Advanced Powder Technology 24 (2013) 871–878

Contents lists available at SciVerse ScienceDirect

Advanced Powder Technology

journal homepage: www.elsevier.com/locate/apt

Original Research Paper

Stochastic analysis on coordination number distribution of particles during powder compaction

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ARTICLE INFO

Article history:
Received 27 September 2012
Received in revised form 29 April 2013
Accepted 3 May 2013
Available online 17 May 2013

Keywords:
Stochastic analysis
Coordination number
Powder compaction
Markov process

ABSTRACT

This paper deals with the change in the coordination number distribution in spherical mono-sized silica powder compacts to discuss its particle-packing process during Cyclic CIP (Cold Isostatic Pressing) with increasing the number of cycles at the maximum CIP pressure of 100 MPa. By measuring the distance between the first closest particles (viz. contact particles) to a center particle, the coordination number of the center particle is determined. The resultant coordination number distributions are analyzed with stationary Markov process. The transition probability matrix obtained by the data at the number of cycles from 1 to 10 gives sufficient predictions for the experimental data at the number of cycles of 100 and 1000.

1. Introduction

Powder compaction is one of the most important industrial routes for metal, polymer and ceramic products, and in particular, its quality strongly affects performance of the final products in ceramics because inhomogeneity in ceramic compacts may partly remain as voids and cracks after sintering. To obtain denser and more uniform ceramic compacts, various approaches have been tried such as effect of powder shape [1], granulation [2], bimodal powder mixtures [3], additives [4], ultra-high pressure [5]. Matsuo et al. [6] also proposed a new process named "Cyclic CIP" (Cold Isostatic Pressing) to obtain better compacts.

The original idea of Cyclic CIP [6] was superimposing cyclically varying pressure onto a static hydraulic pressure of conventional CIP, as shown in Fig. 1. Effects of the maximum CIP pressure, bias (minimum) CIP pressure, frequency, and the number of cycles on ceramic compacts were reported in the previous papers [6–10]. Note that bulk density and homogeneity of Cyclic CIP'ped compacts were monotonously improved with increasing the number of cycles. And also it is worth mentioning that Al_2O_3 and SiC ceramics made by Cyclic CIP showed high reliability in strength after sintering. This process is easily applied to industrial production and we can obtain denser and more uniform compacts at a relatively lower CIP pressure around 100 MPa (not several hundreds MPa in conventional CIP).

Recently, the present authors began to investigate its densification during Cyclic CIP, and showed that it was divided into two specific processes [11]. One was a homogenization (due to granule collapse) operated at the number of cycles below 10, and the other was particle packing (with holding its uniformity) operated at the number of cycles above 10. Moreover, the homogenization was quantitatively interpreted with a multiple shell model proposed by the present authors there. However, the particle packing cannot be explained by collapse of granules itself, and we need another discussion in view of microscopic packing of particles.

Particle packing research was started by Bernal and Mason [12]. They reported that the smallest coordination number in 3-dimensional particle packing was 4 by counting the contact points in ball bearing experiments with etching technique; however, Goodling and Khader [13] pointed out that a small part (0.02%) of polystyrene particles had the coordination number of 3. These researches were developed into plastically-deformed particles in powder metallurgy, and the increase in particle contact area was discussed to attain better sintered metal products. Sundström and Fischmeister [14] reported that the increase in the contact area is more important for the stress required to improve densification than strain hardening of the particle itself in the porosity range of industrial compacts. James [15,16] confirmed that contact flattening for several types of powders to observe the fractured compacts with a secondary electron microscope (SEM). Fischmeister et al. [17] studied non-radial particle motion (particle sliding or restacking) during compaction of spherical bronze particles. They put the bronze powder into a cylindrical die and partially-sintered it at 700 °C in hydrogen to make necking as a marking of the first contact point, and then this compact was compressed in uniaxial (up to 1000 MPa) and isostatic (up to 800 MPa) pressing, respectively. The coordination number of the particles was measured by SEM

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http://dx.doi.org/10.1016/j.apt.2013.05.002

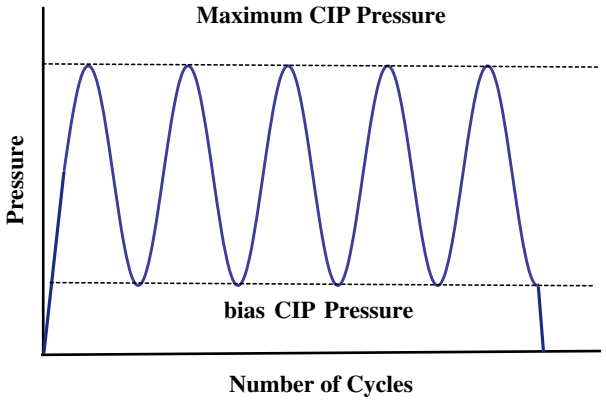

Fig. 1. Concept of cyclic CIP (Cold Isostatic Pressing).

