SOLID-STATE SINTERING SIMULATION: SURFACE, VOLUME AND GRAIN-BOUNDARY DIFFUSIONS

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Abstract. Within the general context of solid-state sintering process, this work presents a numerical modeling approach, at the grain scale, of ceramic grain packing consolidation. Typically, the sintering process triggers several mass transport paths that are thermally activated: surface, grain boundary and volume diffusions. Including this physics into a high-performance computing framework would permit to gain precious insights about the driving mechanisms which are seldom accessible at this scale.

In performing this kind of simulations, several challenges will be faced: the strong topological changes which appear during sintering simulation at the grains scale, the evolution of the structure that is mainly driven by the surface tension phenomena through the Laplace’s law, and the mechanical properties of the grains which could, possibly, be different. The proposed numerical simulations are carried out within an Eulerian Finite Element framework and the Level-Set method is used to cope with changes in the microstructure. The results obtained with this numerical strategy are compared with success to the usual geometrical models.
1 INTRODUCTION

Sintering is one of the stages of the powder metallurgy manufacturing process. Sintering is used for the fabrications of high performances materials and parts in a wide -and still growing- range of domains. Since the 50’s a large amount of work has dedicated to the theoretical and experimental study of this process. However the understanding of the underlying physical phenomena is still a field of active research. Diffusion phenomena are considered to be responsible for the microstructural evolution that takes place during sintering [8]. After the powder has been shaped, under the heat action different diffusion mechanisms are thermally activated. During the first stages of the process the necks between the particles are created. Necks continue to develop allowing the open porosity to become closed, to finally end up by vanishing at the end of the sintering process.

Even if it is possible to distinguish at least six different diffusion mechanisms, this work is mainly concerned by the surface, volume and grain boundary diffusions, which are considered to be the most important diffusion paths. Those diffusion mechanisms can be modeled by using the first Fick’s law. This law establishes a relationship between the matter flux \( \dot{j} \) and the gradient of the chemical potential \( \nabla \mu \):

\[
\dot{j} = m \nabla \mu
\]

where \( m \) is the mobility associated with the diffusion path considered. The chemical potential measures the tendency to diffuse of a substance and its value depends on the region of the particles that is being considered, e.g. surface, volume, grain-boundary, etc.

Table 1 shows the chemical potential as well as the mobility for each diffusion path. In this Table \( D_s \), \( D_v \) and \( D_{gb} \) are, respectively, the surface, volume and grain boundary diffusion coefficient, \( \delta_s \) and \( \delta_{gb} \) the thickness of the layer through which the material diffuses, \( k \) the Boltzmann’s constant, \( T \) the absolute temperature, \( \Omega \) the molar volume, \( \kappa \) the mean curvature, \( \gamma_{sf} \) the surface tension at solid/fluid interface, \( p \) the pressure, \( \sigma_{nn} \) the normal stress and \( f \) a constant of the material representing the ratio between the volume of a vacancy and the volume of an atom [7].

<table>
<thead>
<tr>
<th>Property</th>
<th>Diffusion path</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Surface</td>
</tr>
<tr>
<td>Mobility</td>
<td>( m )</td>
</tr>
<tr>
<td>Chemical potential</td>
<td>( \mu )</td>
</tr>
</tbody>
</table>

Table 1: Chemical potential and mobility for each diffusion path.

The mass flux leads to a deposition of mass at the surface and at the grain boundary. This deposition induces a normal velocity which should satisfy the following mass conservation equation:

\[
\begin{align*}
  v_n &= -\Omega \nabla \cdot \dot{j} & \text{For surface and grain boundary diffusions} \\
  v_n &= \Omega \dot{j} \cdot n & \text{For volume diffusion}
\end{align*}
\]

where \( v_n \) is the normal velocity due to the mass flux \( \dot{j} \) at a given point.

The previous equations are integrated into a continuum finite element Eulerian approach using the numerical strategy presented in Section 2. The surface and volume diffusions problems
are presented in Sections 3 and 4, respectively. In Section 5, the bases toward the sintering simulation by grain-boundary diffusion are stated. The results are presented in Section 7 and finally the conclusions and perspectives are discussed in Section 8.

