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SHORT COMMUNICATION

DENSIFICATION OF POWDER COMPACTS BY VIBRATION

Hern Kim† and Moo-Sil Pyun

Dept. of Chem. Eng., Myong Ji University, Yongin, Kyonggi-Do 449-728, Korea

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Abstract—Various packing methods such as vibration, shaking, etc., in addition to normal gravitational settling, can be often used to densify powder compacts. Many issues relevant to this matter are of great importance in advanced ceramic powder processing. In the present work, the relaxation of structure due to vibration is addressed by using a computer experimental model based on Monte Carlo method. Packing structures, diffraction patterns, radial distribution functions are used for the characterization of structures. Bulk properties such as packing fraction and average height of the deposit are examined. The results agree well with those observed in model experiments, even with more implication.

Key words: Packing, Powder, Vibration, Densification, Microstructure

INTRODUCTION

It has been noted [Kim and Rajagopalan, 1994d] that computer experimental models are good tools for analyzing a number of phenomena and for designing many novel experiments relevant to ceramic powder processing, such as aggregation, packing or deposition, sintering, etc. The effects of some factors such as adhesion and polydispersity have been studied on the resulting microstructures and geometrical properties of the deposits [Kim and Rajagopalan, 1991, 1994a, 1994b]. In the present work the effect of vibration as one of the packing methods is considered.

The compaction of powders is one of the important steps in ceramic powder processing. In most cases the deposition or packing of particles such as ceramic powders is obtained by pouring a collection of particles into a mold or on a substrate, and the final packing structures are determined by 'collective', competitive interactions among the particles as they roll down (even when the particles are deposited individually along ballistic trajectories). Typical structures of deposits of such particles often consist of 'arches' or 'bridges' in the particle networks, even if the particles are nearly spherical and their surfaces are very smooth. Such cooperative effects prevent the formation of dense close packing, and additional actions such as mixing, vibration, shaking, or the like, are necessary to obtain denser and more uniform structures. Most current studies on this topic are experimental (mainly for the packing of coarse particles), rather than theoretical, in view of the complexity of the phenomena involved. The results of such studies (mostly, geometrical properties of the resulting structures) are available only in the form of empirical correlations. Computer simulations have been used very seldom, largely because of the difficulties in simulating the cooperative interactions among particles. On the other hand, little information about the effects of compaction on the variations in the structures of the deposit is available.

The objective of the present work is to develop a computer experimental model which is able to generate the structures, to analyze the resulting properties, and to examine the dynamic behavior during powder compaction.

†To whom all correspondences should be addressed.

COMPUTER SIMULATION PROCEDURE

The packing process may in general include steps such as vibration, shaking, mixing, etc. For this purpose we use a technique [Rosato et al., 1987] used to simulate the effects of shaking. Here, we treat these with a single type of 'disturbance' and assume that all the particles are uniformly disturbed. In this case, the heights of all the particles are increased by a predefined distance (set at one particle radius, 1.0R). Following this, the position of each particle is 'readjusted' using the Monte Carlo procedure based on cooperative packing process outlined elsewhere [Kim and Rajagopalan, 1994c]. The latter step is repeated for each particle for a prespecified number of times; this, we define, as a 'cycle' (The length of one cycle used here was 1,000 MCS, at the end of which all the properties reached asymptotic values.). The above procedure is then repeated until any selected property (such as packing fraction) arrives at a global asymptotic value. Clearly, variations from the above procedure (e.g., randomly chosen displacement, horizontal displacement, etc.) are possible, but we restrict our attention here to the one described above.

In the present work the resulting structures are analyzed using diffraction patterns and radial distribution functions, and the properties such as average height and packing fraction are examined. Details of the characterization of structures are available elsewhere [Kim and Rajagopalan, 1994c].

