Phd position 2024- CEMEF

Title	***Studying rapid solid-state phase transformations by combining controlled pulse heating experiments and Calphad consistent modeling considering the non-equilibrium state of the interface***
Acronym	RAPID-SOLID
Framework	Project carried out within the 2MS team (Metallurgy, Mechanics, Structures & Solidification) of CEMEF (Center for Material Forming, Mines Paris, PSL University). The PhD student will be supervised by researchers from the 2MS team, and will benefit from CEMEF resources, as well as the associated training. Strong interactions will take place with the team carrying out experiments at the Friedrich Schiller University Jena (FSU, Germany).
Global objective of work	The purpose of the project is understanding the influence of the thermodynamic state of the interface on transformation mechanisms and phase selections. The transitions under focus are (massive-type transformation) from diffusion controlled to interface-diffusion controlled and (martensitic-type transformation) from interface-diffusion controlled to interface controlled. The conditions at the interface are characterized analyzing its thermodynamic state by combining experiment and simulation. Partner Friedrich Schiller University Jena (FSU, Germany) will develop controlled pulse heating experiments that allow for an in-situ, high resolution measurement of T-t curves and their assignment to local microstructures as well as high resolution electron microscopy/spectroscopy are employed. Partner Mines Paris will develop a thermodynamic and kinetic model that considers velocity-dependent phase equilibria and interface thermodynamics. Being fully coupled with Calphad databases, simulations of the experiments will be performed to reach direct one-to-one comparisons. The combination of the experimental and numerical investigations will be the foundation for this collaborative project and its final goal: revisit interpretations of the transitions between solid-state transformations involving massive type interface diffusion-controlled reactions.
Context	In rapid solid-state transformations, diffusion kinetics in the bulk are low in both, growing and parent phases, creating a global deviation from equilibrium of the system. However, interface non-equilibrium mechanisms also take place, such as solute drag and attachment kinetics. The energies dissipated by the migration of the interface and the transfer of solute through the interface have to account for these local mechanisms. This leads to a higher amount of undercooling during quenching and a distinct deviation from local equilibrium at the interface. As consequence, a wide variety of solid-state transformations and types of microstructures can be observed as a function of undercooling.
Detailed presentation	The work will consist in developing a numerical model to track the interface between phases during phase transformation with full coupling with non-equilibrium thermodynamic [1]. Figure 1a presents an example of non-equilibrium thermodynamic properties computed as a function of the interface velocity, i.e. the liquidus and solidus lines in the binary Ag-Cu system [2]. The phase diagram boundaries become velocity-dependent as thermodynamic equilibrium is no longer achieved at high velocity. These properties need to be coupled with a numerical description of mass transfers through the interface and

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within the phases in order to explain the various microstructures described in figure 1b, going from Widmannstätten to martensitic morphologies as a result of diffusion-controlled and displacive transformations, respectively [3]. Short stays at FSU in Jena and intense exchanges with experimentalists are planned.

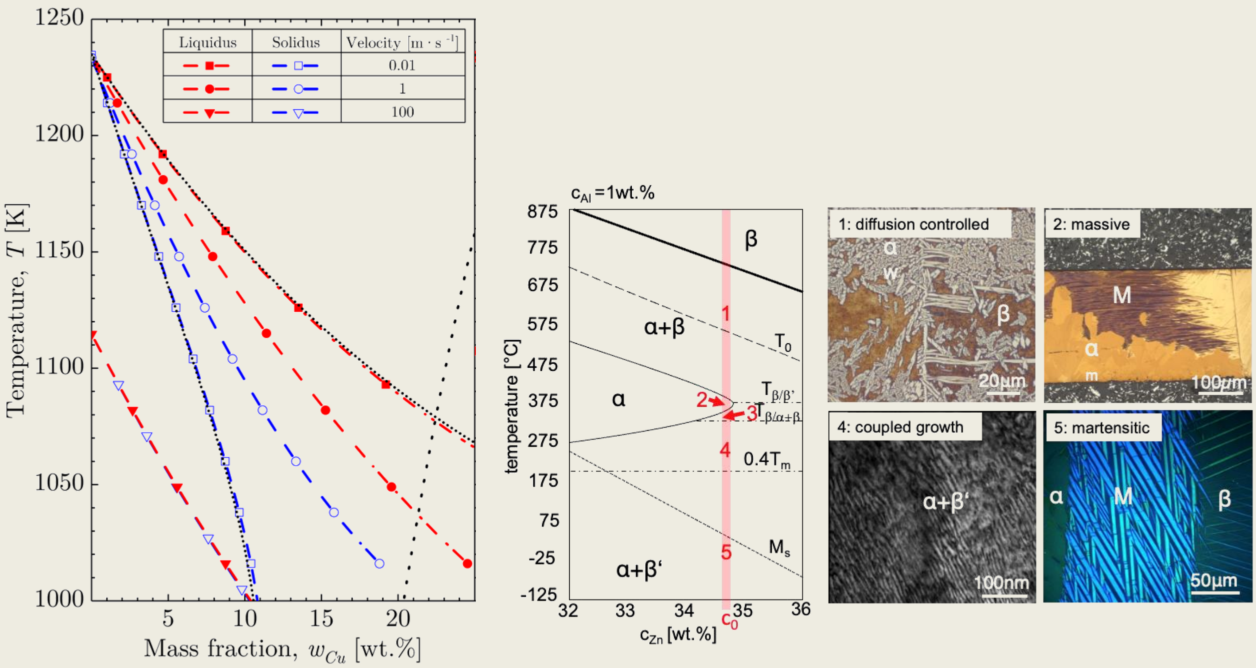

Figure 1. Non-equilibrium phase transformation studies with (left) computed velocity-dependent phase diagram boundaries in the Ag-Cu system [2] and (b) isopleth section of the Cu-Zn-Al system with various types of microstructures [3].

Bibliography references

[1] PhysalurgY library, https://physalurgy.cemef.mines-paristech.fr
[2] P. Martin, G. Guillemot, C.A. Hareland, P.W. Voorhees, C.-A. Gandin, Kinetic effects during the plane-front and dendritic solidification of multicomponent alloys, Acta Mater. 263 (2024) 119473.
[3] S. Lippmann, T. Kaaden, P. Wutzler, M. Rettenmayr, The effect of adding Al on the occurrence and progress of massive transformation in Cu-Zn, Materialia (2019) 100367.

Diffusion

Communication in national and international congresses
Publication in scientific journals

Tools

PhysalurgY library: thermodynamic calculation, front monitoring method, description of metallurgical transformations

Key-words

Phase transformation, Front tracking, Thermodynamic coupling

Skills, abilities requested

Engineer or Master 2, in the fields of physics, materials or mechanics. Student attracted by topics related to modelling and numerical simulation of physical phenomena and materials engineering.
The PhD student will receive the training necessary for his research activities, including scientific computing and programming, in particular to master the dedicated computing tools.

Location	CEMEF, Sophia Antipolis (Site de Mines Paris - PSL)
Gross annual salary	27k€
CEMEF team	Metallurgy, Mechanics, Structures & Solidification – 2MS
Supervisor(s)	Charles-André GANDIN (charles-andre.gandin@minesparis.psl.eu) Gildas GUILLEMOT (gildas.guillemot@minesparis.psl.eu)

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