2 LEVEL-SET STRATEGY

Initially, the numerical strategy for the simulation of sintering by surface and volume diffusion is presented. The strategy for the simulation of sintering by grain-boundary diffusion is slightly different and will be developed in Section 5.

As a first approach only the surface and volume diffusion are considered. For those diffusion paths, the computational domain is formed by only two phases: the particles which are assumed to be solid deformable bodies, and a surrounding medium, which is described as a low viscous Newtonian fluid. Let \( \Psi \) be an open region, \( \Psi \subset \mathbb{R}^d \), where \( d \) is the spatial dimension. The computational domain \( \Psi \) contains two immiscible phases: a set of elastic solids, denoted \( \Psi_s \), embedded into a surrounding fluid \( \Psi_f \). \( \Psi = \Psi_s \cup \Psi_f \) is the closure of \( \Psi \). Furthermore, \( \Psi_s \) is assumed to be completely contained in \( \Psi \), i.e. \( \partial \Psi_s \cap \partial \Psi = \emptyset \). Finally, the interface between the two phases is denoted by \( \Gamma_{sf} = \Psi_s \cap \Psi_f \) (see Figure 1).

![Figure 1: Computational domain \( \Psi \) divided into \( \Psi_s \) and \( \Psi_f \) by the interface \( \Gamma_{sf} \) and bounded by the surface \( \Sigma_f \) (From [12]).](image)

A Level-Set method [6, 11, 13] is used to capture the interface \( \Gamma_{sf} \). This Eulerian approach consists in embedding the surface in a higher dimensional function, the so called level-set function. The level-set approach used in this work was proposed by Coupez et al. in [3]. The basic idea of this method is to solve both the level-set transport and the reinitialization equations in a single step (see [3] for further details).

The level-set function is governed by the following expression

\[
\phi(x) = \begin{cases} 
-\text{dist} (x, \Gamma_{sf}) & \text{if } x \in \Psi_s \\
\text{dist} (x, \Gamma_{sf}) & \text{if } x \in \Psi_f \\
0 & \text{if } x \in \Gamma_{sf}
\end{cases}
\]

where \( \text{dist} (x, \Gamma_{sf}) \) is the distance from any point \( x \) to the interface \( \Gamma_{sf} \).

One of the main advantages of the level-set method is that it is possible to compute the normal \( \mathbf{n} \) and the curvature \( \kappa \) directly from the level-set function \( \phi \):
In the classical level-set method, the level-set function $\phi$ is transported by solving the following transport equation:

$$\frac{\partial \phi}{\partial t} + \nabla \phi \cdot v = 0$$  \hfill (6)

In our case, the velocity $v$ corresponds to the velocity due to the mass flux $j$ and will be computed by using equations (2) and (3). The Finite Elements Method is used to solve the PDEs presented in this work. The computational domain is discretized by using simplexes (triangles in 2D and tetrahedrals in 3D) with linear interpolations. In particular, when using the finite element method for the numerical treatment of equation (6), the Streamline upwind Petrov-Galerkin method (SUPG) is required.

### 3 SURFACE DIFFUSION

In Section 1, equations for modeling the surface diffusion were introduced. As showed in Table 1 the chemical potential on surface $\mu_s$ is proportional to the curvature $\kappa$, which means that the matter flux by surface diffusion $j_s$ is proportional to the first derivative of the curvature $j_s \propto \partial \kappa$. From equation (2), its associated velocity is proportional to the Laplacian of the curvature $v_n \propto \partial^2 \kappa$. Furthermore, the curvature can be computed by using the Level-set function $\phi$, but some difficulties will raise as the curvature $\kappa$ is proportional to the second derivative of $\phi$.

