

Introduction of Adhesive Force to DEM Simulation and Application to Fracture of Fragile Powder Materials

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We introduce an adhesive powder model based on the discrete element method (DEM). By using this model, we investigate how fragile substances consisting of a lot of adhesive powders, powder materials, are fractured. In the powder material, the powders have a weak attraction and are stuck to each other by adhesion. Thus, the powder materials are easily broken by the external force. We investigate the crack morphology of the fractured powder materials by changing two parameters expressing the strength of the adhesive force χ and width of the powder size distribution Δ . The fracture pattern is changed from cracking to crumbling as Δ increases for every χ value. Interestingly, we find that this change seems to start at a particular point of Δ from observations of the fractal dimension of the cracks D_f versus Δ . This result may suggest that the morphological change of the cracks may be related with a transition in the granular systems such as the glass transition.

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1. Introduction

A large number of industrial products are made by compression of powders, e.g. medical tablets, cosmetic foundations, and cookies. Here, we focus on solid-like materials composed by adhesive powders, in which the powders are glued to each other. We assume that the adhesive force is a weak and short-range attractive force; hence the material is fragile, but does not collapse by itself. We call such fragile materials powder material.

We sometimes experience breakage of the powder materials and know that they have their own fracture patterns. For example, the ground will crack if the soil contains appropriate moisture and is made up of grains of almost the same size whereas it may crumble in the opposite case. Roughly speaking, there exists two types of fracture patterns: cracking and crumbling. It is very interesting to investigate how the fracture pattern will change as a function of moisture and grain size distribution.

Moreover, the fracture aspects often provide functionalities of industrial products. For instance, (i) medical tablets should be broken within a given time in the human body; (ii) the fragility of the cosmetic foundation gives softness and affects a good feeling to skin; (iii) the texture of foods corresponds to its breakage behaviors [1]. Additionally, in the granulation process that a rock is crushed into small pieces, the surface area of the granules, which is

directly connected to functionalities of the products, is not the only function of the powder size; the fractal surface dimension is also important [2]. Practically, it is a crucial matter to control the fracture aspects. From the microscopic point of view, however, little is known about powder characteristics which will strongly affect the fractures.

In this paper, we introduce a simulation model of the powders with the adhesive force. We examine the fracture aspects of the powder materials by using this model. We concentrate our attention on the effects of the two characteristics of the powders: strength of the adhesive force and width of the powder size distribution.

2. Simulation Model

Our simulation is based on the discrete element method (DEM) [3,4]. In the standard DEM simulation, the Voight model is employed as a model of the contact force. We denote the contact forces in the normal and shear directions by $f_{n,ij}(t)$ and $f_{s,ij}(t)$, respectively. Hereafter, the suffix n and s mean the normal and shear directions. When i -th and j -th spherical powders with radii a_i and a_j collide at time t , $f_{n,ij}(t)$ and $f_{s,ij}(t)$ are given by

$$f_{n,ij}(t) = K_{n,ij}(t)d_{n,ij} + \eta_n \left(\frac{d}{dt} d_{n,ij} \right), \quad (1)$$

$$f_{s,ij}(t) = \min \left\{ \mu f_{n,ij}, K_s(t)d_{s,ij} + \eta_s \frac{d}{dt} d_{s,ij} \right\}, \quad (2)$$

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where K , η and μ are the spring, viscous and friction coefficients, respectively. d_{ij} is the amount of the displacement from the first contact position, i.e. $d_{n,ij} = a_i + a_j - R_{ij}$ where R_{ij} is the distance between center positions of the i - and j -th powders. We assume $K_{s,ij} = sK_{n,ij}$ and s is chosen to be 0.41.

