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Simulation of sintering using a Non Smooth Discrete Element Method. Application to the study of rearrangement

S. Martin [a,b,*], M. Guessasma [c], J. Léchelle [a], J. Fortin [c], K. Saleh [b], F. Adenot [a]

[a] Commissariat à l'Énergie Atomique et aux Énergies Alternatives, DEN, CAD, DEC, SPUA, LMPC, France
[b] Universite de Technologie de Compiègne, EA 4297, Transformations Intégrées de la Matière Renouvelable, France
[c] Université de Picardie Jules Verne, EA 3899, Laboratoire des Technologies Innovantes, France

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ABSTRACT

The aim of this study is to present an original approach for the simulation of sintering with Discrete Element Method, using a Non Smooth Method called Contact Dynamics.

Recently, there have been numerous papers about the simulation of sintering using Discrete Element approaches. Most of these papers use Smooth Dynamics and their results match well experimental data. However, some limits come from the use of an explicit scheme in which the time step has to be very small. In order to obtain reasonable time steps, the density of particles is dramatically increased which turns out to have an impact on rearrangement. Solving the sintering model with an implicit method such as Contact Dynamics takes into account the real density of particles.

The discrete model of sintering considers spherical particles which overlap due to the sintering stress. In Contact Dynamics, particles are not allowed to overlap. To overcome this issue, the sintering contact law is written using a basic deformation scheme coupled with a cohesion force.

The comparison with experimental data from previous studies shows that Contact Dynamics gives an improved representation of rearrangement when compared with Smooth Dynamics.

1. Introduction

Sintering is a major process in ceramics industry. The main physical phenomenon involved is solid state diffusion. The behavior of two particles in contact has been described several times with numerical approaches. Most of them consider grain boundary and surface diffusion as the principal phenomena [1–8]. Thus, a mechanical approach has been developed to take into account volume diffusion too [9]. In order to get a simpler description of sintering, a some authors introduced geometric assumptions [4,5,7,8,10]. Those led to analytical coupled expressions for the neck growth and center to center approach, as well as for the sintering stress.

Analytical expressions for the sintering of two particles can be used to estimate the behavior of sphere packings, assuming that every particle moves according to the macroscopic strain [5,11].

In contrast, Discrete Element Method (DEM) allows an escape from the mean field strain assumptions. Thus, random packings of spherical particles can be considered. The first DEM simulation of sintering has been presented by Parhami and McMeeking [12]. The authors combined an analytical expression of the sintering stress for spherical particles [4] with Coble's geometrical model [10]. This contact law was implemented into some quasi-static Discrete Element software. The model is based on strict assumptions: the particles are single-crystals and remain spherical. Moreover, only surface and grain boundary diffusion are considered. The resistance to sliding force is taken from Raj's model [13] and is expressed as a viscous law.

Additionally, for the last decade, a couple of authors have presented discrete simulations of sintering. Martin and Bordia [14] have studied sintering on a substrate, Martin et al. [15] the evolution of defects, Henrich et al. [16] have focused on the influence of rearrangement and Wang and Chen [17] have shown the evolution of forces and contact networks. Basic grain growth models have also been implemented by some authors [18,19]. The sintering law has also been completed to take into account the elasticity of the contact [20].

Comparison with experimental data of the stress induced anisotropy has been achieved by Wonisch et al. [19]. Then, a couple of synchrotron X-ray microtomography studies have pointed out the ability of this method to get accurate data on the micro-structure evolution [21,22]. This approach has also been used by Olmos et al. [23,24] to validate the discrete element model.

Hence, DEM simulation appears to be a relevant method to analyze the micro-structure parameters during sintering. Nevertheless, all the previous mentioned studies use either quasi static assumptions [12] or explicit schemes such as Verlet

* Corresponding author at: Universite de Technologie de Compiègne, EA 4297, Transformations Intégrées de la Matière Renouvelable, France. Tel.: +33 344235274.
E-mail address: sylvain.martin@utc.fr (S. Martin).

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Algorithm (VA) [14–16,18,19,23,24]. The first method is very time consuming. Consequently, it is limited to a few hundred particles [16]. VA is able to consider larger assemblies but the motion law integration is based on an explicit scheme that implies very small time steps. According to the application, the size of particles may vary from 100 μm to 0.1 μm. Thus, the inertia of particles is very small compared to the sintering force. Typical time step is about 1.10^{-15} s for 10 μm metallic powders. In order to get reasonable time steps, the density of particles has to be dramatically increased [16,20]. Although this does not change the evolution of density, it appears that some phenomena like rearrangement are very sensitive to the mass of particles. Thus, one can show that VA turns out to underestimate rearrangement [23].

