

Discrete element simulation of powder sintering

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Abstract

This paper presents numerical modelling of powder sintering. The numerical model introduced in this work employs the discrete element method which assumes that material can be modelled by a large assembly of discrete elements (particles) of spherical shape interacting among one another. Modelling of sintering requires introduction of the cohesive interaction among particles representing inter-particle sintering forces. Numerical studies of sintering have been supplemented with experimental studies which provided data for calibration and validation of the model. In the laboratory tests evolution of microstructure and density during sintering have been studied. Comparison of numerical and experimental results shows a good performance of the numerical model developed.

Key words: powder sintering, powder metallurgy, simulation, discrete element method.

Introduction

Sintering is a manufacturing process used for making various parts from metal or ceramic powder mixtures. Sintering consists in consolidation of loose or weakly bonded powders at elevated temperatures, close to the melting temperature with or without additional pressure. This is a complex process affected by many factors. Modelling can be used to optimize and to understand better the sintering process and improve the quality of sintered components.

Modelling of sintering process is still a challenging research task. There are different approaches in modelling of sintering processes, ranging from continuum phenomenological models to micromechanical and atomistic ones. In this work the discrete element method is adopted as a modelling tool. This model employs a discrete model of sintered material and belongs to the class of micromechanical models. It allows us to determine interaction between the grains during sintering and rearrangement of grains during sintering. The numerical model is validated using the results of experimental studies of a sintering process.

Experimental studies of a sintering process

Experimental studies of sintering have been performed in the laboratory of Institute of Electronic Materials Technology. Sintering has been carried out in the Thermal Technology Astro uniaxial hot press shown in Fig. 1a. Morphology of the NiAl powder used for sintering is shown in Fig. 1b. The samples of the sintered material are shown in Fig. 1c. Sintering has been performed under pressure of 30 MPa and at temperature of 1400°C. Variation of temperature is shown in Fig. 2. The process was ended at different time instants in order to

study the evolution and kinetics of sintering. The measurement points are marked on the plot in Fig. 2. The kinetics of sintering can be evaluated by investigation of the bulk density change in time. The macroscopic shrinkage of the porous material during sintering leads to the increase of the bulk density. The evolution of the bulk density obtained in our studies is given in Table 1. The value of the bulk density close to the theoretical density has been obtained. It means that the material with very low porosity has been obtained by sintering.

