36 Months PhD Position:

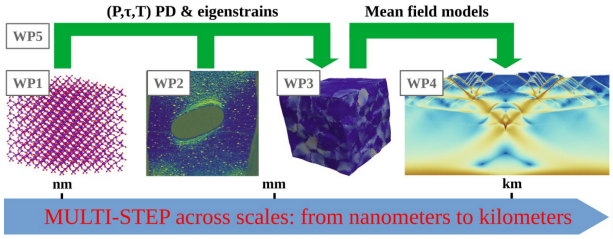
Stress-driven Thermodynamic Equilibrium Predictions

Phase transformations (PT) shape the formation of rocks and determine the mechanical properties of many engineered materials, making them a key area of research in both Earth Science and Metallurgy. When subjected to changes in environmental conditions such as pressure or temperature, rocks and metals undergo PTs to achieve thermodynamic equilibrium.

The mineral phases can be used to trace significant geodynamic processes, such as orogenesis, rifting or subduction. In metallic materials, the development of multiple phases is critical for optimising performance and is an important ingredient in the design of high performance parts in aeronautics, energy, transport and in a variety of other domains.

PT in metals and minerals depend both on temperature and pressure. Phase diagrams, function of pressure and temperature, exist for many materials and allow to know the stable phase of the material for given pressure and temperature conditions. Experimental evidence suggest that plastic strain and stress (deviatoric) might induce a change on the phases stability. The **MULTI-STEP: Multiscale Stress-driven Thermodynamic Equilibrium Predictions** project, involving multiple French and German research laboratories, aims at understanding the effect of deviatoric stress on the phase equilibrium of titanium and silica.

To overcome the classical hypotheses for phase equilibrium calculations using a multiscale numerical approach, from atomistic to large-scale thermomechanical modeling, coupled with micromechanical experiments. Atomistic simulations are optimal tools to compute free energies and infer phase diagram under varying thermomechanical conditions (e.g. deviatoric stress). The methodology will first be developed for the study of PTs in titanium. Then the proposed approach will be applied to the polymorphic quartz-coesite transformation.



MULTI-STEP: Multiscale Stress-driven Thermodynamic Equilibrium Predictions.

Proposed work

In the proposed PhD Position, we will develop a numerical technique that integrates PTs obtained using atomistic simulations into a continuum mechanics framework that accounts for the material microstructure. In essence, we will use the full field mesoscopic tools available at CEMEF to compute the thermomechanical state variables (pressure, temperature, and deviatoric stress) that drive the PT.

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Atomistic simulations are a valuable tool for predicting PTs and for different thermo-mechanical conditions. These simulations enable the calculation of the Gibbs free energy, which can then be used to drive mesoscopic simulations involving phase transformation. A weak coupling between PT and the mechanical balance will be implemented. In this way, we will be able to determine the driving force for PT, we will use the local state variables fields. Two key components are necessary: (i) nucleation criterion & (ii) PT grain boundary migration driving force.

The developed numerical framework will then be used to obtain a homogenization model that can be used at larger scales and that allows to capture the impact of thermo-mechanical conditions (pressure, temperature, and deviatoric stress) on mechanical behavior of the material.

The developments will be carried out using the in-house numerical library developed at CEMEF which is written in C++ and uses distributed memory parallelism (MPI).

Candidate profile

The candidate must hold a Master's degree or an Engineering diploma (or equivalent) in computational mechanics, high performance computing, material science, or a closely related field. The candidate should demonstrate a strong interest in numerical modeling and programming within a high-performance modeling environment.

Partners

The proposed PhD project takes within the ANR Funded project **MULTI-STEP** in collaboration with the University of Potiers, The University of Heidelberg, Goethe University Frankfurt and **Mines Paris**.

The student will be hosted at CEMEF (Mines Paris) in Sophia-Antipolis in the French Riviera. The international nature of the project will give the student the opportunity to spend time in the research laboratories involved in the project in France and Germany.

International Research Collaboration Project