Perspectives on Material Modelling: Porous and Particle-Based Microstructures

An overview on material modeling and its methodological diversity is presented. Representative examples of applications to porous and particle-based microstructures are given.

Abstract
Material modelling has become an indispensable component for designing materials with tailored properties and controlled microstructural quantities. An overview of the methodological diversity is presented, and representative examples of applications to porous and particle-based microstructures are given. The methods contain algorithms to computationally generate granular particle systems and cellular foams with defined porosities and pore distributions. A brief insight into the phase-field method is provided, which enables the simulation of a dynamic microstructure evolution. The approach is applied to describe neck formation, densification and the subsequent grain coarsening. Furthermore, data analysis tools are introduced to determine the porosity and the permeability, for example, as well as to derive dynamic quantities of the evolution. The applications serve as representative examples to indicate the broad variety of material challenges to be addressed by employing advanced material modelling techniques.

Introduction

For the development, the tailoring and the improvement of materials, the integration of computational methods into the processing route has significantly gained in importance. These days, the support through advanced computational methods, in virtual material design, is equally established, compared with experimental measures. Simulations provide a so-called digital twin of the real counterpart. The complexity of material modelling has rapidly increased within the last 5–10 years, due to the requirements of considering multiple physical fields and effects on multiple length and time scales. An essential component in the core position between atomistic and macroscopic methods is a comprehensive understanding of the microstructural evolution and the microstructural properties on a typical length scale of several micrometres.

The current review guides through the spectrum of computational methods operating on the mesoscopic scale. An overview and representative examples are given to indicate the broad range of possibilities of material modelling to characterise and analyse microstructure quantities, and to derive structure-property correlations. The methods capture:

- pre-processing tools to algorithmically generate realistic 3D-microstructures,
- numerical simulation approaches to describe microstructure evolution and dynamics, and
- post processing data analysis tools to quantitatively exploit huge data volumes, and to derive statistically valuable microstructure properties.

The software package Pace3D, which is developed at the institutes IDM and IAM-CMS in Karlsruhe, comprises a compendium of 3D-algorithms to enable an initial pre-processing and post processing of microstructures, as well as highly parallel solvers to enable the use of high-performance computers at their highest performance, to solve multi-physical fields, such as mass and heat transfer, fluid flow, mechanics, etc. At the High-Performance Computing Centre (HLRS), Stuttgart/DE, the Leibniz Supercomputing Centre (LSC), Munich/DE, and the Steinbuch Centre for Computing (SCC), Karlsruhe/DE, large-scale simulations of microstructure for-

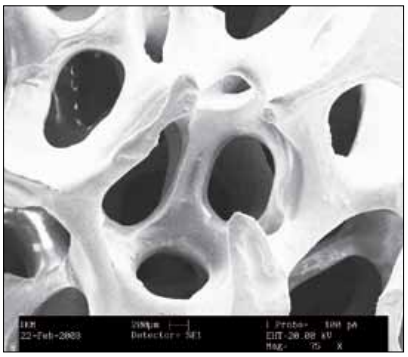

Fig. 1
A photograph of an open ceramic foam (Photo: Michael Hoffmann, IAM-KWT)

Keywords
material modeling, pre-processing tools, numerical simulation, post-processing data analysis tools

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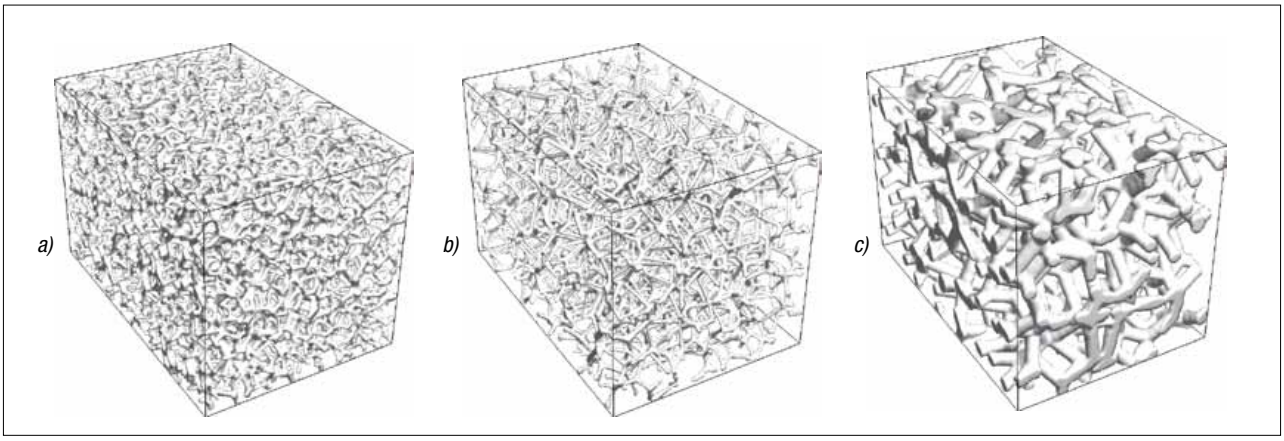

