EUROPEAN MECHANICS SOCIETY

Colloquium Final Report

N. 632 – Data-driven modeling of porous, composite and polycrystalline microstructures for predicting their mechanical and transport properties

Dates and location: **20/09/2023 - 22/09/2023, Ulm, Germany**

Chairperson **Matthias Neumann**

Co-Chairperson **François Willot, Paul Shearing**

Conference fees

What other funding was obtained? **No other funding was obtained**

What were the participants offered? **The conference fee was 640 €. This included 3 overnight stays, 3 breakfasts, 3 lunches, 3 dinners, and 5 coffee breaks at the scientific center "Reisensburg Castle" of Ulm University. Moreover, a printed version of the book of abstract as well as a conference folder and a ball pen.**
Registered participants: 29 (none of them has been a EUROMECH member)
People from Czech Republic (1), France (4), Germany (16), Spain (1), Sweden (3), Switzerland (2), United Kingdom (2) participated at the colloquium.
Due to personal reasons, Davide Cademartori (Genova, Italy) and Antoine Gloria (Paris, France) could not attend in person. They gave their presentations online via zoom and did not follow those of the others. Their abstract is included in the book of abstract, but they do not appear in the list of registered participants and did not pay the fee.

Number of members of Euromech (reduced registration fee) **0**

Number of non-members of Euromech (full registration fee) **0**

Scientific Report

For a wide range of materials, such as, e.g., battery electrodes, alloys or bio-materials, the underlying microstructure strongly influences mechanical and transport processes, which-in turn are key for the functionality of these materials. Thus, methodology for an efficient microstructure optimization is required. During the last decades, stochastic as well as numerical modeling and, in particular, the combination of both turned out to be powerful for virtual materials testing. Stochastic 3D microstructure modeling allows for the generation of so-called digital twins and, moreover, of a wide range of further virtual, but realistic microstructures

on the computer, while numerical modeling enables for the simulation of mechanical and transport properties of those virtual microstructures. In doing so, process-microstructure-property relationships can be quantitatively investigated by means of simulation studies in an efficient way. Ideally, this approach leads to structuring recommendations for experimentalists dealing with the synthesis and manufacturing of materials possessing optimized microstructures.

The EUROMECH colloquium “Data-driven modeling of porous, composite and polycrystalline microstructures for predicting their mechanical and transport properties” focused on recent advances in the interdisciplinary field of data-driven microstructure modeling, where applications to porous, composite and polycrystalline media, mechanical and transport properties have been addressed. The colloquium brought together researchers from different disciplines (mathematics, physics, and materials science) dealing with image analysis, machine learning and stochastic microstructure modeling, the generation of digital twins, numerical simulations of effective properties as well as AI-based methods for characterizing, predicting or optimizing mechanical and transport properties.

The scientific results of the EUROMECH colloquium, which are summarized in the following, are subdivided into 5 categories, which have a strong overlap between each other.

Image analysis as data processing

Raw image data resolving the nano- or microstructure of functional materials has to be pre-processed, in order to reconstruct the material phases by image segmentation. For this purpose, machine learning becomes an important tool which allows for appropriately segmenting image data even in cases when classical methods from image analysis struggle. Applications of machine learning approaches (as the powerful 3D-UNet) are presented, e.g., for battery materials and concrete. For these two types of materials, an important topic is the segmentation of cracks in order to study crack propagation and the influence of cracks on effective properties. Even if machine learning leads to better results of image segmentation, it is error-prone if the learning is only based on hand-labeled data. Thus approaches are presented, where methods from stochastic geometry help to generate semi-synthetic image data as a well-defined ground truth for training. In the special case of concrete, a further challenge is that the thickness of real cracks varies widely, both, within one crack as well as from crack to crack in the same sample. The segmentation method should therefore be invariant with respect to scale changes. A network architecture which is particularly designed for this problem, namely Barisin’s RieszNet has been presented.

Stochastic microstructure modeling and spatial statistics

Stochastic microstructure modeling is a powerful tool for generating virtual micro- and nanostructures. In combination with numerical simulations of transport properties, it can be used as a data-base for an efficient quantification of structure-property relationships. New methodological approaches have been presented for modeling several morphologically different micro- and nanostructures such as, e.g., the arrangement of active material in battery electrodes, the nanostructure within hierarchically structured active materials, the microstructure in fuel cells, polycrystalline structures, short fiber reinforced polymers and foam structures. Recent advances regarding model fitting to image data have been discussed. This involves algorithms to represent polycrystalline materials by tessellation models such as Laguerre tessellations or the more flexible class of general balanced power diagrams. Such representations serve as a basis for fitting random tessellation models. Furthermore, model fitting based on analytical relationships between model parameters and morphological descriptors that can be estimated from image data has been discussed at the colloquium. The latter approach has been presented at the example of fitting an excursion set model of a random field to the nanostructure of active material particles. Besides that, new techniques for modeling foam structures have been presented. In the literature, a common model

