CRACK PROPAGATION MECHANISM IN ROUNDED COHESIVE GRANULAR MEDIA

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ABSTRACT

This work investigates the influence of cohesion on the aspect of fracture and crack propagation in 2D rounded cohesive granular packing simulated by the molecular dynamics method involving simple contact laws with adhesion. 2D numerical "Brazilian" test with samples of 8000 identical radius circular particles suggest that the formation of crystallized agglomerates within samples depends on the value of the cohesive energy between particles. The agglomerate size is increased when the surface energy increases. In the testing phase and for the high values of surface energy, the fissures appear at the agglomerate interfaces in the center of sample and propagate toward to the periphery in parallel to the compressive direction.

1 INTRODUCTION

Granular materials are defined as collections of solid particles for which the macroscopic behavior is governed by some contact forces. There are many examples of granular media, notably in the civil engineering domain: soil, concrete and all of the fragmentation process. In the agro-product, pharmaceutical and chemical industry, many products are constituted from grains or powders. The macroscopic and microscopic properties of granular media are generally complex. Many experimental and numerical studies on the mechanical behavior of granular packing have been undertaken over the last twenty years, with the aim of predicting the macroscopic behavior of granular medium and to investigate the grain scale or the contact scale. These studies indicate that if the whole medium is dense, it is then very strongly structured. This conclusion was first made from the contact force network analysis, of inhomogeneous nature (Radjai et al. [1]), and secondly from the study of the contact directions which characterize the non isotropy of the contact network (Oda and Sudoo [2], Calvetti and al. [3], Cambou [4]). These investigations concern especially the noncohesive granular media.

While cohesion is often taken into account when dealing with macroscopic behavior of granular materials, the microscopic aspects remain only little explored. The aim of this work is to study, by numerical simulation, the influence of cohesion on the aspect of fracture and the crack propagation of the systems by progressively increasing the surface energy (adhesion) between particles, starting with a noncohesive medium. In cohesive granular packing, the cohesion arises from attraction forces of various physico-chemical origins that prevent the loss of contact, together with hard core repulsive force allows a pair of particles in contact to support compressive forces (up to particle cracking).

In this paper, we first present a simple model of adhesion between two circular particles. After a short description of the numerical sample and of the boundary conditions, we present our main results regarding the agglomerate size in the equilibrium state and the crack propagation in the testing phase as a function of surface energy between contacts.

2 ADHESION MODEL

The numerical simulations were carried out on 2D samples using the Molecular Dynamics method (MD) based on the predictor-corrector scheme with Gear's set of corrector coefficients for the integration of Newton's equations of motion (Allen and Tilesley [5]). Principally, the effort of contact

between two particles is defined as a function of the relative displacements and relative velocities of particles. Wuthout considering any distance forces and in the first approximation, the effort of contact is only a function of the overlap depth δ between two particles, (Figure 1). This dependence is generally non-linear, in Hertz's model for example.

In our work, we consider firstly the normal effort of adhesive particles in contact. The adhesion is introduced as a contact resistance to separation effort. With an idea similar to the adhesion model on solid surface of JKR (Johnson and al. [6], Roux [7]), we established a normal interaction model between two particles in which the effort of contact is the sum of a repulsive force an adhesive force. We select the simple elastic linear law for the repulsive part that is given by $k\delta$ (Schäfer and al. [8]), where k is the contact stiffness, and the adhesive force proportional to the contact surface *2a* given by $\gamma\sqrt{r\delta}$, where γ represents the surface energy of particles in contact and *r* the effective radius of the curvature of the interface at δ=0. The dynamic effects are taken in account with a viscous damping term, given by $\alpha\dot{\delta}$, where α is a normal damping coefficient. So the expression of the normal effort f_n as a function of δ is given by (Preechawuttipong and al. [9], Radjai and al. [10]):

$$f_n = k\delta + \alpha\dot{\delta} - \gamma\sqrt{r\delta} \tag{1}$$

This model will referred to as the "geometrical adhesion model" (GA).It is easy to show that threshold of the tensile force F_c (necessary force to separate two particles in contact) is $F_c = r\gamma^2 / 4k$. Note that in contrast with the JKR model, F_c depends here on the elastic modulus *k*.

