IA Cluster ENACT
AMI Thèse IA – Lorraine Nord

PhD position – full time – starting oct. 2025

Generative Machine Learning for Microstructure Design: An Atomic-Scale-Informed Approach to Interfacial Engineering

Supervision

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Keywords

Generative Adversarial Networks, deep learning, grain boundaries, dislocations, mechanics, plasticity, metals

Context

The LEM3 laboratory (Laboratoire d'Étude des Microstructures et de Mécanique des Matériaux: Laboratory of Study of Microstructures and Mechanics of Materials) is a joint research center of the Université de Lorraine, the French National Center for Scientific Research (CNRS), and the engineer school Arts et Métiers. LEM3 is one of the largest research institutes for the physics of materials and engineering in France. It is located in Metz, near the tripoint along the junction of France, Germany, and Luxembourg, and forms a central hub for science in Europe. Over 250 scientists from France and around the world work at LEM3 to perform world-class research in materials science, mechanics, and processes. By conducting both fundamental and applied research, researchers at LEM3 work on long-term solutions for the major challenges facing society, industry, and science. The PhD student will join a team of experienced dynamic researchers from diverse background, including Julien Guénolé (CR CNRS), Stéphane Berbenni (DR CNRS) and Lionel Germain (Prof. UL), with a proven track record in using Artificial Intelligence for material and mechanical engineering (1–5). The selected candidate will have access to multiple high performance computing resources provided by GENCI (https://www.genci.fr/), EXPLOR (https://explor.univ-lorraine.fr/), CASSIOPÉE (https://artsetmetiers.fr/fr/cassiopee-plateforme-hpc) and ENACT (https://cluster-ia-enact.ai/). This PhD offer is provided by the ENACT AI Cluster and its partners. **Application by June 18th, 2025: https://doctorat.univ-lorraine.fr/en/node/100030373**

Summary of the PhD project

Inorganic materials are essential across industries due to their versatile properties, and understanding their mechanical behavior—especially plastic deformation—has been a

key pursuit in materials science. However, the prediction of their mechanical response remains to date a challenge for state-of-the-art modelling approaches, especially for advanced engineering materials that contains a large proportion of interfaces (e.g. grain boundaries…) at various length scales. Indeed, existing models often neglect interface-specific atomic details, severely limiting the ability to predict the mechanics of interface dominated materials. To address this, we envision a data-driven multiscale approach using local defect density fields (Nye dislocation) within an established and highly efficient continuum mechanics framework (Field Dislocation Mechanics), to bridge atomic-scale simulation data and meso-scale continuum models. Within this broader context, this PhD project focuses on the machine learning (ML) generation of the nanostructures of interfaces and defects (dislocations), based on data from classical atomistic simulations.

Atomistic simulations are ideal for modeling interfaces at atomic resolution across various materials, making them central to the generation of the data employed in this project. As we emphasize method development over material specificity, aluminum is chosen for its well-characterized plasticity and available interatomic potentials. The model could be however assessed on more complex materials, like magnesium alloys. Carefully designed simulation setups will control interface and dislocation features, enabling exploration of numerous defect configurations. This will generate the extensive and reliable data required to train the ML model at the heart of this project. The “G-method” recently developed in the team (6), will bridge atomistic results to continuum models via Nye dislocation density tensors, and ultimately provide the data.

The core objective of this PhD project is to enable the generation of defect density fields able to describe material interfaces with atomistic precision thanks to the use of generative ML approaches. More precisely, the prediction of Nye dislocation fields associated with any combination of defects, i.e. interface or/and dislocation. We intend to design and train a data-driven model able to handle the complexity of such configuration space and to generate the required fields.

An excellent candidate for such task is the Generative Adversarial Network (GAN), which is a deep learning approach able to generate data already successful in generating microstructures (7–9). In brief, a GAN is composed of two ML models trained simultaneously and competing through a Nash equilibrium: the generator produces data representing the training dataset and the discriminator distinguished between the data that has been generated and the real one. Original GAN are prone to known issues (mode collapse, vanishing gradient…), which are however widely addressed in the literature by alternative architectures, such as WGAN or CycleGAN. An additional aspect specific to this project is that physical laws governing the generated training data are known (periodicity, equilibrium, etc.). By integrating them within the training dataset or the loss function being minimized during training, we would obtain a physics-informed ML approach that will facilitate the training of the GAN (10).

The expected outcomes of this PhD project are: (i) establish a GAN architecture able to generate defect density fields of interfaces, and (ii) enlighten on the role of interfacial

characteristics on the plasticity in advanced engineering materials. The deep learning approach developed in this PhD project will enable an unprecedented paradigm in multi-scale material modeling and establish a foundation for physics-based interface engineering in crystalline materials.

Profile and skills required

The candidate must have:

- Strong background in Computational science, Material Science, Mechanics, Physics, or equivalent.
- Good background in statistical analysis.
- Good knowledge and programming skills in Python.
- Previous experience in atomistic simulations, molecular dynamics simulations or machine learning, including generative deeplearning technics will be considered as an extra merit.
- The application should include a statement of research interest, a CV with the names of two people to contact for a recommendation, a list of publications and other relevant materials, if available.
- Have exceptional written and verbal communication skills.

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