Discrete Element Analysis of Sedimentary Body Density of Functionally Graded Materials derived from Particle Co-Sedimentation

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Abstract. In this paper, the particle co-sedimentation process is analyzed by discrete element analysis. The formation of deposits of continuous functionally graded materials derived from the particle co-sedimentation method is simulated. The porosity of the deposit is calculated and the variation of the porosity along the deposition direction is obtained. From the simulation, the method to increase the deposit density is firstly generated, which is helpful for preparation of functionally graded materials by particle co-sedimentation method.

1. Introduction

Functionally graded materials (FGM) is a kind of new functional composite materials of which main phase is made of two different materials. By designing the composition and structure of middle layer with continuous gradient variety, the properties of FGM vary gradually along the design direction to meet the requirements of the special features of the material. Due to its widely applicable system, simple preparation and controllable size, co-precipitation process based on the continuous sedimentation of the particles in the liquid phase to obtain the continuous structural changes becomes the most prosperous method [1,2].

To obtain the FGM with efficiently gradient component, the size and distribution of particles is critical to the structure and density of precipitation system. In the previous co-precipitation method, the precipitation system is regarded as no voids (i.e. the accumulation ratio is 1.0) and a continuous, uniform structure, ignoring the effect of discrete particles, size distribution and shape difference on the formation of stacked system voids. In addition, theoretical analysis or calculation also ignores the effect of collision, friction and rolling (among the particles and between the particles and wall) on the porosity of the precipitated system in the liquid medium the precipitation process. Based on the
discrete element method and EDEM discrete element [3], in this paper, the accumulation and precipitation process of the components have been analyze and simulated in the case of full consideration of factors to influence the porosity of stacked system.

Using the EDEM discrete element to simulate particles co-precipitation process is divided into two aspects: firstly, the simulation of particle co-precipitation process by visual presentation to clearly observe co-precipitation process; secondly, the simulation of particles accumulation by using the relationship between the particles of stacked system and the volume of voids to analyze the variation of the gap along the sedimentation direction.

1 Simulation of co-precipitation process

1.1 Component particle characteristics

We take the Al2O3-Cu ceramic-metal FGM prepared by the particle co-precipitation process as an example and the precipitation liquid medium as distilled water [2]. The component distribution of the precipitation system is shown in Fig. 1. The precipitation liquid component parameter settings are shown in Table 1 and the component materials and contact characteristics are shown in Table 2, the gradient material component distribution function is a power function [4,5]:

\[
C_A(x) = a \times \left(\frac{x}{l}\right)^p + b; \quad C_B(x) = 1 - b - a \times \left(\frac{x}{l}\right)^p
\]  

(1)

Where \(C_A(x)\) and \(C_B(x)\) represent the volume percentage content of the lower density component A and the higher density component B component at the point x of the sedimentary system; x is the position coordinate along the gradient in the thickness direction; l is the thickness of the graded layer; p is the component distribution index; a is a nonzero coefficient; b is a constant.

Fig. 1 The schematic graph of the component distribution of the precipitation system

| Table 1 The precipitation liquid component parameter settings |
|-------------------------------------------------------------|
| Density of component A \(\rho_A\) kg m\(^{-3}\) | Density of component B \(\rho_B\) kg m\(^{-3}\) | Density of precipitation liquid \(\rho\) kg m\(^{-3}\) | Viscosity of precipitation liquid \(\mu\) Pa s | Height of suspension \(H_1\) m | Height of clear liquid \(H_2\) m | a | b | p |
|-------------------------------------------------------------|
| Density of component A \(\rho_A\) kg m\(^{-3}\) | Density of component B \(\rho_B\) kg m\(^{-3}\) | Density of precipitation liquid \(\rho\) kg m\(^{-3}\) | Viscosity of precipitation liquid \(\mu\) Pa s | Height of suspension \(H_1\) m | Height of clear liquid \(H_2\) m | a | b | p |
| Material       | Poisson’s ratio | Shear modulus (Pa) | Recovery coefficient | Static friction coefficient | Rolling friction coefficient |
|---------------|-----------------|--------------------|---------------------|-----------------------------|-----------------------------|
| Al₂O₃         | 0.22            | 9.06×10¹⁰         | -                   | -                           | -                           |
| Cu            | 0.33            | 3.9×10¹⁰          | -                   | -                           | -                           |
| Al₂O₃-Al₂O₃   | -               | -                 | 0.45                | 0.45                        | 0.01                        |
| Al₂O₃-Cu      | -               | -                 | 0.48                | 0.40                        | 0.01                        |
| Cu-Cu         | -               | -                 | 0.50                | 0.17                        | 0.01                        |

