A constitutive model and numerical simulation of sintering processes at macroscopic level

Krzysztof Wawrzyk, Piotr Kowalczyk, Szymon Nosewicz, and Jerzy Rojek

Citation: AIP Conference Proceedings **1922**, 030011 (2018);
View online: https://doi.org/10.1063/1.5019045
View Table of Contents: http://aip.scitation.org/toc/apc/1922/1
Published by the American Institute of Physics

A Constitutive Model and Numerical Simulation of Sintering Processes at Macroscopic Level

Krzysztof Wawrzyk[1,a)], Piotr Kowalczyk[1,b)], Szymon Nosewicz[1,c)] and Jerzy Rojek[1,d)]

[1]*Institute of Fundamental Technological Research, Polish Academy of Sciences, Pawińskiego 5B, 02-106 Warsaw, Poland.*

[a)]Corresponding author: kwawrzyk@ippt.pan.pl
[b)]pkowalcz@ippt.pan.pl
[c)]snosew@ippt.pan.pl
[d)]jrojek@ippt.pan.pl

Abstract. This paper presents modelling of both single and double-phase powder sintering processes at the macroscopic level. In particular, its constitutive formulation, numerical implementation and numerical tests are described. The macroscopic constitutive model is based on the assumption that the sintered material is a continuous medium. The parameters of the constitutive model for material under sintering are determined by simulation of sintering at the microscopic level using a micro-scale model. Numerical tests were carried out for a cylindrical specimen under hydrostatic and uniaxial pressure. Results of macroscopic analysis are compared against the microscopic model results. Moreover, numerical simulations are validated by comparison with experimental results. The simulations and preparation of the model are carried out by Abaqus FEA - a software for finite element analysis and computer-aided engineering. A mechanical model is defined by the user procedure "Vumat" which is developed by the first author in Fortran programming language. Modelling presented in the paper can be used to optimize and to better understand the process.

INTRODUCTION

Sintering is a widely used technique of powder metallurgy processes consisting in consolidation of loose or loosely bonded ceramic or metal powders at elevated temperature with or without pressure assistance. During sintering, particulated material is converted into a polycrystal. The process takes place close to the melting point: below melting temperature (sintering with solid phase) or above this temperature (sintering with the presence of liquid phase). In this work we deal with sintering in solid phase only. Sintering is a complex process affected by many factors and there are different ways of classification of sintering models. We can distinguish three main approaches, depending on the scale: atomistic models, micromechanical models and continuum models. Different sintering models are reviewed in [1, 2, 3]. In the continuum macroscopic approach, the porous powder under compaction is treated as continuous medium at the macro-scale. Its deformation behaviour is described by constitutive equations based on a modified plasticity theory of solids. The constitutive model for densification of metal powder compacts under high temperature generally incorporates the mechanisms of power-law creep, diffusional creep, and grain growth. Continuum models of sintering can be classified into two types: continuum phenomenological models reviewed by Olevsky [4], and continuum micromechanics-based models, which were developed in the several papers, such a Scherer [5].

Continuum models do not take into consideration the microstructure of the material. Microstructural changes during sintering are taken into account in micromechanical models. A number of micromechanical models of sintering are based on a particle representation of porous powder material undergoing the sintering process. In particle models, the interaction of particles and the local problems of particle necks are considered [6, 7, 8, 9].

Recently, there is a great potential to perform the simulation of sintering in the atomic-scale. Molecular dynamics (MD) is a method providing a detailed picture of the evolution of atomic positions and velocities as a function of time. The atomic interactions are characterised by the inter-atomic potentials, hence the chemical composition of the material is explicit in the model. Such simulations have been performed by a number of authors, e.g. [10, 11].

Computer Methods in Mechanics (CMM2017)
AIP Conf. Proc. 1922, 030011-1–030011-7; https://doi.org/10.1063/1.5019045
Published by AIP Publishing. 978-0-7354-1614-7/$30.00

Since phenomena at various scales can influence each other, it is possible to model sintering using multiscale modelling, where models can interact with each other. This means that the results of atomistic model can be used as an input data in a micromechanical model [12, 13] and then results from the micromechanical model can be used in a continuum model [13, 14]. Such a multiscale approach is investigated in the MUSINT project, realized at the Institute of Fundamental Technological Research, Warsaw, Poland. The overall objective of the MUSINT (Multiscale numerical modelling of sintering processes) is development of numerical models allowing to analyse at various scales manufacturing processes employing sintering as the main technological stage.

