Abstract for poster presentation

**Modeling the missing carbon phase in X-ray tomographic reconstructions of a metal-based battery cathode**

Lukas Zielke¹, Tobias Hutzenlaub², Dean R. Wheeler³, Chien-Wei Chao³, Ingo Manke⁴, André Hilger⁴, Nils Paust¹,², Roland Zengerle¹,², Simon Thiele¹,⁶

¹ Laboratory for MEMS Applications, IMTEK Department of Microsystems Engineering, University of Freiburg, Georges-Koehler-Allee 103, 79110 Freiburg, Germany.
² HSG-IMIT Institut für Mikro- und Informationstechnik der Hahn-Schickard-Gesellschaft e.V., Georges-Koehler-Allee 103, 79110 Freiburg, Germany
³ Department of Chemical Engineering, Brigham Young University, 350 CB Provo, UT 84602, United States
⁴ Helmholtz Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin, Germany
⁵ FIT, University of Freiburg, Stefan-Meier-Straße 21, 79104 Freiburg, Germany
*Presenting author, email: Lukas.Zielke@imtek.uni-freiburg.de

Metal-based battery cathodes usually contain three phases: The active material (AM) provides ions, the carbon-binder domain (CBD) is the electron conducting network, widely spread throughout the cathode, and the electrolyte filled pore space enables transport of the ions. All of these transport processes take place on multiple length scales.[1] Micro pores (µ-P) and nano-pores (n-P) are shown in the Figure. Representative models in the micro- and nanoscale are therefore needed in order to increase the understanding of ion- and electron transport. To gain representative models, X-ray tomography is the method of choice for battery cathodes and anodes.[2] However when using this method, there is a lack of reliable information on the CBD in metal-based battery cathodes, due to the dominant absorption properties of the active metal domain compared to the CBD in many battery materials. Therefore we apply a stochastic model [3], based on with information of all phases from FIB/SEM images, which models the CBD in a fixed LiCoO₂ domain from X-ray tomographic reconstructions. Furthermore, we apply the same method to obtain the nanoporous structure of the CBD itself. We then incorporate this information into the large model and find significantly different transport parameters. To check if our stochastic model recreates these structures accurately, we validate it with a virtually designed reference structure. This allows quantifying the uncertainties of the applied method.[4]

References