rigid plane walls. Four different the diameter size ratio (D_{stiff}/D_{soft}) was used in the present work, i.e. D_{stiff}/D_{soft} = 1.2, 1.6, 2.2, and 3.0. The ratio between the number of stiff and soft particles (N_{stiff}/N_{soft}) was fixed at 1.0 for all the diameter size ratios. A confined vertical compressive force of 100 N was then applied on the upper wall, while the others were fixed during this stage. Eventually, an initial dense granular packing under static equilibrium condition was obtained.

Next, a vertical constant force of 1000 N was applied to the initial dense packing on its upper wall. During the compression, the other walls were still stationary. It can be seen that in this study the contacts between the particles can be separated into three types: contacts between stiff-stiff, soft-soft, and stiff-soft particles. The effective contact stiffness k_{eff} in Eq. (1) is dependent of the contact types, which was set underlying on the following relations:

$$k_{eff} = \begin{cases} k_{stiff}, & \text{stiff-stiff and wall-any contacts} \\ k_{soft}, & \text{soft-soft contacts} \\ \dfrac{k_{stiff} \times k_{soft}}{k_{stiff} + k_{soft}}, & \text{stiff-soft contacts} \end{cases} \quad (3)$$

When granular systems reached the static equilibrium conditions, it implies that the simulations were finished. The simulation data at the final of this stage were then statistically analysed through granular textures and force transmissions.

3 Geometrical textures

The geometrical textures were essentially used to define the morphology of the granular media by describing in terms of geometrical orientation of the particles and their contacts in space.

3.1 Coordination number

In this context, the coordination number z is defined as the average number of contact neighbours per particle. It can be calculated from $z = 2N_c/N_p$, where N_c is the total number of contacts and N_p is the total number of particles. The results for all the samples regarding the influence of D_{stiff}/D_{soft} ratios on the coordination number are presented in Fig. 1.

Considering the coordination number z_{all} for the whole of contacts, it slightly decreases with the D_{stiff}/D_{soft} ratios (see the black line). In the similar manner, it is observed that the coordination number $z_{soft\text{-}any}$ for only the contacts between soft and any particles decreases quite greatly with the D_{stiff}/D_{soft} ratios (red line). This reduction of z can be explained rationally by the fact that an increasing of the net area of the stiff particles when the D_{stiff}/D_{soft} ratio increased causes a chance of contact occurrences in the system to be decreased. Note that the net area of the soft particles is still the same for all the D_{stiff}/D_{soft} ratios. On the contrary, when only the contacts between stiff and any particles are considered, the coordination number $z_{stiff\text{-}any}$ seems to be steady for all the ratios (blue line).

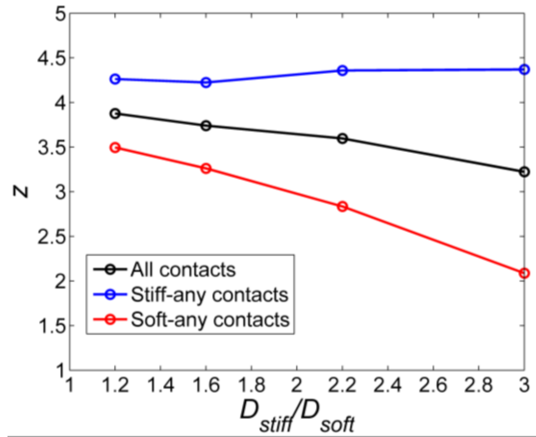

Fig. 1. Coordination number z as a function of the ratio between stiff and soft particle size D_{stiff}/D_{soft}.

3.2 Contact direction

The contact direction is given by the line between the centroids of two particles in contact, measured with respect to the horizontal direction. The angular distribution of the contact directions is used as a statistical quantity to describe and characterize the probability of contacts occurring in each direction of the space. For two-dimensional data, this quantity can be represented by the polar diagrams of the probability distribution $P(\theta)$ of the normal contact directions as shown in Fig. 2. It must be noted that we analysed four different types of contacts: all the contacts, only the stiff-stiff contacts, only the soft-soft contacts, and only the stiff-soft contacts.

First, the spatial arrangement of the particles in the case of D_{stiff}/D_{soft} = 1.2 is taken into account, as presented in Fig. 2 by the green line. In this case, the effect of monodisperse media still exists. That is a reason why we found clearly specific contact orientations, i.e. θ = 0º, 60º, and 120º, for all considerations of the contact types. This phenomenon so-called the "triangular" contact network [8] is logically discovered in the monodisperse media.

