

Master thesis proposal

Simulation of Nanorod Assemblies and SAXS Pattern

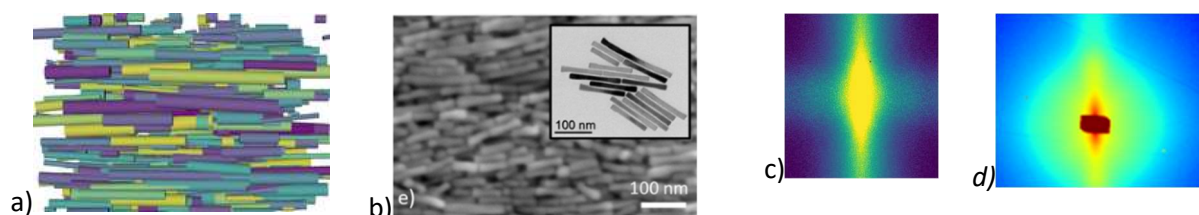
Keywords : nanorods, self-assembly, SAXS simulation, Fourier transform, voxelization, PyBullet, applied mathematics, computational materials science

SCIENTIFIC DESCRIPTION :

The internship will take place at **LPCNO (Laboratoire de Physique et Chimie des Nano-Objets)**, a research laboratory specialized in the **synthesis and exploitation of nanoparticles**, combining expertise in chemistry, physics and materials science. This project is part of the **PEPR Diadem Biman program**, which aims to develop **rare-earth-free miniature magnets with the support of artificial intelligence**.

These magnets are fabricated from assemblies of **magnetic nanorods aligned under an external magnetic field by magnetophoresis**; the degree of misalignment and packing fraction of the nanorods are key parameters controlling the final magnetic properties of the magnets.

Small-Angle X-ray Scattering (SAXS), both in lab and at synchrotron facilities, is the best technique. Indeed, it probes the structure and organization of nanomaterials at the mesoscale on a large volume. It provides access to structural information, such as nano-organizations, by analyzing images of scattered X-ray intensities.



*Fig1: a): Simulated nanorod assembly (Pybullet). b) Scanning Electron Microscope Image
c): Simulated SAXS (3DFFT). d) Experimental SAXS*

The project therefore aims to simulate assemblies of magnetic nanorods under external fields and to generate corresponding SAXS images. Starting from physical parameters (rod size, aspect ratio, misalignment, etc.), the nanorods are modeled and packed using finite-element modeling (PyBullet). The resulting assemblies are voxelized and analyzed in reciprocal space using 3D FFTs (fast Fourier transforms) to compute SAXS intensity patterns. Particular attention will be given to the influence of voxel resolution, apodization filters, and the number of rods on the resulting diffraction patterns.

This process will lead to the creation of a **machine-learning dataset** for predicting misalignment from experimental synchrotron images. This deep-learning approach enables high throughput analyses and therefore optimize strategy of experimental

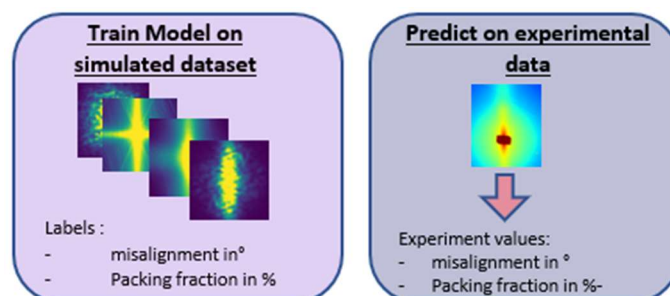


Fig2: Deep learning workflow

parameters for magnet fabrication. Algorithms such as 2D convolutional neural networks have already proven effective in processing SAXS images in a preliminary study.

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The internship will thus provide the student with hands-on experience in both numerical modeling of nanostructured materials and data analysis/AI techniques, contributing to the development of next-generation rare-earth-free miniature magnets.

Techniques/methods in use :

- Numerical simulation of nanorod assemblies (PyBullet physics engine)
- Voxelization and 3D Fourier transforms (NumPy, SciPy)
- SAXS pattern generation and analysis (FFT-based projection methods, apodization)
- Statistical analysis of orientation and order parameters
- Machine learning dataset construction
- Deep learning predictions

Applicant skills :

Background in physics, materials science or applied mathematics; familiarity with python programming; interest in nanostructures and diffraction/diffusion techniques; basic coding skills in Python (NumPy/SciPy).

Internship supervisor(s) :

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Internship location :

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