Call for 2 PhD candidates

Summary of the positions and institute

- Two 3-year PhD positions in the MoSES group
- Thesis director: Prof. Manas V. Upadhyay
- Affiliation: Solid Mechanics Laboratory (LMS), CNRS, Ecole Polytechnique, Institut Polytechnique de Paris
- Funding: European Research Council (ERC) Starting Grant 2020 project G*AM*MA (ID 946959)
- Expected start date for both positions: September 1, 2021

Ecole Polytechnique is one of the most prestigious public institution of higher education and research in France. It was established in 1794, during the French revolution, by the mathematician Gaspard Monge. Among its alumni are 3 Nobel prize winners, 1 Fields Medalist, 3 Presidents of France and many CEOs of national/international companies.

LMS is a joint research unit between the Ecole Polytechnique and the French national research center (CNRS). Research at LMS integrates experimental studies as well as mathematical and numerical modeling of mechanical and multi-physics behavior of materials and structures over a wide range of spatial and temporal scales.

MoSES stands for **Mo**deling **S**imulations and **E**xperimental **S**ynergy. The MoSES group was established by Prof. Manas V. Upadhyay at the LMS. It strives at (i) developing synergies between theoretical models, numerical simulations and advance experimental characterization, to understand the multi-scale behavior of materials, specifically metals and alloys, and (ii) using the knowledge gained to engineer materials with desired properties.

General context of your projects

Additive manufacturing (AM) holds the potential to revolutionize the alloy manufacturing sector through its ability to provide unprecedented control over design of alloy microstructures while building parts. However, the main roadblock preventing its widespread adoption is the inability to design microstructures with desired mechanical response. AM results in the formation of hierarchical microstructures that are extremely sensitive to its process parameters. Minor changes to these parameters can result in very different microstructures that exhibit significant differences in their mechanical response. Controlling the mechanical response requires first understanding microstructure formation during AM. Current experimental and modeling research efforts are heavily focused on studying the role of melt-pool dynamics and rapid solidification during the AM process. Project G*AM*MA aims at tackling the crucial missing link (Fig. 1), which is the microstructure evolution occurring during the long period after solidification and till the end of an AM process, i.e. during Solid-State Thermal Cycling (SSTC), at varying temperature rates and amplitudes.

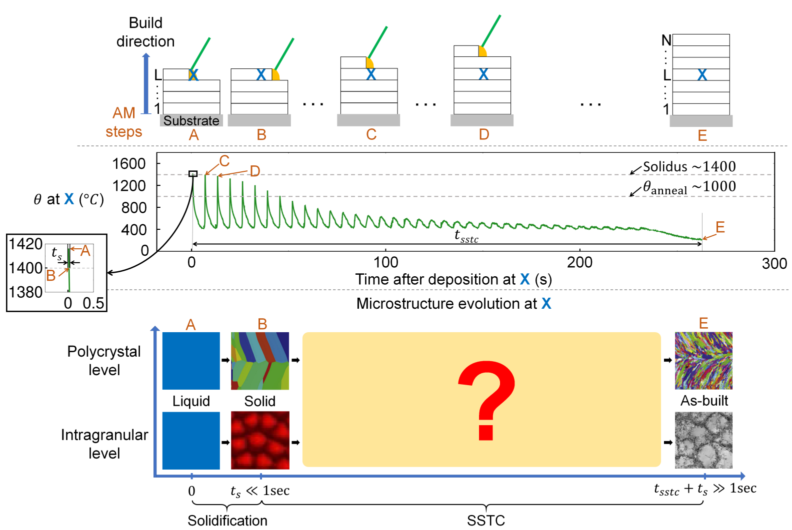

Figure 1: Crucial gap in the current understanding of microstructure formation during an AM process. (Some microstructure snapshots are adapted from Francois et al., Morris Wang et al. and Takaki et al.)