The aim of this study is to present a new algorithm based on a Non Smooth Discrete Element Method called Contact Dynamics (CD). Different Non Smooth methods are proposed in literature, for the modeling of rigid body dynamics [25], deposition of charged cluster-droplets [26] or granular media [27]. They are able to solve non regular contact laws and use an implicit scheme for the motion law integration. Thus, the time step can be very high compared with VA without scaling up the density of particles. CD was first introduced by Jean [28], Moreau [29] and was initially designed for the simulation of large multi-body systems. For two particles in contact, the gap (or velocity) at the contact point and the normal force must be positive [30]. This means that particles are not allowed to overlap. These are called the Signorini conditions. The contact law is then defined by a step function that is not regular. This has to be combined with a shock or a local strain law in order to calculate the normal contact force. This method has been applied to assemblies of spherical or polyhedral particles, deformable or not [31]. Moreover, some studies have shown the ability of CD to model assemblies of cohesive and deformable particles for quasi static phenomena, especially in civil engineering for the breaking strength of granular media [32–34].

In this study, the sintering contact law will be expressed as a translation of Signorini conditions to allow the use of a basic CD solver. Then, an implicit scheme consistent with the CD solver will be proposed for the tangential law.

Numerical aspects will be introduced, and results will be compared with previous numerical and experimental studies. This study focuses on rearrangement of particles in granular assemblies during sintering.

2. Numerical computation methods

2.1. Sintering model

Sintering is due to the excess of surface energy in bulk materials by comparison with dense solids. This produces stress gradients that induce mass transfer. For solid state diffusion, this can occur along different interfaces which are grain boundaries, surface and bulk of grains. In some cases, gas transport phenomena can also play a significant role.

The behavior of two particles in contact is determined by the competition between those diffusions paths. Thus, the sintering model needs to be simplified using extra assumptions.

First of all, only grain boundary and surface diffusion are considered. For two particles in contact, grain boundary diffusion takes mater out of the grain boundary and bring it toward the surface of the neck, this leads to a center to center approach of particles. The extra mater brought at the neck radius is then laid out by surface diffusion.

Moreover, geometric assumptions are introduced to limit the degrees of freedom. Hence, sintering is described as the overlapping of spherical particles, Fig. 1. The grain boundary is assumed to be a disc and the dihedral angle remains constant. This model is only valid for single crystalline particles.

Using these assumptions, analytical or approximate solutions can be written for the sintering force between two particles in contact [5,4]. This is composed of an attractive part which corresponds to the integration of capillarity stress over the surface of particles and a viscous resistance opposed to overlapping which represents diffusion kinetics. Thus, according to Martin and Bordia [14], the normal sintering force is:

$$f_n^{sint} = \frac{\pi r^4}{8\Delta_b} V_n - \frac{9}{8}\pi R\gamma_s \tag{1}$$

where r is the neck radius, γ_s is the surface energy, V_n is the center to center approach velocity and Δ_b is the diffusion parameter defined as follows:

$$\Delta_b = \frac{\Omega\delta_b D_b}{kT} \tag{2}$$

with Ω the atomic volume, D_b the coefficient for grain boundary diffusion and δ_b its thickness.

R is the equivalent radius of particles such that: $R = 2 \times R_1R_2/(R_1 + R_2)$.

The neck grows according to Coble's model [10]:

$$\frac{dr}{dt} = \frac{R}{r} V_n \tag{3}$$

A maximum neck radius is reached when $r = Rsin(\psi/2)$, with ψ the dihedral angle. At this point, the system reaches a local equilibrium and the attractive force of sintering is set to zero in Eq. (1).

As the neck grows, particles are not free to slide. Thus, a tangential force, opposed to sliding has to be implemented. Raj and Ashby [13] showed that when sliding resistance is driven by diffusion, this can be expressed as a viscous force, proportional to the sliding velocity. Hence, the tangential force is given in Eq. (4):

$$f_t = -\eta \frac{\pi r^2 R^2}{8\Delta_b} \dot{u}_t \tag{4}$$

with $\dot{u}_t$ the sliding velocity.

There is no consensus about the value of η, which depends on the grain boundary properties. It must be lower than 0.5, but values ranging from 10^{-3} to 0.3 and can be found in literature [14]. Some authors conducted simulations without any tangential force in order to maximize rearrangement or for simplicity reasons [16,18].

The sintering model defined by Eqs. (1), (3) and (4) is identical to the one developed by Olmos et al. [23]. It allows a comparison between those authors results (using VA) and our simulations (using CD).

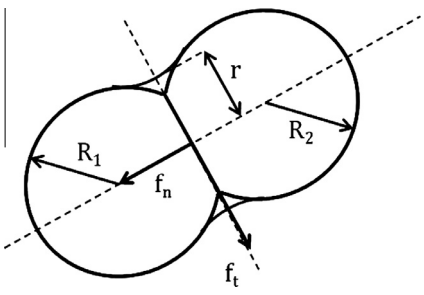

Fig. 1. Discrete element model for the sintering of two spherical particles in contact. R_1 and R_2 are the radii of particles, r is the neck radius, f_n and f_t are the normal and tangential forces applied at the contact point.