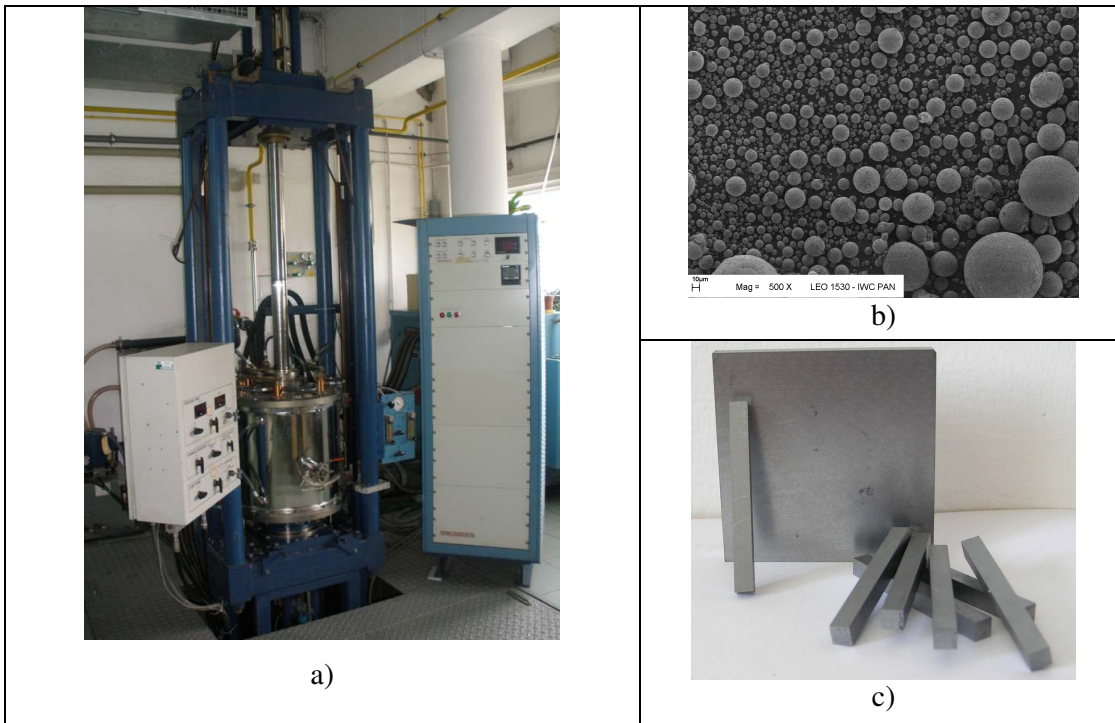


Fig. 1. Experimental studies of sintering: a) Thermal Technology Astro uniaxial hot press, b) NiAl powder, c) samples of sintered material

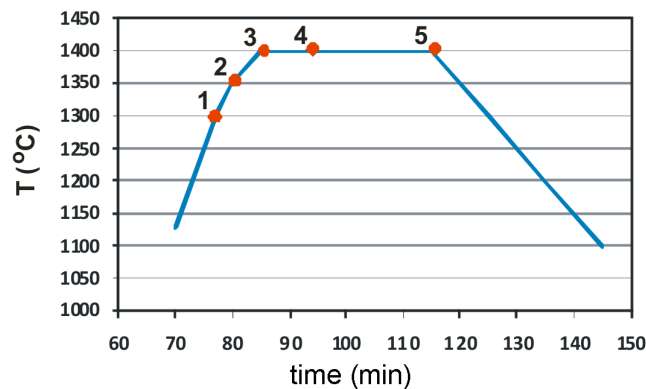


Fig. 2. Temperature variation during the sintering of NiAl with measurement points

Table 1. Density evolution of NiAl during sintering.

Measurement point	1	2	3	4	5
Bulk density (g/cm^3)	5,25	5,35	5,42	5,78	5,86
Relative density* (%)	88,8	90,5	91,7	97,8	99,1

* theoretical density of NiAl $\rho_T=5,91 \text{ g}/\text{cm}^3$

During sintering particulate material is converted into polycrystal. Microstructure evolution during sintering of NiAl is shown in Fig. 3. The microstructure and its change at early stage of sintering is shown in Figs. 1a-c. In the initial stage cohesive bonds (necks) are formed between grains. When the sintering process is continued the necks between particle grow. Grain rearrangement and increase of grain compaction can be observed during sintering. With the advancement grain growth, gradual reduction and elimination of porosity can be observed. Change of the microstructure during sintering can be clearly seen when Fig. 1d is compared with Fig. 1a or 1b.