stereo fractography on the assumption that, one-half of the contact facets can be seen exactly on a fractured surface on average (to meet this assumption, they measured 30–70 particles for each fractured surface). They also checked this method by direct counting method with etching technique (all round counting for around 50 particles in each specimen), indicating that there was not exactly the same but a positive correlation between two methods. In their data by direct counting method, the coordination number of uncompressed compact ranged from 6 to 9 (its average was 7.3) with the porosity of 37.5%, however, at 200 MPa compaction, the coordination number became wider between 7 and 12 (its average was 8.2) with the porosity of around 20%. Finally, at 1000 MPa compaction, the distribution of the coordination number was narrower again between 10 and 14 (its average was 11.8) with the porosity of around 2.5%. The average coordination number was almost linearly increased with the compaction pressure. It was shown that particle sliding occurred up to a pressure at which the initial porosity became in half (up to 20% porosity after 200 MPa compaction) and also that isostatic compaction involved less particle sliding and more plastic deformation than uniaxial compaction. Later on, the same authors developed a densification model by applying a radial density function to their data [18,19], and stated that spherical powder model should be more important because such the powder were increasingly used in industry. In a different perspective, German [20] also gave systematic interpretation on the change in the coordination number of particles from powder compaction to sintering.

In computer simulation, there are a lot of model proposed. One is the central cluster growth model [21–23], assuming that the change in arrangement of particles due to isotropic pressure promotes densification and can be reproduced by Monte-Carlo simulation. Another is discrete element method (DEM) for determining kinematics of particles during compaction by solving Newton's equation of motion for multiple bodies system. This method was proposed by Cundall and Strack [24], and then Thornton and Antony [25] developed DEM to quasi-static deformation of dense packing problems. Recently, many researchers have used DEM method to investigate three-dimensional packing of particle during compaction [26–28].

In these previous studies, however, the coordination number of particles was just discussed with the changes in the bulk density and also the compaction pressure, and there is no consideration on the effects of loading and unloading, and the number of cycles during Cyclic CIP. So, in this study, we pay particular attention to particle packing of Cyclic CIP'ped compacts by measuring the coordination number of particles with a different concept (viz. the average distance between the first closest particles) from Fischmeister et al. [17]. And we try to explain the change in the distribution of coordination number based on a stochastic process model.

2. Stochastic process model

Consider the change in the coordination number of mono-sized spherical particles during powder compaction by Cyclic CIP. As shown in Fig. 2, we may see several types of the changes after one cycle of compaction. For example, the coordination number of a center particle A (gray-colored) is increased from 6 to 7; however, the number is kept at 6 in a particle B. Similarly, the coordination number is decreased from 6 to 5 in a particle C, and the number is changed more than unity in a particle D (from 6 to 8). Bernal and Mason [12] reported that the smallest coordination number in 3-dimensional particle packing was 4 by counting the contact points in ball bearing experiments with etching technique; however, Goodling and Khader [13] found that a small part (0.02%) of polystyrene particles had the coordination number of 3. Therefore, we assume that the coordination number actually ranges from 3 to 12 in 3-dimensional particle packing in this model. Fischmeister et al. [17] reported that, in their measurement, the maximum coordination number was 14 for spherical bronze particle (its size distributes from 250 μm to 315 μm) though, we restrict ourselves here to discuss spherical mono-sized ceramic particles which do not show plastic deformation, so that the maximum coordination number must be 12 in this study.

When we look at one particle, its coordination number widely fluctuates with increasing the number of cycles. However, on the whole of particles with some coordination number, their next coordination numbers must be distributed within numbers from 3 to 12 after all. In order to express such a state transition, it is convenient to use a transition probability matrix P in Markov

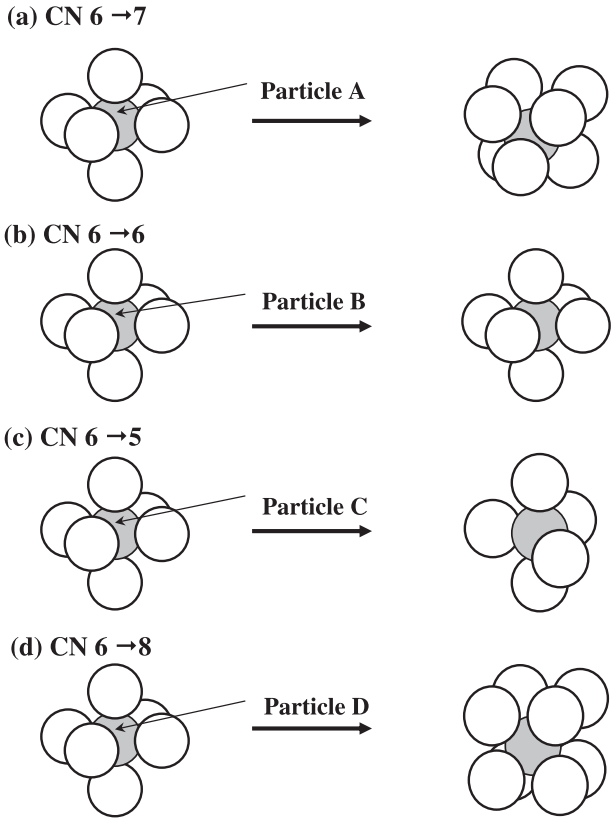

Fig. 2. Changes in the coordination number (CN). The gray particle is the center particle in each case.