Permeability tensor for various columnar dendrite structures

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Abstract. Permeability is a very important parameter determining fluid dynamics in macroscale casting simulations. For a columnar solidification structure, the permeability has anisotropy and becomes a tensor quantity. In our previous study, we proposed a permeability tensor and confirmed its validity. In this study, the applicability of the permeability tensor is shown through a series of permeability computations that are conducted for some columnar dendritic structures with different morphologies.

1. Introduction

In simulations of casting and macrosegregation prediction, we need to know values of a permeability expressing the ease of liquid flow in the mushy region, where solid and liquid coexist [1, 2]. The permeability is computed by Darcy’s law:

\[ \mathbf{U} = -\frac{1}{\mu} \mathbf{K} \nabla P \]  

where \( \mathbf{U} \), \( \mathbf{K} \), \( \nabla P \), and \( \mu \) are the average liquid flow velocity vector, permeability tensor, average pressure gradient vector, and viscosity, respectively. While the permeability tensor, \( \mathbf{K} \), is isotropic for an equiaxed structure [3, 4], it is anisotropic for a columnar structure [5–9]. Permeabilities of flow normal and parallel to a columnar structure have been expressed as a function of primary arm spacing and secondary arm spacing [5, 7, 8]. However, the accuracy of those equations has not been clarified [9] and more efforts are needed to obtain a conclusive equation for expressing the permeability of a columnar structure. Also, no studies concerning the permeability tensor for a columnar structure have been performed to the best of our knowledge.

To predict permeability for various morphologies of solidification microstructure, numerical simulation is a powerful and promising approach [9–12]. In particular, the phase-field method can predict dendritic solidification microstructures with high accuracy. We have developed a permeability prediction method by bridging the phase–field and lattice Boltzmann methods [13]. In this method,
large–scale simulation using a GPU–rich supercomputer enabled the permeability prediction for realistic columnar structures with multiple primary arms [14–16]. Through investigations of the permeability for columnar dendritic/cellular structures, it was concluded that dimensionless permeabilities for normal and parallel flows are well approximated by the Kozeny–Carman (KC) equation [17] with a coefficient $k_c = 9$ and 3, respectively [13, 18]. Here, the KC equation is expressed as

$$K = \frac{(1-f_s)^3}{k_c S_S^2 f_S^2}$$  \hspace{1cm} (2)$$

where $f_s$ is the solid fraction, $S_S$ is the specific interface area, and $k_c$ is a coefficient. The specific interface area, $S_S$, is defined by $S_S = A_{SL}/V_S$, where $A_{SL}$ is the solid–liquid interface area and $V_S$ is the volume of solid. We also proposed a permeability tensor for a columnar structure. The validity of the proposed permeability tensor was confirmed by simulations of flow in various directions to the columnar structure [18]. However, it is important to test the validity of the proposed permeability for different columnar dendritic structures to understand its applicability.

In this study, we carry out testing of the validity and applicability of the permeability tensor by systematically computing permeabilities for some columnar dendritic structures of an Al–15wt%Cu binary alloy.

2. Permeability prediction method

The permeability prediction procedure used in this study consists of the following three steps [13]:

Step 1 A dendrite solidification structure is computed by the phase–field method. In the present study, the directional solidification simulations using frozen temperature approximation are conducted to obtain columnar dendritic structures for a binary alloy.

Step 2 Interdendritic liquid flow in a dendrite structure obtained in Step 1 is computed by the lattice Boltzmann method, where the phase–field variable computed in Step 1 is used to distinguish between the solid and liquid, and a pressure gradient is applied to a direction where the permeability is to be computed.

Step 3 Computing the average flow velocity in the pressure gradient direction; permeability in the pressure gradient direction is computed based on Darcy’s law, equation (1).

The phase–field and lattice Boltzmann simulations in steps 1 and 2 were conducted in large–scale system. For the large–scale simulations, parallel computation was performed using multiple GPUs on a GPU–rich supercomputer (TSUBAME3.0) at Tokyo Institute of Technology [19–23].

