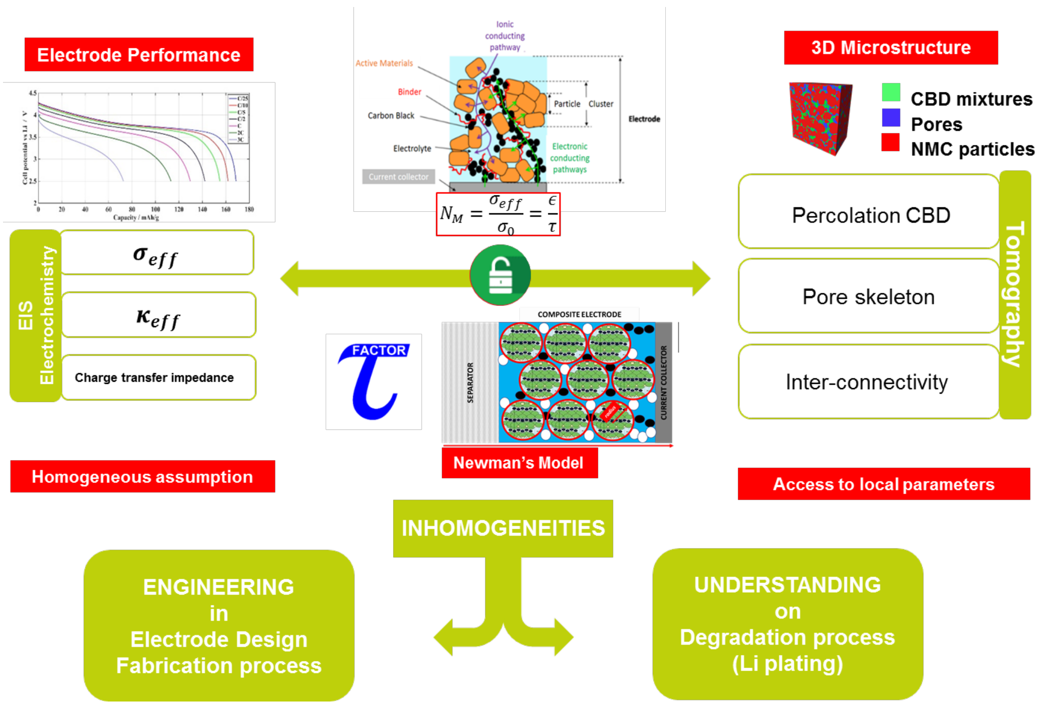
Master Internship in Research
(Materials Science)

Study the effect of tomography data processing on the correlation with transport properties of positive electrodes of Li-ion battery



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Required skills: Image processing, Li-ion Battery, Based skills in Python, FIJI and Avizo softwares.

Contract date: from March 2nd to July 31st

Gratification for internship: 550 euros/month

Research topic :

We already know that for porous electrodes, the electrode microstructure plays a pivotal role in determining its performance, since it has an impact on different electrode's properties such as transport properties via either the electronic or ionic conducting pathways, electrochemical properties via the interface area between phases and mechanical properties due to the non-uniform distribution of phases. As a result, we believe that the electrode microstructure can detrimentally affect its performance, especially at high cycling rate. To bypass this limitation, one need to understand the correlation between these two.

Regarding the electrode performance, we've chosen to focus on the transport properties since they are the most likely to limit the performance at high rate. So far, we already developed a methodology to quantify accurately either electronic or ionic conductivity of our electrodes at multi-scale.

On the other hand, to capture the 3D microstructure, X-ray computed tomography and FIB/SEM were employed. The microstructure data set then gives a valuable basis for the determination of microstructural parameters: (i) interfacial surface area between phases, (ii) volume fractions of the different components and porosity and (iii) tortuosity of the different components. However, these parameters are not ready yet to be exploited due to the lack of a well-defined data processing methodology. Furthermore, to complete the study, a data analyzing methodology is also needed. Only when everything is done, there we can obtain a consistent and relevant correlation between two domains.

