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A Modified Cellular Automaton Model for the Quantitative Prediction of Equiaxed and Columnar Dendritic Growth

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Since the characteristic of dendrite is an important factor determining the performance of castings, a two-dimensional cellular automaton model with decentered square algorithm is developed for quantitatively predicting the dendritic growth during solidification process. The growth kinetics of solid/liquid interface are determined by the local equilibrium composition and local actual liquid composition, and the calculation of the solid fraction increment is based on these two compositions to avoid the solution of growth velocity. In order to validate the developed model, quantitative simulations of steady-state dendritic features over a range of undercooling was performed and the results exhibited good agreement with the predictions of LGK (Lipton−Glicksman−Kurz) model. Meanwhile, it is demonstrated that the proposed model can be applied to simulate multiple equiaxed dendritic growth, as well as columnar dendritic growth with or without equiaxed grain formation in directional solidification of Al−Cu alloys. It has been shown that the model is able to simulate the growth process of multi-dendrites with various preferential orientations and can reproduce a wide range of complex dendritic growth phenomena such as nucleation, coarsening of dendrite arms, side branching in dendritic morphologies, competitive growth as well as the interaction among surrounding dendrites.

KEY WORDS: Cellular automaton; Dendritic growth; Crystallographic orientation; Aluminum alloys

1. Introduction

Solidification of metals is a key process determining the final properties to a large extent[1−3], and studying the formation mechanism of solidification microstructures and controlling them as designed, have been widely concerned[4]. Dendritic morphology is probably the most common microstructure observed during solidification process, which has a significant effect on the final properties. Due to the invisibility of the melt, it is difficult to real-timely observe the dendritic formation process. Although the synchrotron X-ray radiography technology developed in recent years makes direct observation be possible, the difficulty in preparing samples and the high requirements for equipments are also the challenges that the researchers need to face.

In recent decades, with the advancements of computer technology, numerical modeling and simulation have been widely used as a powerful tool to make a better understanding of dendritic evolution[5−7]. At present, various kinds of deterministic and stochastic models have been developed to simulate the evolution of dendritic morphologies during solidification, among which, phase field (PF) and cellular automaton (CA) methods have been employed extensively. PF method, based on a set of thermodynamically-based partial differential equations, deals with the solid/liquid (S/L) interface by introducing a smooth transition variation of order parameter φ, thus avoiding the explicit tracking of S/L interface[8,9]. PF models have been successfully applied to simulate binary or ternary alloys in two or three dimensions and to investigate the growth kinetics and Gibbs energy[10−12]. However, PF models require complex calculations and high computational resources, restricting the application of the models to small regions. CA method, as another computational approach, can reveal a wide range of micro-meso scale dendrite/grain evolution phenomena such as columnar-to-equiaxed transition (CET)[13] and deflection behavior of the dendritic growth in a flowing melt[14]. The simulated results of CA model are similar to those of PF method and it has a higher computational efficiency[15]. Therefore, CA method is rapidly emerging as a choice of simulating the dendritic formation in solidification process[15−18]. A two-dimensional CA model coupled with finite element (FE) to

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obtain the non-uniform temperature field, originally proposed by Gandin and Rappaz[19], was developed to simulate grain nucleation and growth during solidification. This model is capable of predicting the mesoscopic scale grain structure with a random orientation by adopting the decentered square growth algorithm, which was later successfully extended for simulations in three dimensions[20]. However, due to the fact that the model does not take the solute diffusion into account, it is unable to simulate the micro-scale dendritic features. Nastac[21] proposed a comprehensive stochastic CA model including time-dependent calculation of temperature field, solute redistribution both in solid and liquid, interface curvature as well as the growth of anisotropic parameters. This model is capable of explicitly tracking the S/L interface and simulating the evolution of dendritic crystals during solidification. Sanchez and Stefanescu[22] developed a CA model with the ability to simulate quantitatively most of the dendritic features observed experimentally. This model gave a detailed introduction of a new solution for the calculation of interface local curvature instead of using empirical formula[21], which reduced the artificial anisotropy caused by meshes to a certain extent. Sun et al.[23] developed a coupled CA model for the simulation of dendritic growth in the presence of forced and natural melt convection. The melt flow, solute transport and thermal transport were calculated by adopting a kinetic-based lattice Boltzmann method (LBM). Recently, with some certain assumptions, CA models have not been limited to only binary alloys, and many attempts have been made to extend CA models to predict the microstructure of multi-component systems[8,24].