PROBLEM FORMULATION

Microscopic Model

A microscopic model of sintering based on a new generalized viscoelastic model of sintering proposed by Nosewicz et al. [15] [9] is developed within the framework of the discrete element method. The model is schematically depicted in Fig.1. Thermo-viscoelastic model of sintering is introduced as an author's original extension of viscous model. The rheological model of sintering presented in Fig. 1 is enriched by adding elastic and thermal component to the standard viscous model [6, 7, 8].

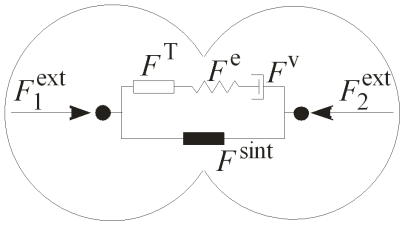

FIGURE 1. Rheological scheme of thermo-viscoelastic model [15]

An addition of elastic part will allow to better redistribute forces in particle assembly with large changes of configuration during sintering. In view of an analogy of a sintered material with a fluid, whose viscoelastic properties are commonly modelled with the viscoelastic Maxwell model, the viscous component is introduced in a series with the elastic element. Furthermore, the rheological model includes the thermal component that allows to include thermal expansion or thermal stresses occurring during temperature evolution.

By analysis of mass transport and stresses at the grain boundary between two sintered particles the following equation for the particle interaction during sintering is obtained [9]:

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

where F_n is the normal force between two particles, v_{rn} – the normal relative velocity, r – the particle radius, a – the radius of the interparticle boundary, Ψ– the dihedral angle, γ_s – the surface energy. The geometrical parameters of the model are defined in Fig. 2 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_{eff} is given by the following formula:

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

where D_{gb} is the grain boundary diffusion coefficient with the width δ, Ω is the atomic volume, k_B is the Boltzmann constant and T is the temperature. The model takes into account the thermal expansion – the particle radius r is calculated as follows:

$$r = r_0 \left(1 + \alpha \left(T - T_0\right)\right) \tag{3}$$

where T_0 is the reference temperature (room temperature), r_0 is the particle radius at the reference temperature and α is the linear thermal expansion coefficient. The rate of radius change due to thermal expansion is taken into account in calculation of the normal relative velocity v_{rn}.

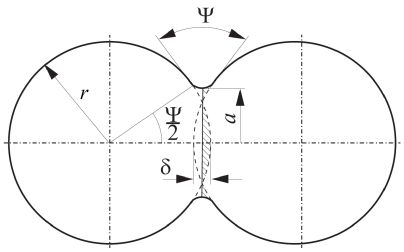

FIGURE 2. Definition of rheological parameters [15]

Macroscopic Model

At the macro scale sintered material is treated as continuous medium. Its constitutive model is tightly related to observations made at the micro scale (single grain level) and fully consistent with microscopic mechanical model described in the above section. The macroscopic model is derived with the use of methodology known from works of e.g. Zhang [16]. The total strain rate is a sum of three parts: thermal, elastic and viscous, as follows:

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^{th} + \dot{\boldsymbol{\varepsilon}}^{e} + \dot{\boldsymbol{\varepsilon}}^{visc} \tag{4}$$

Thus, the constitutive equation has the form:

$$\dot{\boldsymbol{\sigma}} = \mathbf{D}\left(\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}^{th} - \dot{\boldsymbol{\varepsilon}}^{visc}\right) + \dot{\boldsymbol{\sigma}}^{s} \tag{5}$$

where:

- thermal strain

$$\boldsymbol{\varepsilon}^{th} = \alpha T \mathbf{I} \tag{6}$$

- viscous strain rate

$$\dot{\boldsymbol{\varepsilon}}^{visc} = \frac{\boldsymbol{\sigma}'}{2\eta_s} + \frac{tr(\boldsymbol{\sigma}) - 3\sigma_s}{9\eta_b}\mathbf{I} \tag{7}$$

- sintering stress

$$\boldsymbol{\sigma}^{s} = \sigma_s \mathbf{I} \tag{8}$$

$$\sigma_s = \frac{\beta \gamma_s \rho^2}{r_0} \tag{9}$$

where:

$$\rho = \hat{\rho} e^{-(\varepsilon_x + \varepsilon_y + \varepsilon_z)} \tag{10}$$

All parameters in the above equations — viscosity η_s, η_b, initial relative density $\hat{\rho}$, surface energy γ_s etc. — are related to microscopic material properties. For spherical shape of powder particles β is equal 3, η_s and η_b are viscous shear and bulk moduli respectively and these factors are functions of porosity and temperature. These relations are subject to investigation in our research.

