Modeling Morphological Evolution during Dendritic Solidification using a Cellular Automaton

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MODELING MORPHOLOGICAL EVOLUTION DURING DENDRITIC SOLIDIFICATION USING A CELLULAR AUTOMATON

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Abstract

Morphological evolution of a dendritic growth front in a binary alloy is simulated using a cellular automaton approach to establish the feasibility of modeling such growth with a local rule-based scheme. The motivation for this work is derived from the need to predict the development of solidification structures within real components of complex geometry, where significant constraint of the thermal and solutal fields may exist. Such cases present complex boundaries and large domain sizes, which may preclude the effective use of more conventional methods. In this work, a model is presented which couples a two-dimensional alternate-direction-implicit finite-difference diffusion solution with a cellular automaton growth algorithm to simulate morphological evolution in alloys solidifying under directional growth conditions. Temperature, composition, and interface configuration are formulated into a local growth potential which is incorporated into a cellular automaton. Alloy solidification is simulated over a range of experimental conditions, producing various structures. The effects of anisotropic configurational contributions are examined.

We now have a technique for calculating the value of $p$ at each cell, based on the relevant physical parameters. To update the solid morphology, a random number ($0 < r < 1$) is generated for each cell at each time step for comparison with $p$. If $p_i > r$, the cell is set to solid. The composition is then set to $kC$ and the excess solute $(1-k)C^e$ is distributed among the available neighboring cells.

**Modeling Results**

All results presented in the following sections were obtained using input parameters associated with Al-4.5 wt% Cu. Unless otherwise noted, all simulations were performed using a 300x300 mesh over a 2mm square domain, which is permitted to move in space to follow the growth front.

As a method of verifying the solute redistribution techniques, planar growth was forced to occur by specifying $p=1$ for any undercooled interfacial site and $p=0$ for all other sites. This forces the growth front to follow the liquidus isotherm at a prescribed velocity. The solute profiles for the initial transient, steady-state growth, and growth under Scheil conditions compared favorably with analytical solutions, indicating the solute handling technique within the CA is appropriate. Removing the restriction which forced planar growth in the examples given above, we define $p(\phi)$ with (1). The stochastic component of the CA provides the necessary perturbations for morphological instability. If conditions permit, these random perturbations may trigger the breakdown of the growth front. Such a situation occurs in Figure 1. The simulation begins with a planar front at a liquidus temperature. The system cools directionally along a specified gradient and isotherm velocity. As position is calculated, the solid begins to grow at random locations on the planar front with respect to these local perturbations on diffusivity and interface velocity in a realistic fluid. Solute rejected at a growing location decreases the local driving force for growth at neighboring sites. The structure which develops on the $J(S_i^c)$ term in (3), which suppresses the growth of curved features. The coupling between capillarity and kinetic energy evident as the growing structure begins to evolve in time over particular solutions to a well organized waveform. A steady state emerges as solute is channeled away from the liquidus temperature. As the cells deepen, the tips begin to form, determined by their individual shape, indicating the onset of dendritic growth. Side-branches develop gradually due to secondary nucleation and a dendritic structure evolves. Later in the simulation, the structure is reached where the structure consists of an array of dendritic growth regions. As the dendrites grow, the primary dendrites aligned along an isothen.

To show that the model is correctly simulating the anisotropy, a series of 13 simulations were performed with various initial conditions near the stability limit. The results are shown in Figure 2 which shows that the model correctly predicts the transition from stability to instability, as predicted by constitutional supercooling.

Figure 3 illustrates the simulated effect of changing the primary spacing. As expected, higher velocities produce shorter spacings. To quantify the relationship between this spacing and the parameters $G$ and $V$, the growth rate, we now define the proper primary spacing. It is particularly notable that the model not only exhibits agreement with the $V^{-1}$ scaling but also that it provides excellent agreement in parameters as well. Additionally, due to the inclusion of the term $1/\eta$ in expression for $\Delta T_k$, the spacing is not dependent on the resolution, as demonstrated in Figure 5.

Figures 6 and 7 show that the weighting parameter $\alpha$ affects the anisotropy of the growing solid. Figure 6 illustrates the evolution of a single dendrite in a uniform temperature field in constant cooling conditions, with $\alpha=0$. The anisotropy is solely due to the square grid. This grid effect is overcome and the {11} interfaces are favorable for growth under Scheil conditions in favor of {11} interfaces. Figure 7 shows the progression of simulation results for $\alpha=0.5$. In this case, the grid anisotropy is overcome and the {11} interfaces are favored. This grid effect on the anisotropy is overcome and the {11} interfaces are favored. This grid effect on the anisotropy is overcome and the {11} interfaces are favored. This grid effect on the anisotropy is overcome and the {11} interfaces are favored.
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value of $p$ at each cell, based on the relevant physical
parameters. To update the solid morphology, a
random number $(0 < r < 1)$ is generated for each cell at
each time step for comparison with $p$. If $p > r$, the
cell is set to solid. The composition is then set to $c^*$
and the excess solute $(1-k)c^*$ is distributed among the
available neighboring cells.