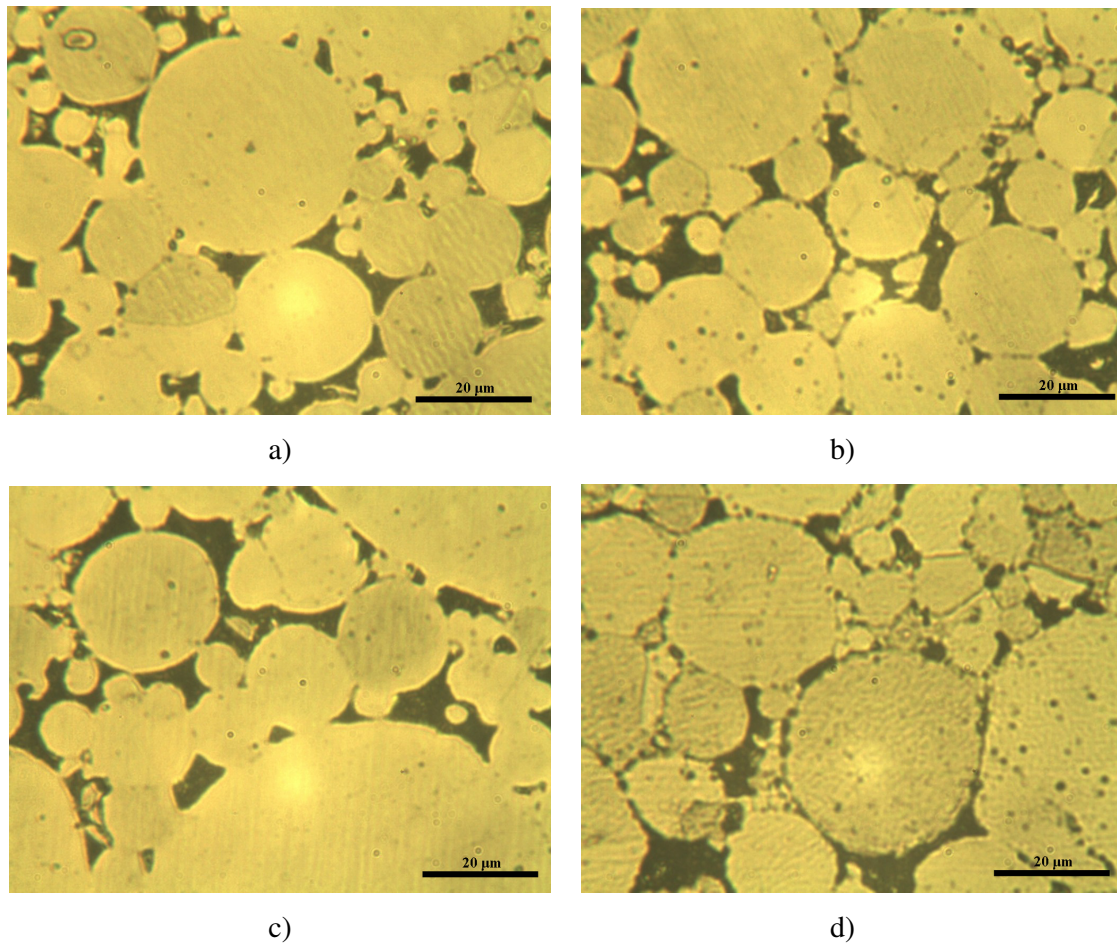


Fig. 3. Microstructure evolution during sintering of NiAl: a) temperature 1300°C (measuring point 1 in Fig. 2); b) temperature 1350°C (measuring point 2); c) temperature 1400°C (measuring point 3); d) temperature 1400°C (measuring point 5).

Sintering mechanisms

Growth of the neck connections between grains during sintering is a result of mass transport by different mechanisms (Hosford, 2006). The main mass transport mechanisms during sintering: surface, volume and grain boundary diffusion, as well as evaporation and condensation are shown schematically in Fig. 4.

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 leading to shrinkage of the system.

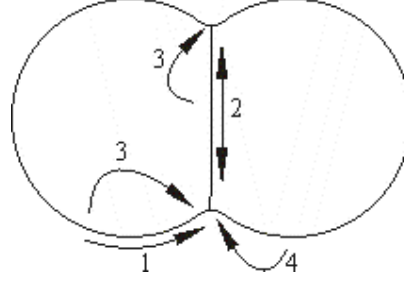


Fig. 4. Mechanisms of mass transport during sintering: 1 – surface diffusion, 2 – grain boundary diffusion, 3 – volume diffusion, 4 – evaporation and condensation

Numerical model of sintering

Considering the relationship between the diffusion and stress state Coble (1958), Johnson (1969), and De Jonghe & Rahaman (1988) formulated mathematical models for sintering force between two particles. The discrete element method provided a suitable framework for more general application of these models (Parhami and McMeeking, 1998, Martin et al, 2006). Discrete element method assumes that material can be represented as a collection of spherical particles interacting among one another (Cundall and Strack, 1979, Oñate and Rojek, 2004), thus the discrete element model takes explicitly into account the particulate nature of the sintered material. The numerical model of sintering has been implemented in the finite/discrete element code Simpack (Oñate and Rojek, 2004).

