Internship MASTER 2/Bac+5 Materials & Mechanics

Academic Year: 2023-2024

Supervisors

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Location of internship

GeM, Institute of Civil Engineering and Mechanics :

- Centrale Nantes (Nantes)
- Nantes Université (Heinlex, Saint-Nazaire)

Title: FFT based full field modeling of crystal plasticity in multi-crystal metallic sheets

Description of the subject:

CONTEXT: The necessary contribution of transport, energy or electronics industries to sustainable development leads 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 internship 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 subsurface 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 giving back to multicrystalline materials the mechanical performances met for polycrystals.

OBJECTIVES: During this internship, a full-field numerical model of crystal plasticity 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.

Fast Fourier Transform (FFT) methods constitute an interesting alternative to finite elements, especially in the context of gradient plasticity, as illustrated in [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), together with a native handling of field gradients. In this internship, we thus propose to implement such a FFT-based numerical model, building upon existing in-house codes for computational plasticity and FFT solvers. Complex microstructures and/or property gradients can easily be treated by FFT (no meshing issues).

FINANCIAL CONTEXT: This internship is part of the MOCAMOR ANR project (2024-2028) 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 candidate will have the opportunity to apply to one of these PhD thesis.

REFERENCES

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Keywords

multicrystals, computational mechanics, plasticity, multi-scale modeling, fast Fourier transform

Required skills

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

Additional information

Duration of the internship: 6 months
Internship scholarship: Yes
Amount: In accordance with the French legislation
PhD opportunity after this internship: YES (ANR project)
Other useful information (housing, …)?
Possibility to provide a financial help regarding traveling costs during the internship

Application procedure

Online application : no application by e-mail, fill the online form
https://questionnaires.univ-nantes.fr/index.php/737823?lang=en
with cover letter, curriculum, grades of the past 2 years, recommendation letter
Application deadline : February 4th, 2024
Interviews and selection : mid-February 2024
Internship starting date : March 11th, 2024