Project 1: Modeling thermally driven dislocation dynamics during alloy additive manufacturing

Dislocations are line-type crystalline defects [1] that are present in all metals and alloys. They are the primary carriers of plastic deformation in all metals and alloys and they have a first order effect in determining the mechanical response of these materials. They are also a primary source of residual stresses in materials.

During alloy AM, dislocations can be formed due to rapid solidification in order to accommodate any lattice mismatch occurring between growing dendrites or grains. Then, during initial stages of SSTC, dislocations can also be generated due to the large thermal stresses formed due to the rapid cooling-heating cycles (Fig. 1). In addition, these thermal stresses can result in dislocation motion and interaction with other dislocations and defects such as precipitates. During later stages of SSTC, where a nearly steady-state response is obtained (Fig. 1), recovery mechanisms can result in dislocation annihilation. All the dislocation-based mechanisms that occur during SSTC can bring about significant changes to the microstructure, which can severely impact a material's mechanical response [2].

In order to engineer AM alloys that exhibit desired mechanical properties, it is crucial to first understand the different type of mechanisms that could occur during the fabrication process. Currently, most research efforts are focused on understanding microstructure formation during rapid solidification. While this is important to study, it is far from being sufficient to understand the microstructural features observed at the end of the AM process.

In this project, your focus will be on understanding what happens to the dislocation microstructure during rapid/gradual SSTC. In order to do this, you will implement a state-of-the-art dislocation dynamics model developed by Upadhyay [2] into a Finite Element (FE) framework. This novel model, known as the Thermal Field Dislocation Mechanics (T-FDM) model, strongly couples the isothermal field dislocation mechanics model with the heat conduction theory. It allows studying dislocation dynamics during any non-isothermal process, e.g. (i) SSTC during AM, (ii) quenching of alloys during conventional processing or post-processing, (iii) cooling of welds, etc.

Your tasks are as follows:

- Develop the theory for the numerical implementation for the T-FDM model in a FE framework
- Implement the T-FDM-FE model inside the "FEniCS" FE tool
- Perform simulations using the T-FDM-FE model and analyze the results
- Collaborate with a national/international team of researchers
- Write and publish scientific articles in relevant journals
- Present your research at national and international conferences
- Write and successfully defend your PhD thesis at the end of the project

References:

[1] D. Hull and D. J. Bacon, Introduction to Dislocations, *Elsevier Ltd.* (2005) 5th Edition.

[2] M. V. Upadhyay, On the thermo-mechanical theory of field dislocations in transient heterogeneous temperature fields, *Journal of the Mechanics and Physics of Solids*, 145 (2020) 104150.

Your profile for project 1

Necessary

- A Master's degree (Bac+5, for French applicants) in Mechanical Engineering or equivalent. Interested candidates graduating before June 1, 2021 can also apply.
- Strong background in continuum mechanics and FE modeling and simulations.
- Background in mathematics, specifically in solving partial differential equations.
- Programming skills in at least one of the following computer languages: Fortran, Python or C++.
- Good communication (oral and written) skills in English.
- You should be able to work independently as well as in a team. You enjoy working on challenging problems. You should be able to think critically, work diligently and rigorously, and present your ideas in a logical manner.
- You enjoy working in a multi-disciplinary team having an international background.

Not necessary, but a plus

- Experience in using FEniCS.
- Research experience and ability to write scientific manuscripts (demonstrated via e.g., master's thesis, article(s) published in scientific journal(s)).
- Experience in the field of metal/alloy AM.

Project 2: X-ray synchrotron and electron diffraction and microscopy to probe microstructure evolution during additive manufacturing

During alloy AM, just after the interactions between a heat-source (laser or electron beam) and feedstock (powder or wire), the feedstock material is melted and experiences complex melt-pool dynamics and rapid solidification. These highly non-equilibrium processes result in the creation of a metastable hierarchical microstructure that exhibits physical and chemical heterogeneities at multiple length scales; depending on the type of alloy, these heterogeneities can be precipitates, microsegregations, dislocation structures, twins, columnar grains, strong texture at the polycrystalline level, multiple crystalline phases, etc., depending on the type of alloy.

