Scientific Area	Synchrotron Light Applications		
Project Title	Microstructure and texture analysis of x-ray diffraction data using Machine Learning		
Recruiting Institution	ESRF		
PhD awarding Institution	Université Grenoble Alpes	PhD Duration	36 Months
Supervisor/Institution	Carsten Detlefs / ESRF		
Co-Supervisor/Institution			
Secondment(s)	ML and HPC training among ENGAGE partners.		

## **Project Description**

This project is a collaboration between the ID03 and Algorithms & Scientific Data Analysis teams at the ESRF to study the microstructure and texture of engineering materials.

Upon plastic deformation, the crystal lattice accumulates defects such as dislocations. With increasing deformation these dislocations self-organize into 3D structures such as grain and subgrain boundaries. Eventually this process leads to work-hardening. Beamline ID03 uses Dark Field X-ray Microscopy (DFXM) to study this microstructure in-situ and in 3D.

The selected candidate will join the Algorithms & Scientific Data Analysis (ADA) group and develop machine-learning techniques to identify and characterize large-scale dislocation structures such as low-angle grain boundaries. He/She will bring much-needed automation of the data analysis workflows for DFXM, enable non-expert users to make better use of their data, and make the techniques more accessible to an even larger scientific community, and especially industry. All work will be carried out in close collaboration with the ESRF Dark-Field X-ray Microscopy beamline ID03.

## **Project Objectives**

- Segment 3D orientation maps acquired with DFXM into cells and subgrains.
- Identify and classify the boundaries between these cells according to their orientation with respect to the neighbouring (sub)grains, orientation change across the boundary, cell size, etc.
- Set up and evaluate the performance of various machine learning models

## **Required Candidate Qualifications**

- Degree allowing enrolment for a PhD (such as MSc, Master 2 de Recherche, Laurea or equivalent) in physics, chemistry, computational science, or a related field.
- Knowledge of computational chemistry/physics software.
- Knowledge of a modern programming language (e.g., Python) and machine learning techniques is an asset.
- Proficiency in English (working language at the ESRF)
- Compliance with the Marie Sklodowska-Curie mobility rule: candidates must not have resided or carried out their main activity (work, studies, etc.) in France in the three years immediately before the applications deadline
- **Eligibility**: Early-Stage Researchers (ESRs) shall, at the time of recruitment by the host organisation, be in the first four years (full-time equivalent research experience) of their research careers and have not been awarded a doctoral degree