Research engineer in image processing for materials characterisation

Fields: software engineering, image processing, materials, solid-state physics
CDD (Non-permanent position) – 24 months

Scientific context:

This 24-month post-doctoral position is proposed in the frame of the European HORIZON project MatCHMaker, dedicated to the characterisation and modelling of advanced materials. The main objective of the MatCHMaker Project is to reduce the time, costs and risks in the development and optimisation of sustainable advanced materials that meet the needs of the EU manufacturing industry.

The main fields covered by the project are materials for construction, energy and for mobility, which are respectively declined in three use cases: cement materials, Solid Oxide Cells (SOCs) and Proton-Exchange Membrane Fuel Cells (PEMFCs). Specific information can be found on the dedicated website: https://he-matchmaker.eu/.

A critical step in the development and optimisation of these materials is their rapid and accurate characterization, which requires addressing specific needs according to the application. The post-doctoral candidate will focus more specifically on the SOC and PEMFC use cases. For these two applications, the characterization of the electrodes is performed either in 2D using a Scanning Electron Microscope (SEM) or a Transmission Electron Microscope (TEM), or in 3D with FIB-SEM or electron-tomography. It should be noted that 3D acquisitions require a large number of good-quality 2D projections, which results in a long measurement time. The analysis of the 2D images can also be time-consuming, especially for extracting quantitative information, such as identifying small features (microcracks) in SOC electrodes, or counting nanoparticles and analysing their characteristics for PEMFC electrodes. Machine Learning (ML) provides promising methods for performing these analysis tasks in an automatic manner, even on high-noise data. This post-doctoral position aims to address these ambitious objectives: the application of ML methods for automatic analysis of SEM and TEM images, and the processing of fast acquisitions, in the context of SOC and PEMFC electrodes characterisation.

The candidate will collaborate with experts in the fields of SOC and PEMFC, at CEA/DRT/LITEN, located in Grenoble, and with specialists in Machine Learning methods at CEA/DES/ISAS, located in Saclay. The position is planned to be located in Grenoble, in close contact with the experts of the use cases.

The candidate will have the opportunity to present his results to the MatCHMaker partners and to communicate through publications and conferences. The methods that will be developed could be transposed to other use cases of interest.

Specific objectives:

The application of Machine Learning approaches to help with SEM and TEM image analysis will focus on specific tasks dedicated to SOCs and PEMFC cases. The specific tasks expected to be improved by Machine Learning approaches are detailed hereafter.

SOC Use Case:

- **Automatic microcracks segmentation:** various operating conditions of the SOCs (leakage, thermal cycling, etc.) can lead to the appearance of microcracks in the Yttria Stabilized Zirconia

(YSZ) ionic conductor backbone. To better understand the impact of this degradation on the cell performances, it is essential to analyse the microcracks' location and their density. In this goal, 3D FIB-SEM characterizations are performed and these properties are extracted after manual labelling of the microcracks. While this manual selection is feasible, it is also time-consuming and prone to human error. Machine Learning models are expected to help automate this task. The learning can be done on real data that are already segmented, or by using data augmentation methods, with the creation of artificial cracks on the images.

- **Phase identification:** the identification of the different phases (porosity, YSZ, metallic and oxidised nickel) currently requires the combination of secondary electron SEM images with Energy-Dispersive X-ray spectroscopy (EDX) mapping. A new ML approach will be investigated to be able to discriminate these phases without the use of EDX information.

PEMFC Use Case:

- **Statistics of sizes of Nanoparticles:** PEMFC electrode characterization requires the analysis of platinum nanoparticles which are the catalysts for the electrochemical reactions. The performance of the electrode is connected to the size of these nanoparticles but can also depend on their spatial distribution. TEM images consist in 2D projections, which imply a loss of information on the 3D geometrical configuration of the nanoparticles. Consequently, several 2D projections are required to be able to reconstruct the 3D configuration of the nanoparticles. This task proposes to use ML algorithms to extract the nanoparticle size distribution and their spatial location by using fewer 2D projections. The training can be done by using simulations, in order to have a sufficient number of examples. Achieving this objective will allow us to scan a larger area of the materials, and get a better global characterization in a shorter time.
- **3D reconstruction using fast acquisitions:** Complementary to the previous task, electron tomography requires the acquisition of a large number of good-quality 2D projections. This task proposes to study the possibility to speed up the acquisition step and improve the quality of the reconstruction by ML. By acquiring multiple frames at each tilt angle, the model can be trained using the reconstruction with the full information as output and the reconstruction obtained with single frames as input.

Special attention will be paid to the validation of the developed models and to their possible generalisation for other applications. When it is possible, the model is expected to provide an uncertainty estimation of the results and a level of confidence, for example by using Bayesian approaches or Ensembling methods.

According to the advancement of the mission, other tasks related to the characterisation of SOC, PEMFC or cement materials could be explored.

Specific skills:

The candidate will hold a PhD in applied mathematics or related to machine learning and data science.

He/she has experience in implementing machine learning and deep learning approaches and carrying out related methodology (training, validation, performance assessment).

Knowledge of material science, SEM and TEM measurements would be an advantage.

Location

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Contacts

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Please send your CV, motivation letter and recommendation letter to the contact persons by

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