Then, during the rest of the AM process, this material microstructure is subjected to multiple heating-cooling cycles at different temperature amplitudes and rates i.e., SSTC (Fig. 1). In the initial stages of SSTC, where fast temperature rates and high temperature amplitudes are encountered, strong thermal stresses can be generated. The resulting thermo-mechanical forces can drive a plethora of microstructure evolution mechanisms such as precipitate evolution, dislocation structure evolution, recrystallization, phase transformations, etc., which manifest as evolution of internal stresses, texture, morphology, dislocation density, etc. During later stages of SSTC, the nearly steady-state heat conduction at elevated temperatures results in mechanisms such as precipitation, recrystallization, grain growth, recovery, etc., which manifest in the form of evolution of internal stress, texture, morphology, dislocation density, etc.

X-ray synchrotron diffraction can be used to probe microstructural evolution in-situ during a process such as mechanical loading to obtain volume averaged information on the evolution of lattice strain, dislocation density, texture, phase transformation, etc. X-ray synchrotron microscopy can be used to obtain volume averaged information on the evolution of phases that demonstrate strong absorption contrast. Meanwhile, Scanning Electron Microscopy (SEM) is a surface probing technique that provides information on evolution of the crystallographic orientation, grain morphology, geometrically necessary dislocations, etc. Transmission Electron Microscopy (TEM) provides information at higher resolution and lower length scales than SEM on thin lamellae.

In this project, the objective is to study microstructure evolution due to SSTC during AM using the aforementioned techniques on different material systems, specifically, Fe-based and Ni-based alloys.

Your tasks are as follows:

- Perform x-ray synchrotron and electron diffraction and microscopy experiments to study microstructure evolution due to SSTC during AM.
- Process and thoroughly analyze the experimental data.
- Collaborate with a national/international team of researchers.
- Write and publish scientific articles in relevant journals.
- Present your research at national and international conferences.
- Write and successfully defend your PhD thesis at the end of the project.

Your profile for project 2

Necessary

- A Master's degree (Bac+5, for French applicants) in Mechanical Engineering, Materials Engineering, Materials Science and Engineering or Physics. Interested candidates graduating before June 1, 2021 can also apply.
- Strong background in diffraction theory and mechanics of materials.
- Programming skills in at least one of the following computer languages: Python, FORTRAN or C++.
- Good communication (oral and written) skills in English.
- You should be able to work independently as well as in a team. You enjoy working on challenging problems. You should be able to think critically, work diligently and rigorously, and present your ideas in a logical manner.
- You enjoy working in a multi-disciplinary team having an international background.

Not necessary, but a plus

- Experience in using LabView.
- Research experience and ability to write scientific manuscripts (demonstrated via e.g., master's thesis, article(s) published in scientific journals).
- Experience in the field of metal/alloy AM.

Application procedure: Deadline 1 April 2021

You are requested to apply for only one position.
Your application will be treated immediately upon receipt.
You are encouraged to not wait until the day of the deadline before applying.

Interested applicants that **fulfill all the necessary criteria**, please send an email to recruitment.ercgamma@gmail.com with the following

- subject line mentioning one of the following:
  - Application for Project 1: Modeling and simulations

  OR
  - Application for Project 2: Experiments
- A 1-page motivational letter
- An up-to-date and detailed CV
- Contact information of at least 2 referees willing to provide recommendation letters on your behalf

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Manas V. Upadhyay, Ph.D.
Assistant Professor
Laboratoire de Mécanique des Solides (LMS), CNRS UMR 7649
Ecole Polytechnique, Institut Polytechnique de Paris
Route de Saclay, 91128 Palaiseau Cedex, France

Website: https://www.manas-upadhyay.com

Other links:
https://portail.polytechnique.edu/lms/en
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