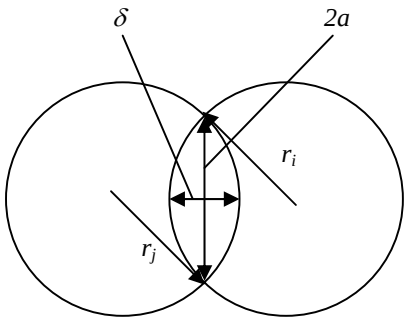

Figure 1: Geometry of the contact between two disks.

The implementation of Coulomb's law in the MD method poses a basic technical problem, i.e. different coefficient of dynamic and static friction (Schäfer and al. [8] and Radjai [11]). In fact, the integration of the equation of motion requires a "smooth" force law such that the friction force f_t is a function of relative sliding velocity v_t. According to Coulomb's law of friction, the set of permissible pairs between f_t and v_t can not be represented as a single-value function, "nonsmooth". The simple way to avoid this difficulty is to adopt a "regularized" from of Coulomb's law and in this case we adopt the simplest regularized Coulomb's law with adhesion defined by:

$$f_t = \min\left\{\beta|v_t|, \mu(f_n + F_c)\right\}\text{sign}(v_t) \tag{2}$$

where μ represent a coefficient of friction and β is a tangential viscosity.

A force law with adhesion in a broad sense involves a pair of adjacent particles that resist not only normal separation, but also relative sliding and rolling. When these conditions are fulfilled, the interparticle contact is "cemented", i.e. the relative degree of freedom of particles in contact are frozen within the range of supportable forces and moments. However, we will not consider here the rolling

friction and stiffness so that contiguous particles may freely roll on one another with no bending moment acting between them.

3 NUMERICAL SAMPLES

For preparing a circular simple well compact, we utilized an original technique which consists of small dispersed particles in a space and expand the radius of particles until the available space is occupied. Our numerical 2D samples are composed of 8000 circular particles with the finall radius of 3 mm. The particles with initial radius of 1.5 mm are randomly distributed (triangular network) without contact at the beginning, and no effect of gravity, in a rounded box. The particle radius grows with a constant velocity until reaching their final size. We wait for the particles to fill up the space and then rearrange them until a static equilibrium is reached. The adhesion between the rounded box and the particles is zero. The surface energy γ is prescribed at contact level for each simulation. The stiffness and the coefficient of damping are the same values for the particle-particle and particle-box contacts. Notice that our samples in this step are really under compression in all directions. As the particle radii are identical, the system presents a global triangular contact network with a coordination number (the average number of contacts per particle) nearly to 6. The next step concerns the release of the sample by slowly increasing the rounded box radius to allow the system to relax to a static equilibrium again. The final state of this preparation step is used as the initial equilibrium state for our analysis and for the Brazilian test. The Brazilian test is realized by placing the system in initial state between two flat plates, (Figure 2). There is no adhesion between the particles and the flat plates but all other parameters of contact are the same values for particle-particle and particle-flat plate contact. The lower flat plate is fixed while the upper plate is pushed down (direction $-y$) with a constant velocity of displacement. The numerical simulations are stopped when the macroscopic strain in the y direction reaches approximately 5%.

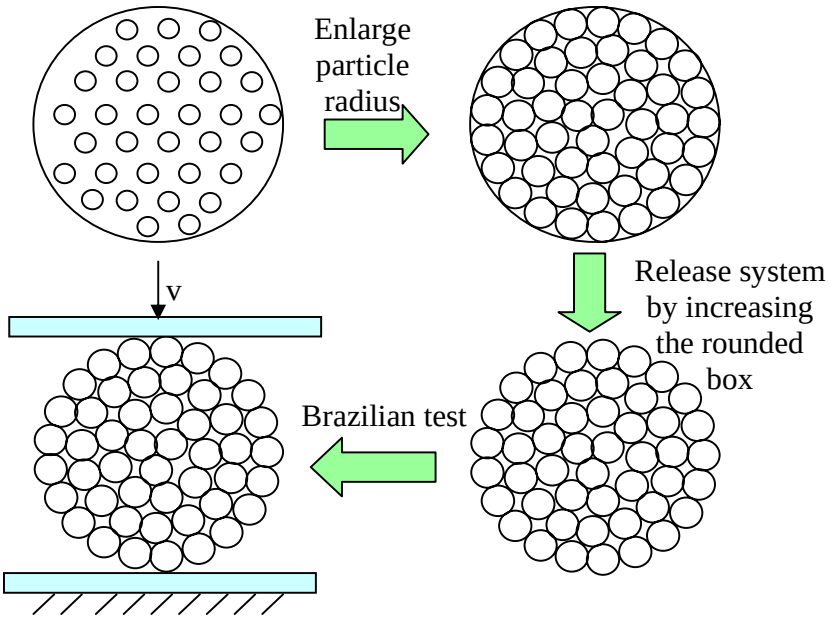

Figure 2: Sample preparation under stress by enlargement of the particle radius and the Brazilian test scheme.

