Labex INTERACTFS (https://labex-interactifs.pprime.fr/)

2022 Projet Proposition d'un module de cours à destination des doctorants

I. Informations générales :

Etablissement d'accueil ***Institution***	**X UP** ☐**ENSMA**
TITRE du cours en français ***French title***	**LA METHODE PHASE-FIELD EN SCIENCE DES MATERIAUX : CONCEPT ET APPLICATIONS**
TITRE du cours en anglais ***English title***	**THE PHASE-FIELD METHOD IN MATERIAL SCIENCE: CONCEPTS AND APPLICATIONS**
Enseignant ***Teacher***	Roberto BERGAMASCHINI **Tel :** +390264485233 **Email :** roberto.bergamaschini@unimib.it

Jours	Horaire	Salle
Sept 26th	14.30-16.30	remote
Sept 29th	14.30-16.30	remote
Oct 3rd	14.30-16.30	remote
Oct 6th	14.30-16.30	remote
Oct 10th	14.30-16.30	remote
Oct 13th	14.30-16.30	remote

II. Brève description du cours proposé

- All teaching will be in English.

The Phase-Field method is nowadays regarded as one of the most powerful approaches for the modelling and simulation of complex microstructure and interface dynamics in multi-phase and multi-component systems, with a wide impact in Materials Science and Engineering. In this introductory course an overview of the method is presented from an applied perspective. The main objective of this lecture will be to teach students how the Phase-Field method can be used for studying problems of relevance on materials structure and properties, as due to diffusion and phase-transformation dynamics across interfaces and free-surfaces. To this purpose, the different topics will be supported by examples from the literature. Also, practical sessions with basic information on coding (in python) simple, demonstrative examples will be proposed so that students could eventually try themselves.

In the first part of the course, the key concepts at the foundation of the Phase-Field approach will be explained both from a physical and a mathematical point-of-view. Basic information about the numerical methods to be used for the model implementation will also be provided. Then, lessons will focus on the application of the Phase-Field method to the dynamics of solid phases and interfaces in-between, dealing with phase-transitions, elastic effects and polycrystalline structures. The peculiar case of free-surfaces and epitaxial growth will also be discussed. Finally, the intriguing approach of Phase-Field Crystal, moving

Phase Field closer to the atomistic scale by accounting for the periodic structure of the crystal, will be reviewed. A list of lesson topics divided by hours follows:

1. General concept of Phase Field - physics
2. General concept of Phase Field - mathematics
3. Basic models: Cahn-Hillard vs. Allen-Cahn dynamics
4. Numerical approaches and examples
5. Phase-transitions: solidification
6. Phase-transitions
7. Elasticity and modelling of stress effects
8. Polycrystalline structure
9. Epitaxial growth and free surfaces
10. Phase-Field Crystal
11-12. Practical sessions

During the practical sessions, simple examples of Phase-Field codes will be implemented in python. The activity will be set according to the students' interest in the most interactive way, offering them the possibility to try implementing parts of the code or simply follow the teacher guidance.