Unfortunately, as a result of artificial anisotropy induced by the CA mesh and the corresponding neighborhood configuration and capture rules, most of the CA models are mesh dependent and can only simulate the dendrites growing aligned with the grid or in 45° orientation. To deal with the problem, the decentered square/octahedron algorithm originally proposed by Rappaz et al., was later modified by Wang et al.[7], through coupling the finite difference model to solve the solute diffusion equations. The algorithm eliminated the effect of grid anisotropy and was adopted by many workers to describe the dendritic growth with arbitrary preferential orientation[3,8,25,26]. On the basis of this technique, the solutal interaction within an advancing columnar dendritic network and columnar-to-equiaxed transition of Al−Cu alloys were investigated by Dong and Lee[13], and the stray grain formation mechanism in the platform region of turbine blades was revealed by Yang et al.[27]. Sanchez and Stefanscu[5] improved their previously developed CA model[22] by using virtual front tracking (VFT) of the shape S/L interface and made the model valid for simulating dendrites growing at an arbitrary crystallographic orientation. Later, Zhu and Stefanescu[6] adopted the virtual front tracking method and calculated the solid fraction increment through the difference between the local equilibrium composition and the local actual liquid composition, rather than by solving the solute conservation equation at the S/L interface to obtain the growth velocity. Wei et al.[17,28] developed a model to reduce the mesh-induced anisotropy by adopting new random zigzag capture rules for interface cells and presented a modified interface curvature calculation method simultaneously. John et al.[29] also investigated the influence of the presence of artificial anisotropy on growth kinetics induced by CA mesh and developed a modified cellular automaton-finite volume model, in which the grid dependent anisotropy was reduced by adjusting the addition of solid fraction and the redistribution of the solute rejected.

Although a lot of efforts has been made to develop CA models for dendrite simulation, the work on this aspect is still far from satisfaction and further efforts are needed. In the current paper, a two-dimensional cellular automaton model is presented to simulate the dendritic growth with different preferential orientations during the solidification process, by adopting the decentered square algorithm to eliminate the mesh-induced anisotropy. The model is compared with the well-established Lipton−Glicksman−Kurz (LGK) analytical model for dendritic tip features of Al−Cu alloys. In particular, a series of simulations including multi-equiaxed dendrites in undercooled melt and columnar dendrites in directional solidification, are conducted to examine the characteristics and capabilities of the model, and the simulated results are compared with the experimental observations published in other papers by *in situ* and real-time synchrotron X-ray radiography technique.

2. Model Description and Numerical Algorithm

CA model for simulating dendrites is a set of algorithms used to describe the evolution of discrete time and space. In the present model, a two-dimensional rectangular calculation domain is uniformly divided into an orthogonal arrangement of square cells with the size of Δx in Cartesian coordinate, and each cell is assigned a pair of integer number (i,j). Each of the spatial cells possess several variables, such as temperature (T), solute content (C_L and C_S), solid fraction (f_S), and crystallographic orientation (θ). According to the solid fraction, the state of the cells can be identified as solid ($f_S = 1$), liquid ($f_S = 0$) and interface ($0 < f_S < 1$). The calculation starts with all the cells in the liquid state. The state transformation from liquid to interface can be achieved through the following ways: stochastic nucleation event, artificially setting certain cell's state as interface or captured by its neighboring solid cells. For partition coefficient $k_0 < 1$ alloys, due to the fact that the local interface equilibrium composition (C_L^*) of a growing cell is larger than its local actual liquid composition (C_L), which is determined from mass transfer, in order to strive for equilibrium, part of the liquid in the cell will solidify to reject the redundant solute, which will diffuse to its neighboring liquid cells. Owing to the growth of interface cells, the temperature field and solute field steadily change in every time step, which will in turn affect the dendritic growth. In order to simulate the dendritic growth process, the governing equations used to calculate the distribution of concentration and temperature, interface curvature, growth kinetics, solid fraction, and nucleation process will be described below.

2.1. Thermal field calculation model

Since the heat diffusivity is several orders of magnitude larger than solute diffusivity, it is reasonable to assume that the heat diffusion has reached an equilibrium state at the scale of dendrite. Therefore, simple and well-defined thermal conditions are applied in the calculation domain. For directional solidification conditions, a schematic illustration is shown in Fig. 1. For an adiabatic boundary condition on both sides, the whole simulation domain cools at a cooling rate R_C with a fixed temperature gradient G. At solidification time t, the temperature $T(t)$ at the point (x,y) can be simply expressed as

$$T(t) = T_{liq}(C_0) + G \cdot y - R_C \cdot t \quad (1)$$