4 NUMERICAL RESULTS

4.1 Initial equilibrium state properties

An interesting result of our investigation is the formation of agglomerate regions in the sample. Figure 3 upper show four initial states of configuration for different surface energy values γ. We observe that the structure forms some crystallized zone or some agglomerates the size of which increases with the adhesion γ. The formation of agglomerates is clearer when we see the images of local coordination number, (Figure 4 middle). The structure is also clarified if we trace the effort between particles in the weak effort zones which form the interfaces of the agglomerates, (Figure 5 lower). Moreover, we found that the coordination number is lower than 4 for the low values of adhesion ($\gamma < k/50$), similar to noncohesive granular media, but exceeds 4 for higher adhesion values.

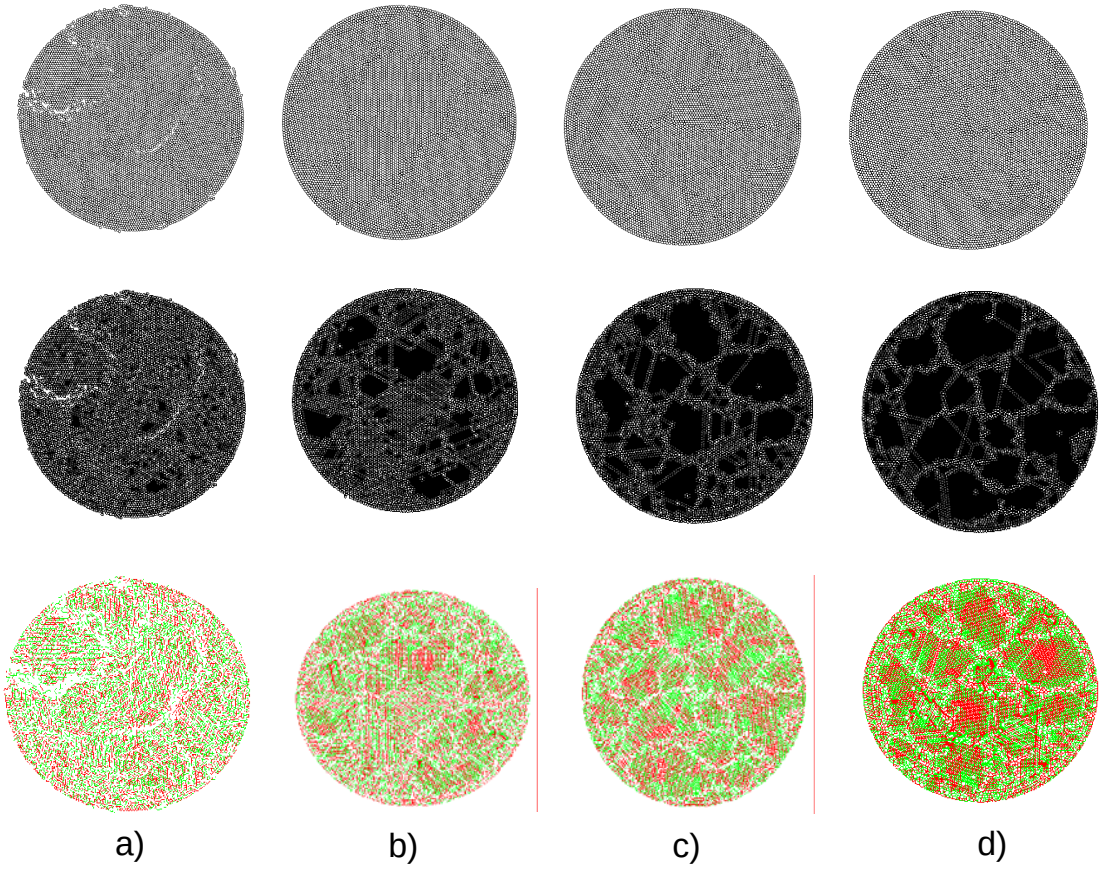

Figure 3: (upper) Initial configuration; (middle) local coordination number coded in greyscale (6 contacts in black, 5 in dark grey, 4 in bright grey and white for less than 4); normal normal contact force network of initial equilibrium state of sample with $\mu = 0.5$ for four different values of adhesion: $\gamma = k/150$ a), $\gamma = k/50$ b), $\gamma = k/20$ c) and $\gamma = k/7$ d). The compressive forces in contact are traced in red and the tensile forces in green.