2.1. Phase-field equations (Step 1)

A quantitative phase–field model for a dilute binary alloy [24] is applied to the directional solidification simulation. Time evolution equations of the temperature $T$ (frozen temperature approximation), phase–field $\phi$ ($\phi = 1$ in a solid and $\phi = -1$ in a liquid), and nondimensional supersaturation $u$ are expressed as

$$T(z) = T_0 + G \left( z - V_r t \right)$$  \hspace{1cm} (3)$$

$$\tau \left( \nabla \phi \right) \left[ 1 - (1-k) u \right] \frac{\partial \phi}{\partial t} = \nabla \cdot \left[ W \left( \nabla \phi \right) \nabla \phi \right] + \sum_{i} \frac{\partial}{\partial x_i} \left[ W \left( \nabla \phi \right) \frac{\partial W \left( \nabla \phi \right)}{\partial \phi_i} \nabla \phi_i \right] \left[ - (\phi + \phi^*) \right] - \lambda^* \left( 1 - \phi^* \right) \left( u + u' \right)$$  \hspace{1cm} (4)$$

$$\frac{1}{2} \left[ 1 + k - (1-k) \phi \right] \frac{\partial u}{\partial t} = \nabla \cdot \left[ D_{i} q \left( \phi \right) \nabla u - j_{i,LT} \right] + \frac{1}{2} \left[ 1 + (1-k) u \right] \frac{\partial \phi}{\partial t} - \nabla \cdot J$$  \hspace{1cm} (5)$$
where $T_0$ is the reference temperature at $z = 0$ and $t = 0$, $G$ is the temperature gradient, $z$ is the spatial coordinate along the direction of $G$, $V_p$ is the pulling velocity, and $t$ is the time. In equation (4), $u' = (z_T - V_p t)/t$ denotes the additional supersaturation, where $l_T = |m|/(1-k)c_0/(kG)$ is the thermal diffusion length, $k$ is the partition coefficient, $c_0$ is the initial concentration in the liquid, $m$ is the liquidus slope, and $z_T$ is the coordinate in the $G$ direction with an origin at $u = -1$. $\tau(\nabla \phi) = \tau_{0i}(\nabla \phi)^2$ and $W(\nabla \phi) = W_{0i}(\nabla \phi)$ are the phase–field relaxation time and interface thickness, respectively, with a crystalline anisotropy $a_{0i}(\nabla \phi) = 1 - 3\varepsilon_i + 4\varepsilon_i(\phi_s^4 + \phi_c^4 + \phi_c^2)/|\nabla \phi|^2$, where $\varepsilon_i$ is the anisotropic strength. Here, $\phi_s$ is the spatial derivative of $\phi$ with respect to $x_i$, $\lambda^*$ is a coupling constant associated with the thermodynamic driving force given by $\lambda^* = a_iW/d_0$, with $a_i = 0.88388$ and the chemical capillary length $d_0 = k\Gamma/(|m|(1-k)c_0)$, where $\Gamma$ is the Gibbs–Thomson constant. The nondimensional supersaturation $u$ is defined as $u = (C_L - C_s^i)/(C_s^i - C_s^e)$, where $C_s$ is the concentration in the liquid, and $C_L^e$ and $C_s^e$ are the equilibrium concentrations in the liquid and in the solid, respectively. We followed the Kim–Kim–Suozzi model [25] and applied the relations $k = C_s^e/C_L^e = C_s/C_L$. The concentration $C$ is given by $C = C_s (1+\phi)/2 + C_L (1-\phi)/2$. In the solute diffusion equation, equation (5), $j_{1i}$ represents the anti–trapping current, given by $j_{1i} = -(1-kD_sD_t)/(2\sqrt{2})W_0(1+1-k)u(\hat{\nabla} \phi\hat{\tau})\nabla \phi\nabla \phi$, in which $D_s$ and $D_t$ are the diffusion coefficients in the solid and in the liquid, respectively. $J$ is the fluctuating current [26] and $q(\phi)$ is an interpolating function given by $q(\phi) = [kD_s + D_t + (kD_s - D_t)\phi]/(2D_t)$.

