Phase-field study on effect of mechanical stress on dendrite fragmentation

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INTROUCTION

Fundamental understanding of the relationship between solidification variables and the resulting microstructure is essential for the development of optimum methods for quality casting. The microstructures of casting product consist of columnar grains formed around the wall and equiaxed grains formed in the middle of the mold. Generally, the equiaxed grains have more dominant effect on the mechanical properties of the product than the columnar grains. Therefore, it is crucial for industrial applications to understand the formation mechanism of equiaxed grain structure. Although the mechanical fragmentation of columnar dendrite due to melt flow and gravity is thought to be a possible nucleation mechanism of equiaxed grains, it has not been clarified yet.

In this study, we investigate stress concentration, which is the indicator of mechanical fragmentation, occurred at dendrite neck due to gravity applying to the vertical direction of dendrite growth direction. The coupling simulations by phase-field method and finite element method are performed.

NUMERICAL MODELS

The dendrite growth from undercooled pure Ni is simulated by a quantitative phase-field model. Then, the calculated dendritic morphologies are transformed to the finite element simulation and the mechanical stress due to gravity are simulated.

< Phase-field method >

Evolution equations of phase-field variable ϕ and temperature T

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

$$\frac{\partial T}{\partial t} = D \nabla^2 T + \frac{1}{2} \frac{L}{c_p} \frac{\partial p}{\partial t}$$

Here,
- ϕ : phase-field variable (ϕ = 1 in solid, ϕ = -1 in liquid)
- a : gradient coefficient
- T_m : melting temperature
- L : latent heat
- T : temperature
- D :thermal diffusivity
- c_p: specific heat
- L :latent heat

Surface anisotropy

$$a(\theta) = \bar{a}\{1 + \varsigma \cos(k\theta)\}$$

- γ: strength of anisotropy
- k : mode number
- θ : angle between surface normal and x-axis

Phase-field parameters $\bar{a}$, W and M_ϕ can be related to the material parameters by following equations.

$$\bar{a} = \frac{1}{2}\sqrt{\frac{3\delta\gamma}{b}}, \quad W = \frac{6\gamma b}{\delta}, \quad M_\phi = \frac{4\sqrt{2} b^2 T_m \kappa}{3 a_1 a_2 \delta^2 L^2}$$

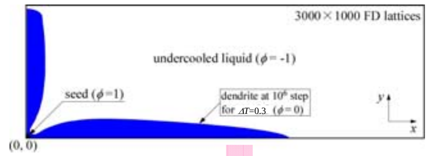
- δ : interface thickness
- γ : interface energy
- κ : thermal conductivity
- b : constant related to δ

< Finite element method >

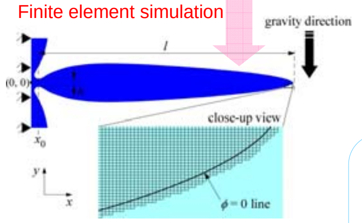
Finite element simulations are performed as liner elastic plane stress problem.

NUMERICAL CONDITIONS

Phase-field simulation



Finite element simulation



The left figure shows computational domain and initial conditions for phase-field simulations of dendrite growth. Initially, all regions are filled with the undercooled liquid and dimensionless undercooling is set to be ΔT=0.3 and ΔT=0.5 . One circular seed with radius r=10Δx is putted on the origin (0,0) or the left bottom corner. By considering symmetrical shape of dendrite, a half region in y-direction is simulated.

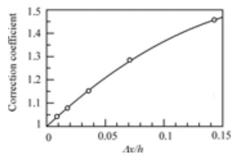
The information of phase-field is transferred to the finite element simulations to evaluate the stress distributions due to gravity. The left figure shows an example of finite element model and boundary condition corresponding to the dendritic morphology shown in left-upper figure.

