Phase-Field Simulations of Columnar Dendritic Structure in Forced Flow

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INTRODUCTION

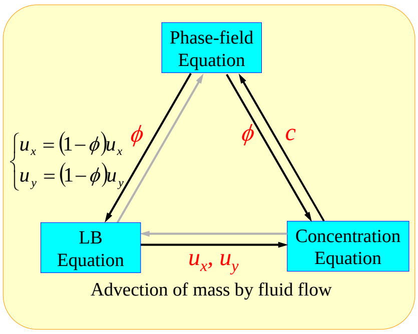
The typical microstructure of ingot consists of the outer chill zone, the intermediate columnar zone and the central equiaxed zone. Although the microstructure is thought to be largely affected by the melt flow, the detail studies have not been reported so far.

In this study, we investigate the effect of the forced flow on the columnar dendritic structure which grow from the multi nuclei on the mold wall with arbitrary crystal orientation. Here, we employ the coupling model of phase-field method and lattice Boltzmann method.

MODEL

Coupling simulations using phase-field equation, concentration equation and lattice Boltzmann equation are performed to investigate the solidification microstructure of binary alloy in forced flow.

The interface migration is simulated by the phase-field equaiton where the thermodynamic driving force is calculated from the local concentration. The concentration distribution is calculated by the diffusion equation of solute with advective term by melt flow. The velocities of melt flow is simulated by the lattice Boltzmann scheme. The coupling of above three equations are schematically shown in the right figure.



Phase-Field Equation

$$\frac{\partial \phi}{\partial t} = M_\phi \left[\nabla(a^2 \nabla \phi) - \frac{\partial}{\partial x}\left(a \frac{\partial a}{\partial \theta}\frac{\partial \phi}{\partial y}\right) + \frac{\partial}{\partial y}\left(a \frac{\partial a}{\partial \theta}\frac{\partial \phi}{\partial x}\right) - 4W\phi(1-\phi)\left\{ \phi - \frac{1}{2} - \frac{15}{2W}\frac{L(T-T_m)}{T_m}\phi(1-\phi) + \chi \right\} \right]$$

Phase-field parameters and material constants

$$\bar{a} = \sqrt{\frac{3\delta\gamma}{b}}, \quad W = \frac{6\gamma b}{\delta}, \quad M_\phi = \frac{\sqrt{2W}}{6a} M$$

Anisotropy equation for interface energy

$$a(\theta) = \bar{a}\left[1 + \varsigma \cos\{k(\theta - \theta_0)\}\right]$$

ϕ : phase-field variable
=1 in solid, = 0 in liquid
T : temperature in domain
T_m : temperature on liquidus line
χ : noise
δ : interface thickness
γ : interface energy
M : interface mobility
ς : strength of anisotropy
k : anisotropy mode
q : angle of interface normal
θ_0 : crystal orientation

Concentration Equation

$$\frac{\partial c}{\partial t} + \left(u_x \frac{\partial c}{\partial x} + u_y \frac{\partial c}{\partial y} \right) = \nabla \cdot D\left[\nabla c + \frac{(1-k)c}{1-\phi+k\phi}\nabla\phi \right] \qquad \begin{cases} c = \phi c_S + (1-\phi)c_L \\ k = c_S / c_L \end{cases}$$

Diffusion coefficient

$$D = D_S + (D_L - D_S)\frac{1-\phi}{1-\phi+k\phi}$$

c : concentration
c_L, c_S : concentration in liquid and solid
k : partition coefficient
D_S : diffusion coefficient in solid
D_L : diffusion coefficient in liquid
u_x, u_y : fluid velocities

Lattice Boltzmann Equation

Pressure distribution function

$$p_\alpha(\mathbf{x} + \mathbf{e}_\alpha \Delta t, t + \Delta t) = p_\alpha(\mathbf{x}, t) - \frac{1}{\tau}\left\{ p_\alpha(\mathbf{x}, t) - p_\alpha^{eq}(\mathbf{x}, t) \right\}$$

Pressure Velocity

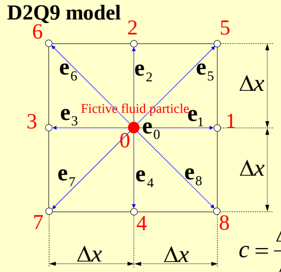
$$p = \sum_{\alpha=0}^{8} p_\alpha, \quad \mathbf{u} = \sum_{\alpha=0}^{8} p_\alpha \mathbf{e}_\alpha \Big/ p_0 \qquad \tau = \frac{1}{2}\left(6\nu \frac{\Delta t}{(\Delta x)^2} + 1 \right)$$

Equilibrium distribution function

$$p_\alpha^{eq}(\mathbf{x}, t) = w_\alpha \left\{ p + p_0 \left[\frac{3(\mathbf{e}_\alpha \cdot \mathbf{u})}{c^2} + \frac{9(\mathbf{e}_\alpha \cdot \mathbf{u})^2}{2c^4} - \frac{3\mathbf{u}^2}{2c^2} \right] \right\}$$

τ : collision relaxation time
w_α : weight coefficient
= 4/9 (α = 0)
= 1/9 (α = 1-4)
= 1/36 (α = 5-8)
ν : kinetic viscosity

