Master thesis and PhD proposal 2026

Quantifying the effect of deviatoric stress on phase equilibrium, a multiscale approach in a geodynamic perspective

Keywords: atomistic simulations, phase equilibrium, free energy, Earth's Sciences

Scientific description:

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. In minerals, investigation of mineral assemblages provides essential insights into their conditions of formation. The mineral phases can indeed be used to trace significant geodynamic processes, such as orogenesis, rifting or subduction. In metallic materials, the development of multiple phases is critical for optimizing performance and is an important ingredient in the design of high performance parts in aeronautics, energy, transport, and plenty of other domains. The theory behind the aforementioned PTs relies on the assumption that the stress has the same effect on phase equilibrium as equivalent hydrostatic pressure, meaning the effects of deviatoric stress are neglected. Such hypothesis, however, have recently triggered discussions in both Earth science and Metallurgy. In fact, there are now several experimental results that show non-trivial relation between mechanical pressure and mineral reactions [1], including the quartz/coesite transformation [2], a PT emblematic of Earth's Science. Similarly, the α/ω transformation of titanium has been shown to be influenced by the applied stress [3].

The master internship and PhD thesis will take place at PPRIME Institute (Poitiers, France) in the context of the international ANR project MULTI-STEP: Multiscale Stress-driven Thermodynamic Equilibrium Predictions, in collaboration with the Centre de Mise en Forme des Matériaux (Mines-ParisTech, Sophia Antipolis, France), the Heidelberg University (Germany) and the Goethe University (Frankfurt, Germany). This project aims at understanding the effect of deviatoric stress on the phase fraction equilibrium of titanium and silica. It proposes 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 (see figure below).

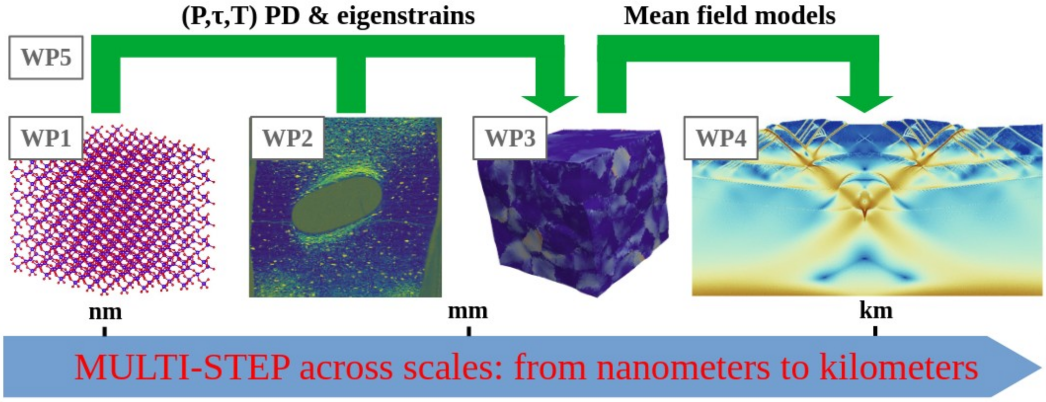

Figure: the different work packages (WP) of the MULTI-STEP project and their interactions.

The master internship and PhD thesis will mostly focus on the WP1 of the MULTI-STEP project lying on atomic scale simulations. The main objective of this WP is to provide deviatoric stress-dependant phase diagram for both titanium and silica. In this aim, atomistic simulations will be used in combination with state of the art approaches for computing Gibbs free energies, such as thermodynamics integration [4] or umbrella sampling [5]. The atomic scale approach will also allow to obtain two main ingredients needed for the homogenization performed in WP5. First, the atomistic simulation will allow to derive equations of state for all phases of interest, which will be used to compute the volumetric part of eigenstrains. Second, the bicrystallography will permits from the atomic structure of the crystals to infer the deviatoric part of the eigenstrains related to the different phase transformations.

Depending on the progress of the subject and the candidate's interests, participation in other WPs of the project may be considered.

References:

[1] : S. Cionoiu and et al. “Impact of interseismic deformation on phase transformations and rock properties in subduction zones”. In: Sci. Rep. 9.1 (2019), p. 19561.
[2] : B. Richter and et al. “Stresses and pressures at the quartz-to-coesite phase transformation in shear deformation experiments”. In: J. Geophys. Res.: Solid Earth 121.11 (2016), pp. 8015–8033.
[3] : K. Dang and et al. “The role of deviatoric stress and dislocations on the α to ω phase transformation in Ti”. In: Acta Mater. 244 (2023), p. 118510.
[4] : P. Y. Chew and A. Reinhardt. “Phase diagrams—Why they matter and how to predict them”. In: J. Chem. Phys. 158.3 (2023).
[5] : Kästner, J. “Umbrella sampling”. Comp. Mol. Sc., (2011), *1*(6), p. 932-942.

Techniques/methods in use: Molecular dynamics, Ab-Initio Molecular Dynamics, Thermodynamics Integration, Umbrella Sampling

Applicant skills: knowledge in material physics, thermodynamics, interest on numerical simulations

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Possibility for a doctoral thesis: Yes, ANR funding secured