Fig. 2
Synthetic open pore structures of different geometric parameters; physical size of the domain: 2 cm × 2 cm × 3 cm

mations, the motion of interfaces and free boundaries, and of phase transitions and multi-physically coupled processes were efficiently carried out on computational domains of high-performance systems, with several billions of computational cells [1].

The high resolution of the computational domain is obligatory to minimise the influence of the domain boundary, and to map effects in the simulation, which are physically relevant. Besides the required high resolution, 3D-simulations are indispensable for the description of microstructure formations, as neighbourly relations have a decisive influence on the morphology. Comparisons between the simulation results and the experimental 3D-tomographic images showed a very good agreement between the microstructural parameters [2, 3]. The phase-field simulation software Pace3D was used as another application to analyse dynamic coarsening of polycrystalline grain structures [4]. The challenge of multiscale modelling enabled the transfer of morphologies and material parameters from the atomistic scale to the mesoscopic scale, and the determination of correlations [5, 6]. During the implementation of large-scale 3D-material simulations, large amounts of data are produced, which require new automated methods of data analysis. In order to analyse three-dimensional data sets of simulated and experimental microstructures, algorithms as well as a unique programming interface were implemented on the basis of principal component analysis (PCA), and were used to evaluate multi-phase microstructures [7], for example, and to characterise porous structures [8].

Design of porous structures

Open-cell solid structures look like an irregular polyhedron grid. An open metal foam sample is made of bubbles – so-called pores – without partition walls in the open-cell structure. Solid material forming the so-called ligaments still remains only in regions where three or more pores meet. Depending on the material and the quality of the foam, the ligaments can show different shapes and thicknesses. The regions between the ligaments – the inside of the earlier gas bubbles – are called pores. Fig. 1 shows an example for an open-cell solid ceramic foam. It can be seen that the pore region is continuous. It is also open to the outside. This enables fluids, such as water, gas or liquid metal, to permeate through such materials. Another advantage of open-cell solid foams is the large surface to volume ratio. This enables an extremely fast heat and mass diffusion.

At the two cooperating institutes IDM and IAM-CMS, processing tools are developed to produce synthetic geometries. By means of Voronoi-based algorithms, the production of open porous structures is possible. Thereby, the solid-state ratio, the pore size and the shape of the ligaments can be varied systematically, and can be generated with specific values. The algorithmic processing route first decomposes the rectangular virtual region into small congruent subregions, which are called cells. Each cell is parameterised with the properties of the material, at an exact location. Virtual spheres are randomly positioned in the three-dimensional domain, and are packed as compactly as possible. The cells occupied by the centres of the spheres define the basis of the Voronoi decomposition. Cells near the regions with more than two Voronoi polyhedrons are parameterised with the values of the solid material. A detailed description of the algorithm can be found in [9].

In Fig. 2, three examples of synthetically generated open-cell structures, with different ligament and pore structures, are shown. Granular structures exhibit a wide range of applications, where multiple particle powders or seed distributions form the base material for subsequent processing steps and multiple physical interactions. Particle-based fillings result in porous structures, where the individual components touch each other or are even connected, for example, as a result of a sintering process. For the digital generation of realistic granular structures, physics engine libraries are employed. During the filling procedure, individual particles are algorithmically produced, and move freely into the computational domain. Specification-oriented particle structures can particularly be designed through the virtual framework, and can be transferred to the real application and process. Moreover, the geometric set-ups serve as an initial microstructure for computational simulations of mechanic, thermodynamic and fluid flow simulations [9, 10]. A synthetically generated structure is illustrated in Fig. 3.

