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Editorial

Recent Advances in Study of Solid-Liquid Interfaces and Solidification of Metals

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1. Introduction and Scope

Solidification occurs in several material processing methods, such as in casting, welding, and laser additive manufacturing of metals, and it controls the nano- and microstructures, as well as the overall properties of the products. Recent advancements in experimental and computational modeling techniques have made it possible to more effectively study atomistic and microscale mechanisms that control the solidification nano- and microstructures, and formation and evolution of solidification defects. Along this direction, this Special Issue solicited articles demonstrating recent advancements in the following areas:

I. Experimental studies of solid-liquid interfaces and solidification nano- and microstructures, including in situ experiments.
II. Computational modeling at different length scales, including atomistic simulations (e.g., molecular dynamics) and mesoscale modeling (e.g., phase-field modeling) of solid-liquid interfaces and solidification structures (e.g., dendritic structures).
III. Experimental and/or modeling studies of solidification defects and their effects on mechanical and physical properties of solidified materials.

2. Contributions

This special issue contains seven research articles and one topical review article.

The first article in this issue by Glicksman and Ankit [1] was to determine by simulation and measurement whether or not interfacial gradients of the Gibbs–Thomson potential distributed along grain boundary grooves also stimulate an energy field along a groove's solid–liquid interface. The distribution of thermo-potentials (such as the Gibbs–Thomson equilibrium temperature) for a variational groove exhibits gradients tangential to the solid–liquid interface. The authors utilized a phase-field modeling approach to quantitatively verify the presence of a capillary-mediated energy field on a stationary grain boundary groove. It is important to note that such energy fields on interfaces can considerably influence the stability and pattern formation dynamics during solidification.

In the second article in this issue, Gatzen et al. [2] utilized both experimental and numerical techniques to investigate the wetting process of an aluminum droplet on a zinc-coated steel surface. The final wetting angle and length were linked to the time where zinc was liquefied during its contact with the overheated aluminum melt, leading to the assumption that the interaction was basically a fluid dynamic effect of liquid aluminum getting locally alloyed by zinc. To further investigate this process, Gatzen et al. [2] developed a numerical model to describe the transient behavior of droplet movement and mixing with the liquefied zinc layer to understand the spreading dynamics. Their simulations revealed a displacement of the molten zinc after the impact of the droplet, which ultimately led to an accumulation of zinc in the outer weld toe after solidification.

Fluid dynamic effects in microscale can also significantly influence the solidification microstructures. To study the dendritic growth during solidification of a binary alloy (Al-Cu) under forced and natural convection, Eshraghi et al. [3] developed a three-dimensional (3D) lattice Boltzmann (LB) model. They used the LB method to solve the solute diffusion and fluid flow equations, and a cellular automaton (CA) scheme to capture new interface cells. Their results showed that decreasing undercooling and increasing solute concentration decelerates the growth in all branches of the dendrite. While increasing fluid velocity did not significantly influence upstream and transverse arms, it decreased the growth rate in the downstream direction considerably. Considering the advantages offered by the LB method in large scale simulations of dendritic solidification, the presented model can be used to predict the 3D microstructures that form during solidification under different convection conditions.

At a larger length scale, Dong et al. [4] studied formation of macrosegregation in continuously cast billets with a newly developed 3D macrosegregation model. The fluid flow, solidification, and solute transport equations were solved in the entire billet region. Their simulation results showed that the solute redistribution occurring with thermosolutal convection at the solidification front contributes significantly to continued macrosegregation as solidification proceeds. They also showed that the equilibrium partition coefficient is mostly responsible for the magnitude of macrosegregation, while comparison between solute P and S indicated that diffusion coefficients also have some amount of influence on macrosegregation.

To study the effects of flow included by in-mold electromagnetic stirring (M-EMS) on solidification and solute transport in bloom mold, Fang et al. [5] utilized a multiphysics numerical model to solve the governing equations of the flow, temperature, solidification, and solute concentration. Their simulations showed that M-EMS can homogenize the initial solidified shell, liquid steel temperature, and solute element in the EMS effective zone. With the rise of current intensity, the bloom surface temperature, level fluctuation, stirring intensity, uniformity of molten steel temperature, and solute distribution increased, while the growth velocity of the solidifying shell in the EMS effective zone declined and the solute mass fraction at the center of the computational outlet decreased. It was concluded that M-EMS with a current intensity of 600 A is more suitable for big bloom castings. In a separate study, Mikolajczak [6] experimentally studied the effect of forced flow induced by EMS on equiaxed solidification of AlMgSi alloys with Fe and Mn alloy elements, and used CALPHAD (Computer Coupling of Phase Diagrams and Thermochemistry) technique to determine the precipitation sequence of the phases. Details on the effects of EMS on transformation from equiaxed dendritic to rosette morphology, secondary dendrite arm spacing, and precipitation process were discussed.

Zhang et al. [7] experimentally investigated the effect of growth velocity on the electric current pulse (ECP)-induced separation of primary silicon in a directionally solidified Al-20.5 wt % Si hypereutectic alloy. Their results showed that a lower growth velocity promotes the enrichment tendency of primary silicon at the bottom region of the samples. It was concluded that with a slower growth velocity, a stronger forced flow is generated to promote the precipitation of primary silicon accompanied by a higher concentration of electric current in the mushy zone.

Finally, a review article by You et al. [8] discussed the progress in modeling of inclusion formation during the solidification of steel. This is a very important subject in metal casting, especially in steel making, where the formation of nonmetallic inclusions during solidification can influence the properties of steels. Computational simulation provides an effective and valuable method to study the process due to the difficulty of online investigation.

3. Conclusions and Outlook

Solidification is one of the most important phenomena occurring in different manufacturing processes of metals and some other material systems. It basically determines the nano- and microstructures and the resultant properties of manufactured materials. Understanding the solid-liquid behavior and determining solid-liquid interface properties [9–11] are essential steps towards predicting the nano- and microstructure patterns. It is clear that further fundamental computational and experimental studies are required in order to acquire enough information on solid-liquid properties for different material systems (e.g., alloys). Besides solid-liquid interface evolution, some rather complex events and features such as formations of crystal defects, meta-stable phases, solute segregation, porosity, oxides, oxide bifilms, and some others, can occur sequentially or simultaneously during solidification. It should be noted that these events and features are effected by composition, process parameters (e.g., cooling rate), boundary conditions, geometry of casting, and external fields affecting the melt flow. Additionally, the complexity of such features may significantly increase in some advanced processes like laser additive manufacturing, where rapid solidification makes the system to go much further away from equilibrium. There is a need for quantitative computational models and accurate experimental approaches to study the mentioned events and features, their interactions, and also their relationships to process parameters.

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