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## MATBOX, an Open-Source Microstructure Analysis Toolbox for Meshing, Generation, Segmentation, and Characterization of 3D Heterogenous Volumes

Thursday, 3 June 2021 19:00 (15 minutes)

Battery performance is strongly correlated with electrode microstructural properties. To account for its impact, lithium-ion battery (LIB) models either abstract the microstructural heterogeneity of composite electrodes using effective macroscopic properties (macro- or meso- scale models) or directly solve the system of equations on the microstructure geometry or mesh (microstructure-scale models). Therefore, to be adequate, both families of models require information from the microstructure geometry, which can be provided by the numerical tool presented in this work.

MATBOX is a MATLAB open-source application [1] developed by NREL for performing various microstructure-related tasks including microstructure numerical generation, image filtering and microstructure segmentation, microstructure characterization and correlation, visualization, and microstructure meshing. MATBOX was originally developed for the analysis of LIB electrode microstructures; however, the algorithms provided by the toolbox are widely applicable to other heterogeneous materials. The toolbox provides a user-friendly experience thanks to a Graphical-User Interface, requires no coding by the user, and is well documented. This presentation will illustrate various MATBOX features for the characterization of a LIB electrode, including a fully automated Representative Volume Element (RVE) analysis, the numerical generation of complex 'virtual' microstructure, including dual-layer electrodes and carbon-binder additive phase, and the meshing of a complex NMC/graphite full cell microstructure suitable for 3D finite-element modeling. Other modules (segmentation, visualization, and correlation) will be briefly presented.

Thanks to its modular, open-source approach, MATBOX can easily incorporate third-party algorithms to eventually build a standard in the field that will benefit the whole scientific community. Effective diffusion coefficient [2], additive phase numerical generation [3], and meshing [4] third-party algorithms have been already integrated in the toolbox with more to come.

### Time Block Preference

Time Block C (18:00-21:00 CET)

### References

- [1] F. Usseglio-Viretta et al., MATBOX: an open-source microstructure analysis toolbox for microstructure generation, segmentation, characterization, visualization, correlation, and meshing (2020) [https://github.com/fussegli/Microstructure\\_analysis\\_toolbox](https://github.com/fussegli/Microstructure_analysis_toolbox)
- [2] S. J. Cooper et al., TauFactor: An open-source application for calculating tortuosity factors from tomographic data. *Software* 5, 203–210 (2016).
- [3] Mistry, A., Smith, K. & Mukherjee, P. P. Secondary Phase Stochastics in Lithium-ion Battery Electrodes. *ACS Applied Materials & Interfaces* (2018) doi:10.1021/acsami.7b17771.
- [4] Q. Fang et al., Tetrahedral mesh generation from volumetric binary and grayscale images. 2009 *IEEE International Symposium on Biomedical Imaging: Nano to Macro* 1142–1145 (2009) doi:10.1109/isbi.2009.5193259.

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