Evolution of polycrystalline grain structures

Grain growth, which accompanies the sintering process, results in a reduction of the porosity of the ceramic material. The phase-field approach serves as a powerful methodology to numerically simulate grain coarsening in a computationally efficient and thermodynamically consistent manner. During solid-state sintering, a pressed body of loose particles, called a green body, is heated up to 70–90 % of the melting temperature. This thermal activation leads to the sintering process, which is driven by surface energy minimization. Thereby, the loose particles bind together and coarsen, while the green body starts to densify.

The sintering process can be divided into three stages [11]. In the initial stage, necks form between the particles of the green body. The simulated structure in Fig. 4 a shows the initial stage in a 400 × 400 × 400 voxel cell domain with 3400 Al_2O_3 particles. At the HLRS, Stuttgart, the simulation was calculated on 1332 cores of the Hazel Hen supercomputer, for 48 h, by using a coupled phase-field and concentration model, which is validated in [14]. In the intermediate stage, the particles impinge upon each other, and build a network of pore channels. As depicted in Fig. 4 b–c, most of the densification occurs in this stage.

During a further densification, the pore channels shrink, which leads to the formation of isolated pores. At this point, the final stage of the sintering process begins. During the ongoing densification and grain growth, the inner pressure of the pores increases until an equilibrium pore size is reached. Fig. 2 a shows a phase-field simulation of the final sintering stage, in a domain of 400 × 400 × 400 voxel cells, with 1492 pores (yellow) and 1000 grains. The grain boundaries are indicated by grey

Fig. 3
Synthetic granular structure: particles of different size (l.) and particle of the same size (r.)

planes. The simulation was also performed on 1332 cores of the Hazel Hen supercomputer, for 12 h, by using a phase-field model with a pressure extension [12, 13, 16].

For the further sintering process, grain growth becomes the dominant driving

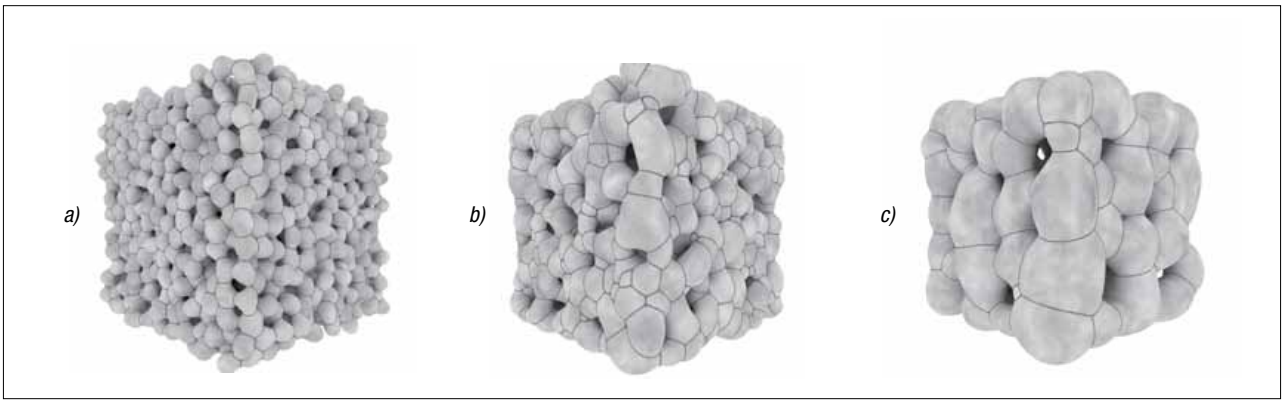

Fig. 4 a–c
Phase-field simulation of solid-state sintering at different stages: a) structure at the initial stage, b) structure at the beginning of the intermediate stage and c) structure towards the end of the intermediate stage