$K_{n,ij}(t)$ is usually calculated by the Hertzian contact theory [3,4]. The formula when two elastic spheres are in contact is given by

$$K_{n,ij}(t) = \frac{2}{3} \frac{E}{1-\nu^2} \left(\frac{3a_i a_j}{2E(a_i + a_j)} F_{n,ij}(t) \right)^{\frac{1}{3}}, \quad (3)$$

where E and ν are the Young's elastic modulus and the Poisson's ratio, respectively. $F_{n,ij}(t)$ is a compressive force between the i -th and j -th powders in the normal direction. The actual equation of the motion and the method of the integration are written in Ref. [4]. We should consider that the contact force is always repulsive while using the formulae (1) and (3).

The adhesive forces between powders arise from very complicated origins, i.e. mechanical, chemical, electrostatic, and van der Waals forces. In granular systems, wetting of liquids such as water plays the most important role. Many models have been proposed to explain experimental observations, but the situation is still complicated [5,6]. At present, it is not our main concern to pursue realistic wetting models. In this paper, we handle a simple model of adhesion by modification of (1) and (3) [7].

We suppose that the contact force differs in two cases that the two powders are getting close and further away. Let us denote the elastic forces in the approach and departure cases by $f_{n,ij}^{\text{in}}$ and $f_{n,ij}^{\text{out}}$. We calculate $f_{n,ij}^{\text{in}}$ by (1) and (3), and $f_{n,ij}^{\text{out}}$ by subtracting a constant value from $f_{n,ij}^{\text{in}}$. Consequently, $f_{n,ij}^{\text{out}}$ takes 0 at $d_{n,ij} = d_0$ and negative values (adhesion) when $d_{n,ij} < d_0$. In Fig. 1, our definition of the adhesive force is schematically explained.

Of course, d_0 must satisfy $d_0 < a_i + a_j$. If we fix the value of d_0 , however, this condition may be violated if a_i and a_j are random numbers. Thus, a normalized distance $\chi \equiv 100 \times d_0 / (a_i + a_j)$ is introduced as a strength parameter of the adhesive force. In this simulation, $\chi = 1, 2, 3, 4$ and 5% are chosen.

Recently, Mitarai and Nakanishi proposed wet granular models for both pendular and funicular states [8]. Our model is very similar to the model for the pendular state (model P). In the model P, $f_{n,ij}$ is given by $kd_{n,ij}$ until $d_{n,ij} \geq (1-\alpha)(a_i + a_j)$, where k is a elastic constant. When $\alpha > 1$, the elastic force becomes attractive and thus α is a control parameter of the adhesive force. Both our and their models include only one parameter to express the strength of the force.

Actually, the two models differ in terms of two points: the attractive force range and the strength of the attractive force. First, the attractive force of our model appears in the positive range of $d_{n,ij}$, i.e. $0 < d_{n,ij} < \chi/100 \times (a_i + a_j)$,

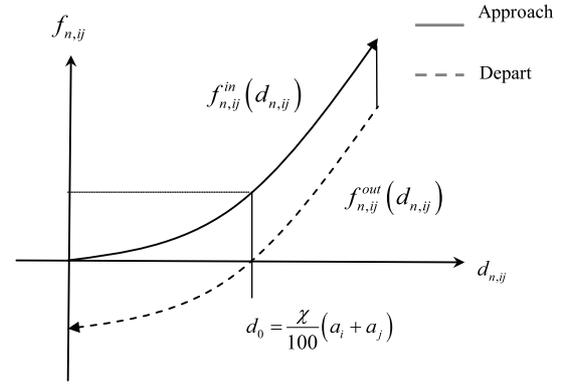


Fig. 1 Schematic explanation of the adhesive force.

Table 1 Parameters of physical properties of powders.

E	a_0	ρ	ν	η_n	η_s
kg/m s ²	m	kg/m ³	-	kg/s	kg/s
4.9 E+9	1.0E-4	2.48E+3	0.23	8.0E-5	5.0E-5

whereas that of their model is negative, i.e. $(1-\alpha) \times (a_i + a_j) < d_{n,ij} < 0$. In addition, our model gives short range forces compared with their model; $\chi/100$ and $(1-\alpha)$ are chosen from 0.01 to 0.05 and from 0.1 to 0.5, respectively. Second, the strength of adhesion in our simulation is stronger than that in their simulation. Although we can not compare the strength of the forces directly due to the difference of the contact force models, the typical particle deformations in our and their simulations are 1 ~ 5% and less than 1%, respectively.

