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Three-dimensional combined finite-discrete element approach for simulation of single layer powder compaction process①

CHEN Pu-qing(陈普庆), XIA Wei(夏 伟), ZHOU Zhao-yao(周照耀),
ZHU Quan-li(朱权利), LI Yuan-yuan(李元元)
(College of Mechanical Engineering, South China University of Technology,
Guangzhou 510640, China)

Abstract: The application of a combined finite-discrete element modeling approach to simulate the three-dimensional microscopic compaction behavior of single-layer metal powder system was described. The process was treated as a static problem, with kinematical component being neglected. Due to ill condition, Cholesky's method failed to solve the system equations, while conjugate gradient method was tried and yielded good results. Deformation of the particles was examined and compared with the results of physical modeling experiments. In both cases, the inner particles were deformed from sphere to polygonal column, with the edges turning from arc to straight line. The edge number of a particle was equal to the number of particles surrounding it. And the experiments show that the ductile metal particles can be densified only by their plastic deformation without the occurrence of rearrangement phenomenon.

Key words: powder; simulation; finite elements; discrete elements
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1 INTRODUCTION

Powder metallurgy(PM) parts are typically produced by compaction, sintering and sizing operations. Since the strength of PM parts and the shrinkage are both strongly affected by the porosity of the green compacts during sintering, various approaches have been presented to reduce this porosity in the compaction process and improve the uniformity of porosity distribution[1-9], including numerical simulation of the compaction process to aid tooling design and optimize processing variables. Some of those methods have been utilized in practice and largely improved the quality of PM parts.

Finite element method(FEM) requires a material model based on continuum mechanics. The peculiarity of powder material hinders its application in powder compaction analysis. Therefore, various material models for powder material have been presented and studied. After comparing the precisions of different methods, Modnet pointed out that powder-forming simulation is entering the phase of industrial implementation[7, 8]. While, to perform the simulation, it is necessary to determine the relationship between the model parameters and the relative density for each kind of powders from experiments. These experiments are usually hard to perform and require special apparatus. Since continuum based approaches do not include parameters of the particles, such as the granularity, shape and the individual mechanical properties, it can not unveil their microscale behavior and the interaction between them.

An alternative is discrete element method (DEM), in which individual powders are modeled as small particles and the interaction between adjacent particles is modeled as a function of the distance between them. In each incremental step, the contact and separation between the particles are detected and processed. Initially presented to analyze the behavior of rock structure and sand, this method omits the deformation of the particles, which doesn't accord with the intrinsic characteristics of metal powders.

The particles both displace and deform in compaction process. To unveil the complicated behavior of the particles, it is necessary to exploit the merits of both FEM and DEM. Therefore a method that combines FEM and DEM was also proposed and studied. The powder bulk was treated as granular material,

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Correspondence: CHEN Pu-qing, PhD Candidate; Tel: +86-20-87112933; E-mail: chpq2000@sina.com

while each particle was discretized into finite elements. The interaction between the particles was calculated based on DEM, and their deformation was calculated with FEM. Up till now, only two-dimensional plain strain models were described in literatures[10-13].

Another approach was by using a special mesh generation method in FEM[14]. Two dimensional plain strain models were analyzed with this method. Physical modeling experiments were performed with commercial pure aluminum rods of 5 and 7 mm in diameter and 25 mm in length. The deformations from simulations and experiments are compared.

However, the shape and arrangement of the particles are both essentially three-dimensional, which is misrepresented by the two-dimensional simplification. Therefore this study attempts to simulate the microscale behavior of the particles with a more precise three-dimensional model.

2 MODEL SIMPLIFICATION AND HYPOTHESIS

The diameter of industrial iron powders often ranges from 50 μm to 200 μm, with irregular shapes. The number of particles involved in each compaction process is very large, from ten million to one billion. It is necessary to make some assumption so that the simulation can be carried out.

2.1 Geometry

Due to the limitation of computing capability, only a small quantity of particles can be included in the simulation. The shapes of the powders are diverse, which makes it unreasonable to use the shape of specific particles in the model. Thus in this study spheres were used to model the particles. For the convenience of preparing the spherical particles and observing the deformation in physical modeling experiments, the diameter of the particles is supposed to be 2.5 mm. Since the behavior of inner particles would be covered by boundary ones if multi-layer particles were included in the experiment, which would make their behavior hard to view, the number and arrangement of the particles were controlled to get them forming a single layer.

