

Effect of Mismatching Interface Energy on γ -Fe Nucleation upon δ/γ Transformation of Carbon Steel

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According to phase diagram, phase transition from δ to γ phase in carbon steel is peritectic reaction, from liquid and δ phases to γ phase, when concentration of carbon is within the range between 0.10 and 0.51 mass%. However, *in situ* observation revealed another type of transformation[1]. This is called massive-like transformation. In this transformation, δ phase changes to γ phase without involving liquid phase after solidification of δ phase is completed. Since crystal structures of δ and γ phases are BCC and FCC respectively and there is no liquid phase which can accommodate the volume change from BCC to FCC, large transformation strain is introduced in massive-like transformation and this may cause crack of carbon steel in continuous casting process. However, the mechanism of massive-like transformation remains unclear, providing no clue to control it. One of the marked characteristics of massive-like transformation is that undercooling is very large[2], over 100 K. In other words, the nucleation of γ phase is very difficult. The interface energy of δ/γ interface may be very large due to mismatch of crystal structures of the two phases, and thus it is plausible that it plays important role in nucleation of γ phase. Therefore we focused on the interface energy and tried to reveal the mechanism of massive-like transformation from viewpoint of interface energy.

In previous study, interface energy between δ and γ phases was calculated as a function of misorientation angle using atomistic calculation [3]. The interface energy has a minimum value when both phases satisfy Nishiyama-Wasserman (N-W) relationship, which is known as one of the most matching relationships between BCC and FCC structure according to studies about martensitic transformation. However, considering γ phase nucleation in matrix of δ phase, it is almost impossible that all of δ/γ interfaces satisfy N-W relationship. Thus, we must consider other various interface energy in a comprehensive manner.

In this study, we defined effective interface energy to take variety of interface energy into account. To obtain effective interface energy, we used Phase Field Modeling (PFM), which calculate temporal evolution of states based on thermodynamics, under the only one condition that total free energy of system decreases. Calculating from initial state shown in Fig. 1(a), in which there are various δ/δ , γ/γ , δ/γ interfaces, we can consider the competition of various interfaces to decrease total free energy of whole system. We defined effective interface energy as the average of interface energies after competition of interfaces is practically completed as shown in Fig. 1(c). Using the effective interface energy, we calculated change of Gibbs free energy for nucleation using following equation based on the classical nucleation theory:

$$\Delta G_t = \Delta T \Delta S_t \cdot V + \sigma \cdot A$$

where ΔT is undercooling, ΔS_t and σ are entropy difference and interface energy

between matrix and nuclei, respectively, and V and A are volume and surface area of nuclei, respectively. Then, we compared undercooling, or driving force, needed for nucleation at fixed critical radius of nuclei.

Fig. 2(a), (b) and (c) are nucleation model for solidification, peritectic reaction and massive-like transformation, respectively. Comparing undercooling on the same standard in both models, peritectic reaction needs more undercooling than solidification and massive-like transformation needs much more undercooling. Changing ΔS_t and σ independently, we found that one of the main reasons why large undercooling is needed for massive-like transformation is because ΔS_t between δ and γ phase is very small compared with that for liquid and δ phase, although the interface energy of δ/γ interface, slightly larger than that for homogeneous grain boundary, also contribute to it. Moreover, intentionally changing δ/δ interface energy in the model of Fig. 2(c) revealed that undercooling needed for the nucleation is significantly changed with δ/δ interface energy within δ phase matrix. This means that if there are δ/δ grain boundaries whose interface energy is large, nucleation of γ phase becomes significantly easier. After solidification is completed, average of δ/δ interface energy decreases as coarsening proceeds, and the progress of coarsening can be controlled by cooling process. Therefore it is suggested that we can control γ phase nucleation, through changing the microstructure of δ phase, by controlling cooling rate, for example.

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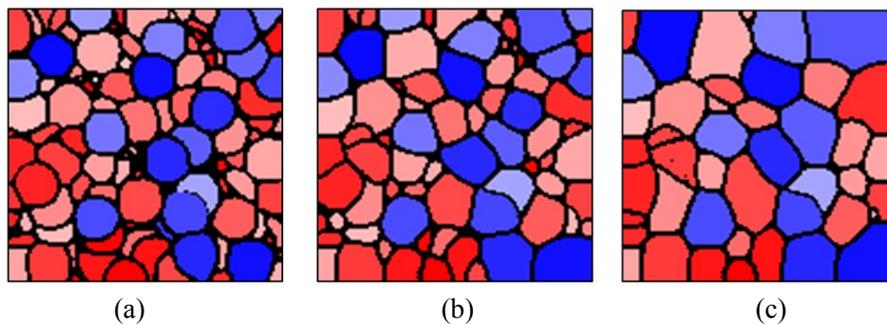


FIG. 1 Temporal evolution of polycrystal of δ (blue) and γ (red) phase: Time step of each figures are (a) initial state, (b) 2000 step and (c) 20000 step. Light and shade means difference of crystal orientation. The competition of all interfaces proceeds with time.

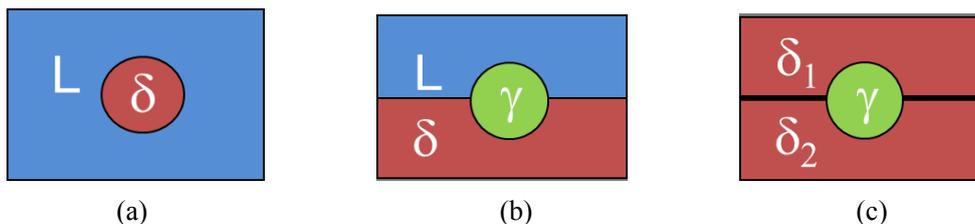


FIG. 2 Nucleation models: (a) solidification, (b) peritectic reaction, (c) massive-like transformation. The shape of all nuclei are spheres.