Considering next the angular distribution of the contact directions for D_{stiff}/D_{soft} = 1.6, 2.2, and 3.0 represented in Fig. 2 by black, red, and blue line, respectively, it must be noted that applying a confined vertical compression on our granular samples prepared inside a square box leads these samples become a quasi-homogeneous system. Several remarkable points can be shown as follows:

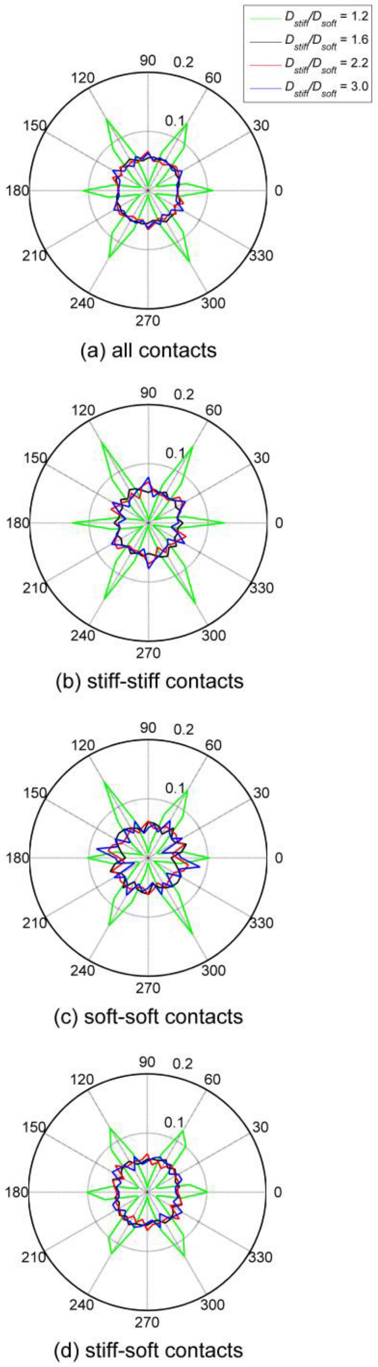

Fig. 2. Polar diagrams of the probability distribution of the normal contact directions for all the D_{stiff}/D_{soft} ratios. The contact networks in each sample are taken into account separately for: (a) all the contacts, (b) only stiff-stiff contacts, (c) only soft-soft contacts, and (d) only stiff-soft contacts.

- In Fig. 2b, the contact orientation between stiff and stiff particles exhibits an anisotropic distribution for most cases, i.e. specific directions are evidently observed in the directions of θ = 30º, 90º, and 150º, excluding the case D_{stiff}/D_{soft} = 1.6. In such case, the contacts between stiff and stiff particles are quite distributed uniformly as observed clearly in both all the contacts (see Fig. 2a) and only stiff-soft contacts (Fig. 2d) for all D_{stiff}/D_{soft} the ratios. We can point out that the specific directions occurred in the contact network between stiff and stiff particles is also caused from the increasing of the net area of the stiff particles, as discussed earlier in the previous section.
- For the contact network between soft and soft particles, the anisotropic distribution is also observed as illustrated in Fig. 2c. It tends to be aligned perpendicular to the compression axis (i.e. the vertical axis), in order to make the granular system in equilibrium by supporting the stiff-stiff contact network.

4 Force transmissions

A strong inhomogeneity of contact forces is a well-known characteristic in granular materials, which is arisen from a force transmission through inter-particle contacts. For all samples, this inhomogeneous contact force is also found in composite granular media, as shown in Fig. 3. It can be observed distinctly that the biggest particles carry the strong forces, similar to what is discovered in granular media made of only one type of base material [9].

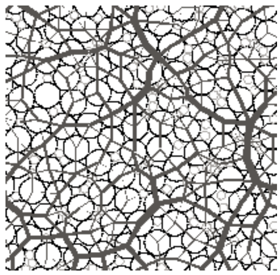

Fig. 3. A snapshot of normal force chains in the sample with D_{stiff}/D_{soft} = 3.0. The stiff particles are represented in black and soft ones in light grey. Note that the magnitude of the normal force is proportional to the thickness of the grey line.

