Internship Master 2:

Image processing based on CNN approaches for nano Computed Tomography reconstruction and semantic segmentation

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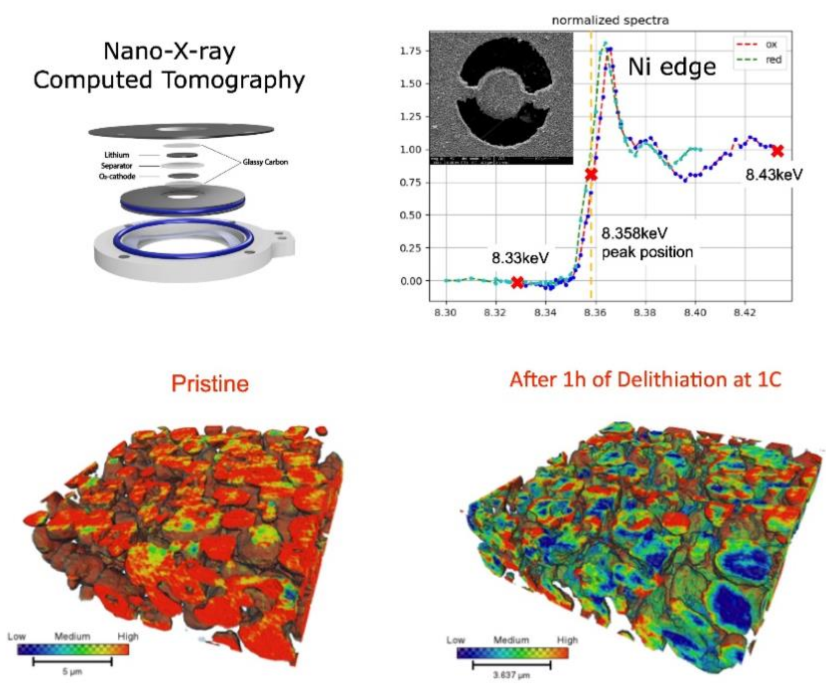
Required skills: image processing, Python coding, deep learning, materials science
Contract dates: from March to July 2022
Salary : 550€/month (net)

Two last decades, a large variety of studies provided valuable information on electrode behaviors, which is in the most cases based on 2D rather than 3D measurements. The development of new tools and methodologies are needed to study dynamical phenomena in 3D. TXM tomography technique (using X-ray synchrotron source) is an incomparable technique to 3D analyze battery materials, which is a no-destructive technique and allows an analysis at 360° without none or very few blind angles. 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) [1]. Moreover, in ideal case, the experiment can be processed in an *Operando* mode that can allows to monitor the structural change (surface and bulk) and degradation of battery electrodes during electrochemical cycles.



On the other hand, X-ray absorption near-edge structure (XANES) spectroscopy is sensitive to chemical and local electronic change of the probed element. As a result, XANES provides a powerful tool to monitor the evolution of these properties at particle scale. Indeed, the change in oxidation state that occurs during the oxidation/reduction process in the probed element can be tracked by detecting shifts in its XANES spectrum. This experiment can also be performed *in situ* or *Operando*, which can enable the mapping and tracking of chemical evolution during electrochemical cycles.

In our group, we proceed the XANES coupling with 3D TXM nanoCT [3] in *Operando* experiment to investigate NMC positive electrode using home-made electrochemical cell (see above). The experiment is aimed at mapping and tracking the chemical evolution of active materials (NMC-$LiNi_xMn_yCo_zO_2$), which can be related to the electrode performance, along with getting 3D microstructural properties under in situ conditions. This experiment is expected to yield a new way to fast direct correlate the microstructural heterogeneities to the electrode performance.

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/).

Goal of this internship:

1. 3D image processing based on CNN approaches for XANES/nano-CT reconstruction
2. Use and develop SegmentPy tool (U-net, LRCS-net) to segmentation nano-CT images.
3. Statistical analysis of 3D volume evolution to extract morphological and chemical modifications as a function of state of charge and time.

Reference:

[1] Nguyen, Tuan-Tu, et al. "3D Quantification of Microstructural Properties of $LiNi_{0.5}Mn_{0.3}Co_{0.2}O_2$ High-Energy Density Electrodes by X-Ray Holographic Nano-Tomography." *Advanced Energy Materials* 11.8 (2021): 2003529. [2] Su, Zeliang, et al. "X-ray nanocomputed tomography in Zernike phase contrast for studying 3D morphology of Li–O_2 battery electrode." *ACS Applied Energy Materials* 3.5 (2020): 4093-4102.

[2] Zeliang Su, Tuan-Tu Nguyen et al. Artificial Neural Network Approach for Multiphase Segmentation of Battery Electrode Nano-CT Images, npj Computational Materials 2022.

[3] Su, Z., De Andrade, V., Cretu, S., Yin, Y., Wojcik, M. J., Franco, A. A., & Demortière, A. (2020). X-ray nanocomputed tomography in Zernike phase contrast for studying 3D morphology of Li–O2 battery electrode. *ACS Applied Energy Materials*, *3*(5), 4093-4102.

This internship can be followed by a PhD.