

Multi-scale simulations of surface dynamics and solidification based on the phase-field approach

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Many desirable properties of a material are determined by its micro structure. Thus contributing to a precise understanding of the micro structure evolution in materials processing is a great challenge to the newly emerging field of computational materials design. From point of view of mathematics this always requires to solve an intriguing and numerically difficult to handle *Stefan* problem.

During the last two decades the phase field method could establish itself within the computational materials science community to tackle such Stefan problems via an implicit formulation overcoming their inherent numerical inaccessibility. Moreover, the phase field method proved to be an important constituent of multi-scale simulation approaches addressing the even greater challenge to

1. predict micro structure evolution in complex material systems quantitatively by taking into account the dynamics contributing from the atomic scale as well, and
2. reveal also the impact of micro structure dynamics at the scale of the full material sample.

Within this talk I will present a brief introduction to the field of phase field modeling in computational materials design with a special focus on scale-bridging modeling. I will then present recent contributions from my group addressing the physics of epitaxial surface growth, corrosion at surfaces and multi-phase solidification involving complex micro structures.