In this case the normal velocity is proportional to the fourth derivative of $\phi$: $v_n \propto \partial^4 \phi$. A classical finite element computation of the normal velocity $v_n$ from $\phi$ would lead to unphysical oscillations of the velocity field. As demonstrated by Bruchon et al. in [1], such oscillations are greatly reduced by solving a mixed $\kappa/\Delta\kappa$ formulation. The proposed mixed formulation is presented in equations (7) and (8):

$$\kappa^t + \nabla \cdot \left( \frac{\Delta t}{A} \nabla v^t_n \right) = \nabla \cdot \left( \frac{1}{A} \nabla \phi^t \right)$$  \hfill (7)

$$v_n \parallel \nabla \phi^t \parallel - C_0 \nabla \cdot \left( P_{\phi^t} \cdot \nabla \kappa^t \right) = 0$$  \hfill (8)

where $\kappa^t$ is the curvature at time $t$, $\Delta t$ is the time step, $\Delta t/A$ is a regularization parameter with $A$ given by $A = \parallel \nabla \phi^t - \Delta t \nabla v^t_n - \Delta t \parallel$, $v^t_n$ is the normal velocity at the time $t$, $\phi^t$ is the level-set function at the time $t$, $C_0$ is a constant containing the diffusion parameter of the material and $P_{\phi^t}$ is the projection operator at time $t$ given by: $P_{\phi^t} = I - n \otimes n$.

Additionally, Bruchon et al. [1] have shown that the velocity field obtained by solving equations (7) and (8) leads to volume conservation.

### 4 VOLUME DIFFUSION

In this case, the matter flux is considered to be proportional to the gradient of the pressure $p$ (Equation (3) and Table 1). This means that the mechanical problem should be solved in order to compute the matter flux and therefore the associated normal velocity. At the particles
scale (microscopic scale), the effect of the surface tension phenomena cannot be considered as negligible. The numerical approach developed to solve the mechanical problem is presented in Section 4.1. According to equation (3), the normal velocity due to the volume diffusion is also proportional to the gradient of the pressure as it will be presented in Section 4.2.

4.1 Mechanical problem

The numerical approach developed to solve the mechanical problem is presented in [12]. The inertia terms and the volume forces are neglected. The momentum conservation can be expressed by the set of equations (9):

\[ \nabla \cdot \sigma = 0 \quad \text{in} \quad \Psi \quad (9a) \]
\[ \sigma \cdot n = g \quad \text{in} \quad \Sigma_t \quad (9b) \]
\[ v = v_c \quad \text{in} \quad \Sigma_v \quad (9c) \]
\[ [\sigma \cdot n]_{\Gamma_{sf}} = \gamma_{sf} \kappa n \quad \text{in} \quad \Gamma_{sf} \quad (9d) \]

where \( \sigma \) is the Cauchy stress tensor for the solid or the fluid. \( g \) is the stress vector on the outer boundary \( \Sigma_t \), velocity \( v \) is equal to \( v_c \) over \( \Sigma_v \), \( [\ ]_{\Gamma_{sf}} \) denotes a jump across the interface \( \Gamma_{sf} \), \( \gamma_{sf} \) is the surface tension coefficient and \( \kappa \) is the main curvature. The outer boundary of \( \Psi \), \( \Sigma_f = \partial \bar{\Psi} \) (showed in Figure 1), is divided into \( \Sigma_t \) and \( \Sigma_v \) where the Neumann and Dirichlet boundary conditions are respectively applied.

For mass conservation issues, the formulation presented in this paper is a mixed formulation, the momentum conservation equation should be complemented with the mass conservation equation. Particles are assumed to have a linear elastic isotropic behavior:

\[ \sigma = 2\mu \dot{\varepsilon}(u) - \left( 1 - \frac{2}{3} \frac{\mu}{K} \right) pI \quad (10a) \]
\[ \text{tr} \left( \dot{\varepsilon}(u) \right) + \frac{p}{K} = 0 \quad (10b) \]

with \( p \) the pressure, \( u \) the displacement, \( \mu \) the shear modulus, \( \dot{\varepsilon}(u) = (\nabla u + (\nabla u)^T)/2 \) the linearized strain tensor, \( K \) the bulk modulus, \( \text{tr} \left( \bullet \right) \) the trace operator and \( I \) the second order identity tensor.

