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Multiscale modelling of powder sintering

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Associate Professor at the Institute of Fundamental Technological Research, Polish Academy of Sciences (IPPT), graduated from the Faculty of Power and Aeronautical Engineering at Warsaw University of Technology in 1985. In 1993 received his PhD in mechanics and in 2008 habilitation at IPPT; employed at IPPT since 1996, since 2011 head of the Division of Computational Methods in Nonlinear Mechanics in the Department of Computational Science. His main research interests include numerical modelling of materials and structures using the finite and discrete element methods, he is the author or co-author of more than 100 peer-reviewed articles, including more than 30 in journals from ICR list.

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 a particulate material is converted into a 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.

A framework for a multiscale model of powder sintering processes will be presented. The multiscale model includes numerical models for three scales relevant for sintering: atomistic, microscopic and macroscopic one. The atomistic modelling has been carried out using the molecular dynamics (1), the microscopic model has been developed within the discrete element method (2), and the finite element method has been a modelling framework for the macroscopic model. The geometric models at the three considered scales are shown in Fig. 1.

Modelling at lower scales provides parametric information to the upper scale while the upper scale models provide boundary conditions for lower scale
analysis. Molecular dynamics simulations have allowed to determine the diffusion coefficient and other parameters for the discrete element model of sintering. The discrete element simulations, in turn, have been used to determine macroscopic viscous moduli which are necessary for the finite element macroscopic model of sintering. The numerical models have been validated using the results of own experimental studies of sintering of NiAl powder.

Fig. 1 Models of powder sintering at various scales: a) atomistic (MD), b) microscopic (DEM), c) macroscopic (FEM)

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