Effect of Fluctuation on Departure of Interface Morphology from Planar Interface during Unidirectional Solidification by Phase-Field Modeling

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Properties of cast materials vary depending on microstructure governed by a solidification process. In this study, we focused on dendrite formation from planar interface during unidirectional solidification [1]. At first, thermal fluctuations or external noises induces perturbation on morphology of a planar interface. Secondly, the perturbation grows and dendrite arms are formed. In other words, the perturbation triggers dendrite formation and, in turn, overall microstructure including unfavorable casting defects. Therefore, to control microstructure, it is important to understand the formation and growth of the perturbation at a planar interface. On the other hand, while the theory of perturbation growth has already been established [2], the generation of the perturbation has not been clarified yet.

Phase-Field Modeling (PFM) is a powerful method based on thermodynamics to examine microstructural evolution [3]. This method assumes that evolution of phases proceeds to reduce total free energy of a system. Since thermodynamics is a macroscopic theory, any fluctuations derived from vibrations of atoms are not considered a priori. It is therefore needed to artificially introduce fluctuations to calculate formation of the perturbation at a planar interface. However, although artificial noises are often used to reproduce experimentally-observed microstructure by PFM, correlation among the fluctuation, the perturbation, and resultant microstructure has not been clarified. Therefore, using PFM, we analyzed the effect of fluctuation on formation and growth of the perturbation at a planar interface in a Fe-C system.

We added a random number to the phase-field parameter, a non-conservative parameter that describes state of phases of a volume element, as in Langevin equation. Here, we defined the maximal random number allowed as the magnitude of fluctuation, a. Anisotropic interface energy with four-fold symmetry was considered in this study. Other physical conditions of the calculations were following: Concentration of carbon was 0.15 mass%, temperature was 28 K below the melting point at the composition, and calculations were started with an initial state: A five mesh-thick planar solid layer was placed at the bottom of the calculation region with the rest filled with liquid phase.

Figure 1 shows time evolution of two concentration profiles, (a) the ones for a = 0.01 and (b) the ones for a = 0.0001. In the former case, small perturbation in the interface morphology at 800 step could be barely visible, with a diffusion layer ahead of solid-liquid interface. At 2600 step, tips of several arms grew through the diffusion layer. Then, growth rate of the arms suddenly increased due to constitutional undercooling resulted from less carbon in liquid in front of the arm ahead of the diffusion layer. This results in drastic change in morphology as observed at 4600 step. Comparing different magnitudes of fluctuation shown in Fig. 1(a) and 1(b), little difference is found in the morphology of planar interfaces in the beginning. However, at later stages when arms grew through the diffusion layer, difference in interface morphology emerged: The number of arms was fewer and the solid-liquid interface was rougher when a = 0.0001.

The interface morphology is governed by the magnitude of the fluctuation itself and the consequent diffusion layer. Figure 2 magnifies the concentration profiles near the solid-liquid interfaces. Comparing both cases, the diffusion layer was thicker and carbon concentration near solid-liquid interface is higher when a = 0.0001. The thicker diffusion layer with higher carbon concentration can be attributed to smaller magnitude of the fluctuation since it takes longer time for the perturbation of interface morphology to grow, building up higher and denser diffusion layer ahead of the interface. In order for solid arms to grow ahead of the diffusion layer, larger magnitude of fluctuation is needed to penetrate thicker diffusion layer. These manifest why less populated arms with various heights were observed when the magnitude of fluctuation is smaller, which would lead to different microstructural evolution at later stages of solidification.

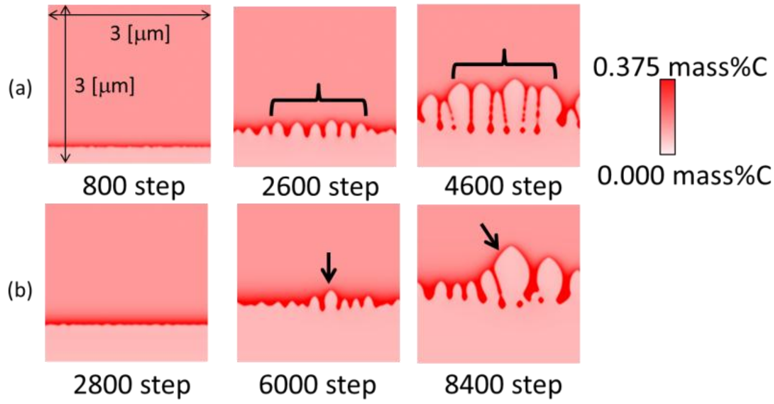

FIG. 1 Time evolution of concentration profile during solidification of Fe-0.15mass%C at 1770 K; (a) a = 0.01, (b) a = 0.0001; Arms grown ahead of diffusion layer are marked.

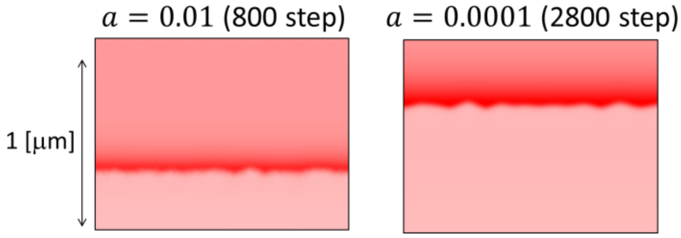

FIG. 2 Magnified concentration profiles near solid-liquid interface at the time when perturbation of interface morphology is grown to the same extent in both cases.

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