Discrete Element Simulation of the Sintering of Composite Powders

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Abstract

The free sintering of metallic powders blended with non sintering inclusions is investigated by the Discrete Element Method (DEM). Each particle, whatever its nature (metallic or inclusion) is modeled as a sphere that interacts with its neighbors. We investigate the retarding effect of the inclusions on the sintering kinetics. Also, we present a simple coarsening model for the metallic particles, which allows large particles to grow at the expense of the smallest.

Keywords : sintering, composites, discrete element simulation, coarsening

1. Introduction

Analytic models are well suited to describe the sintering of powders in simple conditions when all particles are of the same size and of the same material. For more realistic conditions, the Discrete Element Method (DEM) offers an interesting alternative. In DEM, the mechanical equilibrium of each particle is treated by calculating the interactions between contacting particles, hence the rearrangements phenomena that characterize particulate materials are explicitly taken into account. In this work we analyze, using the DEM code dp3D, the effect of non sintering inclusions. We present also a simple model for coarsening that allows the coupling of sintering and particle growth.

The powder compact is modeled as a 3D random assembly of spherical particles interacting through their contacts. A dynamic scheme updates the new position of particles and the new contacts at each time step [1]. Periodic boundary conditions are applied to limit the number of particles necessary to obtain a representative volume element (between 4000 and 40 000 particles were used). Initial relative density is approximately 0.64, which corresponds to the random close pack density for monomodal packings.

The normal contact force model that describes the sintering of metallic particles is derived from the work of Parhami and McMeeking [2] and from the calculations of Bouvard and McMeeking [3] and Pan et al. [4]. It has been described in more detail in [5]. The model considers grain boundary and surface diffusion to be the major mechanisms for mass transport. The contact force includes a sintering term due to surface energy and a viscous part that opposes the normal relative motion of the two particles.

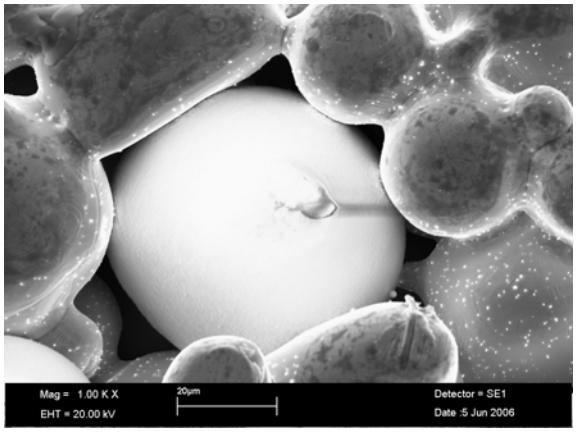

Fig. 1. SEM micrograph of copper particles surrounding an Al_20_3 inclusion after 2 hours at 1000°C.

2. Inclusions

We consider that the sintering of a metallic particle in contact with an inclusion is equivalent to the sintering of this particle on a metallic plane (∞ radius). The rationale of this choice is to mimic the spreading of the metallic particle on the inclusion (fig. 1). The effect of this choice is that, for free sintering, the rate of approach between an inclusion and a metallic particle that have the same size is approximately 16 times slower than the rate of approach that characterizes the sintering of two identical metallic particles. A contact between two inclusions is modeled as elastic.

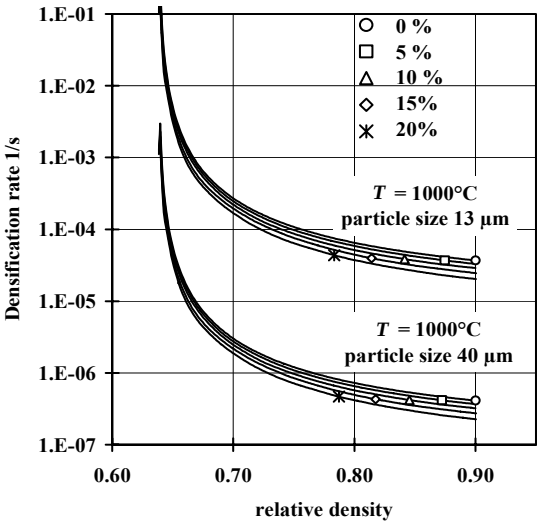

Fig. 2. Densification rate calculated by DEM simulations with various amounts of inclusion volume percentage.