**1.2 Simulation parameters settings**

Based on the EDEM (v2.4.1) software, the simulation parameters are set as follows:

① Defined the contact model: choosing Particle to Particle; setting custom particles in the liquid resistance in Particle Bodyforce.

② Defined the gravity and the material parameters and contact parameters of Al₂O₃ and Cu: wherein taking residual gravity of the particles.

③ Defined the original particles: the radius of the Al₂O₃ and Cu are 1μm multiples and the mass of particles, volume, and other parameters can be automatically calculated dependent on the previously defined density of material.

④ Defined the geometric model: take the entities cylinder infinitesimal with a radius of 50 μm and a height of 500μm as a model.

⑤ Setting the size distribution of Al₂O₃ and Cu: choose Lognormal distribution.

⑥ Setting the particle factory: the particles are generated based on the total mass or the numbers and the way to fill the geometric model. To improve simulation efficiency, 300 particles are selected in simulation demo.

⑦ Setting the calculation parameters: 30 % ideal time step are taken in the test of simulation results.

**1.3 The result of precipitation simulation**

After the simulation, the screenshots are used to clearly show the precipitation process (shown in Fig. 2). The Cu particles are marked as red color area and the Al₂O₃ particles are marked as green color area. The reasons for the long time calculation (for three days) as the follows:

First, the particle size is quite small. The small particles are only of a few micros which requires shorter time step in order to capture the changes in motion of the particles, resulting in the increase of iterative calculations and longer simulation time. The other reason is on the forces acting on particles. The precipitation of particles in a liquid medium by residual gravity and resistance, wherein the resistance is programmed as Laminar flow state of motion resistance coefficient through API contributes to the slow simulation speed.
2 Simulation of accumulated precipitation structure

2.1 Particle size characteristics setting

Component A of raw material is the Al₂O₃-Cu system. The particles are generated by quality, wherein the total mass of Cu is 5000g, Al₂O₃ is 2300g. Set Al₂O₃ component granularity in line with the Gates-Gaudin-Schumann distribution equation [6]:

\[ U_A(D) = 100 \left( \frac{D}{50 \times 10^{-6}} \right)^{0.35} \text{ (\%)} \; ; \; \quad f_A(D) = U'_A(D) \]  \hspace{1cm} (2)

At the time of \( t \), the deposition amount of component A is that:

\[ M_A(t) = m_A \left( \int_{D_1}^{D_{i\text{,max}}} f_A(D)dD - \int_{D_1}^{D_i} \frac{H_2}{H_1} f_A(D)dD \right) + t \frac{dM_A(t)}{dt} \]  \hspace{1cm} (3)

And at the time of \( t \), the deposition amount of component B is that:

\[ M_B(t) = m_B \left( 1 - \left( 1 + \frac{H_2}{H_1} \right) \int_{D_{\text{min}}}^{D_i} f_B(D)dD + \frac{H_2}{H_1} \int_{D_{\text{min}}}^{D_{\text{max}}} f_B(D)dD \right) + t \frac{dM_B(t)}{dt} \]  \hspace{1cm} (4)

Where \( D_i = \sqrt{\frac{18 \mu H_2}{(\rho_A - \rho)gt}} \).