2.2 Material

The iron spheres are difficult to prepare. And with large deformation, they harden severely. So the compaction requires very large force. In the experiments of this study, the stannum particles are used to model the real particles. As both stannum and iron are metal and follow Hook's law and Von-Mises principle, the deformations should be quite similar under the same condition.

The stannum spheres used in the experiments were produced by dripping blobs of liquid-state stannum into cold water. So their shapes were not ideal sphere, but with small tails.

2.3 Boundary conditions

The principle of friction between particles and between particles and die-wall is complicated. The numerical simulation in this study supposed it follows the modified Coulomb principle, and is smoothed by arc-tangent function.

3 NUMERICAL SIMULATION

The theoretical basis of combined finite-discrete element method has been described in Refs. [10-13, 15]. The method proposed treated the particle system as a dynamic system. The effect of inertia and moment of inertia was included in the simulation. Although this may be helpful in high-speed circumstances, the kinematical component was very small in normal compaction process, so that the values of dynamic parameters, such as the density of particles and inter-particle damping, were set at an unreal high value to improve the stability and increase the computing efficiency without yielding too much error[10]. So the current study neglected the unnecessary kinematical component and focused on the static behavior of powders.

Static analysis requires that the rigid body motion should be eliminated, or the system stiffness matrix will be singular or non-positive. However, all the particles in the model are movable. Their movement should be determined in computation. So the displacement boundary conditions cannot be exerted on them. To improve the system stability, the sticky friction is included in simulation. When the relative velocity is smaller than a threshold, the two objects contacted are considered sticking to each other in the next iteration step; or the friction force is calculated with Coulomb model. By this means, the stiffness matrix becomes positive definite, but the system equation is still ill conditioned. Cholesky's method was tried but failed to solve the system equations, while the conjugate gradient method yielded good results.

Simulation was carried out with MSC. Marc software. The geometric model is illustrated in Fig. 1. The spherical particles were filled into a cylindrical die of 20 mm in diameter, formed single layer arrangement. Simulations were carried out with the material's properties set as stannum, iron and copper. With the same other conditions and plastic hardening neglected, the simulations yielded same deformation results but different stress results. The elastic modulus of stannum was set at 43.12 GPa, Poisson ratio

was 0.3 and yield stress was 31 MPa[16]. The upper punch, lower punch and die were treated as rigid body. The contacts between the spheres and between the spheres and die wall were detected and processed. The friction coefficient at the contact surfaces was set at 0.2. This value affects the system stability and the convergence speed of conjugate gradient method. The lower the value is, the more the cycles are required to converge. Here, the maximum cycle number was set to be 10 000, and the tolerance was set to be 0.001. The solution was converged when the maximum residual force over the maximum reaction force was less than the tolerance.

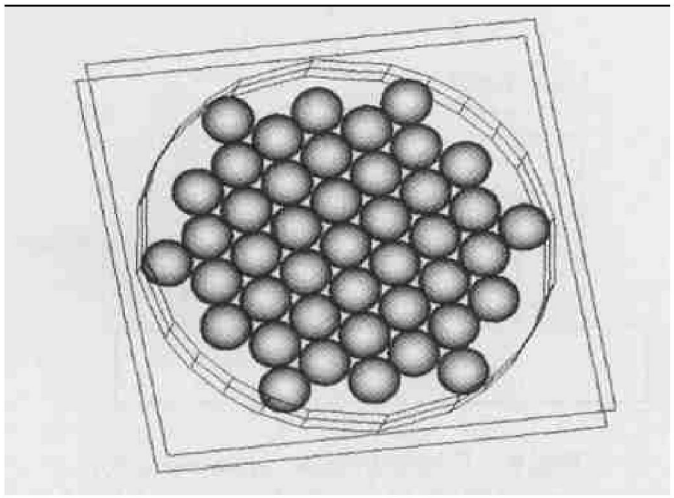

Fig. 1 Initial arrangement of particles and tools

The particles were discretized into four-node tetrahedron finite elements, 1 657 elements for each one. Totally 43 particles, 71 251 elements and 16 426 nodes were included in the model. Fig. 2 shows the finite element model of each particle. From the above data, the initial relative density is

$$\rho_r = \frac{43 \times \frac{4}{3}\pi \times (2.5/2)^3}{\pi \times (20/2)^2 \times 2.5} = 44.79\%$$

This value is close to the experimental data reported in literatures. Totally a period of 0.8 s was analyzed. The process was divided into 250 steps.

