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Numerical simulation of the ball impact process

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article info abstract

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To optimize the operation conditions of the ball impact process, a novel dry surface treatment process developed by the authors' research group, a simulation model was developed on the basis of the discrete element method (DEM). From the calculation results, it was found that the balls impact the top or bottom inner surface as a solid group. When the filling fraction and ball diameter were 19% and 5.0 mm, respectively, the kinetic energy at collision for 1 s was 94 J, and the contact stress on the top inner surface attained an average of 4300 MPa and a maximum of 14,000 MPa. When the ball diameter was above 7 mm, the average contact stress was constant at approximately 6000 MPa, and when the diameter was less than 7 mm, the contact stress had a wide distribution and was notably high for balls with high relative velocity. Therefore, to achieve a significant ball impact, it is reasonable to use a few balls with small diameter so as to obtain high relative velocity and prevent collisions between the balls. In addition, it was shown that there is a strong relationship between the calculated contact stress and the adhesion of actually fabricated hydroxyapatite coatings on Ti substrate.

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1. Introduction

The ball impact process is a novel dry surface treatment of metals that was previously developed by the authors [\[1\]](#page--1-0). Metal or ceramic balls and powder particles are placed inside a vibration chamber, which is mechanically vibrated. This causes the balls to accelerate and repeatedly impact the inner metal surface of the chamber. As a result, the metal surface is rapidly coated with the powder particles. This process is more efficient than the conventional method, in which powder particles loosely adhere to the metal surface prior to vibration in a chamber (pre-coating method [\[2\]\)](#page--1-0).

During the ball impact process [\(Fig. 1\)](#page-1-0), the particles are abraded and sandwiched between the balls and the inner surface of the chamber; the particles bind to each other because of cold welding, thereby forming a particle coating. Using this process, high-density adhesive particle coatings can be fabricated under ambient temperature, normal pressure, and in a standard air atmosphere. Using mechanical vibrations, the authors have successfully fabricated a high-temperature corrosion-preventive coating of $LapO₄$ particles on a stainless steel substrate [\[2,3\],](#page--1-0) a coating of TiN nanoparticles on a metal substrate to improve surface hardness [\[4\]](#page--1-0), and a coating of hydroxyapatite (HAp) particles on a Ti substrate to fabricate a biocompatible material with both mechanical strength and osteoconductivity [\[5\]](#page--1-0). In addition,

instead of powder particles, metal foils such as Mo, Ni, and Ti have been successfully bonded to a metal surface [\[6\]](#page--1-0).

As described above, because the ball impact process is based on a simple principle, the initial and operating costs, energy consumption, and environmental load are comparatively low. Therefore, because of its mechanochemical effect, this process can be possibly applied for not only particle coating but also synthesizing new materials by controlling the atmosphere in the vibration chamber.

However, it is difficult to optimize the operation conditions of this process by trial and error because the process has many variable parameters such as ball material, ball diameter, and frequency and amplitude of the vibration. If operation conditions which provide high process efficiency can be attained by numerical simulations of the process, the number of test productions and experiments can be reduced considerably. This leads to significant decrease in time and cost for a process development. Therefore, in this study, to clarify the effects of the operation condition of the ball impact process on ball impact and its distribution, a numerical simulation model was developed on the basis of the discrete element method (DEM). By using it, the analyses of the behavior of the balls and the contact stress to the wall surface during the process were carried out. The effects of the filling fraction and ball diameter on the calculated results were investigated, and compared with the experimental results of HAp particle coating on a Ti substrate [\[5\].](#page--1-0) If the contact stress acting on the top inner surface of the chamber, which was assumed to be a metal substrate, has some effect on the physical properties of the fabricated particle coatings, it would be possible to fabricate particle coatings with arbitrary properties in an efficient way.

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Fig. 1. Concept of the ball impact process.

2. Numerical simulation based on DEM

2.1. Simulation model

DEM [\[7\]](#page--1-0) is a well-known method for simulating powder behavior in which the behavior of the particles that constitute the powder is calculated using motion equations, which are derived by considering all forces acting on the particles. In DEM, the effects of contact among particles in normal and tangential directions are modeled using the Voigt model [\[7\]](#page--1-0), in which the elastic spring and viscous dashpot are connected in parallel. In addition, a friction slider was introduced to estimate friction in the tangential direction.