In order to simulate powder metallurgy process of two-phase powder it is required to perform some modifications of the material model parameters. The model of sintering of the two-phase powder NiAl-Al_2O_3 is based on mixture theory which is used to predict behaviour of multiphase systems and the basic assumption is that, at any instant of time, all phases are present at every material point. In general, for some material properties it provides a theoretical upper- and lower-bound on properties - Voigt and Reuss model respectively. Formulas for parameter W by Voigt and Reuss model is presented in the Equations (11) and (12) respectively:

$$W = V_1 W_1 + V_2 W_2 \tag{11}$$

$$W = \left(\frac{V_1}{W_1} + \frac{V_2}{W_2}\right)^{-1} \tag{12}$$

where: V_i and W_i are the volume fraction and material property of i-th constituent respectively. In this work theoretical upper- and lower-bound were used to predict surface energy γ_s and shear or bulk viscosity η_s and η_b. In Fig. 3 and 4, the last two parameters as functions of relative density $\hat{\rho}$ are presented for particular components and for the composite (80%NiAl, 20%Al_2O_3) according to Eqs. (11)-(12).

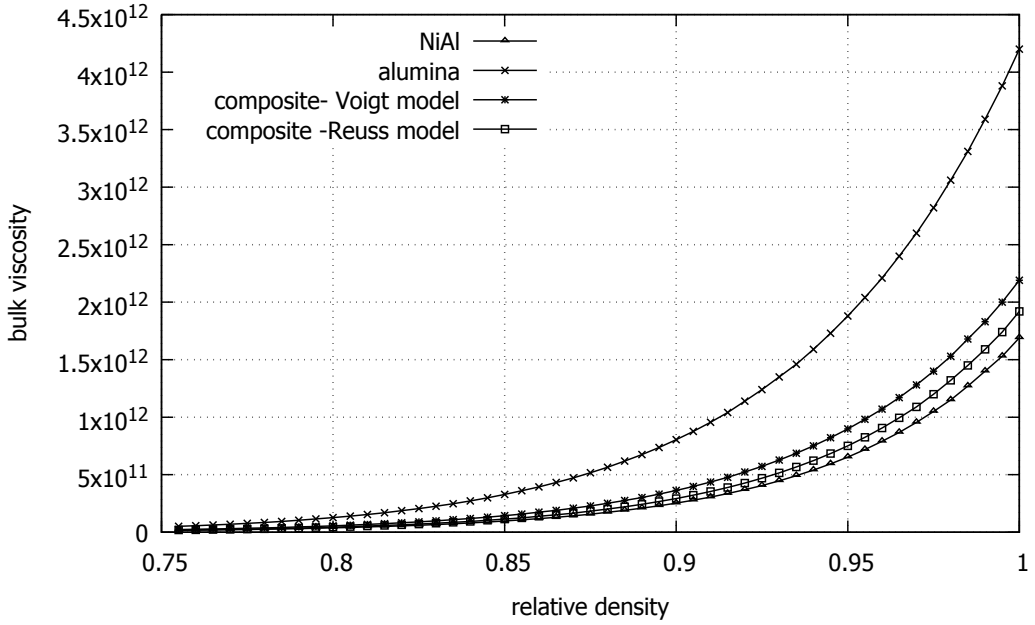

FIGURE 3. Bulk viscosity evolution

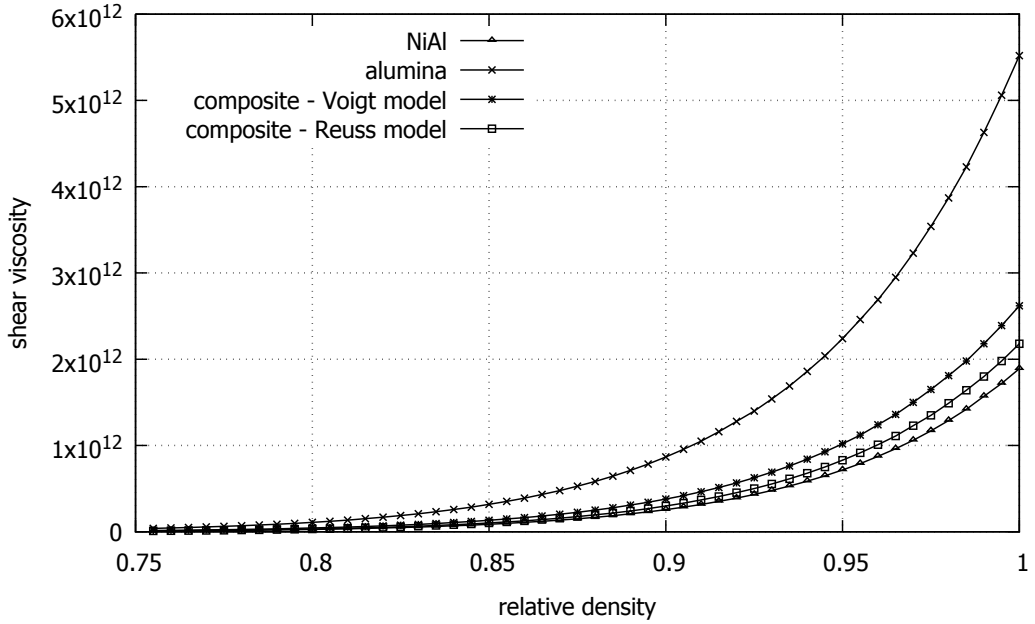

FIGURE 4. Shear viscosity evolution

NUMERICAL SIMULATIONS

In order to verify the model and its numerical implementation, numerical analysis of sintering of one and two-phase powder were performed. Example of the Finite Element Method (FEM) model is shown in Fig. 5. To reduce the number of elements we have dealt with a quater of cylindrical shape with diameter $d = 0.013$ m and total height