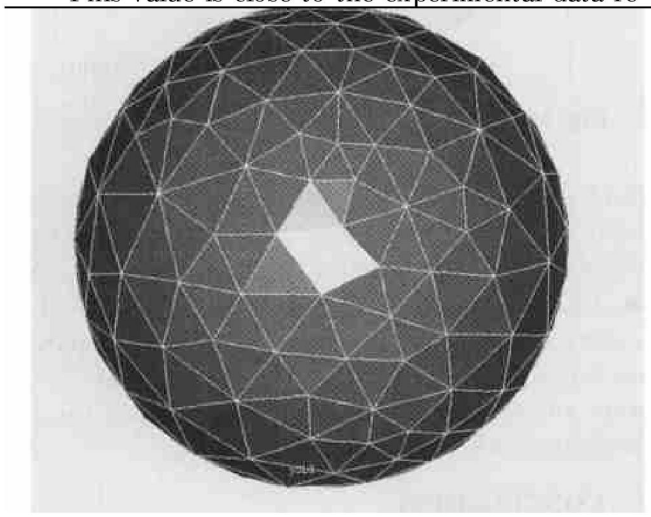

Fig. 2 Finite elements of each particle

Fig. 3 shows the deformation of the particles. After compaction, the relative density turns to be

$$\rho_r = \frac{345}{\pi \times (20/2)^2 \times (2.5 - 0.8 \times 1.6)} = 90\%$$

where 345 mm^3 is the total volume of all the elements after compaction.

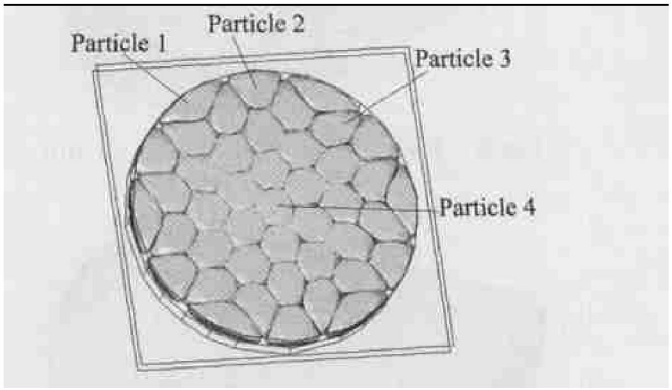

Fig. 3 Deformation of particles

The simulations were carried out on PC platform with a Pentium Ⅳ processor running at 2.4 GHz. Typically one turn of simulation requires about 4 h.

The deformations of the center particle and three particles at the rim are shown in Figs. 4 – 7. The total plastic strain of particle 3 is shown in Fig. 8.

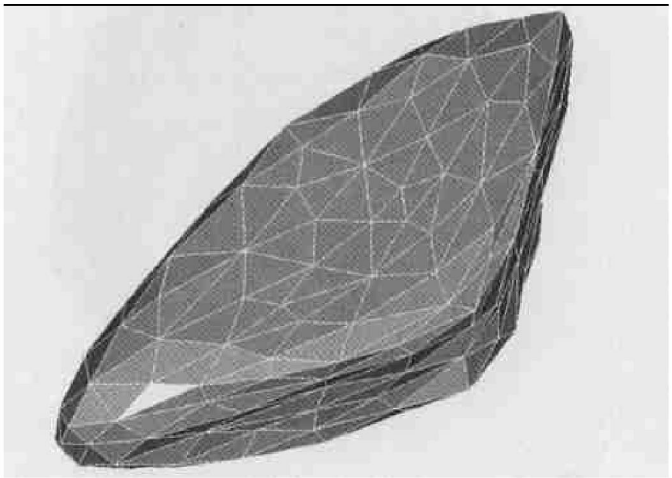

Fig. 4 Final shape of particle 1 at rim

4 EXPERIMENTS AND COMPARISON

The physical modeling experiments were performed to examine the validity of the above simulation approach.