<parameter>

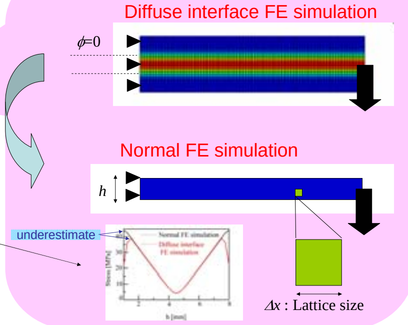
- Interface energy γ = 0.37 J/m2
- Young's modulus E *
- Poisson's ratio ν = 0.3
- Strength of anisotropy ζ = 0.1
- Mesh size: ΔT=0.5 Δx = 3nm; ΔT=0.3 Δx = 13nm
- Time increment $\Delta t = \Delta x^2/6D$

$$* \; E(\phi) = \frac{1}{2}\left(\tanh\frac{\phi}{2\tau} + 1 \right) E_s$$

CORRECT COEFFICIENT TO EVALLUATE MAXIMUM STRESS

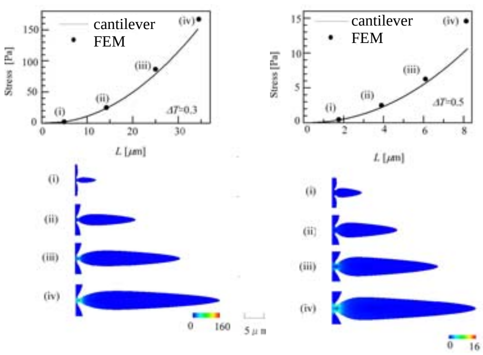


In the present finite element simulations with diffuse interface, the maximum stress is underestimated comparing to the normal simulations where only solid region is meshed. Therefore, the finite element results need to be corrected. So, as shown in upper figure, the correction coefficients are calculated by the simple cantilever simulations beforehand.



SIMULATION RESULTS

RELATIONSHIPS BETWEEN DENDRITE ARM LENGTH AND MAXIMUM STRESS

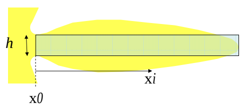


<cantilever model>

The maximum stress in the cantilever model is calculated by

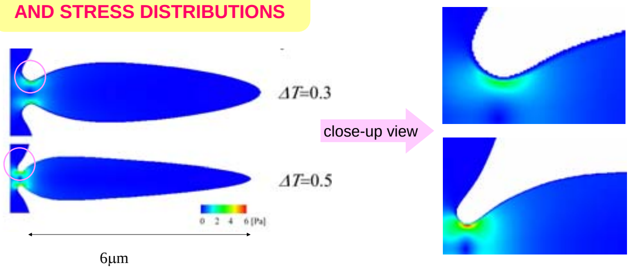
$$\sigma_{\max} = \frac{6}{wh^2} \sum_{i=1}^{N} (x_i - x_0) f_i$$

w: thickness of dendrite (w=1)
N : number of node
f_i : nodal force



These figures show the relationship between dendrite arm length and maximum stress at dendrite neck and dendrite morphologies for each time step. From the dendritic morphologies, although the radius of curvature at the dendrite neck becomes larger with the dendrite growth, the ratio of it to the representative size of dendrite becomes small. Therefore, it is concluded that the dendritic morphology approaches to a shape, which is easy to induce the stress concentration, with growth. As a result, the differences between the cantilever model and the present FE simulation increase with dendrite growth.

DENDRITE MORPHOLOGIES AND STRESS DISTRIBUTIONS



These figures show the dendrite morphologies and stress distributions at an identical length for ΔT =0.5 and 0.3. The radius of curvature and the minimum cross section are smaller for ΔT=0.5 than ΔT=0.3. Therefore, the maximum equivalent stress in case of ΔT=0.5 is higher than that of ΔT=0.3.

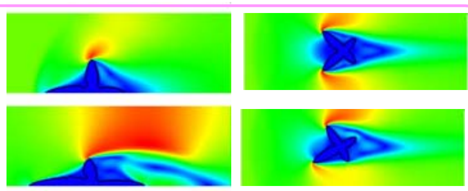
CONCLUTIONS

The stress concentration occurred at the neck of dendrite that grows to the vertical direction for gravity was investigated by coupling phase-field method and finite element method. As a result, it was clearly shown that the maximum stress at dendrite neck increase with dendrite growth and the increasing ratio is higher for high undercooling condition than lower one. Furthermore, to evaluate the maximum stress in the dendrite with high accuracy, the simple cantilever model was concluded to be not enough and finite element method which can directly treat the dendrite morphology is much more powerful.

The developed coupling model of phase-field method and finite element method is anticipated to be applied to the study of mechanical dendrite fragmentation due to the gravity and melt flow.

FUTURE WORK

We will try to develop coupling model of phase-field method, finite element method and Navier-Stokes equation, and to estimate stress distribution in dendrite due to melt flow and gravity force.



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