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Simulation of grain growth and sintering process by combined phase-field/discrete-element method

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Abstract

A combination of the phase-field method (PFM) and the discrete-element method (DEM) is proposed to simulate simultaneously the movement of particles and the grain growth behavior in powder compacts during sintering. To take the mutual interaction into consideration, a precise way of coupling PFM and DEM is developed based on a sintering model. The sintering forces and the contact areas in linked particles are evaluated from the phase field variables, computed in PFM and introduced into the calculation of the rigid motion of particles in DEM. Before treating actual problems as the application, the sintering process of two particles is simulated first for fundamental verification, including the case with different particle sizes. It is confirmed that the changes in the neck size and the center-to-center distance between particles are reproduced well using the proposed method. Secondly, the simulation of microstructural evolution during sintering is implemented for some small clusters of particles. The internal spatial structure and the outer shape of the clusters vary with the shrinkage deformation as well as the grain boundary migration in sintering. The proposed method of simulating the microstructural evolution in sintering bodies may be effective in the computer-aided design of microscale components or thin films produced by powder processing.

Keywords: Sintering; Phase-field method; Discrete-element method; Grain growth; Densification

1. Introduction

Current analytical methods of the sintering process can be divided into three levels – atomic, particle and continuum [1,2] – but may also be roughly categorized into two groups from the viewpoint of the target. One is the group for calculating distortion and stress in the sintering body; the other is suitable for simulating microstructural evolution, such as grain growth. For analyzing macroscopic deformation behavior of powder compacts during sintering, the finite element method (FEM) has been used as a common numerical technique for treating continuum [3]. On the other hand, the discrete-element method (DEM) has recently been used for the simulation of the sintering shrinkage behavior of powder compacts [4–14]. This has the advantage of taking a network structure of particles directory into consideration. It is difficult for current workstations to treat industrial parts with normal size, but the application of DEM to the components of microscale devices may be possible. Conversely, DEM may be a suitable tool for computing deformation behavior of microscale components, because it is critically affected by each particle motion when the powder compacts consist of a small quantity of particles, that is, no longer a continuum. The grain boundary migration, however, cannot be dealt with in DEM itself, though the grain growth is an important phenomenon in the sintering process that affects the shrinkage as well as the microstructure of the components.

For the simulation of grain growth, the Monte Carlo method is commonly used, and applied to the sintering process [15,16]. Although the phase-field method (PFM) has also been applied to it recently [17–19], as a new numerical technique, there remains the problem of how

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to deal with the rigid motion of particles during the initial and intermediate stages of sintering. Since it may be difficult to perform the computation for sintering shrinkage within the scheme of PFM itself, the author has proposed a combined phase-field/discrete-element method to simulate simultaneously the movement of particles and the grain growth behavior in powder compacts during sintering [20]. However, the link-up from PFM to DEM was not considered in this primary study with a simplified sintering model, where the conjugate force in sintering, namely the sintering force, was set to be constant, and the contact area between particles was given by a simple function of the center-to-center distance.

In the present study, a complete way of coupling PFM and DEM is proposed based on a precise sintering model. The sintering forces and the contact areas in linked powder particles are evaluated from the phase field variables, computed in PFM and taken into consideration in the calculation of the rigid motion of particles in DEM. Before treating actual problems as the application, the sintering process of two particles is simulated first for fundamental verification, including the case with different particle sizes. The validity of the calculated results is examined based on a classical model for the early stage of sintering, as a reference. Secondly, the simulations of the sintering process are implemented for some small clusters of particles, as a first step of applied problems, and each motion of the particles is confirmed.