CHARACTERIZATION OF STRUCTURES

The structure of the deposits generated in the simulations is analyzed using diffraction patterns and radial distribution functions of particle positions. For calculating these, only those particles within ± 30% from the mid point are taken so that the influence of the substrate and of the free 'surface' at the top of the packing is avoided. The diffraction patterns are prepared using the structure factor S(**q**), which is defined by [Hansen and McDonald, 1986]

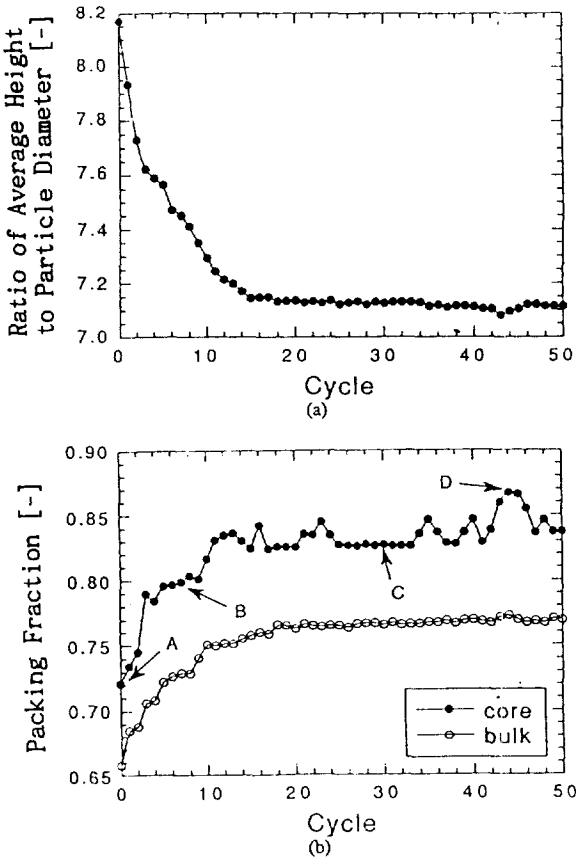

Fig. 1. Effect of vibration on (a) the average height and (b) the packing fraction as a function of vibration cycle.

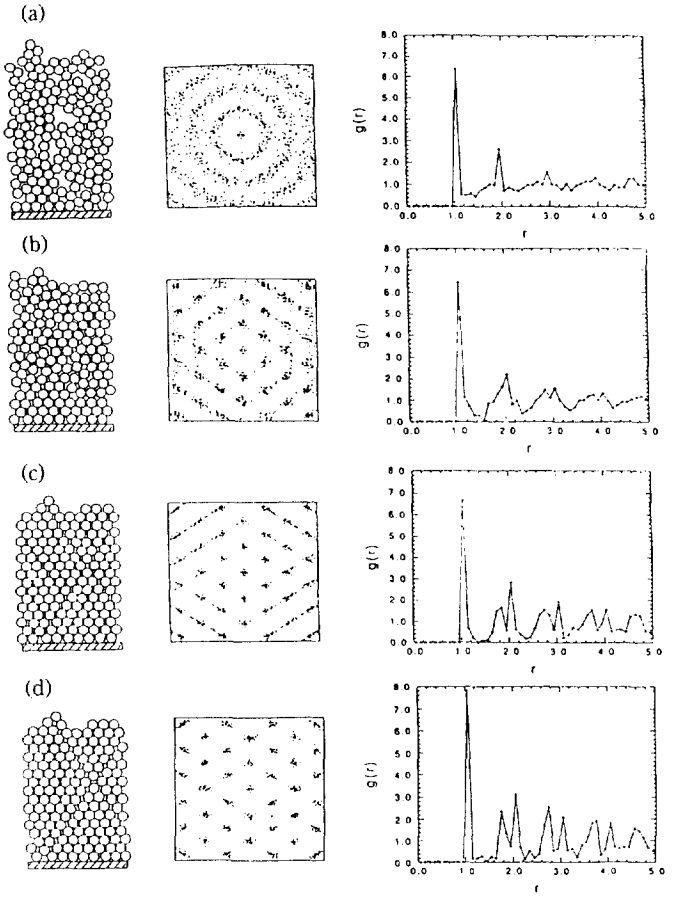

Fig. 2. The packing structures, diffraction patterns, and radial distribution functions obtained for different number of vibration cycles. Number of cycles equal to (a) 0, (b) 7, (c) 30, and (d) 44.

