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Simulation of Solidification Across the Length Scales

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Solidification is an incredibly complex process. At the macroscale, it involves both a liquid phase that may be flowing and a solid phase that may be deforming. At the microscale, it involves pattern selection processes, diffusional effects, grain nucleation, and attachment kinetics. There is also heat and mass transfer to consider at all the length scales of interest. Thus, the process of solidification involves strong coupling between these microscopic and macroscopic views.

The use of computational methods to investigate theoretical and practical aspects of solidification has become quite popular over the past 30 years as they allow for the construction of accurate and detailed models that both include and provide insight into many important phenomena. At the macroscale, geometry and processing conditions determine the solidification sequence. Various modeling techniques based on finite elements and computational fluid dynamics exist to investigate die filling and the subsequent solidification process in components ranging from automotive components to aero engine turbine blades. As the length scale is reduced to roughly 1 μm–500 μm, the characteristic geometry for simulation becomes the microstructure and thus the modeling of grains, dendrites, and solute segregation is of interest. Key techniques at this scale include phase-field, cellular automata, and microsegregation methods in order to investigate the effects of solidification on the final properties of a cast component. A further reduction in the length scale brings us to the atomic level in which the properties of the solid/liquid interface and also the attachment kinetics can be investigated through molecular dynamics, density functional theory and phase-field crystal (to name a few). A significant current area of research is the anisotropy of the solid/liquid interface since this will affect to a large extent the morphology of the final microstructure.

This *JOM* topic explores recent advances in the simulation of solidification at various length scales to examine pattern selection, defects, and processing effects. Five papers are presented that span the length scales described above. In each paper, different methodologies for modeling solidification are described along with the computational resources needed for performing such complex simulations.

The first two papers focus on phase-fields methods to investigate pattern selection and interface effects. The article by I. Steinbach, "Why solidification, why phase-field" provides a wonderful historical perspective on the suitability and application of phase-field to solidification. The article "Atomistic Modelling of Solidification Phenomena using the Phase Field Crystal Model" by H. Humadi, N. Ofori-Opoku, N. Provatas and J. Hoyt focuses on the extension of phase-field to atomic-scale effects at diffusive time-scales. As shown in both contributions, phase-field is a powerful tool for answering questions relating to solidification pattern selection where rigorous theoretical physics are needed.

At the other end of the spectrum, the paper by C. Reilly, J. Duan, L. Yao, D.M. Maijer and S.L. Cockcroft, "Process Modeling of Low-Pressure Die Casting of Aluminium Alloy Automotive Wheels," presents a study of the use of computational modeling to improve industrial casting processes. In this work, the wheel is used as a case study to show both the importance of understanding heat flow in order to minimize shrinkage porosity, as well as the use of criteria functions. In process-level simulations, criteria functions predict defect formation with empirical equations based on local physical conditions such as cooling rate and strain-rate. Criteria functions are useful since they provide the industrial foundry with a strong indication of the likelihood of defect formation at low computational cost and are easy to interpret. In the case of the work by Reilly and colleagues, the Niyama criterion has been applied to the wheel-casting as a whole.

Meso-scale models of solidification attempt to bridge the gap between pattern formation at the

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scale of the dendrite and process models that are strictly interested in thermal and mass transport. The final two papers are examples of such approaches. In the work by Ch.-A. Gandin, T. Carozzani, H. Digonnet, S. Chen, G. Guillemot, "Direct Modeling of Structures and Segregations up to Industrial Casting Scales," the cellular automaton method is applied to simulate grain nucleation and growth. The relevant physical phenomena are included, although not to the detriment of computational cost. The authors then show via simulation how autogenous welding could be utilized to create a columnar grain structure forming the letters TMS. The article "Prediction of Hot Tear Formation in DC Casting of Aluminum Billets using a Granular Approach" by M. Sistaninia, J.-M. Drezet, A.B. Phillion, and M. Rappaz outlines a new modeling approach known as granular modeling of solidification to investigate crack formation during casting. As with the work by Gandin, this modeling approach requires coupling of various physical phenomena with macro-scale effects to quantitatively predict defects.

The ultimate goal of modeling solidification and industrial casting processes is to quantitatively predict both defects and the in-service mechanical performance. As demonstrated through the five complementary articles provided in this *JOM* topic, this goal can be achieved only by combining modeling approaches that span the length scales from the process-level to atomistic. Together, these techniques present a significant opportunity to develop the next generation of cast products.