D2Q9 model



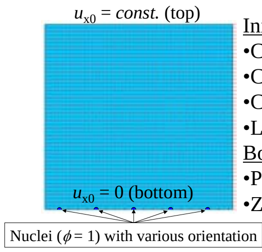
$$c = \frac{\Delta x}{\Delta t}$$

Particle velocities

$\mathbf{e}_0 = \{0 \quad 0\}^T$
$\mathbf{e}_1 = \{c \quad 0\}^T$ $\quad \mathbf{e}_5 = \{c \quad c\}^T$
$\mathbf{e}_2 = \{0 \quad c\}^T$ $\quad \mathbf{e}_6 = \{-c \quad c\}^T$
$\mathbf{e}_3 = \{-c \quad 0\}^T$ $\quad \mathbf{e}_7 = \{-c \quad -c\}^T$
$\mathbf{e}_4 = \{0 \quad -c\}^T$ $\quad \mathbf{e}_8 = \{c \quad -c\}^T$

SIMULATIONS AND RESULTS

We perform the dendrite solidification simulations of Al-10%Si supersaturated alloy in forced flow. Some nuclei with arbitrary crystal orientation are putted on the bottom of computational domain in which the constant fluid flow in x-direction and the constant concentration are set as initial condition. The effects of forced flow on the columnar dendritic structure that grows from the mold wall are investigated.



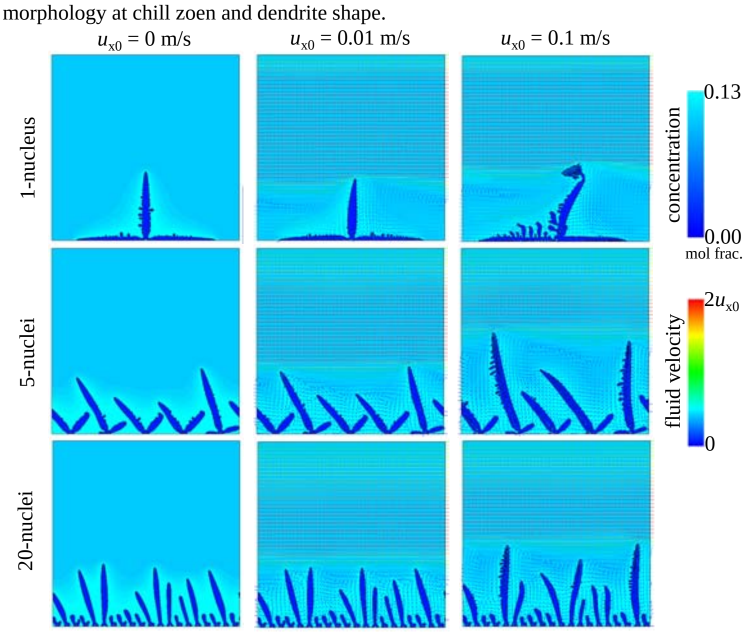
Initial conditions
- Constant fluid flow u_x = 0, 0.01, 0.1 m/s and u_y = 0 m/s
- Constant concentration c = 0.1 mol frac.
- Constant temperature T = 855 K
- Liquid condition ϕ = 0

Boundary conditions
- Periodic in x-direction for all variables
- Zero Nouman on top and bottom for ϕ and c

2000 x 2000 FD lattices (Δx = 50 nm)

Effects of the flow velocity and number of nuclei

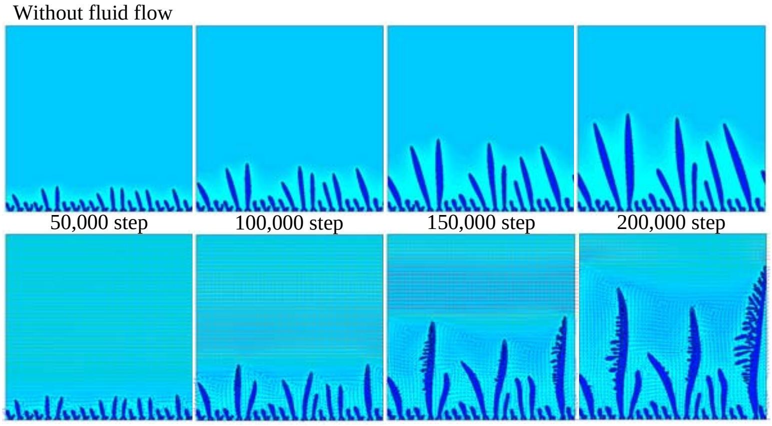
Nine sets of simulations by changing fluid velocity and the number of nuclei are performed. The following figures are the solidification morphologies (solid black line), concentration (color contour) and fluid velocities (vector) at 130,000 step. It is observed that the flow velocity changes the dendritic morphology dramatically especially for high velocity and the number of nuclei changes the solidification morphology at chill zoen and dendrite shape.



Growth processes with and without fluid flow

Without fluid flow, the dendrites grow almost straightly to the preferred growth direction. On the other hand, with fluid velocity, the dendrite changes the growth direction depending on the distance to the nearest-neighbor dendrites.

Without fluid flow



With fluid flow : u_{x0} = 0.1 m/s