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Prediction of the equivalent elastic modulus of mush zone during solidification process coupled with phase field simulations

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ABSTRACT

A phase field model with the consideration of applied and thermal stress is developed in this paper. The elastic stress and strain fields inside the solid skeleton can be calculated out by phase field model together with the phase morphologies. By adding an external constant stress boundary condition, the total strain can be obtained by solving the mechanical equilibrium equations. We can get the equivalent elastic modulus under different phase morphologies from these calculations, which is useful for FEM or FDM simulations on a larger scale. This model is applied to as-cast and semi-solid casting process, respectively. The equivalent elastic modulus under dendritic and spherical solid skeleton are both obtained.

1. Introduction

Casting simulation is now widely accepted as an important tool for product design and process optimization. Casting simulation uses numerical methods to calculate mold filling, cooling and liquid-solid phase transformation. It finally provides some quantitative predictions of defects distribution, thermal stresses and distortions. At the beginning of the casting simulation, the CAD (Computer Aided Design) geometry should be meshed first for the following FEM (Finite Element Method) or FDM (Finite Difference Method) calculations. The cell size changes from hundreds microns to several millimeters, which depends on the complexity of the objective castings. The cells can be divided into three categories during simulation according to the solid fractions inside each mesh, *i.e.* the liquid cell ($f_s = 0$), the solid cell ($f_s = 1$) and the mush cell ($0 < f_s < 1$). The volume average method is usually adopted in order to get the equivalent properties for mush cells, such as density, thermal conductivity, elastic modulus, etc.

Among these properties, the equivalent elastic modulus is very important for residual stress and distortion predictions. But it is not a pure thermodynamics parameter and hard to be measured by experiments at the mush state. So many scientists established a lot of equations to predict the equivalent elastic modulus based on different volume average methods. But most of the equations are only functions of solid fraction or temperature. They did not consider the complexity of solid skeleton network, which can be affected by the processing methods.

Recently, the phase-field model is becoming a powerful tool to describe the complex interface pattern evolutions [1–5]. It describes the microstructure using a set of conserved and non-conserved field variables that are continuous across the interface regions. Phase-field models of solidification have been originally developed for pure materials [6,7] and then extended to alloys [8–13]. The elastic stress and strain fields in the solid skeleton network can also be calculated out directly within the phase field framework, especially the internal stresses caused by the thermal shrinkage. In this work we develop the phase field model by adding an external small stress as mechanical boundary conditions. Using this model we can calculate the stress and strain distributions. The total strain can be calculated out, which is a mechanical response to the external small applied stress. From these calculations we can obtain the equivalent elastic modulus, which is useful for FEM or FDM simulations on a larger scale [14,15].

2. Model descriptions

For multi-grain system, the multi-phase phase field model should be adopted in order to describe the different phases or orientations during solidification process. In this model, different orientations of the same solid phase will be distinguished by separate

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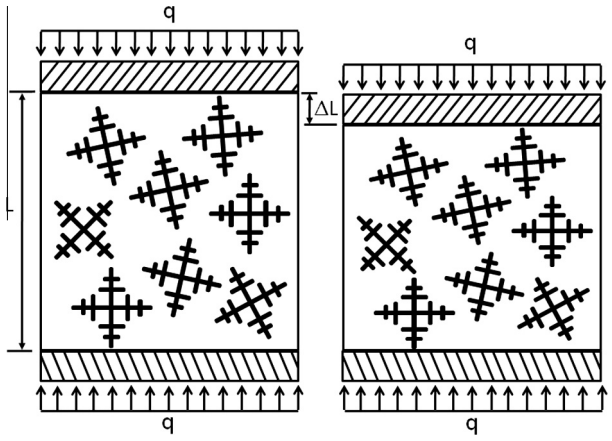

Fig. 1. The calculation sketch for equivalent elastic modulus.

phase-field parameters. The governing equations for phase field evolution can be given as [16–19]:

$$\frac{\partial \phi_\alpha}{\partial t} = \sum_\beta M_{\alpha\beta}\left\{\sigma_{\alpha\beta}\left[\phi_\alpha \nabla^2 \phi_\beta - \phi_\beta \nabla^2 \phi_\alpha + \frac{\pi^2}{\eta^2}(\phi_\alpha - \phi_\beta)\right] + \frac{\pi}{\eta}\sqrt{\phi_\alpha \phi_\beta}\left(\Delta G^{CH}_{\alpha\beta} + \Delta G^{EL}_{\alpha\beta}\right)\right\} \quad (1)$$

where $M_{\alpha\beta}$ is the mobility of the interface, $\sigma_{\alpha\beta}$ is the interface energy, $\Delta G^{CH}_{\alpha\beta}$ and $\Delta G^{EL}_{\alpha\beta}$ are chemical driving force and mechanical driving force, respectively. $\Delta G^{CH}_{\alpha\beta}$ can be written as:

$$\Delta G^{CH}_{\alpha\beta} = -f_\alpha(c_\alpha) + f_\beta(c_\beta) + \mu(c_\alpha - c_\beta) \quad (2)$$

where μ is the solute chemical potentials and can be given as [20]:

$$\mu = \frac{\partial f_\alpha}{\partial c_\alpha} = \frac{\partial f_\beta}{\partial c_\beta} \quad (3)$$