These differences affect the movements of powders. The relative positions of powders in our simulation are almost fixed until the cracks occur whereas those in their simulation are changed for external forces. As a result, the lump of the powders of our model becomes harder and more fragile than that of the model P.

As mentioned before, we introduce another parameter, i.e. the width of the powder size distribution. We randomly generate a_i according to the Gaussian distribution with the mean value a_0 and standard deviation σ . Under fixing a_0 , we change the value of σ . For convenience, we use the following notation: $\Delta \equiv 100 \times \sigma / a_0$. In table 1, we provide the characteristic values of the powders given in Ref. [4].

3. Simulation Procedure

At first, 40,000 powders with different radii are prepared. The powders are uniformly placed in a 200×200 grid so that every powder does not have any contact with the others. Throughout the following simulation, the periodic boundary condition is applied to the left and right sides.

The procedure for the simulation consists of three steps: (1) compression of the powders; (2) relaxation of the structure by vibration; (3) breakage of the powder material sample. These steps and the definitions of the parameters

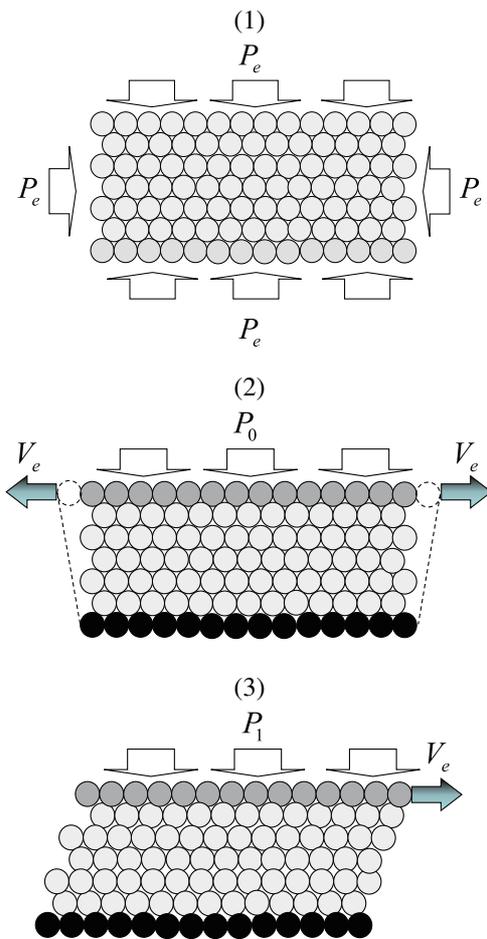


Fig. 2 Illustration of simulation procedures. (1) Compression process. The powders is uniformly compressed with pressure P_e . (2) Relaxation process. The gray powders oscillate horizontally under fixing the black powders at a constant velocity V_e . The maximum strain is γ_0 . The downward pressure P_0 acts on the gray powders. (3) Fracture process. The gray powders slide horizontally with velocity V_e until the material is fractured. The downward pressure P_1 acts on the gray powders.

Table 2 Parameters used in our simulation.

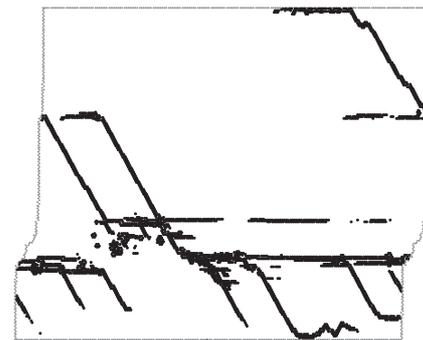
V_e	P_e	P_0	P_1	γ_0
m/s	N/m	N/m	N/m	-
1.6E-1	2.5 E+1	1.0 E+2	1.0 E+1	2.35 E-2

are shown in Fig. 2.