The fluid is Newtonian incompressible:

\[ \sigma = 2\eta \dot{\varepsilon}(v) - pI \quad (11a) \]
\[ \text{tr} \left( \dot{\varepsilon}(v) \right) = 0 \quad (11b) \]

where \( v \) the velocity, \( \eta \) the viscosity and \( \dot{\varepsilon}(v) = (\nabla v + (\nabla v)^T)/2 \) the strain rate tensor.

The numerical method used to solve the mechanical problem (9) to (11), along with the stabilization method is presented in [12]. The numerical treatment of the surface tension term is not straightforward within an Eulerian approach since there is no nodes over the interface \( \Gamma_{sf} \). The Surface Local Reconstruction (SLR) method is used. However, since the interface \( \Gamma_{sf} \) is given by the zero isosurface of the level-set function \( \phi = 0 \), it is possible to locally reconstruct the interface. This is the Surface Local Reconstruction (SLR) method used here: after the intersection between an element and the interface \( \Gamma_{sf} \) has been found, the surface
tension term can then be explicitly computed over this locally reconstructed surface. All the
details concerning the numerical implementation of the method are presented in [12]. It is
important to note that a stabilization method is required in order to satisfy the Ladyzenskaja-
Babuška-Brezzi condition for P1/P1 elements. In this case, a multiscale stabilization method is
used, specifically, the Algebraic Sub-Grid Scale stabilization (ASGS) method.

The surface tension over the interface $\Gamma_{sf}$ induces a jump of the normal stress in the direction
normal to the interface. For this reason, the pressure field also presents a jump at the interface
between the particles and the surrounding medium. Figure 2 shows the jump of the pressure
field computed at $\Gamma_{sf}$ as a result of the surface tension present over this interface.

![Figure 2: Pressure jump [Pa] at the interface $\Gamma_{sf}$ of two spherical particles of radii $R_1 = 0.2\mu m$ and $R_2 = 0.075\mu m$ due to the surface tension.](image)

According to Table 1 and equation (3), the normal velocity $v_n$ due to the volume diffusion
is proportional to the gradient of the pressure. Obviously this pressure gradient should be
computed inside the particles and must not take into account the jump of the pressure at the interface.
The strategy developed to compute $v_n$ is presented in the following Section.

4.2 Flow and velocity computation

Because of the surface tension at the surface of the particles, the pressure field is discontin-
uous. Therefore, it is not possible to compute the matter flux at the interface directly from the
pressure field gradient. The solution consists in computing the matter flux over a layer slightly
below the particles surface in such a way that the pressure discontinuity is disregarded. Having
the matter flux in a layer inside the particles, it must be convected to the interface.

A first approach concerning the velocity computation has been presented by Bruchon et al.
in [2]. Here another method is presented. Let $\lambda$ be a positive constant parameter. the main idea
is to compute the normal velocity inside the solid where the level-set function satisfies $\phi < -\lambda$
and convect those values in the outward normal direction where $\phi > -\lambda$, those regions are
showed in Figure 3.

The normal velocity $v_n$ is directly computed from the gradient of the pressure in the region $\phi < -\lambda$ (darker gray region) and $v_n$ is convected in the outward normal direction in the region $\phi > -\lambda$ (lighter gray region).

The normal velocity $v_n$ is then obtained by finding the stationary solution of the classical convection equation of $v_n$ in the normal direction $n$ for the fictitious time $\tau$:

$$v_n = A \nabla p \cdot n \quad \text{if } \phi < -\lambda$$  \hspace{1cm} (12a)

$$\frac{\partial v_n}{\partial \tau} + \nabla v_n \cdot n = 0 \quad \text{if } \phi > -\lambda$$  \hspace{1cm} (12b)

where $A$ is a constant function of properties of the material.

The stationary solution is found when the first term in the previous equation (12b) vanishes: $\frac{\partial v_n}{\partial \tau} = 0$. In fact, the velocity convection is performed by considering equation (12b) in its stationary form. In this case the SUPG stabilization method is also used to solve equation (12).

