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Dendritic growth of high carbon iron-based alloy under constrained melt flow

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A R T I C L E I N F O

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A cellular automaton (CA) model coupled with momentum, mass and heat transport models was developed to investigate equiaxed and columnar dendritic growth of Fe–0.82 wt%C alloy under four elaborately designed forced flows. During the iterative solution, the evolution of solidification interface and the solute diffusion in solid phase were explicitly tracked and solved, while other transport equations were implicitly solved in staggered grids with the block-corrected TDMA approach. The self-developed codes show a good performance in predicting dendritic growth and melt flow and temperature fields according to the comparisons with LGK analytical model and commercial software. The growth behavior of dendrites under melt flow is determined by the competition between bringing in solute enriched melt from upstream side and carrying away solute rejected at interfaces. The growth of equiaxed dendrites is promoted at the upstream side and inhibited at the downstream side, which becomes more significant with the increase of inlet velocity and the decrease of melt undercooling. Meanwhile, the oblique flow plays an important role in the growth of arms at the downstream side and alleviates the inhibited growth at the lower melt undercooling. Columnar dendrites are under inhibited growth in sequence along the flow direction, except that those near the outlet are promoted under weaker melt flow. Secondary dendrite arms firstly well formed at left sides of columnar dendrites become fatter and better developed compared with those without flow, although those near the upstream side are difficult to be developed. Under the circular flow condition, columnar dendrites at the bottom wall of the modeling domain firstly grow faster than those symmetrically in the right wall, and then become slower as the solidification proceeds under stronger melt flow. Moreover, the effect of melt flow on dendritic growth becomes more significant under the lower melt undercooling condition for equiaxed dendrites and the weaker cooling condition for columnar dendrites. In addition, compared with the effect on the temperature distribution, the effect of the melt flow on the solute distribution around columnar dendrites governs their growth.

1. Introduction

During the solidification of alloys, the melt flow as an inevitable phenomenon is customarily induced by the intrinsic characteristics of alloy solidification such as thermal and solutal variations in die casting process and the external forces such as pouring and electromagnetic stirring (EMS) in continuous casting process [1]. The melt flow not only influences dendritic growth, morphology and distribution of grains and solute distribution in the microscopic and the mesoscopic scale, but also determines solute migration and segregation in the macroscopic scale, and thus plays a critical role in the inner solidification quality of alloy ingots and strands. Moreover, the effect of melt flow on dendritic growth is characterized by dendritic growth direction, primary and secondary dendrite arm spacings and liquid fraction of the porous mushy zone and ultimately exerts on the compactness of columnar and equiaxed dendrite zones, known as the permeability of the mushy zone [1,2], which is the key parameter to accurately investigate the formation and the development of macro segregation. Therefore, the investigation of the dendritic growth of alloys under melt flow during the solidification process is an important and necessary step for the further insight into the formation mechanism of solidification defects and contributes much to control and improve the solidification quality of alloys.

Beckermann and his coworker [3–5] proposed that numerical modeling of dendrite solidification under melt flow should incorporate the microscopic phenomena such as nucleation and dendritic growth and the macroscopic transport phenomena. They were the first to couple classical analytical theories of dendritic

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growth with momentum, heat and mass conservation equations based on the volume averaging approach [6] and they developed a delicate and reasonable mathematical model for equiaxed dendrite solidification which was validated according to experimental results of Al–4 wt%Cu alloy and $NH_4Cl–H_2O$ solution. This method was appropriate to simulate the solute distribution in the macroscopic scale and the formation of macro segregation. However, since the equiaxed dendrite was assumed to be spherical in the model, the effect of melt flow on the morphology and the growth behavior of dendrites could not be described precisely. Fortunately, as phase field method [7–13], front tracking method [14–17] and stochastic methods such as CA approach [18–39] were introduced, the evolution of solidification interface could be tracked directly or indirectly according to physical variables, so that the microscopic solidification phenomena and related parameters could be qualitatively represented and quantitatively predicted, respectively, as well as the influence of transport phenomena such as the melt flow. These researches were mainly carried out through coupling momentum and mass conservation equations of the melt fluid with the growth kinetic equations of dendrites in the microscopic scale.