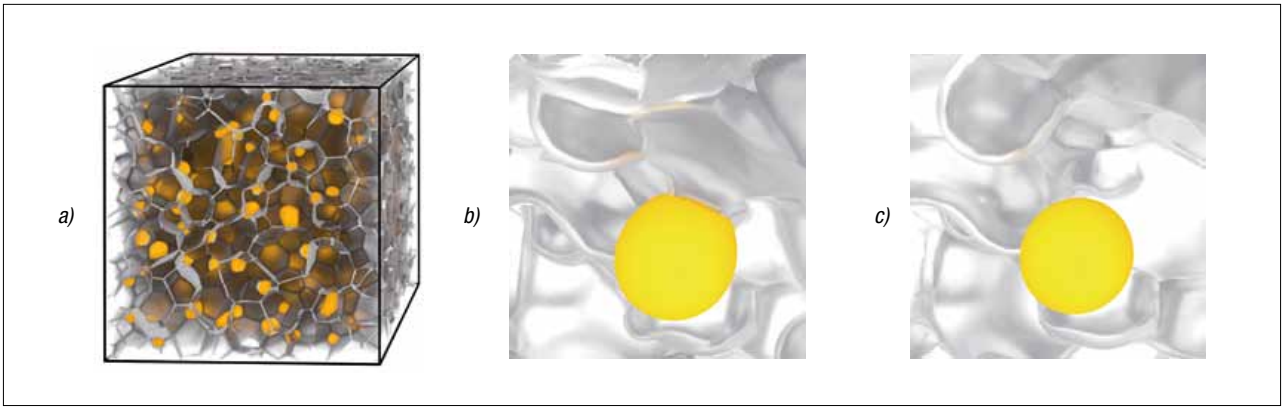

Fig. 5 a–c
Phase-field simulation of pore (yellow) separation from grain boundaries (grey planes) in the final sintering stage: a) polycrystal in the final sintering stage, b) pore before the detachment from the grain boundary, c) pore after the detachment from the grain boundary