By numerical calculation, the undersize cumulative percentage of component B (copper powder Cu) is obtained. Part of the data is given in Table 3 due to the large number of numerical simulation.
Table 3 The cumulative percentage undersize of component B

| Precipitation time t / s | Mₐ(t) / g | Slope of the tangent | The undersize cumulative percentage / % | Particle size/ μm |
|--------------------------|-----------|---------------------|----------------------------------------|------------------|
| ...                      | ...       | ...                 | ...                                    | ...              |
| 1000                     | 6.48762   | 1.28139E-06         | 32.87049                               | 16.72            |
| 1100                     | 6.83014   | 1.05052E-06         | 30.72643                               | 15.94            |
| 1200                     | 7.13312   | 8.78255E-07         | 27.82187                               | 15.26            |
| 1300                     | 7.40376   | 7.46010E-07         | 25.38739                               | 14.66            |
| 1400                     | 7.64755   | 6.42090E-07         | 23.74932                               | 14.13            |
| 1500                     | 7.86871   | 5.58835E-07         | 21.82987                               | 13.65            |
| 1600                     | 8.07058   | 4.91020E-07         | 20.63998                               | 13.22            |
| 1700                     | 8.25585   | 4.35010E-07         | 19.10149                               | 12.82            |
| 1800                     | 8.42669   | 3.88175E-07         | 18.03379                               | 12.46            |
| 1900                     | 8.58490   | 3.48580E-07         | 16.73271                               | 12.13            |
| 2000                     | 8.73196   | 3.14795E-07         | 15.91682                               | 11.82            |
| 2100                     | 8.86913   | 2.85725E-07         | 14.82111                               | 11.54            |
| 2200                     | 8.99748   | 2.60520E-07         | 14.04059                               | 11.27            |
| 2300                     | 9.11789   | 2.38515E-07         | 13.16125                               | 11.03            |
| 2400                     | 9.23117   | 2.19185E-07         | 12.47745                               | 10.79            |

In order to improve the simulation efficiency and easy to observe, all micron particles are amplified × 10³ times to the millimeter, and this treatment does not affect the analysis of the precipitation porosity.

2.2 Simulation results of the precipitation system

After the simulation of the precipitationsystem, the precipitation results are shown in Fig. 3. The precipitationsystem data is obtained at the same time as shown in Table 4, and the porosity of the precipitationsystem is analyzed. Precipitationsystem in the height direction in order to investigate the relationship between porosity in the deposition height, the average is divided into 10 units, respectively, the porosity of each unit is obtained, and can be obtained by the porosity of Fig. 4 with the variation in the height relationship.
As shown in Fig. 4, the bottom of the precipitation system mainly consists of large particles and the porosity of stacked system is relatively large and the density is low. However, the top of the sedimentary body mainly consists of small particles and the porosity of stacked system tends to
decrease and the density increases. The fluctuation of the porosity in this range reflects the effects of two component particles on stacked structure in the size and distribution of particles.

4 Conclusions

(1) Using the EDEM discrete element to analyze a continuous gradient material precipitation process by the co-precipitation particles prepared by the particle co-precipitation method. The effect of collision, friction and rolling (among the particles and between the particles and wall) will be considered to simulate the accumulation and precipitation process of the components, contributing to more accurate and reliable design of continuous gradient material.

(2) Under the condition of particle size distribution of raw materials corresponding with the dense accumulation, the particle size distribution value of another group is obtained by Component distribution function and the precipitation process associated numerical solution. The variation of porosity of precipitation system along precipitation height and the dense precipitation with accumulation rate of 90.98% to 92.18% are attained by the EDEM discrete element simulation.

(3) According to the simulation, if the particle distribution of two components is set as Rosin-Rammler distribution equation, the porosity of precipitation system reaches 48.14% ~ 39.15% when that the uniformity coefficient is set to be 2 and 2.5 makes it significantly deviation from the dense packing conditions (0.5 ∼ 0.7). This indicates that the density of precipitation system can increase more obviously by the dense-graded structure of the particle distribution than that the particle distribution is not controlled and graded.

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