5 TOWARD THE GRAIN-BOUNDARY DIFFUSION

According to Table 1, the chemical potential for grain boundary diffusion is proportional to the normal stress $\sigma_{nn}$. Furthermore, the velocity associated with this diffusion path is function of the second derivative of this normal stress. The first step toward the sintering simulation by grain boundary diffusion is to develop a strategy able to solve the mechanical problem by taking into account, in addition to the surface tension at the free surface of the particles, the surface tension present at the grain boundary. This grain boundary surface tension condition can be written as follows:

$$[\sigma \cdot n]_{\Gamma_{sf}} = \gamma_{gb} \kappa_n$$  \hspace{1cm} in $\Gamma_{gb}$  \hspace{1cm} (13)

where $\gamma_{gb}$ is the surface tension coefficient at the grain boundary $\Gamma_{gb}$. The previous equation (13) should be added to the mechanical problem presented in equation (9).

As a first approach only two particles $\Psi_1$ and $\Psi_2$ are considered. Within an Eulerian context, at least two different level-set functions are required:
\[ \phi_1(x) = \begin{cases} -\text{dist}(x, \Gamma_{sf}) & \text{if } x \in \Psi_1 \\ \text{dist}(x, \Gamma_{sf}) & \text{if } x \notin \Psi_1 \\ 0 & \text{if } x \in \partial \Psi_1 \end{cases} \quad \phi_2(x) = \begin{cases} -\text{dist}(x, \Gamma_{sf}) & \text{if } x \in \Psi_2 \\ \text{dist}(x, \Gamma_{sf}) & \text{if } x \notin \Psi_2 \\ 0 & \text{if } x \in \partial \Psi_2 \end{cases} \]

In this way, the grain boundary \( \Gamma_{gb} \) is defined by the surface where \( \phi_1 = 0 \) and \( \phi_2 \equiv 0 \). The solid/fluid interface \( \Gamma_{sf} \) is defined by the surface where one of the following conditions is satisfied:

- \( \phi_1 \equiv 0 \) and \( \phi_2 \neq 0 \).
- \( \phi_1 \neq 0 \) and \( \phi_2 \equiv 0 \)

The numerical strategy presented by Pino et al. in [12] is slightly modified to take into account the surface tension at the grain boundary. Figure 4 shows the pressure field computed by taking into account both the surface tension at the free surface \( \Gamma_{sf} \) and the surface tension at the grain boundary \( \Gamma_{gb} \).

![Figure 4: (a) Pressure field computed by taking into account the surface tension over \( \Gamma_{sf} \) and \( \Gamma_{gb} \). (b) the jumps of the pressure across the interfaces \( \Gamma_{sf} \) and \( \Gamma_{gb} \).](image)

The numerical strategy allowing to compute the velocity due to grain boundary diffusion is yet to be developed. However, the strategy presented for the mechanical problem with surface tension on the free surface and the grain boundary is an important step toward the sintering simulation by grain boundary diffusion.

### 6 VOLUME CONSERVATION

In the case of volume and grain boundary diffusions, if only the velocities associated with those diffusion mechanisms were considered, the mass conservation equation would not be satisfied\(^1\). To overcome this problem, the solution consists in adding a correction velocity \( v_c \), in order to ensure the mass conservation [15, 14]. Considering that the density of the material

\(^1\)It has been shown by Bruchon et al. in [1] that the velocity induced by surface diffusion leads to mass conservation.
remains constant, the mass conservation leads to the conservation of the volume of the particles. This volume conservation is in agreement with the experimental results that can be found in the literature.

In order to satisfy the volume conservation, the correction velocity is computed after each time step and is used to restore the initial volume of the structure. Let $V_0$ be the initial volume of the structure. After a time step, the volume at the time $t$ ($V_t$) may be different from $V_0$. The correction velocity is assumed to be normal to the surface of the particles and is also assumed to be constant over all the computational domain. Considering this, $v_c$ is given by:

$$v_c = \frac{V_0 - V_t}{S \Delta t}$$  \hspace{1cm} (14)

where $S$ is the total area of the surface of the structure and $\Delta t$ is the time step. Finally, equation (14) is introduced into the convection equation (equation (6)) to recover the initial volume of the structure.

