The emergence of complex microstructures during solidification: A multiscale challenge

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Metallic Alloy Solidification *Microstructures* *Multiscale Modeling*

Abstract Microstructures are crucial to the properties, performance, and often lifetime of structural components. In most technologically critical components, solidification is the first stage of microstructure development. Hence, the understanding, modeling, and predictive simulation of solidification processes is crucial to the development of novel alloy chemistries or processing routes, in order to obtain microstructures "on demand" and reach outstanding properties and performance levels. Yet, the underlying mechanisms of solidification are fundamentally multiscale. Relevant scales span from the nanoscopic cluster of atoms nucleating in the liquid to macroscopic heat, mass, and solute transport. From a theoretical standpoint, a major challenge is that all these scales are intricately linked to one another in various ways depending on the alloy or process at hand.

In this talk, I will give a brief overview of the most prominent tools for computational modeling and simulation of solidification across scales (see Figure 1), including molecular dynamics, phase-field, and cellular automaton methods, highlighting their advantages and limitations. I will then illustrate computational simulation studies that have allowed gaining further insight into some mechanisms of microstructure selection during solidification, namely: (a) grain growth competition during polycrystalline dendritic solidification [1-4], and (b) the occurrence of microstructure transitions due to rapid solidification in fusion-based additive manufacturing processes [5]. Finally, I will give my subjective evaluation of the most critical challenges ahead in the quantitative modelling of solidification across scales and highlight some recent studies opening interesting routes for combining computational and experimental research.

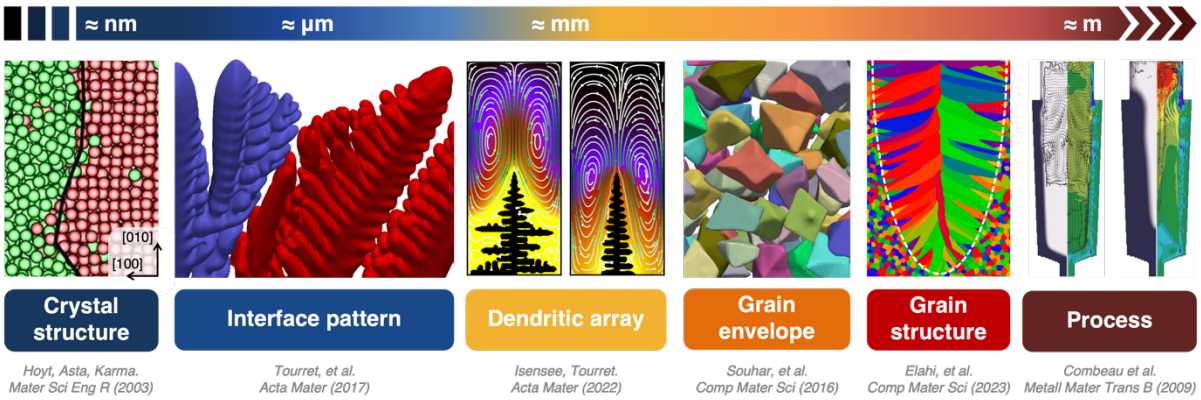

Figure 1 *– The different scales of solidification, illustrated with relevant computational simulations (from left to right) : Molecular Dynamics [6], Phase-Field [1], Dendritic Needle Network [7], Grain Envelope Model [8], Cellular Automaton [3], Volume-averaging [9].*

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