For contact involving metallic particles, the contact grows according to Coble's geometric model [6], while Hertz model describes the geometry of inclusion-inclusion contacts. When the contact grows to attain the equilibrium value defined by the dihedral angle for two sintering particles, the contact force is reduced to its viscous part and no sintering tensile force is included.

The material parameters in the model have been chosen to represent cupper powder [5] while the inclusions are typically ceramic with elastic constants E=200GPa and ■=0.2. The sintering particles and the inclusions have been chosen of the same size although it is possible to generate packings with bimodal or lognormal size distributions. Two sizes were tested: 13 and 40 µm.

Figure 2 shows the sintering kinetics of the cupper powder without inclusion and with 5, 10, 15 and 20 volume % inclusions. The retarding effect is clear, with a densification rate approximately half for the 20% volume inclusion packing as compared to the copper powder compact. The effect of particle size on the densification kinetics is also clearly demonstrated. Densification rate scales approximately with $1/R^4$. No coarsening effect is included in the simulations presented in this section.

3. Coarsening

A simple coarsening mechanism has been included in the DEM code to account for particle growth during sintering. For each contact, the larger particle gains a volume ΩV (equal to the increment of indentation between the two spheres) at the expense of the smaller one. Particles stay spherical and radiuses are updated accordingly. Eventually, some particles shrink to negligible size and they are removed from the simulation box, mimicking coalescence (Fig. 3). Starting from 40 000 particles, the number of particles decreases to 740 in the periodic box at the end of the simulation (relative density 0.95). This causes an increase of the average particle size from 13 µm to 48 µm.

Fig. 3 illustrates the growth of particles that this simple coarsening model is able to provide. The particle growth curve is well fitted by an equation of the type $\overline{R}^n - \overline{R}_i^n \propto$ time where n=3 at the beginning of the growth process while n = 2 at the end. Fig.3 also shows that most of the coarsening occurs at the end of sintering when densification kinetics is very slow.

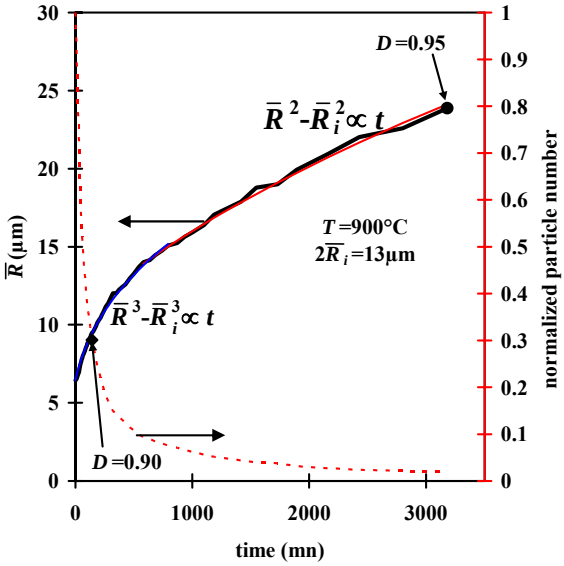

Fig. 3. Particle growth kinetics due to the coarsening mechanism. Particle number in the simulation box (---) decreases as coarsening proceeds.

We have shown that this simple model allows taking into account the retarding effect of particle growth on sintering kinetics [5]. Of course, the model is too simple to account rightly for grain boundary migration that characterizes coarsening. Some further work is needed to input some more physics into the coarsening model.

4. References

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