Development of generative models for synthetic material microstructures

1 Digital materials

Machine learning approaches have become ubiquitous in material science and for characterizing and simulating microstructures, as a result of two main breakthroughs: (i) formidable advances in imaging techniques that allow sub-micron resolution, 3D, in-situ, non-destructive imaging, 3D+time etc. [1]; (ii) their ability to take into account realistic material images representing complex heterogeneous microstructures [2]; (iii) identifying patterns in images without making specific assumptions on the geometry or the probability distribution of shape or dispersion of heterogeneities, as is implicit in parametrized well-defined models from integral geometry [3, 4]. Furthermore, microstructures at the mesoscopic scale are essential in numerous applications for understanding, simualting or designing materials properties, or their reverse-design (see e.g. [5]). Applications include polycrystals, porous materials, nanomaterials, bio-sourced or additive manufacturing, which are especially sensitive to structures. This is due to our recognition that optimal properties in nature (or industry) are achieved by materials with heterogeneous structures [6].

Nevertheless, to account for the materials' complex behavior, e.g. nonlinear and irreversible phenomena, simulation tools using digital twins must incorporate key details of a material's microstructure (e.g. percolation, particle size distribution), whereas other geometrical features are not necesarily important w.r.t. the application. In granular materials for instance, the full-field strain and stress distribution depends on gaps or bottleneck regions in-between grains, much less on the exact shape of the grains [7]. As a consequence, in industrial applications, one must take into account physical or mechanical properties to train machine learning methods. This feature is essential in inverse homogenization approaches or optimal design problems where one seeks to explore the variability of microstructures and their properties. Despite their versatility, the development of variational auto-encoders (AE) and adversarial architectures (GANs) frameworks rest to a great extent on observational knowledge and numerical experiences. This emprirical approach remains essential in practice, yet it hampers efforts to justify or interpret

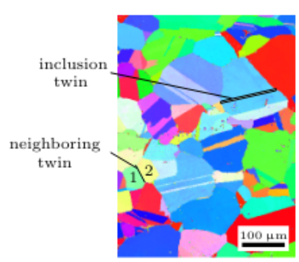

Figure 1: Electron backscatter diffraction (EBSD) scan of a γ-TiAl sample. Pairs of twin grains with different morphologies can be observed.

the good-behavior (or lack thereof) of machine learning pipelines – nothwistanding progress made on domains such as parcimonious neural networks and explainable models [8, 9].

2 Goal of the internship

The present project aims to develop and explore machine-learning neural networks adapted to the simulation of realistic material microstructures and conditional to their physical properties. To achieve this, we will use both experimental images as well as mathematicaly well-defined models from random set theory, that can be used to provide a large number of data sets.

The research program is centered around a set of images of two types of microstructures of different origins: grey-level tomography or 2D SEM images of porous cold-spray or anode materials (Fig. 1). These images are to be used in the project as demonstrators of the method. They represent multi-phase and porous materials with complex shape and structure and have been studied in previous works and used in widely-different applications.

The program will include the folloing steps:

- Collecting and processing images, generation of virtual 2D images using morphological models with few parameters (Boolean random sets or Gaussian excursions)
- Development of a diffusion based machine-learning framework consistant with the morphological models from the previsou task
- Generation of models with increasing complexity and training of the corresponding machine-learning framework
- (if time permits) Physical and mechanical characterization with FFT-based method. Assessment of the consistency of the ML framework w.r.t. the material properties.
- (if time permits) Analysis of the constraints for using 3D images in a supervised machine-learning frameworks

3 Students application

The research program will be undertaken in cooperation with the reasearchers who provided the images from the center of materials of Mines Paris and supervised by E. Decencière, F. Willot (Centre of Mathematical Morphology) and P. Kerfrdien (Center of Materials). The internship will be located in Fontainebleau, at the CMM laboratory and held for 6 months. The internship student will be paid by Ecole des Mines during the 6 months.

Please send your application with CV, master grades and any relevant document (recommendation letters, ingeneering project etc.) to `francois.willot@minesparis.psl.eu`

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