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液滴浮遊法における内部対流が結晶粒成長に及ぼす影響

Effects of internal convection on grain growth structure in levitated droplets

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1 Introduction

In metal additive manufacturing techniques, adding heterogeneous nucleation site particles is known to improve grain structures, resulting in the strength of manufactured objects. The Hetero-3D project is being carried out in an electrostatic levitation furnace (ELF) in the International Space Station (ISS) to investigate the refinement effects of heterogeneous nucleation sites on microstructures. Although the experiment in the ISS allows us to extract the effect of refinement in pure form due to the absence of the buoyant convection in the droplet, opportunities are limited because of the cost of the ISS mission. Thus, ground experiments are also carried out through electrostatic levitation (ESL), aerodynamic levitation (ADL), and electromagnetic levitation (EML). In these levitation methods, the intensity of the droplet internal convections may be significantly different, and it may affect the grain structures. This study aims to clarify the effect of convection on crystal grain structures and, consequently, to extract the effect of adding heterogeneous nucleation sites on grain refinement.

2 Methods of investigation

2.1 Multi-phase-field model

In this study, a multi-phase-field (MPF) model is applied in numerical simulation to describe the microstructure evolution of multiphase and polycrystalline materials. In the MPF model, the sum constraint is considered for the phase fields ϕ as

$$\sum_{i=1}^{n} \phi_i = 1, \tag{1}$$

where n is the number of grains locally present. The dynamics of the interface are derived from the generalized free energy F, which is integration of sum of the double well potential f_{doub}, the gradient energy density f_{grad}, and the chemical energy density f_{chem} as

$$F = \int_V \left(f_{\mathrm{doub}} + f_{\mathrm{grad}} + f_{\mathrm{chem}}\right) dV = \int_V \left[\sum_{i=1}^{n}\sum_{j=i+1}^{n}\left(W_{ij}\phi_i\phi_j\right) + \sum_{i=1}^{n}\sum_{j=i+1}^{n}\left(-\frac{a_{ij}^2}{2}\nabla\phi_i\cdot\phi_j\right) + f_{\mathrm{chem}}\right] dV. \tag{2}$$

Based on the Gibbs-free energy, the time evolution equation of ϕ is formulated as follows:

$$\frac{\partial \phi_i}{\partial t} = -\frac{2}{n}\sum_{j=1}^{n} M_{ij}^{\phi}\left[\left\{(W_{ik} - W_{jk})\phi_k + \frac{1}{2}(a_{ik}^2 - a_{jk}^2)\nabla^2\phi_k\right\} + \left(\frac{\partial f_{\text{chem}}}{\partial \phi_i} - \frac{\partial f_{\text{chem}}}{\partial \phi_j}\right)\right], \quad (3)$$

where $M, W,$ and a denote phase-field mobility, energy barrier, and gradient coefficient, respectively. For quantitative simulation, these coefficients are determined from physical properties of materials. The chemical driving force during the solidification process in pure substances is defined as the difference in free energy density between the solid and liquid phases:

$$\Delta f = -(f_S - f_L) = -\frac{L(T - T_m)}{T_m}, \quad (4)$$

where $f_S, f_L, L,$ and T_m represent free energy of solid phase and liquid phase, latent heat, and equilibrium temperature, respectively. Binary alloys are considered by calculating the Gibbs free energy from a linearized phase diagram.

$$\Delta f_{ij} = -S_{ij}\Delta T_{ij} = -S_{ij}(T - T_{ij}), \quad (5)$$

with

$$T_{ij} = m_{i:ij}(c_i - c_i^r) + T^r = m_{i:ij}(c_j - c_j^r) + T^r. \quad (6)$$

Here S denotes the entropy of fusion, $m_{i:ij}$ and $m_{i:ij}$ the gradient of phase lines, c_i and c_j the concentration, c_i^r and c_j^r the reference concentration, T^r the reference temperature.

2.2 Numerical methods and implementation

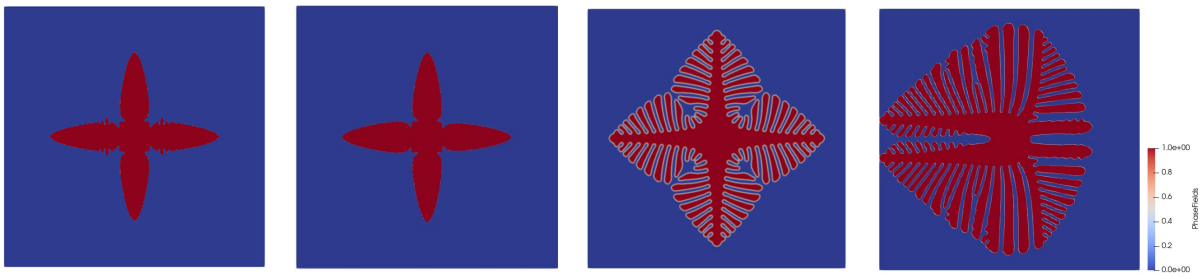
A series of numerical simulations are carried out based on the MPF methods using the Academic version of the OpenPhase. Pure titanium and the titanium alloy Ti-Al, which is often used in additive manufacturing, were considered as materials to be simulated. The time evolution of the orientation fields and concentration field are coupled with the standard MPF model. One or several nuclei are generated within the computational domain at the initial state. These nuclei are then grown according to the driving force of the Gibbs energy. The convections are solved by the Lattice Boltzmann method, and the concentration and temperature fields are advected by the flow.