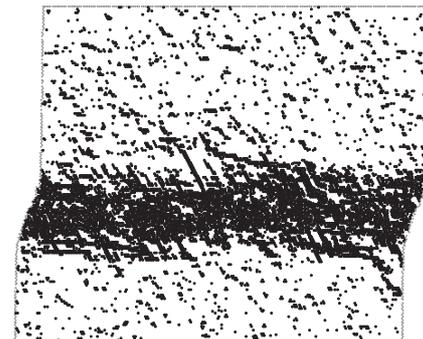
We should note that appropriate values of P_e , P_0 and P_1 must be chosen so that the powder materials may not be broken before the proper shear force. The parameters used in the simulation are listed in Table 2.

4. Result and Discussion

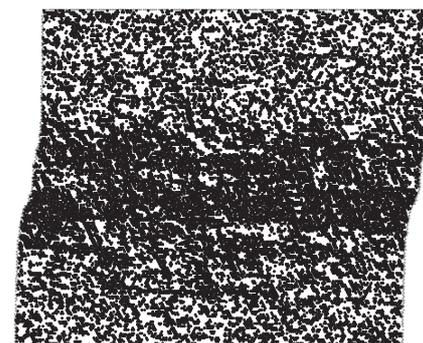
Typical figures of the fracture aspects for $\Delta = 0.0, 1.4$ and 3.0 are shown in Fig. 3. There are roughly three types of fracture aspects. For $\Delta \leq 0.3$, some large cracks are formed throughout the powder material and its shapes are almost straight lines. In the region of $1.0 \leq \Delta \leq 1.7$



(a) $\Delta = 0.0$



(b) $\Delta = 1.4$



(c) $\Delta = 3.0$

Fig. 3 Figures of fractured powder materials for $\Delta = 0.0, 1.4$ and 3.0 at $\chi = 1.0$. In the figures, the black circles denote the powders of cracks. Small cracks involving less than 7 powders are extracted from the figures. The periodic boundary condition is applied to the left and right sides.

the powder material splits into the upper and lower parts. The cracks are partially concentrated in the boundary. For $\Delta \geq 3.0$ many small pieces of the cracks are distributed everywhere. This means that the fracture aspect becomes crumbling.

One may suspect that the result of Fig. 3 depends on the system size. In the previous study [7], we have investigated the dependence of D_f on χ under $\Delta = 0.0$ by using a smaller system, 100×80 powders. Although the cracks in Ref. [7] are shorter and fewer, D_f is within the range of about 1.2 to about 1.6 for all χ values. This is consistent with the observation of Fig. 3. Thus we expect that the error bar of D_f by the size effect will be small if the system size is considerably large.

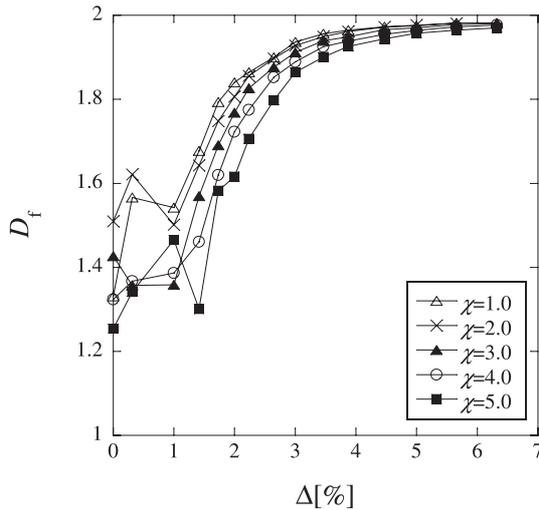


Fig. 4 Plot of fractal dimension D_f versus Δ . D_f looks to start increasing at a particular point of Δ .

The fractal dimension of the cracks D_f versus Δ is depicted in Fig. 4. D_f is calculated by the box counting method. For all χ values, the behaviors of D_f are very similar: in the region of $\Delta < 1.0$, the value of D_f fluctuates between about 1.2 and 1.6, and after that, D_f increases and finally reaches to 2.0. Since the system is 2D, $D_f = 2.0$ means that the powder material completely crumbles. This is quite consistent with the observation in Fig. 3.