7 NUMERICAL RESULTS

All the developments have been implemented in the finite element library CimLib. CimLib is a highly parallel C++ library developed at Center for Material Forming (Mines ParisTech, CNRS UMR 7635) by the team of Professor Coupez [4]. As in [2], the simulations presented in this work have been performed by using a mesh adaptation strategy aiming to obtain accurate results while keeping a “reasonable” number of mesh elements. The mesh is refined over a narrow band around the surface of the particles, the detailed strategy is presented in [10]. The element size is computed as a function of the second derivative of a primal variable such as a filtered level-set function or the pressure field. This approach has successfully been applied within the sintering simulation context by Bruchon et al. in [1, 2].

The material properties used in the following simulations correspond to the properties of Alumina ($\text{Al}_2\text{O}_3$) and are summarized in Table 2.

<table>
<thead>
<tr>
<th>Constant</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_s \Omega \gamma sf \delta_s / kT$</td>
<td>$1 \cdot 10^{-7}$</td>
<td>m mol/s</td>
</tr>
<tr>
<td>$D_v \Omega (1 - f) / kT$</td>
<td>55.16</td>
<td>m mol/N s</td>
</tr>
<tr>
<td>$K$</td>
<td>260</td>
<td>GPa</td>
</tr>
<tr>
<td>$\mu$</td>
<td>156</td>
<td>GPa</td>
</tr>
<tr>
<td>$\eta$</td>
<td>1e-3</td>
<td>Pa/s</td>
</tr>
<tr>
<td>$\gamma sf$</td>
<td>0.9</td>
<td>N/m</td>
</tr>
<tr>
<td>$\Omega$</td>
<td>$8.55 \cdot 10^{-6}$</td>
<td>m$^3$/mol</td>
</tr>
</tbody>
</table>

Table 2: Material properties used.

7.1 Two particles sintering: surface and volume diffusions

The first step toward the simulation of sintering process at the particles scale consists in studying the growth of the neck formed between two particles during the early stages of sintering. There exists different models attempting to predict the evolution of the radius of the neck $X$ as a function of time. Those models\(^2\) are mainly based on some geometrical hypotheses of

\(^2\) Also called power laws.
the evolution of the neck and the particles. In general those geometrical models can be written as follows:

\[
\left( \frac{X(t)}{r} \right)^n = At
\]  

(15)

where \( r \) is the radius of the particles (supposed to remain constant) and \( A \) and \( n \) are parameter depending on the radius of the particles and the diffusion path being considered. Even if the validity of these models is restricted to necks radii smaller than 30\% of the radius of the particles, they represent a very useful tool concerning the validation of the kinetic obtained from more elaborated numerical approaches. For graphical purposes, equation (15) can be slightly modified by introducing the dimensionless time \( t^* \):

\[
\left( \frac{X(t)}{r} \right)^n = A' t^*
\]  

(16)

where \( A' \) is a constant and no longer depends on the radius of the particles.

Figure 5: Growth by surface diffusion of the dimensionless neck radius \( X/r \) over the dimensionless time \( t^* \) for different values of \( r \) [1].

Figure 5 presents the evolution of the dimensionless radius \( X/r \) as a function of \( t^* \) during sintering by surface diffusion for particle radii between 0.1 and 2.5. According to Exner et al. [5], the exponent \( n \) on equation (16) ranges between 3 and 7 for surface diffusion, which is in agreement with the simulations performed here. The dashed line showed in Figure 5 (referred to as “Simulation, 1/7”) corresponds to the best fitting curve obtained by least-squares and for comparison purposes, the line corresponding to \( n = 6 \) in equation (16) is also plotted (referred to as “1/6 law”).

The same kind of simulation has been performed for volume diffusion. Figure 6 shows the kinetics of the growth of the dimensionless neck \( X/r \) by volume diffusion as a function of the dimensionless time \( t^* \) for particle radii ranging from 0.1 to 0.4. For volume diffusion, the exponent \( n \) in equation (16) ranges between 4 and 5 [5]. This time the best fitting curve in Figure 6 corresponds to an exponent \( n \) equal to 5.6 (referred to as “n = 5.6”).

