Phase-field simulations of crystal growth in a two-dimensional cavity flow

Seunggyu Lee [1] , Yibao Li [2] , Jaemin Shin [3] and Junseok Kim [4]

1) *National Institute for Mathematical Sciences, Daejeon 34047, REpublic of Korea*

2) *School of Mathematics and Statistics, Xi'an Jiatong University, Xi'an 710049, China*

3) *Institute of Mathematical Sciences, Ewha W. University, Seoul 120-750, Republic of Korea*

4) *Department of Mathematics, Korea University, Seoul 138-713, Republic of Korea*

Corresponding Author : Juneok Kim, cfdkim@korea.ac.kr

ABSTRACT

In this paper, we consider a phase-field model for dendritic growth in a two-dimensional cavity flow and propose a computationally efficient numerical method for solving the model. The crystal is fixed in the space and cannot be convected in the most of previous studies, instead the supercooled melt flows around the crystal, which is hard to be realized in the real world experimental setting. Applying advection to the crystal equation, we have problems such as deformation of crystal shape and ambiguity of the crystal orientation for the anisotropy. To resolve these difficulties, we present a phase-field method by using a moving overset grid for the dendritic growth in a cavity flow. Numerical results show that the proposed method can predict the crystal growth under flow.

1 INTRODUCTION

Convection of the crystal in the melt is of great interest for the practical processes to understand the dendritic solidification. The convective effects on free dendritic crystal growth have been investigated experimentally and numerically. In numerical investigation, the phase-field method is a flexible mathematical tool to describe the interfaces in dendritic crystal growth with convection. However, the crystal is fixed in the space and cannot be convected, instead the supercooled melt flows around the crystal, which is hard to be realized in the real world experimental setting in the previous studies. The main purpose of the present paper is to resolve these difficulties by using a moving overset grid. The fluid domain is covered with a fixed Cartesian grid, while a moving overset grid is used to represent the crystal growth. The motion of the crystal is derived by calculating the translational and rotational force of the crystal phase.

2 MATHEMATICAL MODELING

The governing equations for crystal growth in the flow are given as

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla p + \frac{1}{Re}\nabla\cdot[\eta(\phi)(\nabla\mathbf{u}+\nabla\mathbf{u}^T)], \tag{1}$$

$$\nabla\cdot\mathbf{u} = 0, \tag{2}$$

$$\epsilon^2(\phi)\frac{\partial\phi}{\partial t} = \nabla\cdot(\epsilon^2(\phi)\nabla\phi) + [\phi - \lambda U(1-\phi^2)](1-\phi^2) + \left(|\nabla\phi|^2\epsilon(\phi)\frac{\partial\epsilon(\phi)}{\partial\phi_x}\right)_x + \left(|\nabla\phi|^2\epsilon(\phi)\frac{\partial\epsilon(\phi)}{\partial\phi_y}\right)_y, \tag{3}$$

$$\frac{\partial U}{\partial t} + \mathbf{u}\cdot\nabla U = D\Delta U + \frac{1}{2}\frac{\partial\phi}{\partial t}, \tag{4}$$

where $\mathbf{u}$ is the velocity, p is the pressure, $\eta(\phi)$ is the variable viscosity, and U is the temperature. Note that Eqs. (1) and (2) are the Navier–Stokes equations [1] and Eqs. (3) and (4) are the governing equations for dendrite growth [2]. Here, $\eta(\phi) = 0.5[\eta_s(1+\phi)+\eta_m(1-\phi)]$, where η_s and η_m are viscosities of solid and melt, respectively. We take the increased viscosity approach [2] which uses a very large viscosity in the solid to describe the resistance to the flow. The dimensionless parameters are the Reynolds number Re, λ, and D. For the four-fold symmetry, $\epsilon(\phi)$ is defined as:

$$\epsilon(\phi) = (1-3\epsilon_4)\left(1 + \frac{4\epsilon_4}{1-3\epsilon_4}\frac{\phi_x^4+\phi_y^4}{|\nabla\phi|^4}\right), \tag{5}$$

where ϵ_4 is a parameter for the anisotropy of interfacial energy.

In this section, we propose a hybrid numerical method using an overset grid for the simulation of the crystal growth in a cavity flow. Let $\Omega_f = (a,b)\times(c,d)$ be a domain for the fluid velocity $\mathbf{u} = (u,v)$, pressure p, and temperature U with proper boundary conditions. Also, let $\Omega_c = (0,\alpha)\times(0,\beta)$ be another domain for the phase-field function ϕ with interpolated boundary conditions. Ω_{moving} is the coordinate transformation of Ω_c, and it represents the location and rotation of Ω_c on Ω_f. Let $\mathbf{X}_1$, $\mathbf{X}_2$, $\mathbf{X}_3$, $\mathbf{X}_4$ be corners of Ω_{moving} on Ω_f corresponding to points $(0,0)$, $(\alpha,0)$, (α,β), $(0,\beta)$ on Ω_c, respectively. We determine the location of Ω_{moving} by setting its center as $\mathbf{m}_c = (\mathbf{X}_1+\mathbf{X}_2+\mathbf{X}_3+\mathbf{X}_4)/4$ and the rotation θ_c as the signed angle measured from the horizontal axis to the vector $\overrightarrow{\mathbf{X}_1\mathbf{X}_2}$ (see Fig. 1).

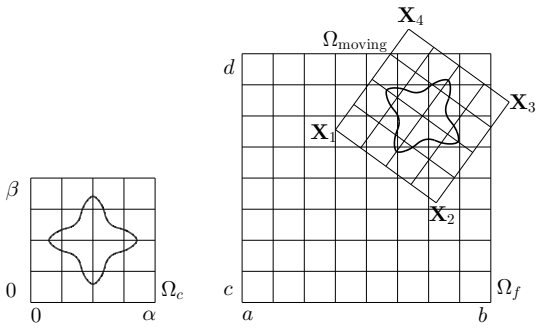

Figure 1. Schematic illustration of the fluid domain Ω_f, the crystal domain Ω_c, and the moving domain Ω_{moving}.

REFERENCES

1. Choi, Y., Jeong, D., Lee, S., Kim, J., "Numerical Implementation of the two-dimensional incompressible Navier–Stokes equation", *Journal of the KSIAM*, Vol. 9, 2015, pp. 103–201.
2. Dantzig, J.A., "Modelling liquid-solid phase changes with melt convection", International Journal for Numerical Methods in Engineering, Vol. 28, 1989, pp. 1769–1785.