In the discrete element method, the translational and rotational motion of rigid spherical elements (particles) is governed by the standard equations of rigid body dynamics. For the i -th spherical particle we have:

$$m_i \ddot{\mathbf{u}}_i = \mathbf{F}_i \quad (1)$$

$$J_i \dot{\boldsymbol{\omega}}_i = \mathbf{T}_i \quad (2)$$

where \mathbf{u}_i is the element centroid displacement in a fixed (inertial) coordinate frame \mathbf{X} , $\boldsymbol{\omega}_i$ – the angular velocity, m_i – the element mass, J_i – the moment of inertia, \mathbf{F}_i – the resultant force, and \mathbf{T}_i – the resultant moment about the central axes. Equations (1) and (2) are integrated in time using the explicit central difference time integration scheme.

Vectors \mathbf{F}_i and \mathbf{T}_i are sums of all forces and moments applied to the i -th element due to external load and contact interactions with neighbouring spheres. Modelling of sintering requires introduction of the cohesive interaction among particles representing inter-particle sintering forces. In our model the translational motion will be considered only, assuming that the rotational motion is negligible in sintering. The particle interaction model assumed for sintering employs the equation derived by Parhami and McMeeking (1998):

$$F_n = \frac{\pi a^4}{8D_b} V_n - \pi \gamma_s \left[4R \left(1 - \cos \frac{\Psi}{2} \right) + a \sin \frac{\Psi}{2} \right] \quad (3)$$

where F_n is the normal force between two particles, V_n – the normal relative velocity, R – the particle radius, a – the sintering contact radius, Ψ – the dihedral angle, γ_s – the surface energy and D_b – the grain boundary diffusion coefficient. The geometric parameters used in Eq. (3) are defined in Fig. 5. The second term on the right-hand side of Eq. (3) represents the attractive interaction between the particles, while the first term described the viscous resistance opposing the relative motion.

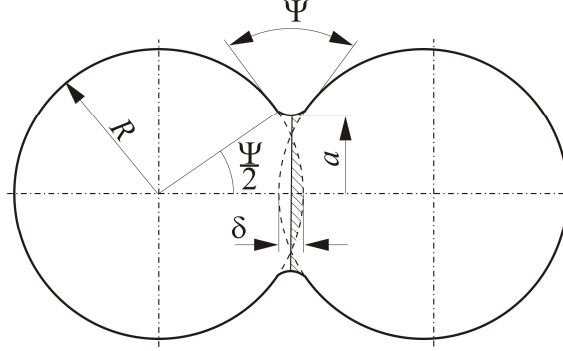


Fig. 5. Two particle interaction model – model parameters definition.

The effective grain boundary diffusion coefficient D_b is determined from the following relationship (Martin et al, 2006):

$$D_b = \frac{\Omega}{kT} \delta D_g \quad (4)$$

where Ω is the atomic volume, T – temperature, k – Boltzmann constant, δ – thickness of the diffusion area, D_g – temperature dependent coefficient.

The growth of the neck radius is calculated according to the following evolution equation (Martin et al, 2006):

$$\dot{a} = \frac{RV_n}{a} \quad (5)$$

The end of sintering is controlled by the limit value of the neck radius:

$$r_{\max} = R \sin \frac{\Psi}{2} \quad (6)$$

The dihedral angle Ψ is determined according to the Young's law which assumes that in the system consisting of two grains and a gas in the pore in the equilibrium we have equilibrium of surface tensions.

Sintering of two particles

The model implementation has been verified and calibrated using a simple example of free sintering of two particles. Figure 6a shows two equal particles touching each other at the beginning of sintering. The particles can move freely along the line passing through their centres, no other load except that due to sintering is involved. Figure 6b shows the particles at the equilibrium at the end of sintering. The model parameters have been taken from the literature and then the viscosity has been changed so that the sintering process takes about 35 minutes. The final results have been obtained for the following data: $R = 22.5 \cdot 10^{-6}$ m, $\rho = 5910$ kg/m³, $\gamma_s = 1.72$ J/m², $\Omega = 1.18 \cdot 10^{-29}$ m³, $T = 1673$ K, $\delta D_g = 3.832 \cdot 10^{-19}$ m³/s, $\psi = 146^\circ$. Evolution of the interaction force calculated according to Eq. (3) is presented in Fig. 7, and evolution of the velocity is plotted in Fig. 8. The logarithmic scale is used for time axes in both plots in order to better present changes occurring in the initial period.

