Book of Abstracts of the XXIV International Conference on Computer Methods in Materials Technology KomPlasTech 2017

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Modelling of sintering at atomistic, microscopic and macroscopic 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 phenomena at atomistic, microscopic and macroscopic 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 various scales

At the macroscopic level during sintering, one can observe changes of mechanical properties and geometry (shrinkage) 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 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 Figure 1a. The model incorporates mechanisms of thermal and elastic deformation and viscous creep flow. The creep strain rate $\dot{\boldsymbol{\varepsilon}}^{v}$ is given by the following realtionship:

$$\dot{\varepsilon}^{v} = \frac{\mathrm{dev}(\boldsymbol{\sigma})}{2\eta_S} + \frac{\mathrm{tr}(\boldsymbol{\sigma}) - \sigma^{sint}}{3\eta_v} \tag{1}$$

where $\boldsymbol{\sigma}$ is the total stres, σ^{sint} – the sintering stress, η_s – the shear viscosity modulus, η_v – 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 Figure 1b. It includes elasticity, thermal expansion, viscosity (creep) and the sintering driving force, which is consistent with the macroscopic model. The bulk and shear viscous moduli can be determined from the following formula:

$$\eta_S = \frac{\|\mathrm{dev}(\sigma)\|}{2\|\mathrm{dev}(\dot{\varepsilon}^{v})\|}; \qquad \eta_v = \frac{\mathrm{tr}(\sigma) - \sigma^{sint}}{\mathrm{tr}(\dot{\varepsilon}^{v})} \tag{2}$$

where the symbol $\|.\|$ denotes the norm of a second order tensor, and the stress and strain rates are obtained by averaging procedure applied to the discrete element results. The constitutive parameters of the DEM model of sintering, in turn, 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.

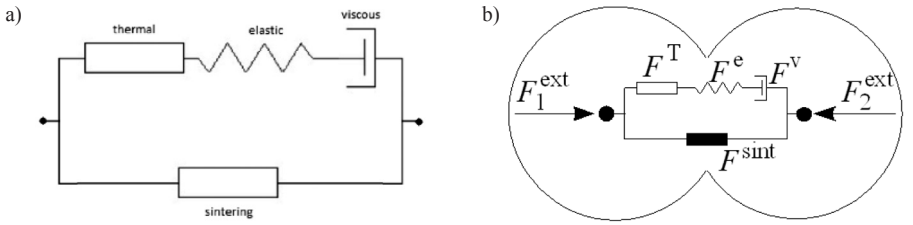

Figure 1. Rheological schematics of the macroscopic (a) and microscopic (b) models of sintering.

4. Numerical results

Sintering of NiAl powder has been analysed as a case study using the multiscale approach. At the atomistic level grain boundary diffusion as the main mass transport mechanism in sintering has been investigated using the molecular dynamics (MD) models representing bicrystals of NiAl with different crystal orientations as that shown in Figure 2. MD simulations have been performed using the LAMMPS program. The embedded-atom method potential EAM2009 [3] has been used in the atomistic model. Grain boundary diffusivity for different bicrystals is shown in the form of the Arrhenius plot in Figure 3.

Diffusivity parameters estimated by molecular dynamics simulations have been used in the discrete element simulation of sintering as initial data. Figure 4 shows the numerical density evolution curve in comparison with experimental data. It can be seen that the numerical simulation with initial diffusivity parameters has predicted a slower densification. The final values of micromechanical parameters have been established by fitting the numerical evolution of the relative density with the experimental results.

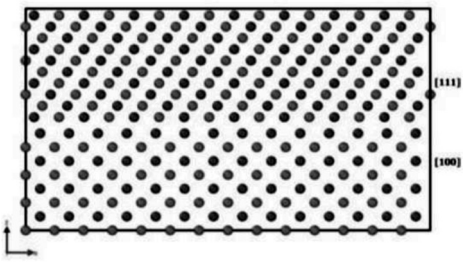

Figure 2. Atomistic model for grain boundary diffusion calculation.

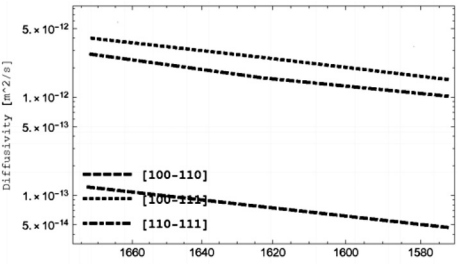

Figure 3. Diffusivity Arrhenius plot.

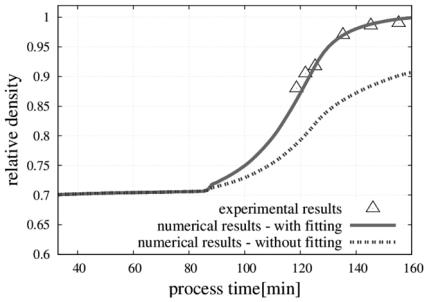

Figure 4. Evolution of the relative density during the process.

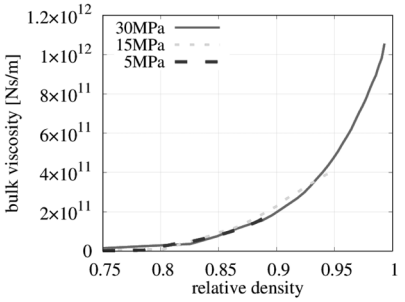

Figure 5. Bulk viscous modulus as a function of the relative density.

The DEM results obtained with diffusivity parameters determined as described above have been used to calculate macroscopic viscous moduli of the sintered material. The bulk viscous moduli obtained for different pressure levels have been plotted as functions of the relative density in Figure 5. It can be easily noticed that the curves corresponding to different pressures coincide very well. This confirms correctness of our simulations, since the micromechanical model does not assume any pressure dependence of the constitutive parameters and this is reflected in the macroscopic constitutive properties. It can be seen from Figure 5 that the numerical calculations predict an increase of the viscous moduli with increasing density. This increase, especially in case of the volumetric viscous modulus, becomes faster when the relative density tends to unity.

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