### 2.2. Lattice Boltzmann equations (Step 2)

The lattice Boltzmann equation is expressed by [13]

$$f_i(x, t + \Delta t) = f_i(x, t) - \frac{1}{\tau_{BM}} \left[ f_i(x, t) - f_i^{eq}(x, t) \right] + \rho W \left[ \frac{5c_i^2 - U}{c_i} + \frac{9(c_i \cdot U)c_i}{2c_i} \right] G_{i\Delta} - 3\rho W_i (\nabla P)_{\Delta i} \quad (6)$$

where $f_i$ is the particle distribution function, $f_i^{eq}$ is the equilibrium distribution function, $\tau_{BM}$ is the relaxation time, $w_i$ is the weight function, $c = \Delta x/\Delta t$ is the lattice velocity, $\Delta t$ is the grid size, and $\Delta t$ is the time increment. The density $\rho$ and flow velocity $U$ are computed by 

$$\rho = \sum_{i=0}^{\phi+4} f_i$$

and

$$\rho U = \sum_{i=0}^{\phi+4} c_i f_i$$

with the number of discrete velocities $Q$. In this study, $Q = 19$ because the D3Q19 model is employed. The kinetic viscosity $\nu$ can be computed by $\nu = \Delta t c^2 (\tau_{BM} - 0.5)/3$. To satisfy the no–slip condition at the solid–liquid interface, the dissipative drag force $\mathbf{G} = -2\rho \nu \mathbf{V}/W_0((1 + \phi)/2)\mathbf{U}$ [27, 28] is introduced to a diffuse interface, where $\nu$ is the kinetic viscosity and $h = 2.757$ [27]. The forced convection is caused by applying a constant pressure gradient $\nabla P$ [29].

### 2.3. Permeability computation (Step 3)

When computing the average flow velocity $U_{a}$ in the pressure gradient direction, the permeability in the $x_i$–direction is computed by $K_{ai} = -\mu U_{a} dx_i/(dP/dx_i)$.

### 3. Permeability tensor

In our previous study [18], a permeability tensor for a columnar structure was proposed as

$$K = R^T K_x R \quad (7)$$

where $K_x$ is the diagonal permeability tensor and $R$ is the coordinate transformation matrix. Here, $K_x$ and $R$ are expressed as
$K_n = \begin{bmatrix} K_x & 0 & 0 \\ 0 & K_y & 0 \\ 0 & 0 & K_z \end{bmatrix}$, $R = \begin{bmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$

where $K_x$, $K_y$, and $K_z$ are the permeabilities of flow in the $x$-, $y$- and $z$-directions, respectively. It is convenient that the $x$-, $y$- and $z$-directions correspond to the preferred growth directions $[100]$, $[010]$ and $[001]$ of a cubic material. Thus, $K_x$ and $K_y$ are the permeabilities for normal flow, and $K_z$ is the permeability for parallel flow, as the temperature gradient, $G$, is set to the $z$-direction. After coordinate transformation, the permeability for the $(\theta, \psi)$ direction can be expressed by

$$K(\theta, \psi) = K_{11} = (\cos \theta \cos \psi)^2 \cdot K_x + (\sin \theta \cos \psi)^2 \cdot K_y + \sin^2 \psi \cdot K_z$$

By comparing this equation to simulation results, the validity of the permeability tensor, equation (7), is confirmed.