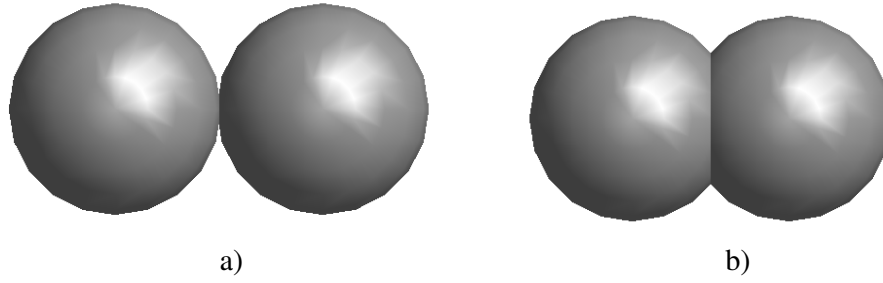


Fig. 6. Simulation of sintering of two particles: a) at the beginning of the sintering, b) at the end of the sintering

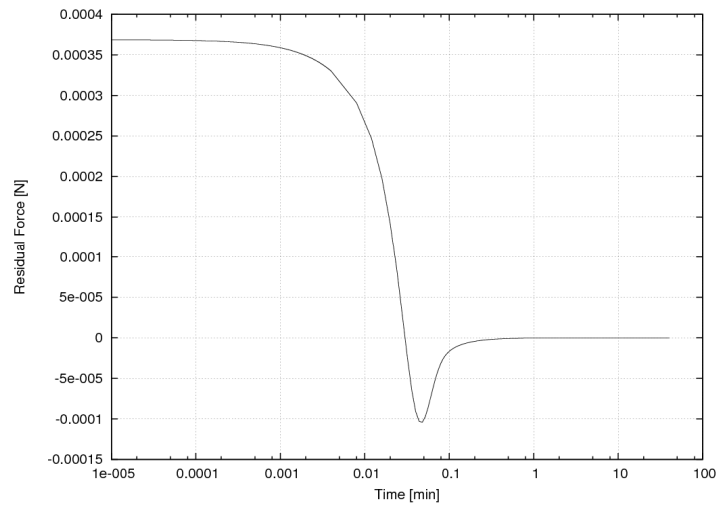


Fig. 7. Evolution of interaction force during sintering of two particles

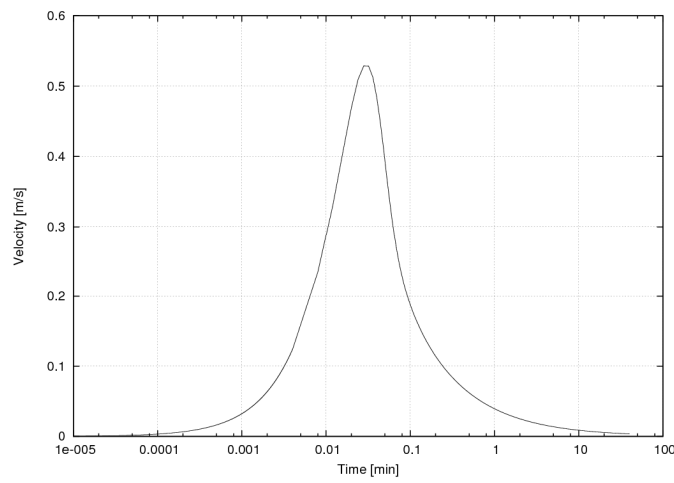
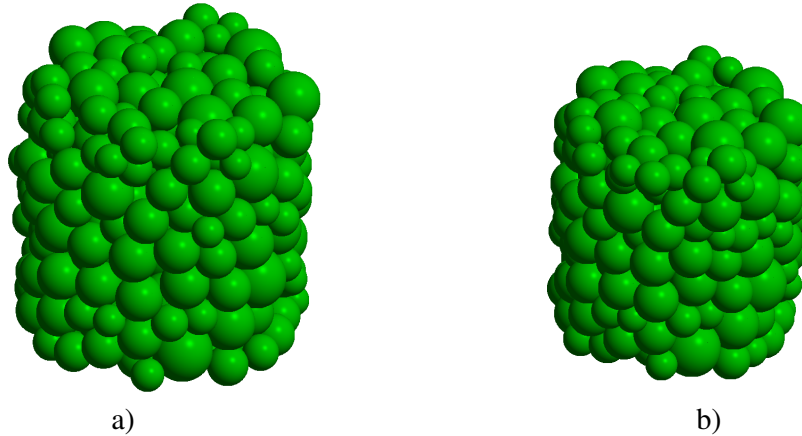