4.2 Crack mode and propagation

The sample in initial equilibrium state is effectuated by the Brazilian test for studying the crack mode and propagation. Of course, the ultimate failure load of the system increases when the local surface energy between particles increases. We observe that faults appear and are manifested near the circumference for low values of adhesion. In contrast, for high values of adhesion, the first fissure occurs at the centre of the sample and propagates throughout the periphery. This high cohesive behaviour reconciles the results of elasticity theory in which the tensile stress is maximum at the centre of the sample (Timoshenko and Goodier [12]). A spectacular aspect of the fissures is their initiation and their propagation in the agglomerate joints where the structure is less compact. The initial agglomerate remains intact, (Figure 6) and the crack is oriented along the axis of compression. Moreover, we found that the fissures are more diffuse in the system with low adhesion but they are more localized for the highly cohesive sample.

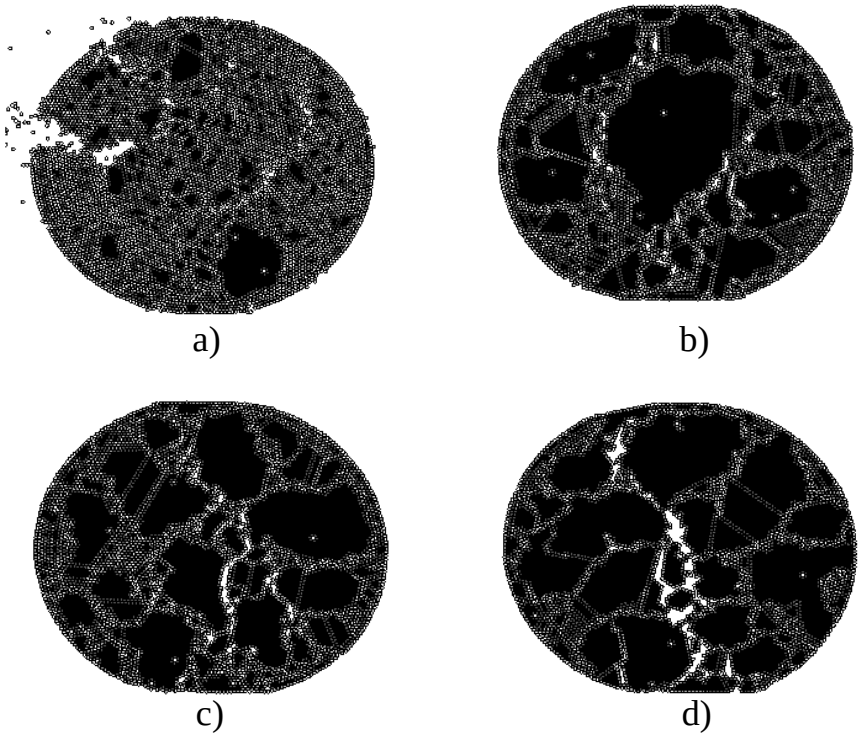

Figure 4: Configuration of the sample at 5% of macroscopic stress for four values of adhesive energy: (a) $\gamma = k/150$, (b) $\gamma = k/50$, (c) $\gamma = k/20$ and (d) $\gamma = k/7$. The greyscale represents the coordination number: black for 6, dark grey for 5, bright grey for 4 and white for less than 4.

5 CONCLUSION

The result of the numerical investigations described demonstrate the feasibility of the indirect tensile test using the suggested method. We can obtain the auto-equilibrium geometry of enough regular form. The choice of a homogeneous system allowed samples to be generated that present a disorderly type “joints of agglomerate” and to observe that the weak effort or contact zones which guide essentially the fissure and the fracture of the medium. The values of adhesive energy between particles changes the macroscopic behaviour, in particular the crack mode and propagation. The investigation presented here could be extended for characterizing an evolution of stress in the ruin phase of a structure.

ACKNOWLEDGEMENT

This work is supported by Chiang Mai University and The Thailand Research Fund under grant number MRG4608185.

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