$$S(\mathbf{q})=(1/M)<|\Sigma\exp(i\mathbf{q}\cdot\mathbf{r}_j)|^2>;\ j=1,\cdots,M \quad (1)$$

where $\mathbf{r}_j$ is the position vector of the j-th particle, the summation is over all M particles in the chosen region, and the bracket $<\cdots>$ denotes the statistical average over the configurations.

The radial distribution function, g(r), is a measure of the probability of finding two particles at any center-to-center separation r and is given by

$$g(r)=[\Delta n(r)/2\pi r\Delta r]/\rho_{avg} \quad (2)$$

where $[\Delta n(r)/2\pi r\Delta r]$ is equal to $\rho(r)$, the local particle density, with $\Delta n(r)$ equal to the number of particles in the interval $[r, r+\Delta r]$ and ρ_{avg} is the overall average density of the packing.

RESULTS AND DISCUSSION

A starting powder compact with a low packing fraction is generated for sticking probability of 0.25 using the noncooperative packing method [Kim and Rajagopalan, 1991] (One can consider such a powder compact to be similar to an agglomerate of weakly interacting particles.). The powder compact is then vibrated using the scheme described above (We take the Peclet number to be 10^{16}.). Fig. 1(a) shows the change of the average height of the deposit as a function of time, where the average height is expressed in multiples of the diameter of particle. The average height of the deposit shows a rapid decrease initially and becomes nearly constant after a certain relaxation period (of approximately 15 cycles), the constancy of the height indicating that compaction is almost completed. Fig. 1(b) shows the change in the corresponding packing fraction. Initially, a rapid densification is observed. The packing fraction reaches essentially an asymptotic value (between 0.83 and 0.87) after a certain period (of approximately 15 cycles). The figure does show some fluctuations in the packing fraction in this asymptotic region, but this is very possible due to the small size of the simulations used here. In addition, these abrupt fluctuations can also be caused by the intensity of vibration used in the simulations (which has been taken to be high for the results in the above figure). One can expect to reduce such fluctuations in the packing fraction in the core region of the sediment by reducing the intensity of vibration.

The computer simulation scheme used in this work is quite general and is appropriate for studying densification or relaxation phenomena related to a variety of packing processes. As an example, one of the current issues in ceramic powder processing is the use of high-intensity ultrasound to promote the improvement of geometrical and structural properties of the deposits. This method has been proposed as an innovative molding method [Lange, 1989], with a recommendation that attenuation of the ultrasound is one problem that must be addressed. The intensity of vibration (or relaxation) introduced in the simulation is one of the important factors that can determine the degree and the rate of densification [Kim, unpublished work].

Fig. 2 shows the packing structures, diffraction patterns, and radial distribution functions for different times during the vibration. One can observe that the deposits densify gradually as a result of vibration. The gradual increase in ordering and the increasing resemblance of the structure to a perfect hexagonal structure can also be seen from the appearance of Bragg peaks in the diffraction pattern with increasing time. From the radial distribution functions we find that, with increasing time, positional correlations appear over longer distances and new peaks appear between those already present (e.g., at $r=\sqrt{3}d$), with the old ones becoming sharper. These results are consistent with what one would expect in practice, and therefore the computer simulation methods proposed here can be used for studying and predicting the phase behavior of particle assemblies as a function of densification. Currently, such attempts are made using model experiments [Pieranski, 1984; Lemaitre et al., 1991]; the model experiments, however, are limited in their ability to isolate individual phenomena whose effects need to be examined closely.

NOMENCLATURE

d : particle diameter
g(r) : radial distribution function
N : total number of particles
q : scattering vector
r : radial distance
R : particle radius
S(**q**) : static structure factor

Greek Letters

ρ_{avg} : overall average packing density
$\rho(r)$: local particle density

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