# TWO-SCALE MODELLING OF POWDER SINTERING

S. Nosewicz[1], J. Rojek [1], G. Maciejewski[2], M. Maździarz [1], and M. Chmielewski[3]

[1]*Institute of Fundamental Technological Research, Polish Academy of Sciences, Pawinskiego 5B, 02-106 Warsaw, PL*
[2]*Institute of Aviation, Al. Krakowska 110/114, 02-256 Warsaw, PL*
[3]*Institute of Electronic Materials Technology, Wólczyńska 133, 01-919 Warsaw, PL*

*e-mail: snosew@ippt.pan.pl*

## 1. Introduction

Sintering is a manufacturing process in which loose or weakly bonded metal or ceramic powders are consolidated into a solid compact body by heat treatment which can be combined with mechanical pressure. Macroscopically during sintering, one can observe changes of the bulk material volume (shrinkage) and, associated with this, densification and decrease of porosity. The macroscopic phenomena result from processes undergoing at the microscopic level. The microstructure during sintering undergoes an evolution characterized by grain rearrangement and increase of grain compaction. In the initial stage, cohesive bonds (necks) are formed between powder particles. When the sintering process is continued the necks between particle grow due to mass transport. Surface and grain boundary diffusion are normally dominant mechanisms of mass transport in sintering.

This paper will present a two-scale framework for numerical modelling of sintering phenomena. The proposed approach bridges simulations performed at the atomistic and microscopic scales. The two-scale model has been validated using the results of own experimental studies of pressure-sintering of NiAl powder.

## 2. Atomistic modelling

The atomistic modelling has been carried out using the molecular dynamics (MD). The methodology to estimate parameters of a microscopic sintering model by MD simulations has been developed in [1]. The parameters include temperature dependent diffusion parameters, surface energy and linear thermal expansion. These parameters define material behavior during sintering and are used in the microscopic model of sintering.

## 3. Microscopic model of sintering

The authors' own original viscoelastic model [2] developed within the framework of the discrete element model have been used for simulation of the powder sintering process at the microscopic level. The discrete element models consider the powder as a collection of spherical particles (discrete elements) interacting with one another by contact forces. The two-particle model of sintering is derived considering diffusion as the main mechanism of sintering.

$$F_{\mathrm{n}} = \frac{\pi a^4}{8 D_{\mathrm{eff}}} v_{\mathrm{rn}} + \pi \gamma_S \left[ 4r \left( 1 - \cos \frac{\Psi}{2} \right) + a \sin \frac{\Psi}{2} \right] \tag{1}$$

where $F_{\mathrm{n}}$ is the normal force between two particles, $v_{\mathrm{rn}}$ – the normal relative velocity, $r$ – the particle radius, $a$ – the radius of the interparticle boundary, $\Psi$ – the dihedral angle, $\gamma_{\mathrm{S}}$ – the surface energy.

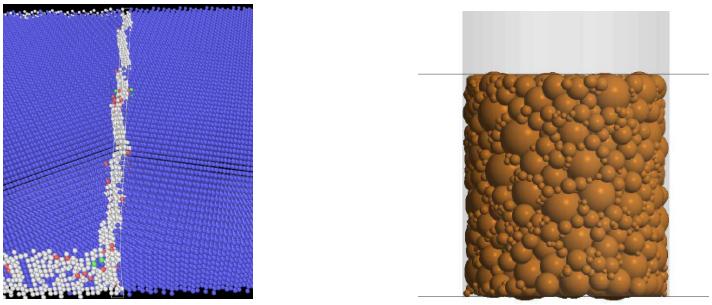
The value of diffusion parameter directly depends on certain diffusion mechanism, which is considered at the constitutive model of sintering. Assuming that the grain boundary diffusion is a dominant mechanism in the neck growth and shrinkage of the system the effective grain boundary diffusion coefficient $D_{\mathrm{eff}}$ is given by the following formula:

$$D_{\mathrm{eff}} = \frac{D_{\mathrm{gb}} \delta \Omega}{\mathrm{k_B T}} \tag{2}$$

where $D_{\mathrm{gb}}$ is the grain boundary diffusion coefficient with the width $\delta$, $\Omega$ is the atomic volume, $\mathrm{k_B}$ is the Boltzmann constant and $T$ is the temperature.

## 4. Numerical results

Pressure assisted sintering of an intermetallic NiAl powder has been simulated using the methodology described above. First, the molecular dynamics simulations have been carried out to derive sintering parameters from an atomic scale level. The simulations have been performed with LAMMPS program [3] using the embedded-atom method (EAM) potential developed for Ni-Al system [4]. The MD model for grain boundary diffusion simulation is shown in Figure 1a. The GB diffusion coefficient $D_{\mathrm{gb}}$ has been extracted from the Einstein relation $\langle x^2 \rangle = 2D_{\mathrm{gb}}t$, where $\langle x^2 \rangle$ is a mean-squared displacements of atoms within the GB core region.



a) b)

Figure 1: Numerical models: a) MD model for grain boundary diffusion simulation, b) DEM model of powder sintering process

The parameters estimated in the MD simulations have been used in the microscopic DEM model of sintering. The DEM model of sintering is presented in Figure 1b. The evolution of the relative density obtained numerically has been compared with the experimental data. in Figure 2. A good agreement can be observed, which demonstrates a good performance of the presented two-scale model of powder sintering.

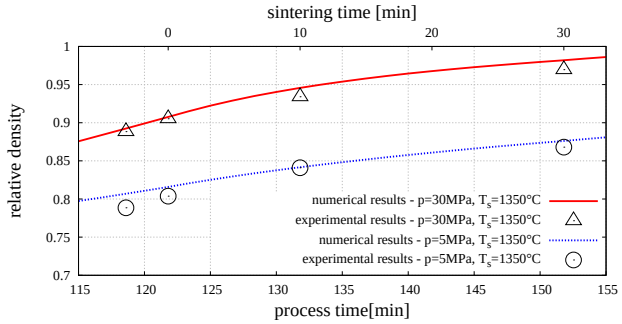



Figure 2: Comparison of experimental and numerical results – density evolution during sintering.

**Acknowledgments** This work has been financed from the funds of Polish National Science Centre (NCN) awarded by the decision number DEC-2013/11/B/ST8/03287.

### References

[1] M. Maździarz, J. Rojek, and S. Nosewicz. Estimation of micromechanical NiAl sintering model parameters from the molecular simulations. *International Journal for Multiscale Computational Engineering*, 15:343–358, 2017.

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

[3] S. Plimpton. Fast parallel algorithms for short-range molecular dynamics. *J. Comp. Physics*, 117:1–19, 1995.

[4] G.P. Purja Pun and Y. Mishin. Development of an interatomic potential for the Ni-Al system. *Philosophical Magazine*, 89:3245–3267, 2009.