PhD position

Advanced FFT-based crystal plasticity framework for microstructure-sensitive mechanical behaviors

Context and description

The present PhD proposal is part of the project **AMMETIS**[1] (AI-assisted Simulations of Microstructure driven Mechanical properties from high Throughput and multiscale analysIS), in the framework of **PEPR DIADEM**[2], which aims to develop an advanced characterization platform for innovative materials by combining advanced experimental techniques, physics-based mesoscopic modeling, and artificial intelligence. Within this context, high-throughput experiments will provide detailed information on local deformation mechanisms at the microscale, while numerical simulations and data-driven approaches will enable the development of predictive models capable of linking microstructural features to macroscopic mechanical behavior.

The objective of this PhD project is to develop advanced mesoscopic crystal plasticity models capable of capturing microstructure-dependent plastic deformation mechanisms. Classical crystal plasticity models provide a powerful framework to describe anisotropic plasticity in crystalline materials, but they rely on local constitutive laws that cannot fully capture key physical phenomena such as strain localization, dislocation accumulation near interfaces or influence of microstructural length scales. To overcome these limitations, the project will focus on the development of non-local crystal plasticity formulations incorporating internal length scales associated with dislocation structures and microstructural interfaces (like grain boundaries).

Based on recent developments by the project team regarding advanced crystal plasticity models, different modeling strategies will be explored, including strain gradient plasticity [1,8,9], micromorphic approaches [2], and mesoscale field dislocation mechanics [3-5]. The proposed models will be calibrated and validated using high-resolution experimental measurements obtained within the AMMETIS project, including HR-DIC, HR-EBSD and nanoindentation mapping, providing detailed information on strain localization, lattice rotations and local mechanical properties.

The developed models will be implemented in AMITEX-FFT [6,7], a massively parallel FFT-based simulation platform for polycrystalline plasticity, enabling efficient simulation of the mechanical response of realistic 3D microstructures. These simulations will be used to generate a large database

[1] https://www.pepr-diadem.fr/projet/ammetis-2/
[2] https://www.pepr-diadem.fr/

linking microstructural descriptors to macroscopic mechanical behavior. This database will be used for the development of AI-based surrogate models enabling fast prediction of material properties at the structural scale within the AMMETIS framework.

Overall, this PhD project aims to contribute to the development of next-generation predictive tools capable of linking microstructure, deformation mechanisms and mechanical performance, ultimately enabling more efficient design and optimization of advanced structural materials.

Required skills

- Master’s degree (or equivalent) in Mechanical Engineering, Materials Science Engineering, Applied Mathematics or Computational Mechanics.
- Solid background in continuum mechanics and advanced plasticity modeling
- Strong interest in micromechanics and microstructure-based modeling
- Experience with numerical methods for PDEs
- Programming skills in Python (knowledge of C++, Fortran or HPC is a plus)
- Scientific curiosity and critical thinking
- Ability to work in interdisciplinary environments
- Motivation for collaborative academic-industrial research

Starting date, duration and location of the PhD

The PhD position is available starting in September 2026 (flexible date). The research will be conducted primarily at LEM3 (Laboratoire d’Études des Microstructures et de Mécanique des Matériaux), Metz, in collaboration with CEA (Commissariat à l'énergie atomique et aux énergies alternatives), Saclay, and PIMM (Laboratoire Procédés et Ingénierie en Mécanique et Matériaux), Paris. The duration of the PhD is three years, with a gross salary of around € 2300 per month.

Application

Applications (including a CV, transcripts of Master’s years 1 and 2 (or equivalent), a cover letter describing the candidate’s interests and skills related to the proposed PhD topic, the contact details of two academic referees, and, if possible, two letters of recommendation, all compiled into a single PDF file) should be sent to:

- Mohamed Jebahi (mohamed.jebahi@ensam.eu)
- Stéphane Berbenni (stephane.berbenni@univ-lorraine.fr)
- Lionel Gélébart (lionel.gelebart@cea.fr)

References

[1] Amouzou-Adoun, Y. A., Jebahi, M., Forest, S., & Fivel, M. (2024). Advanced modeling of higher-order kinematic hardening in strain gradient crystal plasticity based on discrete dislocation dynamics. Journal of the Mechanics and Physics of Solids, 193, 105875.

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[3] Berbenni, S., Taupin, V., & Lebensohn, R. A. (2020). A fast Fourier transform-based mesoscale field dislocation mechanics study of grain size effects and reversible plasticity in polycrystals. Journal of the Mechanics and Physics of Solids, 135, 103808.

[4] Berbenni, S., & Lebensohn, R. A. (2021). A numerical study of reversible plasticity using continuum dislocation mechanics. Comptes Rendus. Physique, 22(S3), 295–312.

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[6] Gélébart, L. (2024). FFT-based simulations of heterogeneous conducting materials with combined non-uniform Neumann, periodic and Dirichlet boundary conditions. European Journal of Mechanics - A/Solids, 105, 105248.

[7] Gélébart, L. (2025). An accurate and robust FFT-based solver for transient diffusion in heterogeneous materials. Comptes Rendus. Mécanique, 353(G1), 113–125.

[8] Jebahi, M., & Forest, S. (2023). An alternative way to describe thermodynamically-consistent higher-order dissipation within strain gradient plasticity. Journal of the Mechanics and Physics of Solids, 170(September 2022), 105103.

[9] Marano, A., Gélébart, L., & Forest, S. (2021). FFT-based simulations of slip and kink bands formation in 3D polycrystals: Influence of strain gradient crystal plasticity. Journal of the Mechanics and Physics of Solids, 149(January), 104295.