PhD thesis at Mines Paris

Generative models for metal microstructures

Thesis directors

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Location

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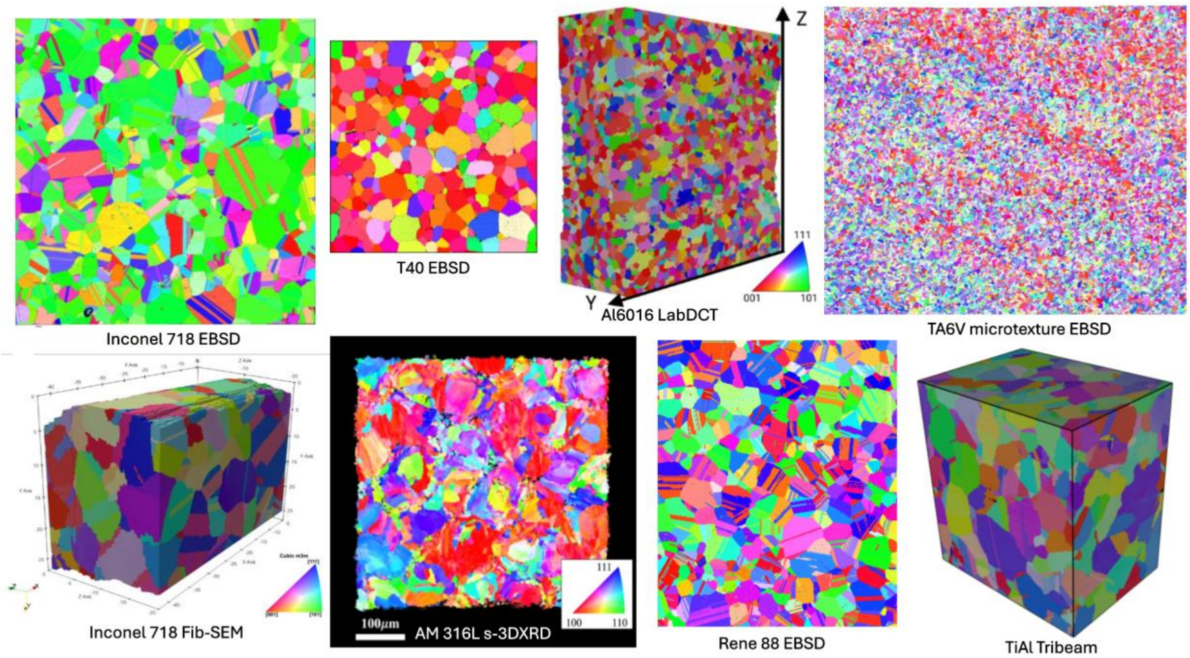
Context and objectives of the PhD thesis

Our modern world is made possible by structural materials, they transport us, protect us, help us grow our food, etc and to a large extend, they gain their mechanical properties thanks to their small scale structure: the microstructure. This PhD thesis focuses on AI-based generation of synthetic metallic material microstructures -- creating numerical instances of polycrystalline microstructures that replicate the statistical properties of observed ones. The goal is not only to generate microstructures that visually resemble real materials but also to create models that yield accurate mechanical responses when simulated in finite element codes. In particular, the mechanical behavior of materials is highly sensitive to morphological singularities, which act as stress concentrators and impact mechanical responses at first order.

Improving synthetic generation capabilities for crystal microstructures is highly challenging, because of the deeply rooted limitations of existing models. For instance, Voronoi diagrams, while useful for some applications, offer overly simplistic geometries that fail to represent the complex interplay between deformation and damage mechanisms at the boundaries of grains in metallic alloys. The problem is compounded by the fact that the geometrical modelling of polycrystalline materials must incorporate statistical descriptors that operate at multiple scales. The morphology of individual grains (spatial domain with a single crystal orientation depicted by a uniform color in the figure below) is the smallest length-scale that will be considered in this PhD thesis and we seek to build models capable of generating representative volumes for mechanical properties (typically that span one millimeter).



Above figure: examples of various metallic polycrystalline microstructures, including steel, aluminium, titanium and nickel based alloys; these microstructure were characterized by electron of X-ray diffraction, in 2D (surface) or 3D (tomography). All images are depicted using inverse pole figure coloring related to the crystal orientation.

The present PhD thesis will rely on a rich dataset of material images obtained using advanced techniques that allows sub-micron resolution, such as Electron Backscatter Diffraction (EBSD), three-dimensional data like X-ray computed tomography, and even four-dimensional data where materials' microstructures are imaged during mechanical testing. The following tasks will be undertaken to achieve our objectives:

(i) **Dataset generation** by collecting and processing both synthetic and experimental images. We will generate virtual 3D images using the Voronoi-diagram-based approaches. We will also collect and process a large amount of experimental data by leveraging automated microscopy. Laboratory based DCT micro-tomography and 3D EBSD using automated serial sectioning will be leveraged to image polycrystalline microstructures that exhibit different scales, complex grain morphology and granulometries, as well as texture and correlation in space of the crystal orientations. Thanks to these new experimental methods, we aim to create the largest microstructure database in the world.

(ii) **Development of a diffusion based machine-learning framework** for synthetic and experimental polycrystalline structures (with transfer learning from the first to the second case)

(iii) **Model optimization** by investigating the more efficient way to generate polycrystals with correlated mechanical properties between grains, starting from a graph representation of the polycrystalline aggregate as a coarse vector for fast diffusion.

(iv) **Compare of the statistics of mechanical simulations** (with the FFT method) carried out on Voronoi-based polycrystalline structures as well as on experimental microstructures to that obtained when using the proposed AI-based microstructure generators.

How to apply

We are looking for highly-motivated Master 2 students in artificial intelligence or equivalent with excellent mathematical background, and the ability to work with a team. Please include in your application a CV, motivation letter, master grades and any relevant document (recommendation letters, engineering projects, articles etc.) to: francois.willot@minesparis.psl.eu, henry.proudhon@minesparis.psl.eu

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