ulm university universität ulm

Fakultät für Mathematik und Wirtschaftswissenschaften
Institut für Stochastik

Universität Ulm | 89069 Ulm | Germany

Professor Dr. Volker Schmidt

Helmholtzstraße 18
89081 Ulm, Germany

Tel: +49 731 50-23532
Fax: +49 731 50-23649
volker.schmidt@uni-ulm.de
http://www.uni-ulm.de/stochastik/

21. Juni 2016

Einladung zum Vortrag

von

Samih H. Ibrahim
Warsaw University of Technology, Poland

Modeling the microstructure of open-porous materials for high-temperature gas catalysis

Microstructure, apart from chemical composition, is one of the major factors influencing materials properties. This is especially important for open-porous materials used in catalysis applications, where the volume fraction of pores, their size distribution and specific surface area influence the diffusion of reactants and the kinetics of catalytic reactions. In this talk, numerical microstructure models of open-porous electrodes for Molten Carbonate Fuel Cells (MCFC) will be presented. These models simulate the fabrication routes of real materials including mixing of powders, tape casting and sintering processes. The substrate powders are represented by spheres with defined size distributions. Mixing and compaction of powders with polymeric binder is simulated by a granular model implemented in LAMMPS code. The polymeric phase represented by fine particles and larger porogen additives is later removed to form pores. The sintering process is simulated by geometry smoothing which results in an aggregation of spheres. The models presented in this talk were compared with tomographic 3D images of real MCFC materials. Quantitative analysis of μ-CT images was performed and it was shown that the algorithms used in our studies are able to realistically design materials with desired porous microstructures.

The talk is based on joint work with T. Wejrzanowski.

Termin: **Dienstag, 19. Juli 2016, 15.00 Uhr**

Ort: **Universität Ulm, Helmholtzstr. 18, Raum E60**

Der Vortrag findet im Rahmen des Forschungsseminars des Institutes für Stochastik statt.
Alle Interessenten sind herzlich eingeladen.

gez. V. Schmidt