Postdoc position: 3D crystal orientation imaging in STEM
(with possible extension to synchrotron X-ray)

Scientific background: Many physical properties of polycrystalline materials are closely related to their grain microstructure and hence a complete description including size, three-dimensional shape, and orientation of the grains is necessary to model the behaviour of these materials. The ambition of the bi-national (Franco-German ANR - DFG) project 3D SPED-APT [1] is to analyse elemental segregation (measured by Atom Probe Tomography) as a function of 5 macroscopic grain boundary parameters. Accurate mapping of the 3D grain boundary network in nanocrystalline agglomerates is a prerequisite for this.
We have recently developed of a variant of Scanning Precession Electron Diffraction (SPED) in the Transmission Electron Microscope (TEM) which enables this type of 3D characterization with down to nanometre spatial resolution [2]. The method is based on the Automated Crystallographic Orientation Mapping tool (ASTAR) and involves indexing of superimposed electron diffraction patterns, reconstruction of virtual dark field images and tomographic reconstruction of the 3D grain shapes from a tilt series (Figure 1). In its current version the method is bound to microstructures exhibiting small intra-granular orientation spread. Our ambition is to explore the possible generalization of the method, explicitly accounting for the presence of intragranular orientation spread within the individual grains.

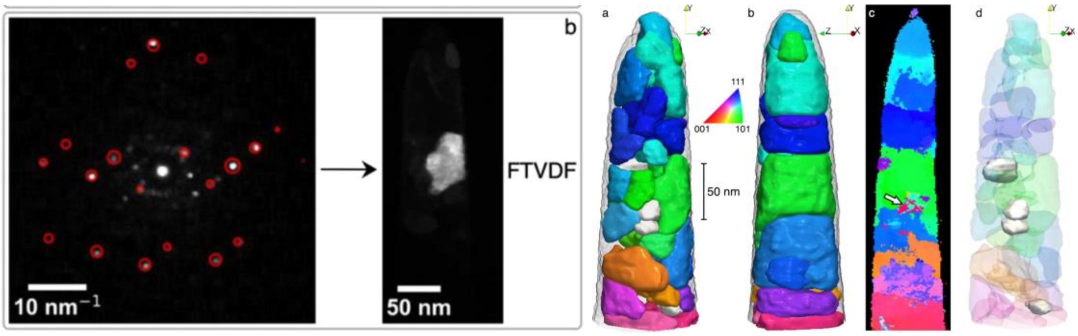

Figure1: (left) electron diffraction pattern with superimposed indexing solution; middle: virtual darkfield reconstruction of 2D grain projection; right: rendering of 3D grain structure in pearlitic steel tip [2].

Project description: Considering a discrete sampling of local orientation space for each grain, we have implemented a forward model which can be used to “fit” experimental diffraction patterns of a deformed grain as a superposition of patterns with slightly different crystal orientation. The reconstruction of the 3D orientation field from a tomographic tilt series can be formulated as a convex optimization problem, similar to recent work in synchrotron X-ray orientation mapping [3]. After initial tests and optimization of the framework on synthetic diffraction data (known ground truth with varying levels of complexity), we intend to apply this concept to experimental data, acquired by our project partners. Further extension of the algorithmic framework to the case of scanning 3DXRD (synchrotron X-ray data) data will be envisaged in a follow-up project, via possible extension of the current contract, covering a 12 month period, initially.

Candidate: We are looking for a postdoctoral researcher with a PhD in physics (applied mathematics, materials science). The candidate should have experience with one or more of the following topics: electron and/or X-ray diffraction, digital image processing, inverse problems. Programming skills in Python are a mandatory requirement. Applications should include a motivation letter and contact details of two referees.

Conditions: time limited contract (12 month) with a possibility for extension; working place in Grenoble (ESRF / SIMAP), application deadline 15 February 2022.

Contacts:
W. Ludwig, MATEIS, ludwig@esrf.fr, +33476882973; E. Rauch, SIMAP edgar.rauch@inp-grenoble.fr +33476826340

[1] https://anr.fr/Projet-ANR-19-CE42-0017 ; https://gepris.dfg.de/gepris/projekt/431450858
[2] P. Harrison, et al. ,*Ultramicroscopy*, , 2022, 238, pp.113536
[3] N. Vigano et al. Scientific Reports, 2016, 6 (1), 1-9