2. Numerical methods

2.1. Phase-field method

Grain growth behavior with advection flux was described by Wang [18], based on the Cahn–Allen equations [21]:

$$\frac{\partial S_k}{\partial t} = -L\frac{\delta G}{\delta S_k} - \nabla \cdot \vec{J}_s \tag{1}$$

where S_k is the phase-field variable, t is the time, L is the constant characterizing grain boundary mobility, G is the total free energy and $\vec{J}_s$ is the advection flux. The subscription k of S_k denotes the different crystallographic orientations of grains ($k = 1, 2, ..., p$). S_k is equal to 1 or -1 inside the grain and 0 outside it, with orientation k, and is taken to have intermediate values at the grain boundaries. For the conservation of mass, a relative density field is also treated based on the Cahn–Hilliard diffusion equation [22]:

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left(B\nabla \frac{\delta G}{\delta \rho} - \vec{J}_r \right) \tag{2}$$

where ρ is the relative density, B is the constant characterizing surface mobility and J_r is the advection flux. The total free energy G is assumed to be expressed as

$$G = \int \left\{ G_0 + \frac{\alpha}{2}(\nabla\rho)^2 + \sum_{k=1}^{p}\frac{\beta}{2}(\nabla S_k)^2 \right\} dV \tag{3}$$

$$G_0 = -\frac{a_1}{2}\left(\rho - \frac{1}{2}\right)^2 + a_1\left(\rho - \frac{1}{2}\right)^4 + \frac{2a_3 - a_2}{4}\rho^4 + \sum_{k=1}^{p}\left\{ \frac{a_2}{2}(\rho-1)^2 S_k^2 - \frac{a_3}{2}\rho^2 S_k^2 + \frac{a_4}{4}S_k^4 + \frac{a_5}{4}\sum_{l\neq k}^{p} S_k^2 S_l^2 \right\} \tag{4}$$

where G_0 is the local free energy density (Appendix A), α and β are gradient coefficients and a_1–a_5 are constants [17]. The calculation of Eqs. (1) and (2) is implemented by using the two-dimensional (2-D) finite difference method (FDM).

2.2. Discrete-element method

For the calculation of DEM, a model proposed by Parhami and McMeeking [6] is employed, but a 2-D version is used to meet the 2-D phase-field simulation. The transfer and the rotation of each particle are given by

$$\{f\} = [C]\{v\} + \{f_s\} \tag{5}$$

$$\{f\} = \{ f_n^1 \quad f_t^1 \quad M^1 \quad f_n^2 \quad f_t^2 \quad M^2 \}^T \tag{6}$$

$$\{v\} = \{ v_n^1 \quad v_t^1 \quad \dot{\theta}^1 \quad v_n^2 \quad v_t^2 \quad \dot{\theta}^2 \}^T \tag{7}$$

$$\{f_s\} = \{ f_s^1 \quad 0 \quad 0 \quad f_s^2 \quad 0 \quad 0 \}^T \tag{8}$$

The components of $\{f\}$ are the conjugate forces and the moments at the nodes of each element, where f_n and f_t are the normal and the tangential forces, respectively, M is the moment and superscript 1 or 2 is to make the distinction between adjoining particles. $\{v\}$ contains the velocities and the rotational rate of the nodes corresponding to the forces and the moments, where v_n, v_t are the normal and the tangential velocities, respectively, and $\dot{\theta}$ is the rotational rate. $\{f_s\}$ is the sintering force vector, which produces the rigid motion of particles, where f_s^1 and $f_s^2 (= -f_s^1)$ are the normal forces acting between particle 1 and 2. Matrix $[C]$, correlating $\{f\}$ with $\{v\}$, is formulated as follows:

$$[C] = \begin{Bmatrix} a & 0 & 0 & -a & 0 & 0 \\ 0 & b & \frac{bl}{2} & 0 & -b & \frac{bl}{2} \\ 0 & \frac{bl}{2} & \frac{bl^2}{4}+c & 0 & -\frac{bl}{2} & \frac{bl^2}{4}-c \\ -a & 0 & 0 & a & 0 & 0 \\ 0 & -b & -\frac{bl}{2} & 0 & b & -\frac{bl}{2} \\ 0 & \frac{bl}{2} & \frac{bl^2}{4}-c & 0 & -\frac{bl}{2} & \frac{bl^2}{4}+c \end{Bmatrix} \tag{9}$$

where l is the center-to-center distance of the particles and a, b, c are parameters derived by a classical sintering model for grain boundary diffusion as follows:

$$a = \frac{2X^3}{3\overline{D}_{gb}}, \quad b = 2X\eta, \quad c = \frac{2X^5}{45\overline{D}_{gb}} \tag{10}$$