Scientific Area	Synchrotron Light Applications		
Project Title	Bragg coherent diffractive imaging driven by Machine learning: from data collection through reduction		
Recruiting Institution	ESRF – The European Synchrotron		
PhD awarding Institution	University Grenoble Alpes	**PhD Duration**	36 Months
Supervisor/Institution	Tobias Schulli, ESRF		
Co-Supervisor/Institution	Vincent Favre-Nicolin, Steven Leake, ESRF		
Secondment(s)	ML and HPC training with the ENGAGE network. Experiments in other synchrotrons		

Project Description

The ESRF ID01 beamline is a strain microscope, which exploits the intrinsic coherent properties of the X-ray source to image the strain in materials at high spatial resolution (<10nm) using the Bragg Coherent Diffraction Imaging (BCDI) method. This characterization tool provides a route to materials design through strain engineering. With the realisation of the ESRF-EBS and improvements in data acquisition, a data deluge is imminent for BCDI experiments at the ID01 beamline, ESRF. It is timely that a solution is sought with regards to all aspects of the data pipeline; from sample selection and data acquisition, through data pre-processing and the subsequent image generation and analysis. Machine learning (ML) has the potential to unlock the sought physical parameters and rapidly put them at the fingertips of the scientist, dramatically improving both the throughput, design and output of such experiments.

At the core of the proposal is the BCDI method. BCDI allows the scientist to image the strain distribution in 3D, *operando* or *in-situ*. Strain signatures are common in the presence of defects and typically extend beyond the spatial resolution of the method, thus the defects themselves can be located and identified, alongside strain associated to facets, substrate interactions, phase changes and so forth.

Project Objectives

Several attempts have already been made to use ML methods to tackle the phase retrieval step, the image creation, but there is significant work to be done before less tailored samples can be routinely solved. Specifically, the goals of the project are to augment:

- Sample selection and data acquisition
- Experiment design (optimise date collection parameters)
- Fast (on-the-fly) 2D and 3D strain image reconstructions
- Data pre-processing (e.g. automatically filter spurious signals)
- Data post-processing (e.g. identify crystalline defects from the strain map)

The ML developments will be applied to experimental datasets collected on metal (Pt, Ni, Au, Cu) nano-crystals, and will also be tested within the scope of the ERC project Carine.

Required Candidate Qualifications

- Degree allowing enrolment for a PhD (such as MSc, Master 2 de Recherche, Laurea or equivalent) in physics, materials science, computer science or closely related science
- A background in machine learning is desirable, the ability to code in Python is considered an asset.
- In order to succeed in such an international team, you must be both independent and a team player, and bring the drive and willingness to make your research shine.
- English proficiency (working language at the ESRF)