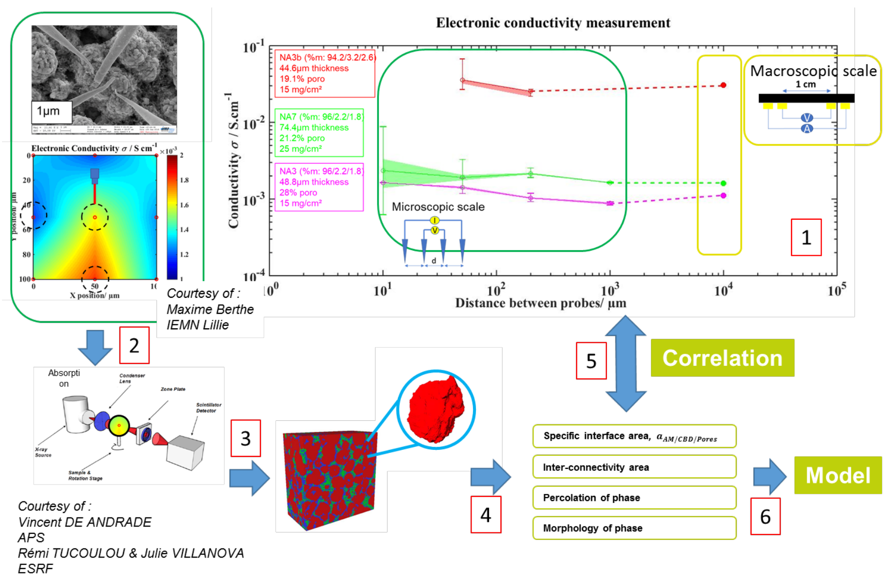

Figure1 : Schematic showing workflow to correlate the electrode microstructure to its performance, here is the electronic conductivity measured by 4points method at multi-scale.

It is worth noting here that the data processing already begins at the moment we get the raw tomography data. As a result, it covers a complete study of different aspects such as: reconstruction, artifact removal, filtering, segmentation. On this matter, the Master student is expected to be consistent but also not afraid to explore different approach to find a best and efficient way to accomplish the mission. Then, the data analyzing step requests the Master student to have a good sense of rationality and a good understanding on the physics of battery in order to find a relevant correlation from different parameters from both domains.

Complexity of these composite features as well as presence of multiple phases demands careful segmentation in order to get usable data for 3D analysis. Machine learning [3] provides a robust solution to automate segmentation processes by learning from existing model data relationships and is suitable to analyze of high-dimensional complex data problems. Its implementation in this field can make segmentation almost an entirely automated process. Among different approaches, convolutional neural network (CNN) [4] is a popular deep learning technique for image processing. It is capable of classifying structural features in images similar to the way the human visual system operates. Its accuracy and efficiency for feature recognition and classification have been proved for various applications. Different hierarchical levels of the trained network are used to identify features of varying complexity. The trained network is then used to segment the entire 3D image stack.

3D reconstructions will be performed using Tomopy and specific libraries for filtering. Subsequent 3D segmentation, quantification and visualization will be carried out in Avizo and FIJI softwares. A Python toolbox named Xlearn [5] was used to implement the CNN model. The project will focus on NMC electrodes with different loading conditions.

References:

[1] Pietsch, P., & Wood, V. (2017). X-ray tomography for lithium ion battery research: a practical guide. Annual Review of Materials Research, 47, 451-479.

[2] Schluter, S., A. Sheppard, K. Brown, and D. Wildenschild (2014), Image processing of multiphase images obtained via X-ray microtomography: A review, Water Resour. Res., 50, 3615– 3639, doi:10.1002/2014WR015256

[3] Yang, X., De Andrade, V., Scullin, W., Dyer, E. L., Kasthuri, N., De Carlo, F., & Gürsoy, D. (2018). Low-dose x-ray tomography through a deep convolutional neural network. Scientific reports, 8(1), 2575.

[4] Kaira, C. S., Yang, X., De Andrade, V., De Carlo, F., Scullin, W., Gursoy, D., & Chawla, N. (2018). Automated correlative segmentation of large Transmission X-ray Microscopy (TXM) tomograms using deep learning. Materials Characterization, 142, 203-210.

[5] https://github.com/tomography/xlearn

[6] S.J. Cooper et al. / Journal of Power Sources 247 (2014) 1033e1039