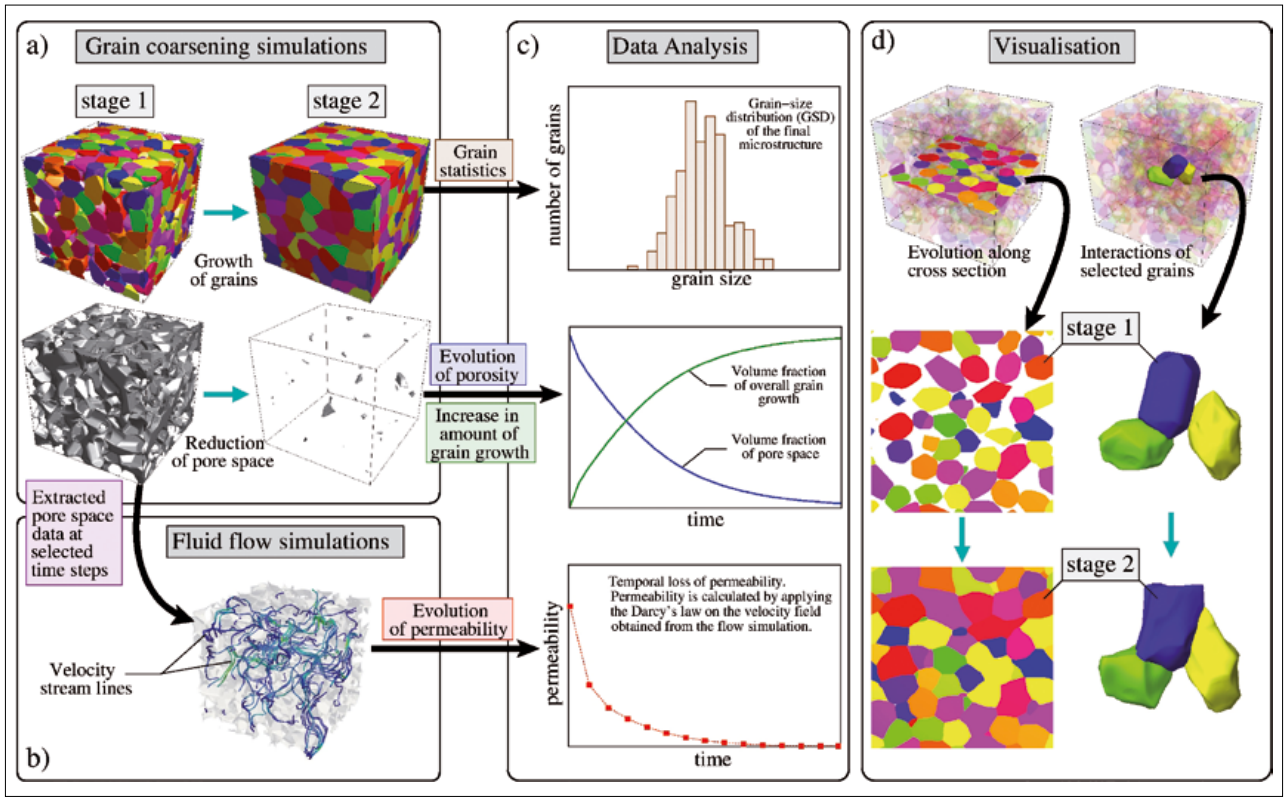

Fig. 6 a–d
Exemplary work flow: a) simulated grain coarsening (in BRG colours), and the corresponding loss of pore space (in grey), for two progressive stages of growth; b) fluid flow simulations are performed for the pore space data extracted from the coarsening simulations at successive time steps; c) from the coarsening simulations, we can obtain the data pertaining to (1) the grain size distributions (GSD) and (2) the temporal evolution of the porosity, as well as the amount of grain growth; from the flow simulations at different stages of coarsening, the temporal evolution of the permeability can be derived; d) advanced visualisation techniques illustrating (1) the evolution of grains along a plane cross section, and (2) the analysis of grain boundary interactions of selected grains

force. Depending on their size, the remaining grains grow with different velocities. Larger grains grow faster than smaller grains, and finally overgrow them. The growth of the grains is further influenced by the pores attached to their boundaries [15]. Pores with a high mobility can be dragged with the growing grain (Fig. 5 b), whereas pores with smaller mobilities can detach from the grain boundary (Fig. 5 c). The detached pores remain stable inside the grain, and their porosity cannot be reduced. In [12–16], the pore drag-drop interaction was investigated in detail with this model.

Data analysis of grain structures

Fig. 6 a illustrates the two different stages of the evolution of grains (in BRG colours) and the evolution of pore space (in grey), which are simulated by using a multiphase-field model. From the coarsening simulations, inferences can be drawn with regard to the grain statistics, as well as the kinetics of growth and porosity loss. Fig. 6 c depicts the histogram plot of the grain size distribution (GSD) at "stage 2". Furthermore, the authors plot the temporal evolution of the pore space (in blue) and the overall grain growth (in green) to study the kinetics of coarsening, as shown in Fig. 6 c. Moreover, the phase-field (coarsening) simulations can be coupled with the fluid flow simulations to estimate the flow behaviour of the evolving microstructure, as shown in Fig. 6 b. By using the velocity field obtained from the flow simulations at successive stages of coarsening, and by applying Darcy's law, the temporal evolution of the permeability can be derived (Fig. 6 c). In order to gain insights into the dynamic microstructure evolution, and the complicated grain boundary interactions, visualization techniques have been developed to analyse the evolution along arbitrary cross sections, and the mutual grain boundary interference of selected grains, as demonstrated in Fig. 6 d.

Summary and perspectives

The software framework Pace3D contains a broad variety of computational methods for the algorithmic generation of microstructures with tailored characteristics, for the simulation of dynamic microstructure evolution processes, incorporating multi-physical interactions, and for advanced analysis methods of huge (3D+t) data volumes. Representative examples of virtual cellular foams and granular powders are given to indicate the possibilities of structure design. The algorithms are developed in a general form, and allow a computational design of arbitrary structures and complex topologies. The digital models may directly serve as a digital twin to be copied for the production of a real material microstructure. In addition, the generated data can be used as an initial phase distribution to conduct simulations of dynamic processes, such as mass and heat transfer, phase transformations, fluid flow, mechanical loading, and the evolution of a magnetic and electric

field. The presented application to a sintering process of particle-based ceramic powder considers the densification and the accompanied change of the porosity. Finally, examples of the large compendium of data analysis and visualization methods are presented. The post-processing library includes a large number of data analysis tools to derive statistical measures and various combinations of structure-property linkages. The framework further offers specialized visualization applications.

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