To analyze the behavior of the balls in the vibration chamber using DEM, we used R-FLOW, a versatile software program developed by R-flow Corporation, Ltd. In the simulation model, the existence of the powder particles used to fabricate the coatings was not considered.

The material of the balls and chamber was assumed to be $ZrO₂$, and the normal and shear stiffness coefficients were set at $5.5\times$ 10^9 N/m and 2.1×10^9 N/m, respectively. These stiffness coefficients can be calculated from Hertz elastic contact theory equations [\[8\]](#page--1-0) using the ball diameter of 5.0 mm, Poisson's ratio of 0.31, and Young's modulus of 2.1×10^{11} N/m². There is no experimental data available for the restitution coefficient of ball–ball and ball–wall contacts; therefore, 0.5 was used after considering the values for stainless steel measured by the authors (0.57) [\[9\]](#page--1-0) and the effect of particle existence. The friction coefficient of ball–ball and ball–wall contacts was assumed to be 0.6 with reference to the relationship between the repose angles of powders and friction coefficients used in DEM simulations, obtained by Kano et al. [\[10\].](#page--1-0) This is because the repose angle of HAp particles was approximately 35°. The time step Δt [s] was set on the basis of the following equation [\[11\]](#page--1-0) (5.3 × 10⁻⁷ s for ball diameter of 5.0 mm), which guarantees calculation stability in unsteady DEM calculations. In this equation, m and K_n are the mass of a ball and the normal stiffness coefficient, respectively. The physical properties used in the simulation model are summarized in Table 1.

$$
\Delta t \leq 2 \sqrt{\frac{m}{K_n}}
$$

2.2. Calculation method

A prescribed number of balls were arranged spatially at equal distance in a static cylinder, which simulated the vibration chamber, both with a diameter and height of 40 mm; the balls were then allowed to fall freely and the calculation was started. Within 1 s, all the balls had fallen and were at rest, and the state in which the balls came to rest was considered as the initial packing condition for the calculations. From this initial condition, the calculations were started using the prescribed vibration amplitude and frequency. As the balls were assumed to be in an almost steady state within 1 s, the calculations were continued for 5 s.

For the fabrication of particle coatings by the ball impact process, the repeated ball impacts on a substrate surface are believed to be highly relevant to the coating characteristics considering the process mechanism. Therefore, at each time step, the contact stress was calculated by dividing the normal contact force acting on the top inner surface of the cylinder, which simulated a substrate surface, with the instant contact area for each contact point, and the time variation of the calculated stress was obtained. The time step used in this study was shorter than the time before the ball starts to impact a wall surface, changes shape, bounces, and rebounds completely from the wall; therefore, the change of each ball impact could be estimated correctly.

2.3. Calculation conditions

The variable parameters in the calculations were the filling fraction and ball diameter. The amplitude and frequency of the vibration chamber were fixed at 40 mm and 20 Hz, respectively. First, the ball diameter was set to 5.0 mm and the filling fraction was varied from 9.3% to 44%. In these cases, the mass and number of balls were 25–120 g and 64–307, respectively. Second, after fixing the filling fraction at 19% and mass at 50 g, the ball diameter and number of balls were varied in the range of 1.0–25 mm and 15,921–1, respectively, for the calculations. The calculation conditions are summarized in Table 2.

3. Results and discussion

3.1. Behavior of balls

[Fig. 2](#page--1-0) shows the typical time variation in the ball behavior by DEM simulation for filling fraction of 19%, mass of 50 g, ball diameter of 5 mm, and 125 balls. In the figure, time passes clockwise. When the vibration frequency was set at 20 Hz, it took 0.05 s for one run. The balls impact the top or bottom inner surface every 0.025 s. When 125 balls are used, they impact as a solid group.

3.2. Kinetic energy of balls at collision

[Fig. 3](#page--1-0) shows the time variation (4.8–5 s) of the kinetic energy of balls at collision with the top inner surface of the vibration chamber for the case previously described. The kinetic energy of a ball was

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