MODELLING OF POWDER SINTERING AT VARIOUS SCALES

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1. Introduction

Sintering is a technique of powder metallurgy consisting in consolidation of loose or loosely bonded ceramic or metal powders at elevated temperature with or without pressure. During sintering particulate material is converted into compact solid material. At sintering, processes at different levels interact with one another, therefore in numerical modelling we should consider physical phenomena occurring at various scales.

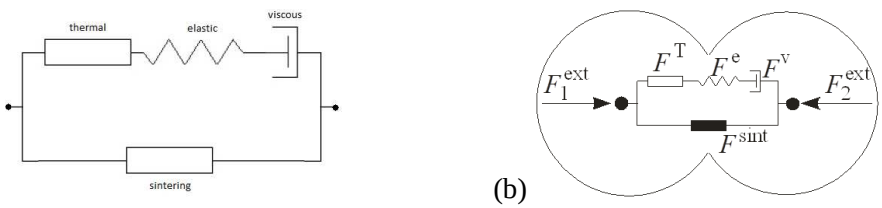
In this work, development of numerical models allowing us to analyse sintering at various scales will be presented. Theoretical formulations and numerical models for three scales relevant for sintering: atomistic, microscopic and macroscopic one will be presented. Modelling at lower scales will provide parametric information to the upper scale while the upper scale models provide boundary conditions for lower scale analysis. The numerical model will be validated using the results of own experimental studies sintering of NiAl powder.

2. Sintering phenomena at different scales

At the macroscopic level during sintering, one can observe change of mechanical properties, change of geometry (volume) leading to change of bulk density. The macroscopic changes are the result of phenomena occurring at the microscopic level. Under microscope, it can be seen that sintering is initiated by forming of cohesive bonds between particles in the form of necks. When the sintering process is continued, the necks between particles grow. The main driving force of sintering is reduction of the total surface energy of the system. As a result of the stresses in the neck and the surface tension the particles are attracted to each other, which leads to the shrinkage of the system (macroscopic effect of sintering), grain rearrangement, and gradual reduction and elimination of porosity. Microscopic phenomena are the result of processes of diffusion occurring at atomistic level. Grow of connections between particles during sintering is caused by mass transport. Surface and grain boundary diffusion are dominant mechanisms of mass transport in a sintering.

3. Formulation of sintering models

The macroscopic model employed for sintering is based on the formulation proposed in [1]. It has been derived from the continuum formulation of the problem. In the continuum approach, the porous powder under compaction is treated as a continuous medium at the macro-scale. The rheological schematic of the model is shown in Fig. 1a. The model incorporates mechanisms of thermal and elastic deformation and viscous creep flow. The creep strain rate $\dot{\varepsilon}^v$ is given by the following realtionship:



(a) (b)

Figure 1. Rheological schematics of the macroscopic (a) and microscopic (b) models of sintering

$$\dot{\varepsilon}^v = \frac{\boldsymbol{\sigma}'}{2\eta_s} + \frac{\mathrm{tr}(\boldsymbol{\sigma}) - 3\sigma_s}{9\eta_b}\mathbf{I} \tag{1}$$

where $\boldsymbol{\sigma}'$ is the deviatoric stress, $\mathrm{tr}(\boldsymbol{\sigma})$ – the trace of the stress tensor, σ_s – the sintering stress, η_s – the shear viscosity modulus η_s – the bulk viscosity modulus.

In the multiscale approach, macroscopic constitutive properties, including the elastic moduli, bulk and shear viscosity, as well as the sintering driving stress are determined from micromechanical simulations of sintering. The micromechanical model of sintering has been developed within a framework of the discrete element method [2]. The DEM considers large assemblies of particles which interact with one another through contact forces. The rheological scheme of the contact model for sintering is shown in Fig. 1b. It includes elasticity, thermal expansion, viscosity (creep) and the sintering driving force, which is consistent with the macroscopic model.

The constitutive parameters of the DEM model of sintering depend on the parameters which can be determined using atomistic models. The methods of molecular statics and dynamics will be used to determine the elastic constants, surface energy and diffusion coefficients used as input data in microscopic sintering models.

4. Case study

Sintering of NiAl powder has been analysed as a case study using the multscale approach. Figure 2 shows selected mechanisms of diffusion considered in the molecular statics analysis. Average shear viscous modulus determined from the DEM simulations is plotted in Fig. 3 as functions of sintering time and relative density.

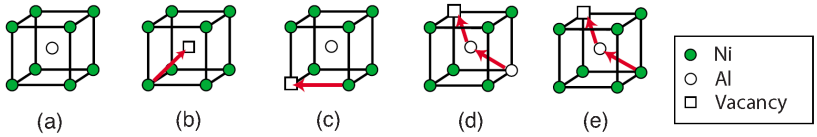


Figure 2. Schematic representation of NiAl crystal structure and selected hop mechanisms [3]

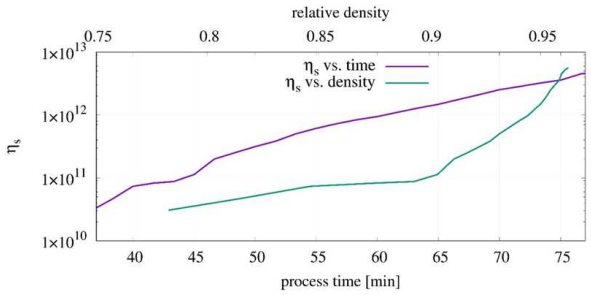


Figure 3. Average shear viscous modulus determined from the DEM simulations

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5. References

[1] R. Zhang (2005). *Numerical Simulation of Solid-State Sintering of Metal Powder Compact Dominated by Grain Boundary Diffusion*, PhD Thesis, The Pennsylvania State University.

[2] S. Nosewicz, J. Rojek, K. Pietrzak, and M. Chmielewski (2013). Viscoelastic discrete element model of powder sintering, *Powder Technology*, **246**, 157–168.

[3] Q. Xu and A. Van der Ven (2010). Atomic transport in ordered compounds mediated by local disorder: Diffusion in B2-Ni_xAl_{1-x}, *Physical Review B, Condensed matter*, **81**, 064303.