4. Simulations and results

4.1. Columnar dendritic structures

We prepared columnar dendritic structures by performing phase-field simulations for directional solidification of a single-crystal Al–15wt%Cu binary alloy. The temperature gradient $G$ and pulling velocity $V_p$ in the $z$-direction were set as $G = 50$ K/mm and $V_p = 20$ $\mu$m/s, respectively. The material and simulation parameters are summarized in table 1. From a preliminary simulation in a large computational domain which allows growth of multiple primary arms, we obtained the average primary arm spacing $\lambda_{ave} = 174.7$ $\mu$m ($= 447.3 \Delta x$) by a counting method assuming a regular hexagonal array. In our previous study, we confirmed that the permeability computed for a columnar structure with multiple primary arms becomes nearly the same as that of a columnar structure with periodic regular hexagonal array with the same primary arm spacing. This means that we can drastically reduce the computational cost for permeability computations. Thus, a minimum domain to express the regular hexagonal array was employed as shown in figure 1. In addition, to obtain columnar dendritic structures with different morphologies, four computational domains with different size were used as shown in figures 1(a–d). Here, the primary arm spacing, $\lambda = (L_x^2 + L_y^2)^{0.5}$, becomes (a) $0.68 \lambda_{ave}$, (b) $0.93 \lambda_{ave}$, (c) $1.22 \lambda_{ave}$, and (d) $1.47 \lambda_{ave}$ for each model. The number of grid points in all directions was set to a multiple of 8 for efficient computation, and the size in the $z$-direction covers the solid fraction $f_S = 0 \sim 0.55$. Figures 1(a–d) also show dendrite morphologies at a steady-state growth ($\sim 10^7$th step). Many computational steps were required to achieve steady-state growth due to the low pulling velocity. Since a moving frame algorithm was employed, the top region with $1068 \Delta x$ consists of only liquid. As shown in figure 1, we can see different dendritic morphologies depending on the domain size. For a larger computational domain, the secondary arms grow longer and competitive growth among secondary arms is observed.

| Table 1. Material and simulation parameters. |
|---------------------------------------------|
| Quality            | Symbol | Value          | Reference |
|---------------------|--------|----------------|-----------|
| Initial concentration| $c_0$   | 0.0697 at.frac.|           |
| Pulling velocity    | $V_p$  | 20 $\mu$m/s    |           |
| Temperature gradient | $G$    | 50 K/mm        |           |
Diffusion coefficient in liquid \( D_L \) \( \times10^{-9} \) m\(^2\)/s [30]

Diffusion coefficient in solid \( D_S \) \( \times10^{-13} \) m\(^2\)/s [30]

Partition coefficient \( k \) 0.14 [31]

Anisotropic strength \( \varepsilon_4 \) 0.012 [32]

Gibbs-Thomson constant \( \Gamma \) \( \times10^{-7} \) Km [33]

Liquidus slope \( m \) \( \times10^{-7} \) K/at.frac. [34]

Reference temperature at \( z = 0 \) \( T_0 \) 885.89 K

Grid size \( \Delta x \) 0.3906 \( \mu \)m

Interface thickness \( W_0 \) \( \Delta x/0.6 = 0.651 \) \( \mu \)m

Time increment \( \Delta t \) 9.083\( \times10^{-6} \) s

Figure 1. Columnar dendritic structures at a steady-state growth condition (~10\(^7\)th step) for four different domains with a periodic regular hexagonal array. The computational domain sizes are also indicated in this figure as the number of grid points.

4.2. Interdendritic liquid flow

To compute interdendritic liquid flow in the dendritic structures presented in figure 1, four models shown in figure 2 were developed. These models were constructed by mirror symmetry of a red domain shown in figure 1 in all axial directions, which enabled us to compute the liquid flow in arbitrary directions [18]. The size in the \( z \)–direction of the red region shown in figure 1 was determined as a length
Figure 2. Models with \( f_S = 0.4 \) to compute interdendritic liquid flow in arbitrary directions: (a) Model A, (b) Model B, (c) Model C and (d) Model D. These models were constructed by mirror symmetry of the red region shown in figure 1 in all axial directions. Domain sizes are also indicated in this figure as the number of grid points.

of roughly five secondary arms. The solid fraction \( f_S \), interface area density \( S_V \), and specific interface area \( S_S = S_V / f_S \) for the four models shown in figure 2 are indicated in table 2. The value of \( f_S \) for all models is a constant of 0.4. \( S_V \) and \( S_S \) increase as the domain size increases. This means that the complexity of solid morphology becomes greater with domain size.