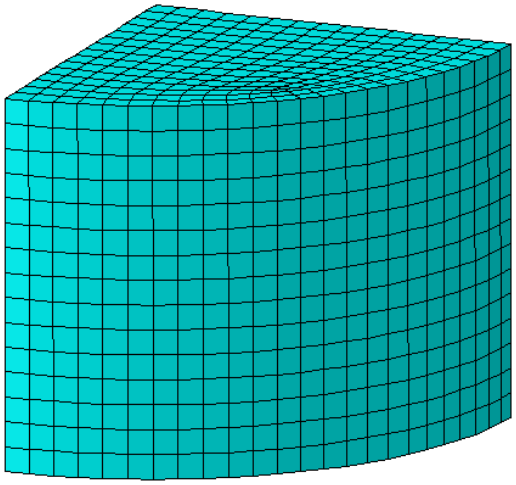

FIGURE 5. Finite element method model

$h = 0.028$. The sample was subject to uniaxial compression p at sintering temperature $T_{sint} = 1400°C$.

TABLE 1. Input data

	E[GPa]	ν	β	γ_s[J/m^2]	r_0[m]	ρ[kg/m^3]
NiAl	183	0.34	3	1.5	3.97e-6	5910
alumina	404	0.232	3	1.28	2.48e-6	3970
composite	219	0.286	3	1.46	3.01e-6	5520

The input data are presented in the Table 1. The values of elastic constants, Young's modulus and Poisson's ratio and also densities, has been taken from [17], which considered the experimental investigation of NiAl and NiAl-based composite. Mean value of particle size has been taken from [15], and surface energy has been calculated on the basis of mixture theory. The both viscous parameters - bulk and shear viscosity - are taken from micromechanical model.

In this model the following displacement boundary conditions were assumed: radial displacements on the lateral wall and all displacements at the bottom are zero. As a result shrinkage of the element and changes of relative density were obtained. Evolution of relative density for NiAl sintering process is presented in Fig. 6, which presents comparison of the FEM simulation against the results of the Discrete Element Method analysis with the microscopic model implemented. In this figure one can see the results for various pressure loads: 5, 15 and 30 MPa. The dashed lines represent results of macroscopic model, and the normal lines are results of microscopic model. Different colors correspond to different values of pressure p. Good agreement between the two model results is observed for all pressure levels.