The mechanical driving force $\Delta G^{EL}_{\alpha\beta}$ can be obtained using the following equations:

$$\Delta G^{EL}_{\alpha\beta} = -\left(\frac{\partial}{\partial \phi_\alpha} - \frac{\partial}{\partial \phi_\beta}\right) f^{EL} \quad (4)$$

$$f^{EL} = \frac{1}{2}\sum_\alpha \phi_\alpha \left[\varepsilon^{ij}_\alpha - \left(\varepsilon^0_\alpha\right)^{ij}\right] C^{ijkl}_\alpha \left[\varepsilon^{kl}_\alpha - \left(\varepsilon^0_\alpha\right)^{kl}\right] \quad (5)$$

where $\left(\varepsilon^0_\alpha\right)^{ij}$ is the transformation strain and C^{ijkl}_α is the elasticity tensor.

In order to get the finial strain in Eq. (5) at the mechanical equilibrium state, the following equations should be solved:

$$0^i = \nabla^j \sum_\alpha \phi_\alpha C^{ijkl}_\alpha \left[\varepsilon^{kl}_\alpha - \left(\varepsilon^0_\alpha\right)^{kl}\right] \quad (6)$$

By adding an external constant stress boundary condition, the mechanical response can be obtained by solving the mechanical equilibrium equations. The grids at the top boundary are set to keep the same displacement, which can be seen in Fig. 1. The equivalent elastic modulus can be described as:

$$E_{eq} = qL/\Delta L \quad (7)$$

Table 1
The parameters used in the simulation.

Parameters	Liquid	Solid
Diffusion coefficient	2×10^{-8} m^2 s^{-1}	1×10^{-12} m^2 s^{-1}
C_{11}	20 MPa	7198 MPa
C_{12}	10 MPa	3876 MPa
C_{44}	5 MPa	1660 MPa
Initial concentration	1.5 at%	0.21 at%
Interface energy	0.1 J m^{-2}	
Mobility of the interface	4×10^{-10} m^4 J^{-1} s^{-1}	
Mesh size	2×10^{-6} m	

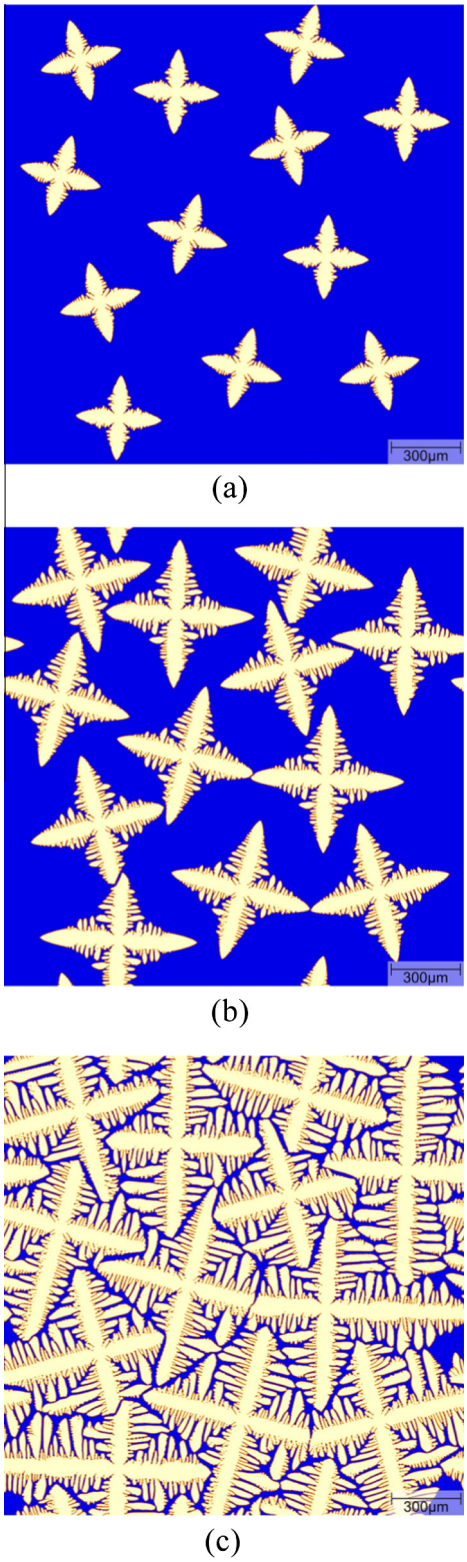

Fig. 2. The dendrite morphology at different solid fractions. (a) $f_s = 0.12$, (b) $f_s = 0.32$, (c) $f_s = 0.75$.