Table 2. Solid fraction \( f_S \), interface area density \( S_V \), specific interface area \( S_S \) and permeabilities in all axial directions for four models shown in figure 2.

| Model | \( f_S \) | \( S_V [\mu m^2] \) | \( S_S [\mu m^3] \) | \( K_x [\mu m^2] \) | \( K_y [\mu m^2] \) | \( K_z [\mu m^2] \) |
|-------|-----|----------------|----------------|----------------|----------------|----------------|
| A     | 0.398 | 0.0479         | 0.120          | 26.4           | 15.2           | 48.6           |
| B     | 0.399 | 0.0571         | 0.143          | 33.7           | 21.1           | 58.0           |
| C     | 0.399 | 0.0732         | 0.183          | 35.1           | 21.4           | 67.0           |
| D     | 0.399 | 0.0729         | 0.183          | 40.6           | 21.8           | 76.7           |

4.3. Permeability

Computed permeabilities in the \( x- \), \( y- \) and \( z- \) directions for models shown in figure 2 are indicated in table 2. For all models, the permeability is largest for \( K_z \), followed by \( K_y \) and then \( K_x \). Thus, the liquid can flow more easily in the \( z- \) direction, followed by the \( x- \) and \( y- \) directions shown in figure 2. Because the liquid flow path in the \( z- \) direction is established as being straight, it would be reasonable to conclude that the parallel direction to the columnar structure is the easiest flow direction. The same tendency has been observed in other studies [7, 9]. The relation of \( K_x > K_y \) depends on the primary arm spacing in the \( x- \) and \( y- \) directions as shown in figure 2. As the primary array in real columnar structures is not regular, the permeabilities in the \( x- \) and \( y- \) directions should be the same for columnar structures with massive number of primary arms. We confirmed this point in our previous study for columnar structures with multiple primary arms [13, 15]. It is also observed all the permeabilities increase with increasing domain size, because the spacing among solids becomes larger for a larger domain size.
Figure 3. Permeabilities computed for different angles of $\theta$ and $\psi$ for (a) Model A, (b) Model B, (c) Model C and (d) Model D shown in figure 2.

4.4. Permeability tensor

To confirm the validity and applicability of the permeability tensor defined by equation (7), we conducted 16 lattice Boltzmann simulations for each model shown in figure 2 by changing the angles of $\theta$ and $\psi$ from 0° to 90° with an increment of 30°. The results are shown in figure 3. Here, the horizontal axis is the angle $\psi$, and the vertical axis is the permeability $K(\theta, \psi)$ in the $(\theta, \psi)$ direction. The marks are the simulation results, and the solid lines correspond to equation (9). Equation (9) agrees well with the simulation results in all cases. Thus, it can be confirmed that the permeability tensor, equation (7), can be applied to various columnar dendritic structures.

5. Conclusions

To express the applicability of the permeability tensor proposed in the previous study, permeabilities were computed for four columnar dendritic structures with different morphologies. Here, the columnar dendritic structures were obtained by conducting the phase–field simulations during directional solidification of a single–crystal of Al–15wt%Cu binary alloy, and the interdendritic liquid flow in the columnar dendritic structures were computed by the lattice Boltzmann simulations. As a result, for all dendritic structures, the computed permeabilities agreed well with the results of the permeability tensor equation. Thus, the wide applicability of the permeability tensor equation could be confirmed. In conclusion, it was shown that we need only two components $K_n$ and $K_p$, where $K_n$ is the permeability of normal flow and $K_p$ is for parallel flow to the columnar structure. The $K_n$ can be computed as an average value of $K_x$ and $K_y$ shown in equation (8), $K_n = (K_x + K_y)/2$. 


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