It is worth mentioning that D_f seems to begin increasing not monotonously but suddenly. In order to consider this behavior in detail, the fractional free volume S_f is introduced by

$$S_f = \frac{V - \sum_{i=1}^N \pi a_i^2}{V}, \quad (4)$$

where V and N are the volume of the system and the number of the powders. S_f expresses the fraction of the free area where the powders can move freely. Fig. 5 shows the dependence of S_f on Δ . We find that for every χ value the slope of the line is changed at a particular point of Δ , Δ_g . Comparing Figs. 4 and 5, we see that the point at which D_f starts to increase is close to Δ_g (≤ 1.0) at every χ value. This result will suggest that the crack morphology is closely related with S_f .

Now, we consider the fracture mechanism of the powder materials in terms of the fractional free volume. We can imagine two limits of $\Delta \sim 0$ and $\Delta \gg \Delta_g$. When $\Delta \sim 0$, almost all the powders have a close packed structure like a crystal and have very little free space. In such a case, the powders must move cooperatively for the external force, i.e. the powder material will behave as a brittle solid. According to the Griffith theory [9], small cracks in the brittle solid enhance the strength of the inner stress and will grow into large cracks if the internal stress exceeds a critical stress. On the other hand, when $\Delta \gg \Delta_g$ there are many defects everywhere. Then, the powders have enough

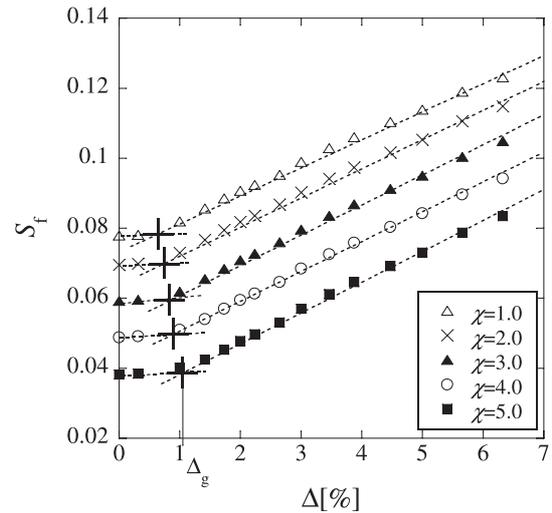


Fig. 5 Plot of fractional free volume S_f versus Δ . For every χ , the point of Δ where the slope of the line is changed is indicated by the symbol + and defined as Δ_g .

spaces to move independently. For the external force they can rearrange their position according to the force balance principle [10]. Therefore, no stress concentration will occur and small cracks can not get large, i.e. the powder material will crumble.

Actually, the similar behavior of the Δ dependence of S_f is found in the glassy materials. It is well known that the fractional free volume f of the particles in the glassy materials has the following T dependence [11]

$$f(T) \sim \begin{cases} f_g & (T \leq T_g) \\ f_g + \alpha(T - T_g) & (T > T_g) \end{cases}, \quad (5)$$

where T_g is the glass transition temperature. f_g and α are constant values. Remember that the particles change their movement from cooperatively to independently at $T = T_g$ [12]. Although both the phenomena are completely different, there is a common factor concerning the mobility of the powders, which is indicated by the fractional free volume. Following this analogy, we may suggest that if the powder material is in a solid-like state, it cracks; if in a molten-like state it crumbles.

5. Summary

We introduced the adhesive force model into the DEM simulation. By using this model, the fracture morphologies of the powder materials were investigated. We found that as increasing Δ the morphological change from the cracking to crumbling occurs around $\Delta = \Delta_g$.

We also proposed a hypothesis that the morphological change may be related with a kind of transition in the powder or particle systems such as the glass transition. If this hypothesis is confirmed, the powerful tools developed in the theories for the glass transition may be applied to the fracture mechanism of the fragile powder materials.

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