Next, the two-phase powder ($80\%\mathrm{NiAl}, 20\%\mathrm{Al_2O_3}$) sintering tests were performed. In Fig. 7 one can see comparison of three models: two macromechanical models (one using parameters from the Voigt model, and the second model for parameters from the Reuss model) against the micromechanical model. One can see good agreement of these three models.

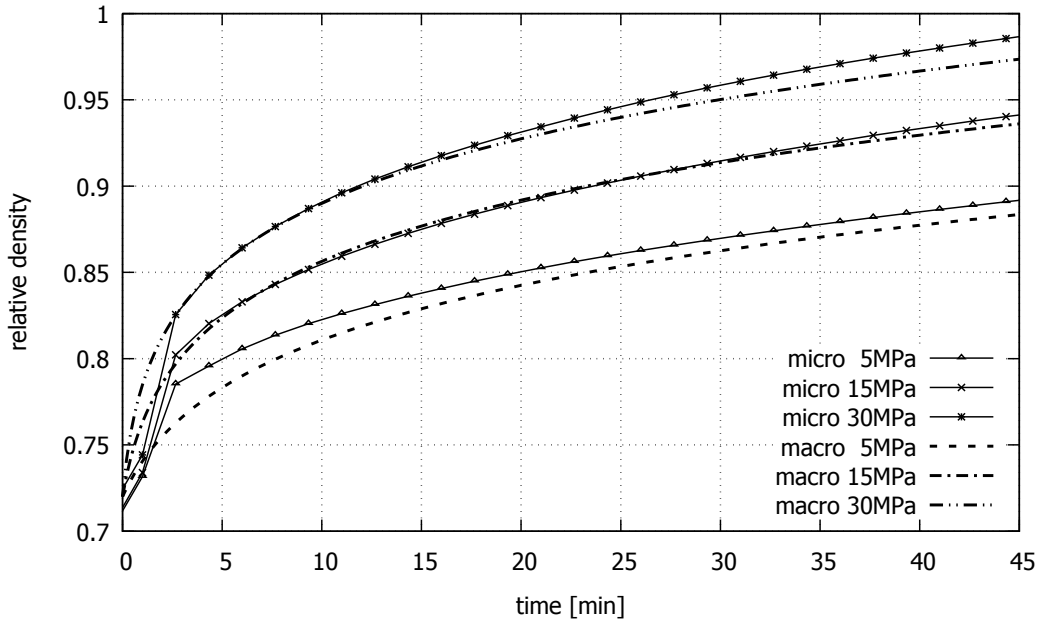

FIGURE 6. Relative density evolution in time at the uniaxial compression of NiAl sample - comparison with numerical results of micromechanical model analysis

