The 8th European Congress on Computational Methods in Applied Sciences and Engineering
ECCOMAS Congress 2022
5-9 June 2022, Oslo, Norway

MULTI-FIDELITY MODELING OF SINGLE DENDRITIC CRYSTAL GROWTH OF BINARY ALLOYS

Josef M. Winter[1,*], Jakob W. J. Kaiser[1], Meike Tütken[1], Stefan Adami[1] and Nikolaus A. Adams[1]

[1] Technical University of Munich, TUM School of Engineering and Design, Chair of Aerodynamics and Fluid Mechanics, Boltzmannstraße 15, 85748 Garching, Germany
[*] Mail: josef.winter@tum.de, URL: https://epc.ed.tum.de/aer

Keywords: *Dendritic growth, Binary alloys, Multi-fidelity modeling, Gaussian processes*

Microstructure evolution during solidification strongly affects the thermo-mechanical properties of the solidified part and influences its behavior in subsequent manufacturing steps. Modern manufacturing processes such as metal additive manufacturing may involve strong thermal gradients resulting in rapid solidification exhibiting peculiar dendritic growth patterns. Relating characteristic parameters of a dendrite with process parameters, such as undercooling or species concentrations of solidifying alloys, has been in the focus of research for decades [1]. In this work, we generate a stochastic surrogate model for the tip velocity of single dendritic growth of binary alloys. Therefore, we extend our earlier work [2] to simulate non-isothermal liquid-solid phase transition of binary alloys using a semi-implicit conservative sharp-interface model. We integrate the model in the open-source simulation framework ALPACA, which is used to generate the multi-fidelity dataset relating tip-velocities with process parameters and local segregation patterns. The dataset contains a large number of coarse/low-accurate estimates of the tip velocity (low-fidelity data) and only a few high-fidelity measurements. We fuse data from different fidelity levels and employ multi-fidelity deep Gaussian processes to train an accurate stochastic surrogate model for the tip velocity. Due to the strong nonlinear relation between tip velocity and process parameters, model convergence and quality can be improved by applying input warping functions to regularize the model-parameter space. The accuracy of the multi-fidelity tip velocity model is assessed by using cross-validation techniques. The stochastic nature of the surrogate model allows for quantifying predictive uncertainty. This motivates its application in Bayesian-optimization algorithms for inverse problems or to create problem-tailored improvements by using exploration and exploitation approaches.

REFERENCES

[1] J. Strickland, B. Nenchev, and H. Dong, On directional dendritic growth and primary spacing-a review. *Crystals*, Vol. **10(7)**, pp 1–30, 2020.

[2] J. W. J. Kaiser, S. Adami, I. S. Akhatov, and N. A. Adams, A semi-implicit conservative sharp-interface method for liquid-solid phase transition. *International Journal of Heat and Mass Transfer*, Vol. **155**, pp. 119800, 2020.