Development of 3D X-ray spectral ptychography for the hyperspectral characterization of technical catalysts

Context:
This 36-months Ph.D. project is funded by an ANR (French National Research Agency) JCJC project, entitled "Adding Spectral capabilities to ptychographic imaging of Technical Catalyst". The innovation of this project is the combination of 3D X-ray phase-contrast imaging via ptychography and spectroscopic techniques to give rise to a novel 3D hyperspectral nanoimaging. This methodological develop will have an immediate impact in the catalysis industry by enabling the characterization of technical catalysts at different life stages. Progress in catalysis has always been motivated by societal needs, such as environment, energy, and fuels, with the goal of improving the efficiency of the catalytic process on a technical scale. Technical catalysts are complex multicomponent bodies, ranging from dozens of μm to several cm, consisting of active phases, supports, and additives in shaped forms suitable for their application. They differ strongly from a research catalyst, i.e., the laboratory-developed materials constituted by a single bulk or supported active phase, which is the predominant focus of academic investigations. Yet despite the tremendous relevance, understanding the complexity of their structure-property-function relationships is very challenging, mainly due to the limitations of the characterization techniques. Ptychographic X-ray Computed Tomography (PXCT) is the 3D X-ray nanoimaging technique that overcomes these shortcomings and has revolutionized the characterization of technical catalysts (Fig. 1). However, access to the localization and state of individual chemical elements within the sample structure is not yet directly possible. By adding spectral capabilities to ptychography and PXCT, this project aims at bridging this gap between the morphological and spectroscopic characterization of technical catalysts.

Objectives and means available:
The main goal of this Ph.D. project is the development of a novel 3D hyperspectral nanoimaging methodology for the characterization of technical catalysts by combining X-ray computed tomography and spectral-ptychography. The addition of spectral capabilities, similar to near-edge structure spectroscopy, to ptychography will provide the locations and chemical state of the metals that promote or poison the catalysts with high sensitivity and high spatial resolution within the 3D microstructure. This project comprises samples of hydrocracking and Fluid Catalytic Cracking (FCC) catalysts. The data will be obtained in synchrotron source facilities. High-performance computing resources will be available and Python-based software will be developed for simulation, data analysis, 3D image rendering, and segmentation. Machine and deep learning will be also used for data analysis.

Possible collaboration and networking:
She/he/they will develop the project in collaboration with scientists and engineers from NÉEL Institute CNRS/UGA, French CRG beamlines at ESRF, and KAUST catalysis center (KCC), Saudi Arabia. Working trips to different synchrotron source facilities for data collection will be organized. Additionally, Grenoble is an important scientific hub hosting important research institutions and technological companies.

Required profile: A degree in Physics, Chemistry, Materials Science, Electrical Engineering, or related sciences, and allowing enrolment for a Ph.D., such as an MSc, Master 2 de Recherche, Laurea, or equivalent. Interest in working with imaging processing and material characterization. Good
INSTITUT NEEL Grenoble

PhD student

experimental and programming skills are highly desirable and important for the development of this project. Experience with X-ray imaging or catalysis is considered an asset. English proficiency.

**Duration**: 36 months

**Salary**: According to the university/CNRS salary grid for a Ph.D. student (~2135 euros/month gross).

**Foreseen start**: the beginning of 2021

Applicants should send a CV, a motivation letter, and at least one recommendation letter to:

**Contact**: Julio Cesar DA SILVA

**Phone**: +33 4 76 88 74 11  **e-mail**: julio-cesar.da-silva@neel.cnrs.fr