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Advances in Modeling of Solidification Microstructures

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In different manufacturing processes, such as casting, welding, and additive manufacturing, metallic materials go through solidification to produce parts with different sizes and shapes. Microstructures that develop during solidification control the property and performance of the manufactured parts, thereby predicting the solidification microstructures as functions of alloying composition and processing parameters is essential to control the quality of products.

The multiscale nature of solidification microstructures, which depend on temperature distribution, solute concentration, capillary forces, and kinetic length,[1] make the understanding and prediction of these microstructures exceptionally difficult. In recent years, and because of emergence of new and powerful supercomputers, it has become more feasible to computationally simulate the materials nano- and microstructures in large scales and with finest details. The computational models for solidification of metallic materials need to be developed based on the actual multiphysics of solidification, while considering the need for efficient numerical algorithms to solve the governing equations of the models. To quantitatively predict solidification microstructures, computational models at mesoscale need information from theory, experiments, lower scale models (e.g., density functional theory calculations, molecular dynamics simulations, etc.), and phase diagram calculations.

The current computational models for simulating dendritic growth at the microscopic scale are based on different methods such as phase field (diffusive interface),[2–8] level set,[9,10] direct interface tracking,[11,12] and cellular automaton[13–15] methods. Each of these methods has its advantages and disadvantages: some can simulate the finest details of solidification microstructures with high accuracy, while others can simulate dendritic growth in large-scale domains with high computational efficiency.

In this *Journal of Metals* topic, we present recent contributions in modeling of solidification microstructures.

Damien Tourret et al. present a three-dimensional (3D) version of the dendritic needle network (DNN) model for directional solidification. They apply the DNN model to predict the stable range of primary dendritic spacings for an Al-9.8 wt%Si alloy over a range of growth velocities. They compare their predictions to spacings measured from in situ x-ray imaging of directional solidification experiments.

Mohsen Eshraghi et al. present a parallel 3D lattice Boltzmann-cellular automaton model to simulate dendritic growth during solidification of metallic binary alloys. Their large-scale simulations show a great scale-up performance up to 40,000 computing cores and an excellent speed-up performance on up to 1000 computing cores. Yasushi Shibuta and co-workers performed simulations of solidification from atomic to microstructural levels using a graphics processing unit (GPU) architecture. They use million-atom molecular dynamics simulations to study nucleation of solid phase in undercooled melt and to capture evolution of anisotropy for solid seeds. Using a quantitative phase-field model, they simulate dendrite growth in directional solidification at millimeter scale in two–dimensional (2D) and 3D by multi-GPU computation on a supercomputer. These two articles present promising techniques to predict solidification microstructures in large macro-scale domains with good computational efficiency.

Alexander Monas et al. present 3D phase-field simulations of solidification microstructures of Mg-Al alloy. They use the Calphad method to obtain the phase diagram and necessary parameters for their simulations.

Michael Rappaz and Güven Kurtuldu discuss a new nucleation mechanism in liquid metallic alloys based on thermodynamics arguments. They explain that the two-step nucleation mechanism starts with

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formation of small icosahedral quasicrystals due to spinodal decomposition of the liquid, which is followed by heteroepitaxy of the fcc phase on facets of these quasicrystals due to a transformation of these quasicrystal precursors into multiple-twinned-fcc nanocrystals. Their explanation sets up guidelines for finding solute elements and composition ranges that favor grain refinement.

Qiang Wang, Hongguang Yan, Fang Wang, and Baokuan Li present a 2D cellular automaton -finite element model to study electromagnetic stirring on the grain morphology of the electroslag remelting ingot.

The articles presented in this *Journal of Metals* topic provide a narrow view of how modeling and simulation are substantially impacting our understanding of solidification microstructures of metallic materials. It is expected that such predictive models will help us to understand the mechanisms controlling the solidification microstructures, and therefore enable us to predict their effects on the properties of solidified materials. It is evident that there is a need for continued advancement and research in the field of modeling of solidification microstructures, because these efforts continue to better describe the processing–microstructure–properties relationships for materials produced by manufacturing processes that involve solidification.

The following papers being published under the topic of Advances in Modeling of Solidification Microstructures provide excellent details and research on the subject. To download any of the papers, follow the url http://link.springer.com/journal/11837/67/8/page/1 to the table of contents page for the August 2015 issue (vol. 67, no. 8).

- "Three-Dimensional Multiscale Modeling of Dendritic Spacing Selection during Al-Si Directional Solidification" Damien Tourret, Amy J. Clarke, Seth D. Imhoff, Paul J. Gibbs, John W. Gibbs, and Alain Karma
- "Large-Scale Three-Dimensional Simulation of Dendritic Solidification Using Lattice Boltzmann Method" Mohsen Eshraghi, Bohumir Jelinek, and Sergio D. Felicelli
- "Solidification in Supercomputer: from Crystal Nuclei to Dendrite Assemblages" Yasushi Shibuta, Munekazu Ohno, and Tomohiro Takaki
- "Divorced Eutectic Solidification of Mg-Al Alloys" Alexander Monas, Oleg Shchyglo, Se-Jong Kim, Chang Dong Yim, Daniel Höche, Ingo Steinbach
- "Thermodynamic Aspects of Homogeneous Nucleation Enhanced by Icosahedral Short Range Order in Liquid fcc-Type Alloys" Michael Rappaz and Guven Kurtuldu
- "Impact of Electromagnetic Stirring on Grain Structure of Electroslag Remelting Ingot" Qiang Wang, Hongguang Yan, Fang Wang, and Baokuan Li

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