Equations (15) and (16) are obtained by making strong geometrical hypotheses [9, 8], for this reason it is hard assess a numerical approach with respect to these power laws, though
those laws are very useful to analyze the kinetics of a specific diffusion path in a qualitative way. Considering this, it is fairly safe to say that our approach is able to group the main mechanisms controlling both surface and volume diffusions, and is especially robust although pressure discontinuities are to be computed numerically and volume has to be conserved. Nevertheless, a better understanding of the volume diffusion requires a deeper study of this diffusion path and this study is yet to be done.

Surface and volume diffusions are coupled to simulate the sintering of two particles by these two diffusion mechanisms. Figure 7 shows the evolution of two particles as they sinter together by surface and volume diffusions. Figure 7a presents the initial state of the particles, they are set to be quasi-tangent. After 50 time steps, the neck between the particles is $\sim 30\%$ of the particle radius, as it is shown in Figure 7b. The power laws presented can be used for values of the neck radius $X < 0.3r$. It is interesting to see how the two particles evolve beyond this limit (Figure 7c), they can not be considered to remain spherical any longer.

Coupling between these two diffusion mechanisms is shown in Figure 8, and as expected, the neck grows significantly faster when surface and volume diffusion take place simultaneously.

7.2 Particle packing

A sintering simulation by volume diffusion over a more realistic particles packing is presented. A set of 154 particles with radii ranging from $0.0633 \, \mu m$ to $0.0797 \, \mu m$ is embedded into a computational domain given by a cube of side $1.2 \, \mu m$. In order to obtain accurate results,
the element size is refined near the surface of the particles [10]. Figure 9a. shows the initial particles packing as well as a cut of the refined mesh that is made up tp about 2 millions nodes and about 11 millions tetrahedral elements.

The evolution of the structure is showed in Figures 9a to 9d. In the initial geometry (Figure 9a) particles are set to be quasi-tangent. As the volume diffusion takes place, the necks between the particles grow up to a point (Figure 9d) where the particles can not be distinguished any more.

As neither the mass nor the density of the particles change during the sintering process, the volume of the particles must remain constant. Considering the simulation shown in Figure 9, the change of total volume of the particles after 200 time steps is about 0.12%, which is negligible. This simulation involves 200 time steps and has been performed in 100 h by using a parallel computing strategy on 24 cores.

8 CONCLUSIONS AND PERSPECTIVES

A numerical approach for the sintering simulation by surface and volume diffusion has been presented. The level-set Eulerian framework adopted allows to take into account all the topological changes that can appear during the sintering. The level-set method also provides very useful tools for the computation of the surface and volume diffusion, and at the same time it allows to handle 2D and 3D simulations with ease. The mesh adaptation strategy used allows to perform simulations while keeping a “reasonable” number of nodes and elements, and is specially useful when dealing with 3D simulations as the number of mesh element is dramatically increased compared with a 2D simulation.

The results concerning the sintering of two particles by surface and volume diffusion has been compared with analytical power laws. The comparison showed that both approaches (surface and volume diffusion) lead to a good simulation of the kinetics of each process. Furthermore, the results of the evolution of the neck between two particles by surface and volume
diffusions are in agreement with the predictions obtained from power laws. The simulation of sintering by coupled surface and volume diffusions has been presented. Even if the results of this coupling seem to be in agreement with the kinetics of the process, it is very difficult to validate the results as there is no experimental data available for these two routes. Finally the capabilities of the numerical approach has been demonstrated by performing a simulation of the sintering of more realistic 3D particle packing.

A large amount of work is yet to be done, mainly concerning the grain boundary diffusion. But the bases for the treatment of the diffusion path has been presented as the approach developed to solve the mechanics can also be used to take into account the surface tension at the grain boundary. The mechanical problem has been solved by considering the particles to respond as linear elastic isotropic materials, it would be very interesting to study how differently the structure would evolve if another material model would be considered or if the mechanical properties of each particle were different. The global goal of this work is to simulate the sintering process of fully 3D granular packing, which would open huge perspectives regarding the computational materials design.

REFERENCES