Phase field approach was the first to be employed to investigate the impact of melt flow on the growth behavior of equiaxed dendrites of pure materials in two dimensional (2D) domains, and then was extended to the application in three dimensional (3D) domains and binary alloy systems [7–9]. Lan and Shih [10] developed a 2D phase field model with adaptive meshes to investigate the growth behavior of equiaxed dendrites of Ni–Cu alloy in undercooled melt under forced flow and non-isothermal conditions and found that the upstream dendritic arm grew faster with more developed secondary dendrite arms compared with other ones. Chen et al. [11] developed 2D and 3D phase field models and analyzed different influences of melt flow on the growth behavior of equiaxed dendrites controlled by the thermal diffusion. Zimmermann et al. [12] used the flow field calculation software CrysMAS and the phase-field code MICRESS to investigate the effect of melt flow on the growth behavior of columnar dendrites of $AlSi_7$ based alloys during the directional solidification process and presented the asymmetric dendritic morphology under melt flow. Guo et al. [13] adopted the parallel-multigrid approach to solve the coupled thermal-solutal-convective equations and investigated the phenomena such as dendrite tilting and arm splitting of equiaxed dendrites under melt flow. Since the solute diffusion layers over dendritic branches were sharp during the solidification of alloys, fine meshes in solute diffusion layers were needed to accurately describe the dendrite solidification with phase field approach [14]. In addition, the iterative solution of the momentum conservation equation and the continuity equation would impose more burdens on the computation with finer meshes. Although the adaptive mesh method and the parallel-multigrid approach were introduced, phase field model was still confined to the application in small modeling domains. Therefore, front tracking method [15–17] was employed to simulate the growth behavior of equiaxed dendrites and columnar-to-equiaxed transition (CET) under melt flow. Although it avoided the fine mesh in thermal and solutal diffusion layers, complexity and difficulty induced by explicitly tracking the position of solidification interface hindered its wide application to conditions such as multi-dendritic growth with well developed side branches, let alone under 3D conditions [14].

As a result, CA approach based on the stochastic capture mechanism of interface cell and known for relatively less computational cost, was competent to deal with the coupled problems of transport phenomena with dendritic growth kinetics and of great interest to researchers. Firstly, Shin and Hong [18] developed a CA model to consider the dendritic growth kinetics and introduced the diffusion interface from the phase field model to solve momentum and mass conservation equations of melt flow, accordingly investigated the growth behavior of equiaxed dendrites of Al-Cu alloy with melt flow. Subsequently, Zhu and her coworkers [19–28] contributed a lot to the development of CA models for dendritic growth and solidification microstructure, especially under melt flow. Zhu et al. [19–22] coupled transport equations directly with the CA model and solved these equations with SIMPLE algorithm and tri-diagonal matrix algorithm (TDMA), accordingly investigated the growth behavior of equiaxed dendrites with different crystal orientations and columnar dendrites of Al–Cu alloys under melt flow. In order to improve solution stability and efficiency of transport equations, Sun et al. [23–27] adopted the Lattice Boltzmann method to solve transport equations and developed CA-LBM and ZS-LBM models with the corporation of different dendritic growth models to describe equiaxed dendritic morphology and solute distribution of binary alloys under natural and forced convection conditions. Coupled with CALPHAD (Calculation of Phase Diagram), the CA-LBM model was extended to equiaxed dendritic growth of ternary alloys with melt convection afterwards [28]. In addition, Liu et al. [29] developed a CA-FDM (Finite Difference Method) model to investigate the effect of stirring melt flow on the morphology of equiaxed dendrites of the Al–Si alloy. Yin et al. [30] also developed a CA-LBM model to investigate the growth behavior of equiaxed dendrites with multi-orientations and the splitting phenomenon of dendritic tips. Recently, Jelinek et al. [31] adopted the parallel computation algorithm and developed a large scale CA-LBM model which showed a good performance in the simulation of the growth behavior of more than ten millions equiaxed dendrites under forced convection. However, the growth kinetics of dendritic growth in above mentioned models was completely based on the linear relationship with the local undercooling or the local liquid concentration at solidification interface, so that, these models neglected the solute balance at solidification interface [32–34]. Shi et al. [35] introduced solute balance equations in separate forms with coordinates [32,33] to determine interface evolution velocity and investigated 3D equiaxed dendritic growth under forced convection and 2D columnar dendritic growth under natural convection in the $NH_4Cl–H_2O$ solution. Meanwhile, Zhang and Zhao [36] employed the normal velocity from solute balance at solidification interface [34] and analyzed the effect of forced convection on equiaxed dendritic growth of Al-Cu alloy under the 3D condition. Li et al. [37] applied a volume averaged technique to predict the evolution of solidification interface according to the solute conservation there and presented the morphology and the solute distribution of equiaxed dendrites of Fe-C alloy under forced melt flow. Lee and his coworkers [38,39] calculated the increase of solid fraction of interface cells directly from equivalent diffusion equations there rather than indirectly from interface velocities, and they developed a CA-FVM (Finite Volume Method) model to investigate the dendrite solidification of binary alloys under natural and forced convection and found that the natural convection induced by the buoyancy would promote the development of secondary dendrite arms of columnar dendrites at the upstream side. Moreover, Karagadde et al. [40] used the volume of fluid (VOF) method and the immersed boundary method (IBM) to track growth and movement of solid dendrites and solve N–S equations and the enthalpy method to deal with the heat transfer problems and investigated the motion and growth behavior of equiaxed dendrites of pure Al under melt flow.

All of the models utilized to describe the effect of melt flow on dendritic growth are on the basis of momentum, heat and mass transport equations and the evolution kinetics of solidification interface. On the one hand, the melt flow field influences solute and temperature distribution in the modeling domain, especially near the solidification interface, and thus changes the growth behavior of dendrites. On the other hand, as dendrite grows, the flow field is