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Computational homogenization of liquid-phase sintering with seamless transition from macroscopic compressibility to incompressibility ☆

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ABSTRACT

Liquid phase sintering of particle agglomerates is modeled on the mesoscale as the viscous deformation of particle–particle contact, whereby the single driving force is the surface tension on the particle/pore interface. On the macroscale, a quasistatic equilibrium problem allows for the prediction of the shrinkage of the sintering body. The present paper presents a novel FE^2 formulation of the two-scale sintering problem allowing for the transition to zero porosity, implying macroscale incompressibility. The seamless transition from compressibility to incompressibility on the macroscale is accomplished by introducing a mixed variational format. This has consequences also for the formulation of the mesoscale problem, that is complemented with an extra constraint equation regarding the prolongation of the volumetric part of the macroscopic rate-of-deformation. The numerical examples shows the sintering of a single representative volume element (RVE) which is sheared beyond the point where the porosity vanishes while subjected to zero macroscopic pressure.

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1. Introduction

Powder metallurgy is a versatile technology for the manufacturing of components to (near) net-shape with high product quality. For a hardmetal (such as WC-Co) cold compaction of the powder to a "green body" is followed by liquid-phase sintering from the subsequent heating. This means that the binder metal Co is heated to melt in order to obtain sufficient mobility via capillary action, i.e., via surface traction, stemming from stored surface energy. The resulting flow causes gradual filling of the pore space and brings about a macroscopic shrinkage of the particle compact until a completely dense state is obtained, at least ideally. To model and quantitatively simulate the sintering process is a challenging task. The goal is to (i) estimate the final resulting quality (i.e., in terms of porosity) and (ii) to predict the final net shape and size of the sintered component.

A wealth of literature has been devoted to the modeling and simulation of the sintering process. From a mesoscale viewpoint, a classical approach is to consider socalled "unit problems", whereby the constitutive modeling is based on diffusion and, most importantly, flow models. Among the early attempts to numerically simulate the surface-tension driven reshaping of contacting particles are those by Jagota and Dawson [1,2] and van de Vorst [3]. In a series of papers, [4,5] emphasize efficient finite element algorithms to trace the complex 3-dimensional flow of multi-particle interaction. The main challenges are the complex subscale geometry and the moving free boundary giving rise to very large deformations and severe topology changes. Recent developments of free-boundary tracing FE-strategies for large deformations (without severe topological changes) are discussed by Dettmer and Perić [6] and Saksono and Perić [7,8]. All the mentioned work consider surface tension effects in fluids. A recent extension to include surface tension in the context of solid modeling, where anisotropic surface energy may be present, is due to [9,10].

Attempts have also been made in the literature to use macroscopic models based on nonlinear viscoelasticity and viscoplasticity. In such models the densification process is driven by the "sintering stress", which is the macroscale manifestation of the stored surface energy. From a thermodynamical viewpoint, it is the dissipative stress that is conjugated to the current macroscale porosity, e.g., [11,12]. Among the literature on macroscale modeling, we mention [13–15].

Since computational homogenization has proven useful in a wide variety of applications, e.g., [16–20], it is natural to exploit this technique even for the present type of complex deformation process. In a previous paper, Öhman et al. [21], liquid phase sintering of particle agglomerates was modeled on the mesoscale as the viscous deformation of particle–particle contact. A FE^2-strategy was outlined; however, the variational setting was applicable only under the restriction of non-vanishing macroscopic porosity (corresponding to a not fully dense end-product). The present paper

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generalizes this situation such that it allows for the transition to zero porosity, which is accomplished by introducing a mixed variational format of the macroscale problem. We (still) assume that the particles are homogeneous and deform as a viscous fluid with sufficiently high viscosity to motivate the neglect of all acceleration terms. Moreover, the simplifying assumption is introduced that the flow properties are unaffected by temperature changes, i.e the sintering process is only modeled during the fully heated part of the process.

The paper is structured as follows: The various features of subscale modeling (surface tension, particle arrangements within the RVE, etc.) are briefly summarized in Section 2. This is followed in Section 3 which describes the transition to macroscale and RVE problems through computational homogenization. Numerical examples, based on a single RVE, are presented in Section 5. Conclusions and an outlook to future developments are given in the final section.