Fig. 8. Relative particle velocity during sintering of two particles

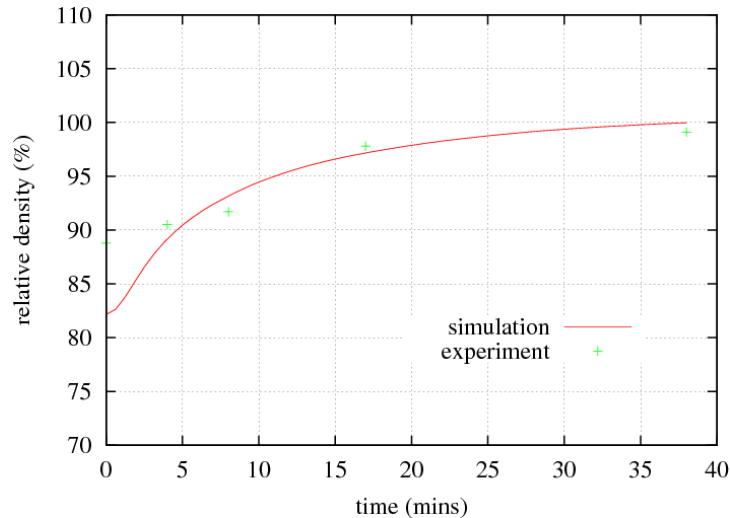
Simulation of intering of a cylindrical specimen.

The initial configuration of the discrete element model consisting of 350 particles is shown in Fig. 9a. It has been assumed that the kinetics of sintering is the same as in the laboratory test of sintering presented above. The model parameters found in the previous example have been applied in this example. The objective of this study was to check if with these parameters we can match the results obtained in the laboratory test. Figure 9b shows the specimen at the equilibrium after sintering. The shrinkage can be clearly observed.



Rys. 9. Numerical simulation of sintering of a cylindrical specimen: a) at the beginning of the sintering, b) at the end of the sintering

The relative density evolution obtained in the numerical simulation has been compared with experimental measurements in Fig. 10. It can be seen that the change of the density obtained in the simulation agrees quite well with experimental results.



Rys. 10. Evolution of relative density during sintering process – comparison of numerical and experimental results

Concluding remarks

The discrete element method is a suitable tool to model powder sintering. Particulate nature of the sintered material is taken explicitly into account in the discrete element model.

Presented results show a big potential of the developed numerical model in modelling of sintering processes, although further developments and validation are necessary.

Acknowledgements

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Symulacja spiekania proszków metodą elementów dyskretnych

Streszczenie

W artykule przedstawiono badania doświadczalne oraz modelowanie numeryczne procesu spiekania proszków metalicznych. W części eksperymentalnej pracy badano ewolucję mikrostruktury oraz gęstości spieku w trakcie procesu spiekania. Jako metodę modelowania wybrano metodę elementów dyskretnych, w której zakłada się, że materiał jest reprezentowany przez liczny zbiór elementów dyskretnych (cząstek) o kształcie sferycznym oddziałujących między sobą. Modelowanie spiekania wymaga wprowadzenia oddziaływania kohezyjnego między cząstkami reprezentującego naprężenia powstające między ziarnami w trakcie spiekania. W artykule przedstawiono wstępne wyniki numeryczne pokazujące ewolucję gęstości pozornej w trakcie spiekania.