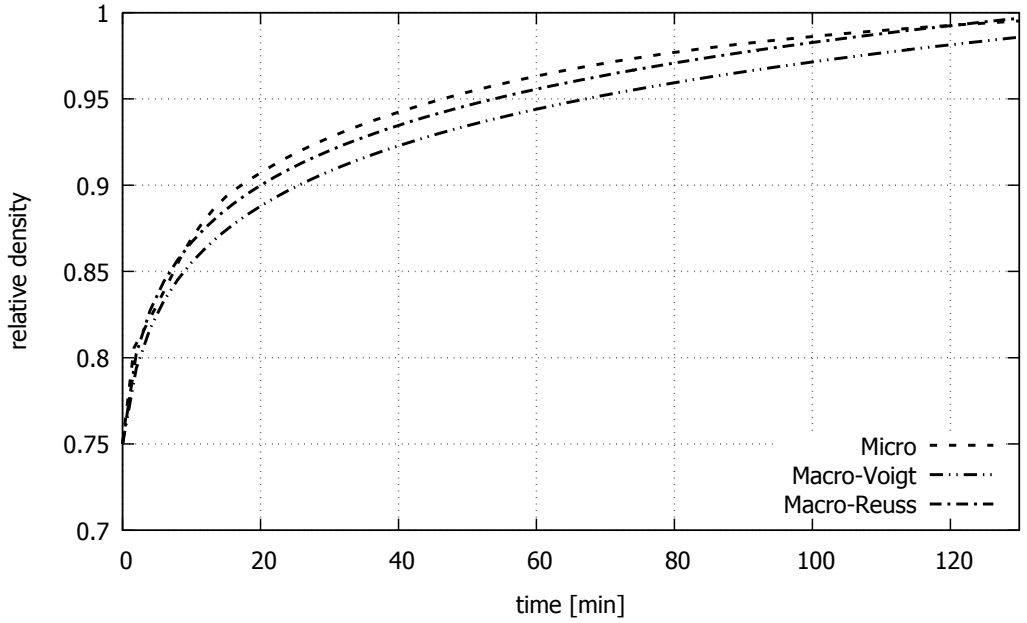

FIGURE 7. Relative density evolution in time at the uniaxial compression of composite sample - comparison with numerical results of micromechanical model analysis

Conclusions

The formulation of macroscopic model of sintering has been developed based on material data obtained in numerical micro scale simulations within the discrete element method. The formulation concerns one- and two-phase powders

and in the second case, in order to obtain certain material parameters either experimental data or mixture theory were used. For both (one- and two-phase) powders finite element implementation has been performed with the use of an authors's own material procedure. The model formulation and numerical tests presented in the paper are just preliminary, however good qualitative and quantitative agreement of the results with those obtained with the microscopic model indicates that the presented macroscopic model may be suitable for macroscopic simulations of sintering processes.

In further research, possibilities of more precise formulation of macroscopic properties of two-phase sintered composite are going to be investigated as, at the present stage, only approximate results based on upper and lower bounds formulae are available. Besides, the model will be extended to simulate all other stages of powder metallurgy, in particular to take into account heating and cooling stage, with corresponding thermal strain and stress considered. Our final objective is to obtain macroscopic model of entire (industrial) sintering process.

ACKNOWLEDGMENTS

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

REFERENCES

[1] J. Missiaen, Rev. Met. Paris **12**, 1009 – 1019 (2002).
[2] H. Exner and T. Kraft, In Powder Metallurgy World Congress 1998 **2**, 278–283 (1998).
[3] J. Pan, International Materials Reviews **2(17)**, 69–85 (2003).
[4] E. Olevsky, Mater Sci Eng R **23**, 41–100 (1998).
[5] G. Scherer, J. NonCrystalline Solids **34**, 239–256 (1979).
[6] F. Parhami and R. McMeeking, Mechanics of Materials **27**, 111–124 (1998).
[7] C. Martin, L. Schneider, L. Olmos and D. Bouvard, Scripta Materialia **55**, 425—-428 (2006).
[8] A. Wonisch, O. Guillon, T. Kraft, M. Moseler, H. Riedel and J. Rode, Acta Materialia **55**, 5187–5199 (2007).
[9] S. Nosewicz, J. Rojek, K. Pietrzak, and M. Chmielewski, Powder Technology **246**, 157–168 (2013).
[10] M. Zachariah and M. Carrier, Journal of Aerosol Science **30**, 1139–1151 (1999).
[11] H. Zhu and R. Averback, Materials Science and Engineering A **A204(1-2)**, 96–100 (1995).
[12] M. Maździarz, J. Rojek and S. Nosewicz, International Journal for Multiscale Computational Engineering **15(4)**, 343–358 (2017).
[13] J. Rojek, S. Nosewicz, M. Maździarz, P. Kowalczyk, K. Wawrzyk and D. Lumelskyj, Procedia Engineering **177**, 263–270 (2017).
[14] M. Chmielewski, J. Rojek, S. Nosewicz, International Journal for Multiscale Computational Engineering **15(4)**, 323–342 (2017).
[15] S. Nosewicz, J. Rojek, K. Pietrzak and M. Chmielewski, Advanced Powder Technology **28**, 1745–1759 (2017).
[16] R. Zhang, "Numerical simulation of solid state sintering of metal powder compact dominated by grain boundary diffusion," Ph.D. thesis, The Pennsylvania State Univeristy 1998.
[17] S. Nosewicz, J. Rojek, S. Mackiewicz, M. Chmielewski, K. Pietrzak and B. Romelczyk, Journal of Composite Materials **48(29)**, 3577 – 3589 (2014).
[18] L. D. Jonghe and M. Rahaman, Acta Metallurgica **36**, 223–229 (1988).
[19] D. Johnson, Journal of Applied Physics **40**, 192–200 (1969).
[20] R. Coble, Journal of Applied Physics **32**, 787–792 (1961).