Due to the inhomogeneity of the contact forces, in order to characterize explicitly the distribution of the normal contact forces in composite granular media, the probability distribution function P of the normalized normal contact forces F_{norm} is plotted as shown in Fig. 4. In this figure, the contact force networks can be divided into two complement networks [10]: the strong network presented in Fig. 4a and the weak network presented in Fig. 4b. The former consists of the contacts transmitting the forces greater than the average force $<F>$, contrary to the latter that the contacts carry the forces lower than the average force.

It is obvious that the probability distribution function of the normalized normal forces for all the samples is distributed as an exponential decay for the strong network and a power-law for the weak network. These distribution shapes found in this study for composite granular media are also discovered in non-composite granular media made of only one type of base material [11]. Moreover, both strong and weak networks in the cases of stiff-stiff, soft-soft, and stiff-soft contacts are characterized by the exponential fall-off and the power-law, respectively. It can be that the law of the force distributions for both strong and weak networks is a common feature of granular media, which is not only dependent on the effect of particle size but also the types of contact.

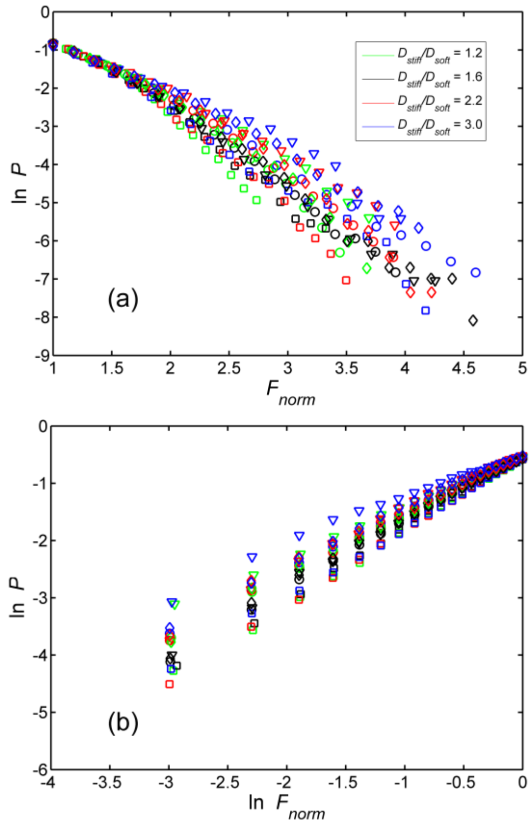

Fig. 4. Probability distribution function P of the normalized normal contact forces F_{norm} for all the samples: (a) the strong network is presented in a semi-logarithmic scale and (b) the weak network is presented in a logarithmic scale. Note that considering the whole set of contacts is represented by the "circle", only stiff-stiff contacts represented by the "square", only soft-soft contacts represented by the "triangle", and only stiff-soft contacts represented by the "diamond".

In addition, it must be noted that the contacts carrying the forces lower than the average force is almost 60% of the total number of contacts. This property is also observed for whatever the type of contact is taken into account.

5 Conclusions

The influence of the particle size on behaviours of 2D composite granular media under a confined vertical compression is methodically investigated in terms of the texture and force transmission. The molecular dynamics (MD) simulations were employed for this purpose. The composite samples were established from two different types of disks with rigidity ratio of four: the larger stiffness is referred to as stiff particles and the lower one as soft particles. Four different ratios between stiff and soft particles (D_{stiff}/D_{soft} = 1.2 - 3.0) were varied in this study. Under static conditions, the numerical results can be concluded that the influence of the particle size ratio on the texture and force transmission is only observed for the contact sub-networks. These can be summarized as follows:

- The coordination number for the whole set of contact decreases when the D_{stiff}/D_{soft} ratios increase, similar to what observed in the soft-any case. On the other hand, the coordination number remains constant in stiff-any case.
- Due to a confined vertical compression, the contact distributions between stiff particles is anisotropic with specific directions in almost cases, while the other types of contact, i.e. soft-soft and stiff-soft contacts, play a role to sustain the granular system in equilibrium. It must be noted that the effect of monodisperse media is observed for the case of D_{stiff}/D_{soft} = 1.2.
- The particle size ratio does not affect force transmissions in composite granular media in terms of the distribution laws and the percentage of the number of contacts characterized for both strong and weak networks. These features are similar to what observed in non-composite granular media.

In a future work, it would be interesting to study the texture and force transmission in composite granular media subjected to a complex mechanical loading such as biaxial compression. Furthermore, the net area of each particle type should be the same for the further study, in order to eliminate its effect.

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