2. Subscale modeling

2.1. Preliminaries

We consider a sintering body with current macroscale configuration $\Omega(t)$ in space for any given time $t \geqslant 0$. The boundary of $\Omega(t)$ is denoted $\partial\Omega(t)$, and we adopt standard Dirichlet and Neumann boundary conditions on the (external) boundary parts $\partial\Omega_{\mathrm{D}}$ and $\partial\Omega_{\mathrm{N}}$, respectively. In particular, no prescribed tractions is considered, as is the case in free sintering. Our aim is to exploit the concept of computational homogenization in order to determine the unknown $\Omega(t)$ and certain mechanical fields on $\Omega(t)$, such as the current macroscale velocity field, $\bar{\boldsymbol{v}}$, the macroscale true stress field, $\bar{\boldsymbol{\sigma}}$, and the macroscale porosity field, $\bar{\phi}$ (which is the ratio of pore volume and bulk volume). We note that the initial configuration $\Omega(0)$ represents the so called "green body", obtained after cold compaction and characterized by the inhomogeneous (macroscopic) porosity $\bar{\phi}_0$. In the case of "free sintering", i.e., sintering without any external loading, it is clear that $\bar{\boldsymbol{\sigma}}$ represents the macroscopic residual stresses at every instant in time.

Subsequently, we shall adopt modeling on the subscale in terms of an Eulerian description of the motion, which means that it will be possible to trace the development of the current macroscale configuration $\Omega(t)$ by computing the macroscale velocity field $\bar{\boldsymbol{v}}(\bar{\boldsymbol{x}}, t)$ for $(\bar{\boldsymbol{x}}, t) \in \Omega \times (0, T)$.

In a 3D representation of the microstructure the assembly of sintering particles create an open pore system (at least initially). With reasonable accuracy one may then assume that the pore surfaces are "free" surfaces, i.e., the pore gas does not impose any resistance on the motion. The situation is, of course, different in the (physically unrealistic) case of a 2D representation of the microstructure. However, in this paper, gas flow and pore pressure from trapped gas is not taken into account. In any case the pertinent surfaces associated with surface tension are particle/pore and particle/particle (contact) surfaces, as indicated in Fig. 1.

2.2. Surface tension

The "surface tension" along particle/particle and particle/pore interfaces (the latter denoted pore boundaries) is considered to be the sole "driving force" of the sintering process, and it is defined in terms of a "surface tension force" acting in the tangent plane of the surface. In the simplest (and most common) case of isotropic surface tension, this traction is characterized by the constant surface-specific surface energy γ_{s} in the current configuration as the single material parameter. Although we adopt this simplified model below in the numerical results, it is possible to consider the more general situation of anisotropic "surface stress" that may also depend on the surface deformation via a suitable constitutive assumption, cf. [22].

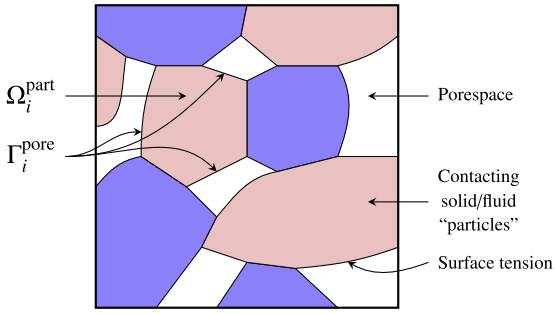

Fig. 1. Microstructure of porous particulate material with sintering particles in contact. The sintering body is subjected to Dirichlet and Neumann boundary conditions on the external boundary.

As shown in, e.g., Öhman et al. [21], it is possible to represent the surface tension force by an equivalent surface traction, henceforth denoted $\boldsymbol{t}_{\mathrm{s}}$, acting on the surface (or interface). In the presently assumed case of isotropic surface tension, $\boldsymbol{t}_{\mathrm{s}}$ is directed in the normal direction to the surface and is given as

$$\boldsymbol{t}_{\mathrm{s}} \stackrel{\mathrm{def}}{=} -\kappa\gamma_{\mathrm{s}}\boldsymbol{n}, \tag{1}$$

where $\kappa \stackrel{\mathrm{def}}{=} -\boldsymbol{n} \cdot \hat{\boldsymbol{\nabla}}$ is the curvature. Here, $\boldsymbol{n}$ is the taken positive outwards from a convex surface, whereas $\hat{\boldsymbol{\nabla}} \stackrel{\mathrm{def}}{=} \boldsymbol{\nabla} - [\boldsymbol{\nabla} \cdot \boldsymbol{n}]\boldsymbol{n}$ is the surface gradient operator.