3 Results

In this study, simulations were carried out in 2-dimensional domain by changing flow velocities listed in Table 1. These velocity values are drawn from results of Usui et.al.[1)] Figures 1 shows the growth of single Ti. In these cases, heat conduction is much faster than the convection heat transfer, so the temperature field is almost not affected by the convection. Thus, the effect of the convection on the final grain structures is vanishingly small.

Table 1. The magnitude of internal convective flow velocity in droplets during the levitation methods

Levitation methods	ESL	ADL	EML
Velocity order [m/s]	$v \approx 1.0 \times 10^{-3}$	$v \approx 1.0 \times 10^{-1}$	$v \approx 1.0 \times 10^{0}$



No convection EML condition

Figure 1. Pure titanium solidification

No convection ESL condition

Figure 2. Titanium alloy Ti-30at%Al solidification

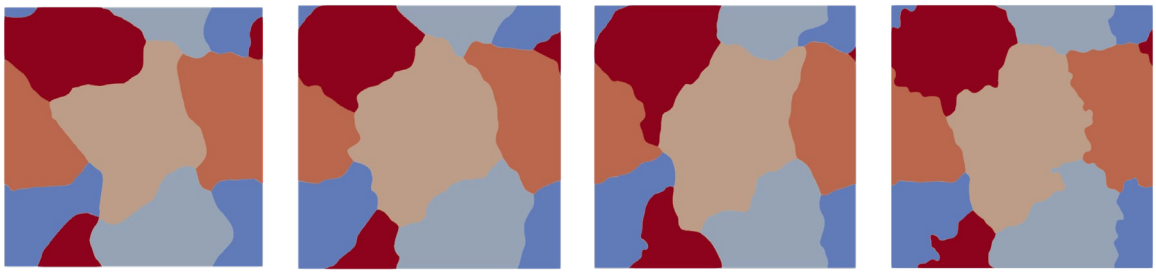


Figure 3. Multi-dendrite simulation of TiAl alloy with flow

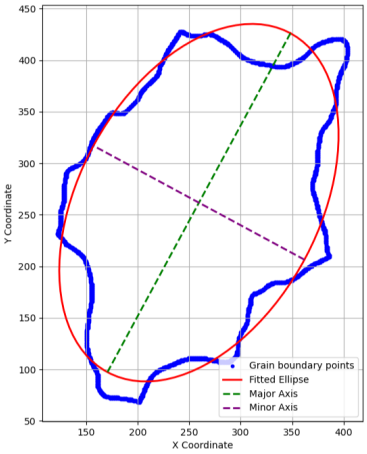


Figure 4. The elliptical fitting

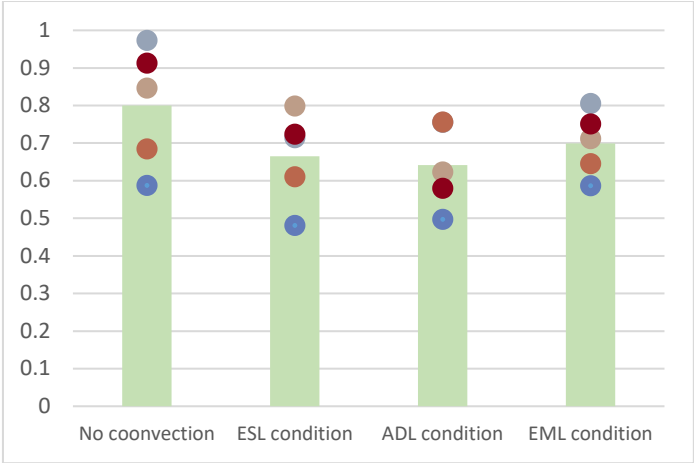


Figure 5. Aspect ratio of grains

Figures 2 shows the dendrite growth of Ti-30at%Al alloy. In these cases, the concentration gradient becomes steep at the grain boundary faced orthogonal to flow, leading to faster solid growth. Figure 3 shows the growth of multiple grains of Ti-30at%Al dendrites simulated in 2D. To investigate the effect of convection on the grain structures, grain interfaces are fitted by ellipses, as shown in Fig.4. The shape of the structures is evaluated as the aspect ratio, which is defined as the ratio of the minor to the major axes. Figure 5 shows the aspect ratios of the five grains in the computational domain and their average for each levitation method condition. The average aspect ratio of the grain generated under ADL conditions was 1.25 times larger than that for the case of no convection. The tendency of the aspect ratio can be explained by the gradient of the concentration field due to the mass transport by the convection.

4 Conclusion

The effect of liquid convection on grain shape was elucidated through MPF simulations. The results of the present study showed that the final grain structures may be affected by the droplet internal convection in the levitation methods.

References

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2) T. Takaki & A. Yamanaka: Phase-field method -Microstructure design through numerical simulation, 1st ed., Yokendo (2012).