PHD THESIS PROPOSAL

Full field modeling of crystal plasticity in crystal improved miniaturized metallic components

Start: Fall 2024

Research Lab: GeM, UMR CNRS 6183 Institut de Recherche en Génie Civil et Mécanique

Location: Nantes, Saint-Nazaire

Keywords: computational mechanics, plasticity, multi-scale modeling, FFT-based methods, multicrystals

CONTEXT

The necessary contribution of transport, energy or electronics industries to sustainable development drives them to lighten structures and/or reduce the dimensions of their parts, particularly in terms of sheet thickness, but also to use materials with a mechanical behavior remaining efficient, even when they are miniaturized. However, a dramatic degradation of mechanical properties is observed during dimensional reduction [Hall 1951, Petch 1953, Thompson et al. 1973, Miyiazaki et al. 1979, Dubos et al. 2013]. The ambition of the MOCAMOR ANR project, within which this PhD thesis is proposed, is to remove these hindrances by an original approach and methodology combining experiments and modeling.

To do so, a Physical Vapor Deposition (PVD) method is proposed to coat a material on a substrate with the same chemical composition (deposit thickness in the order of one micron on a sheet with only few grains in its thickness) in order to restructure the sub-surface area of the substrate by a gradual evolution of this type of deposit [Dubos et al. 2022]. The challenge of MOCAMOR is to understand the physical mechanisms of the plastic deformation taking place in the newly generated subsurface zone. A particular attention will be paid to the film/substrate interfacial zone with the aim of restoring the mechanical performances of polycrystals to multicrystalline materials.

OBJECTIVES

During this thesis, a full-field numerical model of non-local crystal plasticity [Gurtin 2002, Evers et al. 2004a,b] will be implemented. This tool will allow to obtain a better understanding of mechanisms acting at the intragranular level (i.e. within the dislocation microstructure) in terms of stress heterogeneities and dislocation densities, which will, in turn, allow to evaluate the contribution of PVD surface deposits on the confinement of dislocation structures.

This model will be based on the description of plastic strains generated by dislocations gliding on slip systems. It will predict the evolution of dislocation densities, while enabling to distinguish between dislocations resulting from homogeneous plastic deformation accommodation by mutual trapping process (SSD) and geometrically necessary dislocations which accumulate in plastic strain gradient fields to maintain the strain compatibility across microstructures (GND) [Evers et al. 2004].

WORK PLAN

In order to simulate the behavior of polycrystalline and multicrystalline sheets, numerical samples will be generated, accounting for the size, geometry, crystal orientation, and distribution of grains.

The aim of this model is to understand the softening mechanisms occurring within the material by investigating the distribution of stresses and SSD / GND dislocation densities while considering the surface microstructure of the deposits. The microstructure description of the sheets with and without the PVD deposit will benefit from experimental SEM and XRD observations at the granular level carried out by members of the project.

A non-local model of crystal plasticity [Gurtin 2002, Evers et al. 2004a,b] will be implemented in a Fast Fourier Transform (FFT) based solver. FFT-based methods constitute an interesting alternative to finite elements, especially in the context of gradient plasticity, as illustrated in [Berbenni et al. 2014, Lebensohn and Needleman 2016, Marano et al. 2021, Zecevic et al. 2023].They indeed allow handling of up to several billions of unknowns thanks to a matrix-free resolution and a good scalability for high performance computing (HPC). Complex microstructures and property gradients can easily be treated by FFT (no meshing issues). In this thesis, we thus propose to implement such a FFT-based numerical model, building upon existing in-house codes for computational plasticity and FFT solvers. A particular attention will be payed to the handling of free edge effects, through the introduction of a layer of gas-filled voxels at the edge of the simulated sample and appropriate treatment of the non-local terms [Zecevic et al. 2023].

In order to understand the origin of the impediment to the dislocation motion by the microstructure of the deposits, simulation results will be compared to an electron microscopy characterization of the structures (stacking length, cell size, wall density) that will be carried out post mortem by members of the project, near the surface zones and in the core of pre-strained specimens, at different steps characteristic of work hardening stages. Additional experimental results will consist in nanoindentation analyses, achieved through the specimen thickness in order to ensure their accuracy. Thanks to quantitative gradient analyses, the improvement of macroscopic mechanical properties, generated by PVD deposition onto multicrystalline structures, will be explained combining these state-of-the-art microstructural analyses and simulations.

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FINANCIAL CONTEXT

This thesis is part of the MOCAMOR ANR project (2024-2028, N° ANR-23-CE08-0036-01) involving 1) the manufacturing of multicrystals and two-sided coatings manufactured with different strategies 2) the mechanical and microstructural characterization of coated multicrystals combined with an analytical work hardening modeling 3) the full field modeling of crystal plasticity considering the sheet microstructures. To fulfil this project, two Master students, two PhD students (starting fall 2024) will be recruited. The applicant will be able to take advantage of the new regional supercomputing facility Glicid and the concomitant experimental PhD work of a second thesis.

Required skills

- Highly motivated by scientific research, serious, curious
- Continuum mechanics, Numerical modeling, Constitutive laws, Computer Programming (python/julia/c++), Multi-scale modeling

Application should be made online at:

https://questionnaires.univ-nantes.fr/index.php/769348

with the following enclosed documents:

Letter of application

CV

Diplomas and transcripts

Letter(s) of recommendation

Additional information

Duration of the thesis: 36 months

Gross salary per month: 2250 € (Net salary >1850€)

PhD supervisor	**Co-supervisors**	
STAINIER Laurent Phone: (+33)2 40 27 35 86 laurent.stainier@ec-nantes.fr	**BIGNONNET François** Phone: (+33)2 49 14 22 24 francois.bignonnet@univ-nantes.fr	**GLOAGUEN David** Phone: (+33)2 72 64 87 67 david.gloaguen@univ-nantes.fr