type for foam structures is based on the strut system of random tessellation. It has been shown that post-processing by means of Brakke's surface evolver enables for more concentrated distributions of edge lengths and facet shapes. The model also allows to generate realistic structures of partially closed foams.
Moreover, the crucial topic of estimating morphological descriptors from image data has been vividly discussed during the colloquium. Novel descriptors quantifying spatial correlations in polycrystalline materials as well as novel descriptors for quantifying bottleneck effects and connectivity properties in porous materials have been presented. The latter descriptors are based on the computation of shortest (geodesic) paths through a material. Finally, new stochastic microstructure models are presented for generating virtual structures with predefined types of bottlenecks.
In general, the choice of suitable and meaningful morphological descriptors for the prediction of mechanical and transport properties has been discussed. This is an important issue as a wide range of morphological descriptors is a available in the literature. A clear terminology as well as an understanding of relationships between these descriptors is an important issue for the community to make results comparable, which concerns also the notion of tortuosity (as detailed below).
The role of machine learning
During this colloquium, three different applications of machine learning are presented. First, machine learning is used for data-processing, i.e. image segmentation, which is required for computing morphological descriptors as well as effective properties from 3D image data. Second, as an alternative to models from stochastic geometry, generative machine learning models are used for generating virtual microstructures that are statistically similar to the structures observed by 3D imaging (digital twins). Compared to methods from stochastic geometry, generative machine leaning models might be more prone to overfitting. Third, machine learning is a powerful tool for data-driven predictions of effective properties based on structural input. Here, neural networks are either used for non-parametric regression establishing a link between aggregated morphological descriptors and effective properties or, by means of convolutional neural networks, effective properties are predicted taking the full 3D information of the image into account. Interpretability of the machine learning methods has been discussed compared to classical (low) parametric regression models. Open source software, in which the considered machine learning models are implemented, has been presented and discussed.
The concept of tortuosity and effective transport properties
The main topic of this session is the structural influence on effective transport properties. In this context, the notion of tortuosity plays an important role. However, there are many different notions of tortuosity (e.g. effective tortuosity, geometric tortuosity, hydraulic tortuosity) around in the literature. During this session, a possible nomenclature for tortuosity has been proposed and discussed. As examples, microstructures in solid oxide fuel cells and batteries are discussed. In particular, a homogenized model for hierarchically structured materials for lithium-ion batteries is presented, where the effective transport properties (effective tortuosities) of nanostructured active materials are considered to obtain an improved accuracy of the model. Besides the nano-scale, the micro-scale, i.e. the arrangement of the active material and the carbon binder domain is crucial for the performance of battery electrodes. This issue, and particularly the role of the carbon binder domain, have also been discussed at the colloquium. Modeling approaches of effective transport properties with a spatially resolved carbon binder domain have been presented that are applied to 3D image data representing cathodes in lithium-ion batteries. In the context of transport properties, the software GeoDict, which can be considered as a the digital material laboratory, has been presented. It provides tools for the complete chain of data-driven modeling and simulation of effective properties based on 3D image data. Algorithms for analyzing the morphology as well as the technologies behind the solution of the partial

differential equations, that help computing material properties, have been discussed, including AI, grid coarsening and parallel computing.
Data-driven modeling of mechanical properties
Regarding the prediction of mechanical properties, data-driven model-free fracture mechanics has been presented. The fracture-related material modeling assumptions are removed from the formulation, while retaining the epistemic laws of fracture that stem from variational principles. This data-driven approach delivers results in excellent agreement with those of their standard fracture mechanics counterparts.
Moreover, a combination of extensive image analysis with finite element modeling is presented that elucidates the role of geometric defects during additive manufacturing on the performance of metallic cellular materials. For this purpose, laser powder bed fusion is used as an additive manufacturing technology to fabricate metallic cellular architectures. The morphology of the latter, exhibiting heterogeneous, yet precisely-controlled, pore features has been virtually designed on the computer.
The influence of morphological descriptors on mechanical properties has been discussed at the example of short fiber reinforced polymers which have been manufactured by injection molding. For this purpose, virtual fiber reinforced polymers are generated, which serve as an input for the computation of effective material properties, carried out in conjunction with computational homogenization methods. The influence of the distribution of the fiber length on mechanical properties has been discussed, before the model is finally validated comparing it with industrial short fiber reinforced polymers.

Please send this report in electronic form to the Secretary General of EUROMECH, within one month after your Colloquium.