Fig. 9 illustrates the apparatus used in the experiment. The stannum balls were filled into the cylindrical die, formed one layer, and compacted. The diameters of the balls were about 2.5 mm. The diameter of the die was 20 mm. After compaction, the balls deformed severely and adhered to each other,

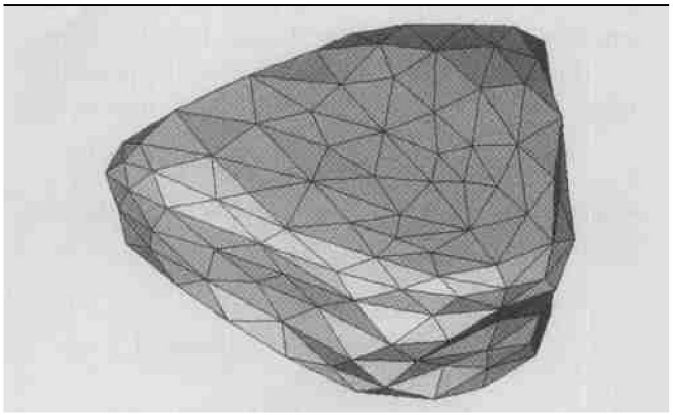

Fig. 5 Final shape of particle 2 at rim

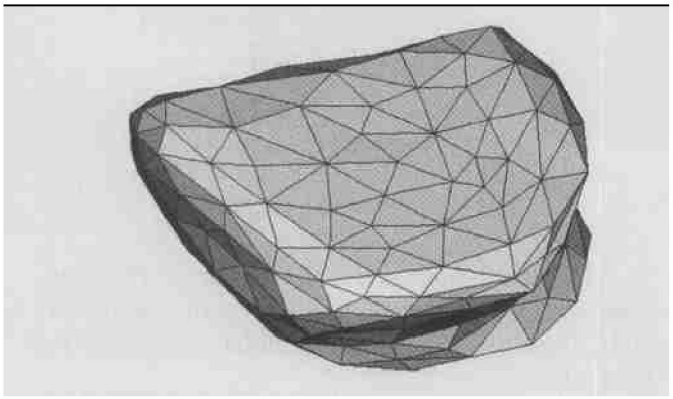

Fig. 6 Final shape of particle 3 at rim

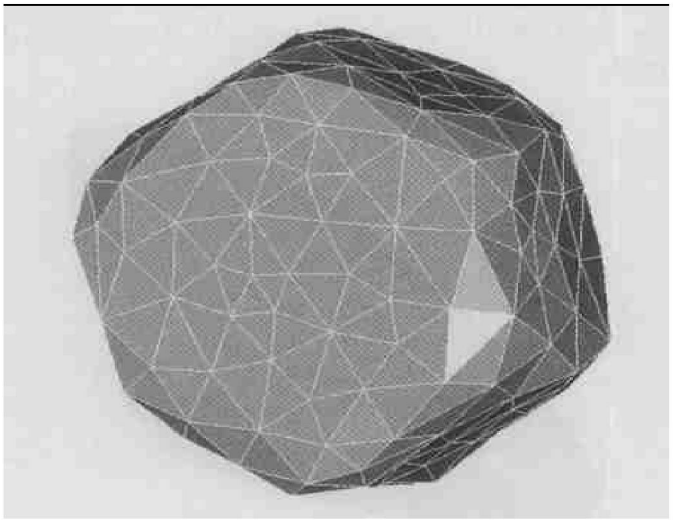

Fig. 7 Final shape of particle 4 in center

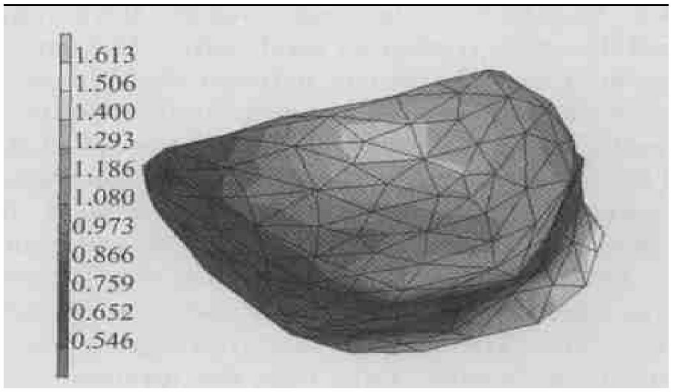

Fig. 8 Distribution of total equivalent plastic strain in particle 3

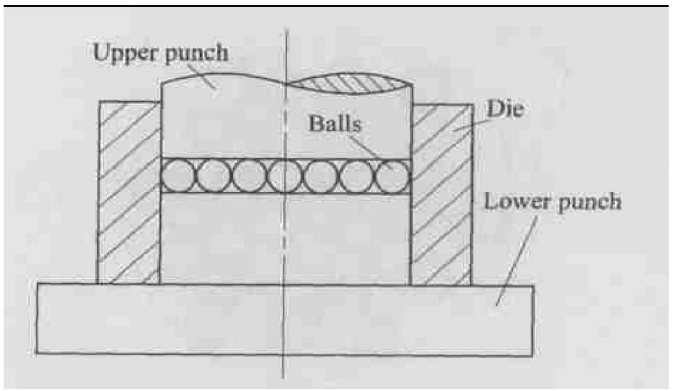

Fig. 9 Experimental apparatus for compaction of single-layer particles

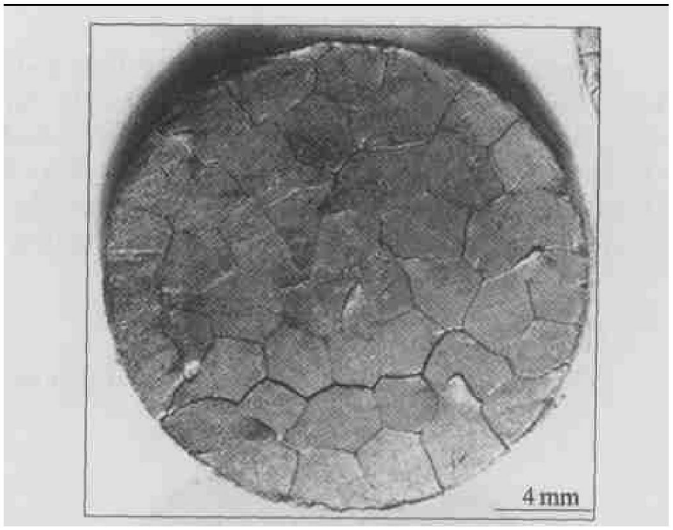

Fig. 10 Picture of particles after compaction

forming a disk-like object. The disk was spited and assembled together again to make the gaps prominent to observe. The picture of particles after compaction is shown in Fig. 10. It shows that the sections of the particles turned from circles to polygons. The number of the particles was equal to the initial number of the balls. This demonstrates that when rearrangement phenomenon is eliminated, particles of ductile material can still be densified by only their plastic deformation.

The particles used in the experiment were not ideal spheres, and their initial arrangement was random, so the deformation was not exactly the same as that in simulation. While, in both cases, the deformation had similar characteristics. Most of the particles were deformed into polygonal columns. The initial curving boundary of the particles turned to be straight lines. Particles at the rim were pressed by die wall, which makes their deformation different from inner ones.

5 CONCLUSIONS

The compaction process of metal particles was simulated. The deformation of the particles was examined and compared with experimental results. The result shows that:

1) In both cases, the inner particles deformed from spheres to polygonal columns. Their edges turned to be straight line. The number of edges of each polygon is equal to the number of other spheres touching it.

2) Ductile metal particles can be densified only by their plastic deformation, without the occurrence of rearrangement phenomenon.

3) In the numerical simulation, unnecessary dynamic components were neglected, which made the system unstable and the system stiffness equations ill conditioned. The conjugate gradient method can be used to solve the equations.

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