Master 2 internship at CNRS in LRCS Lab (Amiens, France)

Multiphase Segmentation for Tomography data using Convolutional Neural Network and Morphological Study of Cathode Secondary Particles

Laboratories: LRCS (CNRS)
Address: 15 Rue Baudelocque, 80000 Amiens, France
Supervisors: Dr. Arnaud Demortière (CR-CNRS) and Valentine Destarkeet (PhD student)
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Required skills: image processing, Machine/deep Learning, X-ray tomography, Python coding
Contract dates: from February/March/April to July 2023
Salary : 550€/month (net)

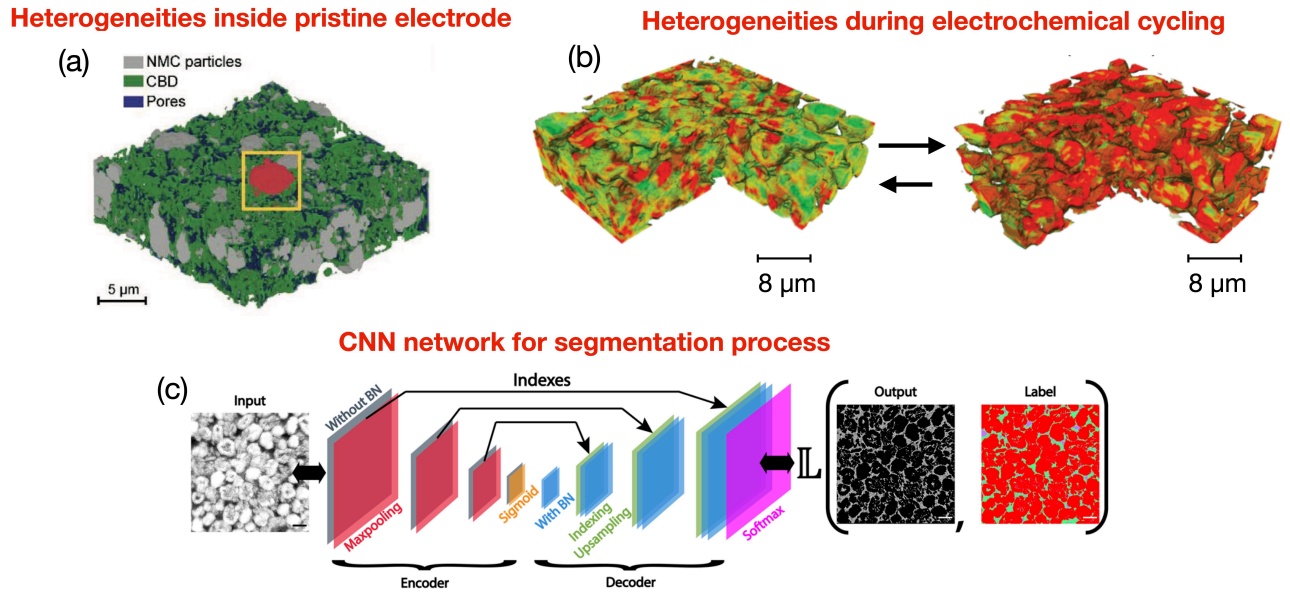

Figure 1: (a) NanoXCT 3D volume of cathode electrode with complex architecture containing NMC secondary particles, CBD phase and porosity [6]. (b) XANES nanoCT before and after lithiation process [6]. (C) CNN network built for multiphase segmentation of XCT images [7].

Research topic: X-ray nano Computed Tomography (CT) with a spatial resolution of 20-60 nm is a strong new tool to probe Li-ion battery materials in a non-destructive mode **[1]**. Nano CT allows us to distinguish in 3D different phases of composite electrode such active particle, carbon-binder (CBD) and porosity, which is crucial to properly get insight into electrochemical properties of Li-ion battery. 3D morphological parameters, such as porosity, tortuosity, connectivity, specific surface, and surface contact, directly drive ion diffusions and electronic conductivities as well as electrochemical reactions. 3D quantitative characterization of these complex materials using X-ray computerized tomography can provide a fingerprint of the 3D microstructure of battery electrodes, which can be used as input parameters in numerical model (continuous and multi-scale model developed in our laboratory LRCS/RS2E).

Complexity of these composite features as well as presence of multiple phases demands careful segmentation 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.

A development on the convolutional neural network (CNN) to segment multiphasic XCT image has been made last 3 years. An open-source software segmentPy, based on CNN approach, has been built to make segmentation of multiphase image (https://segmentpy.readthedocs.io/en/latest/) **[7].** 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

However, the amount of data generated by such analysis in a synchrotron is incredibly huge. Therefore, we propose also to develop a workflow to implement every step needed for the dataset processing such as filtration, reconstruction, 3D visualisation, 3D analysis and quantification of morphological properties using CuPy and DragonFly.

This project is in collaboration with Umicore company. You will be working within the Image & Diffraction team in LRCS lab leading by Dr. Arnaud Demortière, CNRS researcher. The internship will be under the supervision of Dr. A. Demortière and Valentine Destarkeet (PhD student).

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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]** Gürsoy D, De Carlo F, Xiao X, and Jacobsen C. Tomopy: a framework for the analysis of synchrotron tomographic data. *Journal of Synchrotron Radiation*, 21(5):1188–1193, 2014. **[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]** T-T Nguyen et al., Advanced Energy Materials, 2003529, 2021, **[6]** T-T Nguyen et al., ACS Energy letter, 2022 (In reviewing). **[7]** Su, Z., Decencière, E., Nguyen, T. T., El-Amiry, K., De Andrade, V., Franco, A. A., & Demortière, A. (2022). Artificial neural network approach for multiphase segmentation of battery electrode nano-CT images. *npj Computational Materials*, *8*(1), 1-11.