Deep learning for 3D+t datasets in material science: Application to the analysis and quantification of the evolution of the 3D morphology of Li-ion batteries

3-year PhD position

In the Centre for Mathematical Morphology, Mines Paris – PSL University

General Context and Challenges

Over the past ten years, driven by the need to reduce our dependence on fossil fuels, significant efforts have been made to develop high-performance Li-ion batteries for both electric vehicles and storage of renewable, wind and solar energy. However, the use of liquid electrolytes in conventional Li-ion batteries has many disadvantages such as their limited potential stability window, the dissolution effects of transition metals and their flammable nature which leads to high fire risks. These problems can be overcome by replacing the liquid electrolyte with a solid electrolyte [1].

The objective of this project is the analysis and quantification of the evolution of the 3D morphology of all-solid-state Li-ion batteries during i) their manufacture and then ii) their use through electrochemical cycling. We aim at detecting and understanding the changes in the microstructure of batteries that lead to degradation and loss of electrochemical performance. The analysis of the morphology of the microstructure will be based on the use of X-ray tomography imaging techniques at different scales (µ and nano) [2] and from different sources (laboratory CT and synchrotron). Indeed, the non-destructive aspect, the possibility of coupling between imaging and spectroscopy and the recent improvements in terms of spatial resolution and rapid acquisition make X-ray tomography an ideal tool to follow in operando the morphological modifications within the solid-state Li-ion batteries [3], [4].

Project description

3D tomographic images will be segmented and analyzed using deep learning. A specific development will be necessary to segment a large quantity of 3D data [5], especially since the temporal aspect (3D+time) will have to be considered. The 3D+time data will be used to calculate 3D displacement maps thanks to measurements by 3D volume correlation (Digital Volume Correlation) [6] which will allow by derivation to obtain 3D deformation maps and thus to follow the sintering phenomena or the appearance/propagation of cracks as a function of pressure and cycling parameters. The segmented images will be used to develop models faithful to the initial microstructure, which can be used for additional calculations and verification. The mechanical properties quantified from these calculations can be related to the evolution of the electrochemical performances, to detect the primary origins of the polarizations and the losses in capacities.

The processing of massive data (3D+time) acquired during cycling experiments (operando tomography) necessarily involves a semi- or fully automatic approach. Deep learning has become the methodology of choice for 2D or 3D image segmentation [7], both in computer vision and in the bio-medical field. These approaches are beginning to be applied to battery domains [8]. However, batteries raise unprecedented challenges, since complex architectures/morphologies and connections between different material phases play critical roles in electrochemical reactions. Guaranteeing the good connectivity/percolation of the segmentation is essential but remains for the moment an open problem. Approaches seeking to ensure that purely convolutional networks such as U-Net can exploit global information, such as topology and connectivity, open interesting perspectives [9].

The challenges raised by this task will be addressed by (a) reducing the need for annotated images through transfer learning [10] and self-supervision [11], [12], [13]; (b) the study of the appropriate level of precision for the reference segmentations, (c) the adaptation of 3D convolutional networks applied in the medical field to the problem of the project and the proposal of 3D+t networks. In order to avoid the explosion of the size of the model, we will take inspiration from lightweight architectures which seek to factorize the convolutions, such as

MobileNet [14]. We will also study the interest of spatio-temporal convolutions to integrate 3D dynamics intrinsically in segmentation networks.

The obtained microstructural properties will be correlated with the evolution of the electrochemical performances, to detect the origins of the polarizations and the losses in capacities. These results will allow better understanding of underlying phenomena and will open new avenues for optimization in the manufacturing of all-solid-state batteries, to quickly acquire greater technological maturity and approach the deployment to the market.

PhD Advisors
Petr DOKLADAL, Jesus ANGULO, Etienne DECENCIERE, Mines Paris, PSL - University.

Location
Centre for Mathematical Morphology, MINES Paris PSL https://www.cmm.minesparis.psl.eu/

Doctoral School
ISMEE Mathématiques et Systèmes, École doctorale 621, Ingénierie des Systèmes, Matériaux, Mécanique, Énergétique

Application condition
finished M2 programme, image analysis, AI coding skills (tensorflow or pytorch), excellent academic records

Application procedure
a prospective candidate should send his curriculum, academic track, motivation letter, two reference letters to petr.dokladal@minesparis.psl.eu

References:

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