2.3. Incompressible viscous flow of the Stokes' type

We shall adopt a model for the subscale deformation within the solid particles undergoing the time-dependent sintering process. The model is simplified in the sense that elastic deformation is neglected a priori. This is a common and reasonable simplification for free sintering since the plastic deformation is dominant. It is then possible to consider a viscoplastic (fluid-like) material with intrinsic incompressibility (within the particles). Such incompressibility is expressed as $\boldsymbol{v} \cdot \boldsymbol{\nabla} = 0$ and, hence, $\boldsymbol{d}_{\mathrm{dev}} = \boldsymbol{d} \stackrel{\mathrm{def}}{=} [\boldsymbol{v} \otimes \boldsymbol{\nabla}]^{\mathrm{sym}}$. An isotropic and associated viscoplastic flow rule of the classical Perzyna type is proposed as follows:

$$\boldsymbol{d}_{\mathrm{dev}} = \frac{1}{2\mu}\boldsymbol{\sigma}_{\mathrm{dev}} + \boldsymbol{d}^{\mathrm{p}}_{\mathrm{dev}}(\boldsymbol{\sigma}_{\mathrm{dev}}), \quad \boldsymbol{d}^{\mathrm{p}}_{\mathrm{dev}} = \frac{1}{t_*}\eta(\Phi(\sigma_{\mathrm{e}}))\frac{\mathrm{d}\Phi}{\mathrm{d}\boldsymbol{\sigma}}, \tag{2}$$

where t_* is the relaxation time, $\eta(\Phi)$ is an overstress function, $\Phi(\sigma_{\mathrm{e}})$ is the quasistatic yield function and $\sigma_{\mathrm{e}} = \sqrt{\frac{3}{2}|\boldsymbol{\sigma}_{\mathrm{dev}}|}$ is the equivalent stress. Upon introducing the abbreviated notation $k = \frac{\eta}{t_*}\frac{\mathrm{d}\Phi}{\mathrm{d}\sigma_{\mathrm{e}}}$, we may solve for σ_{e} in terms of the equivalent rate of deformation $d_{\mathrm{e}} \stackrel{\mathrm{def}}{=} \sqrt{\frac{2}{3}|\boldsymbol{d}_{\mathrm{dev}}|}$ from the equation

$$\frac{1}{3\mu}\sigma_{\mathrm{e}} + k(\sigma_{\mathrm{e}}) = d_{\mathrm{e}} \tag{3}$$

and we, finally, obtain the "Newtonian-like" constitutive relation

$$\boldsymbol{\sigma}_{\mathrm{dev}}(\boldsymbol{d}) = 2\tilde{\mu}\boldsymbol{d}_{\mathrm{dev}}, \quad \tilde{\mu} \stackrel{\mathrm{def}}{=} \frac{\sigma_{\mathrm{e}}}{3d_{\mathrm{e}}}. \tag{4}$$

The corresponding tangent stiffness $\mathbf{E}_{\mathrm{T,dev}}$ in the relation $\mathrm{d}\boldsymbol{\sigma}_{\mathrm{dev}} = \mathbf{E}_{\mathrm{T,dev}} : \mathrm{d}\boldsymbol{d}$ (representing the linearization of the subscale constitutive problem), is given as follows:

$$\mathbf{E}_{\mathrm{T,dev}} = 2\tilde{\mu}\mathbf{I}_{\mathrm{dev}} + \frac{4}{9d_{\mathrm{e}}^2}\left[d_{\mathrm{e}}\left[\frac{1}{3\mu} + k'\right]^{-1} - \sigma_{\mathrm{e}}\right]\boldsymbol{d}_{\mathrm{dev}} \otimes \boldsymbol{d}_{\mathrm{dev}} \tag{5}$$

with

$$k' = \frac{1}{t_*}\left[\eta\frac{\mathrm{d}^2\Phi}{\mathrm{d}\sigma_{\mathrm{e}}^2} + \frac{\mathrm{d}\eta}{\mathrm{d}\Phi}\left[\frac{\mathrm{d}\Phi}{\mathrm{d}\sigma_{\mathrm{e}}}\right]^2\right]. \tag{6}$$

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