**Modeling Results**

All results presented in the following sections
were obtained using input parameters associated with
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simulations were performed using a 300x300 mesh
over a 2 mm square domain, which is permitted to
move in space to follow the growth front.

As a method of verifying the solute redistribution
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follow the liquidus isotherm at a prescribed velocity.
The solute profiles for the initial transient, steady-state
growth, and growth under Scheil conditions compared
favorably with analytical solutions, indicating that the
solute handling technique within the CA is
appropriate. Removing the restriction which forced
planar growth in the examples given above, we define
$p(\phi)$ with (1). The stochastic component of the CA
provides the necessary perturbations for morphological
instability. If conditions permit, these random perturbations will
wedge the breakdown of the growth front. Such a situation is shown
in Figure 1. The simulation begins with a planar front sitting at the
liquidus temperature. The system cools directionally, according to
a specified gradient and isotherm velocity. As positive undercooling
develops, the solid begins to grow at random locations. The stability
of the planar front with respect to these local perturbations is dictated
by diffusivity and interface velocity in a realistic fashion, since the
solute rejected at a growing location decreases the probability for
growth at neighboring sites. The structure which develops depends
on the $\lambda s_1$ term in (3), which suppresses the growth of sharply
curved features. The coupling between capillarity and diffusion is
evident as the growing structure begins to evolve from random
perturbations into a well-organized waveform. A cellular structure
emerges as solute is channeled away from the fastest growing
regions. As the cells deepen, the tips begin to grow at a rate
determined by their individual shape, indicating the onset of dendritic
growth. Side-branches develop gradually due to secondary instability
and a dendritic structure evolves. Later in the simulation, a steady-
state is reached where the structure consists of an array of uniformly
spaced primary dendrites aligned along an isotherm.

To show that the model is correctly simulating morphological
instability, a series of 13 simulations were performed, using a range
of conditions near the stability limit. The results are summarized in
Figure 2 which shows that the model correctly simulates planar
stability or instability, as predicted by constitutional supercooling.

Figure 3 illustrates the simulated effect of velocity on the
primary spacing. As expected, higher velocities promote finer
spacings. To quantify the relationship between this simulated steady-
state primary spacing and the parameters $G$ and $V$, two sets of tests
were run for various values of $V$. For each set, $G/V$ was held
constant. The results of these tests, shown in Figure 4, are compared
with the analytical prediction of Kurz and Fisher. This figure
clearly indicates that the model accurately simulates the evolution of
the proper primary spacing. It is particularly noteworthy that the
model not only exhibits agreement with the $V^{1/4}G^{1/2}$ dependence,
but also that it provides excellent agreement with the values
themselves. Additionally, due to the inclusion of $(\Gamma/\Delta z)$ in the
expression for $\Delta T_a$, the spacing is not dependent on the mesh
resolution, as demonstrated in Figure 5.

Figures 6 and 7 show that the weighting parameters in the
configurational undercooling, particularly the $\alpha_1$ term, can be used to
affect the anisotropy of the growing solid. Figure 6 shows the
evolution of a single dendrite in a uniform temperature field, under
constant cooling conditions, with $\alpha_1=0$. The anisotropy of the growth
is solely due to the square grid. This grid effect promotes $(01)$
interfaces in favor of $(11)$ interfaces. Figure 7 shows the same
progression of simulation results for $\alpha_1=0.5$. In this case, the grid
anisotropy is overcome and the $(11)$ interfaces are favored over the $(01)$ interfaces. The resulting $<01>$
growth direction is necessary to achieve steady-state dendritic growth conditions in the directional
solidification simulations. The grid anisotropy can also result in unnatural rectangular features at the
interface during the development of a dendritic front. As shown in a previous paper, this is most evident
in the cellular regime where cells maintain flat fronts with corners near the cell divisions. The
progression of $(01)$ interfaces, the transition is delayed. The cells begin to develop instabilities on their flat fronts until
dendritic growth emerges from these. In contrast, the cellular to dendritic transition in Figure 1 consists of
a gradual increase in cell curvature, followed by secondary instability and side-branch generation.

Figure 3. Simulation results showing the difference in
primary spacing selected for $V=0.2$ mm/s (upper) and $V=0.5$ mm/s (lower). For both: $G=5$ K/mm. Black to white
indicates 0 to 5 wt% Cu.

Figure 6. A simulation progression of
the growth shape for $\alpha_1=0$. The
cellular regime where cells maintain flat fronts with corners near the cell divisions.

Figure 7. The physical size of the shown frame
increases from top to bottom.
Conclusions

A cellular automaton was applied to the growth of dendritic structures in an alloy under conditions for directional solidification. With the incorporation of growth anisotropy, the method reproduces many features of dendritic solidification and can operate with realistic values of G and V. This technique can predict solidification structures at a large enough scale to make it practical for simulating real casting processes, and because the growth algorithm used here depends only on local conditions, this model may be well suited for application to systems with complex geometry, where other methods may be difficult to implement. These features indicate the potential usefulness of the CA as a tool for the simulation of dendritic growth in actual castings.

References


Figure 7. A simulation progression of the growth shape for $\alpha=0.5$. The physical size of the shown frame increases from top to bottom.