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On the application of multi-phase field modeling to the micro-stractural change in welding process†

TERASAKI Hidenori*, MORIGUCHI Koji and KOMIZO Yu-ichi*****

Abstract

The problems were discussed when a multi-phase filed modeling (MPM) was applied to the weliding phenomena, such as solidification. In order to generate the second phase during solidification, the nucleation principle and place should be decided.Both the enrgy balance search and Neumann rejection method are candidate to overcome the problems. Furthermore, the importance of interafce migrating rate was enhanced. In order to assess the validity of applied interface migrating rate, the usage of in-situ observation technique is useful The importance of in-situ observation method to assess the simulation results was also enhanced in this report. For instance, austenite formation from the delta-ferrite phase in low carbon steel was simulated using MPM and the morphology of microstructure and the interface migrating rate was assessed using LSCM images.

KEY WORDS: (Solidification), (multi-phase field modeling), (In-situ observation), (TRXRD)

1. Introduction

A phase field modeling is a promising technique to express the pattern of microstructural change. The change occurs based on the variation of total energy in calculating domain. For instance, the double-well potential of chemical energy is defined with an order parameter and it defines the potential density with the term expressing the interface energy (static term and dynamic term)[1]. For the chemical energy, the CALPHAD method[2] can be applied. Integrating the potential density gives total energy and the variation process corresponds to microstructural change. The concept for the multi-phase field model was suggested by Steinbach et al[3] and microstructural changes between many phases can be treated in the frame work of phase-filed modelling. Then, applying the phase-field model to the welding research is possible by treating multi-phases in the solidification process and solid-state transformation process.

However, there is a problem about nucleation of phases in the simulation. In the experimental work, many mechanisms of second phase nucleation were found during solidification processes of welding. That is eutectic, peritectic and independent two phase growth mechanisms[4]. In order to consider the second-phase generation in the phase-field model, the nucleus has to be put in the calculation domain based on the theory of second phase nucleation. It is a little artificial. Since second phase governs following micostructural change the same as in real welding, the theory how to put the second phase nucleaus governs the micorstructural pattern derived by phase-field simulation. However, in the paper of Steinbach, a detailed explanation of second phase generation was not provided.

Another problem is the setting of the calculation parameter. In the phase-field model, the interface mobility is the parameter. In some case, there is a literature-based value. However, in many cases, there is no reference value. Then in order to assess the rate, a calibration technique is needed to verify the accuracy of the migrating rate.

In the present work, the solidification process of low-carbon steel (the Fe-C system) is simulated and the method of second-phase generation during peritectic reaction is suggested as a simple instance. Furthermore, it is discussed that in-situ observation techniques can be used for verifying the simulation model and selecting the calculation parameter such as interface mobility. The tracing of microstructural change in the solid-state transformation from delta-ferrite to gamma-austenite is introduced as an instance.

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2. Theory

The theory of multi-phase field modeling is detailed in the original paper[3]. Furthermore, carbon diffusion in the Fe-C system is also taken into account. The technique is detailed in the work by Tiaden et al[5]. In this section, the point of theory is briefly summarized.

In the multi-phase field model, the fraction of the phase becomes an order parameter as:

$$\sum_{\alpha}^{N} \phi_{\alpha} = 1 \qquad (1)$$

The static f_{pot} and kinetic f_{kin} potential density term is defined and integrated in the calculation domain Ω, giving total energy F as:

$$F = \int_{\Omega} f_{pot} + f_{kin} d\Omega \qquad (2)$$

The phase parameter is changed with the following variation rule developed to multi-phases:

$$\tau_{ik} q_{ik} = -\frac{\delta F}{\delta \phi_i}$$

$$\frac{\partial \phi_i}{\partial t} = \sum_{k(k \neq i)} q_{ik} \qquad (3)$$

For the carbon diffusion, the amount of carbon is related with the phase parameter as:

$$c = \sum_{\gamma}^{N} \phi_{\gamma} c_{\gamma} \qquad (4)$$

The time development of carbon content is governed by the phenomenological equation shown as:

$$\dot{c} = \nabla \cdot \sum_{\alpha=1}^{N} \phi_{\alpha} D_{\alpha} \nabla c_{\alpha} \qquad (5)$$

, where D is the diffusion coefficient. By using a partition coefficient related to the reference phase, the equation (5) become simple. In the present calculation, the CALPHAD data in Gustafson's paper[6] is used as a chemical potential. For example, **Fig. 1** shows the chemical free energy at 1767.8 K and 1750 K. Then the partition coefficient can be derived from the CALPHAD data during calculation.

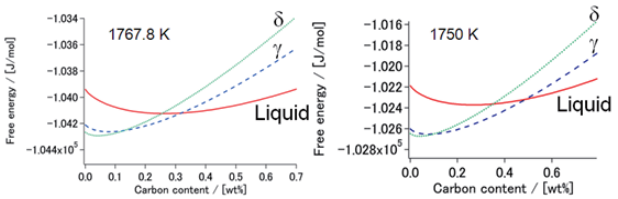

Fig. 1 Free energy in Fe-C system (at 1767.8 K and 1750 K).

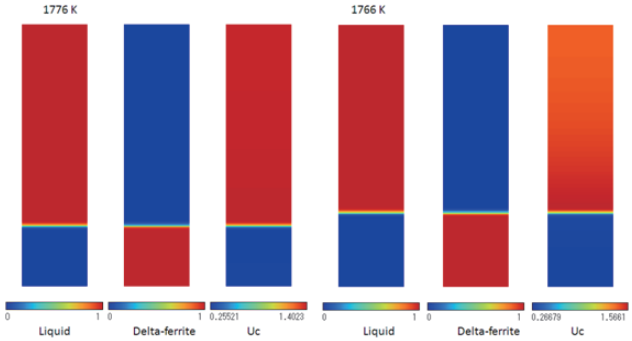

Fig. 2 The phase fields and carbon density of delta-ferrite and liquid phase at 1776 and 1766 K.

3. Results and discussion

The simple solidification process was calculated in a multi-phase field model. The thermal cycle is a cooling rate of 0.5 K/s from 1781 K. The carbon concentration of delta-ferrite was 0.0577 wt% and 0.3 wt% for liquid phase.

Figure 2 shows the phase field of delta-ferrite and liquid phase at 1776 and 1766 K. The amount of delta-phase and carbon density at the interface was increasing through the cooling process. Throughout the calculation time, the energy balance was also calculated to judge the possibility of second phase nucleation in the peritectic reaction. It is the energy balance during heterogeneous nucleation of austenite phase in the shape of a cylinder. The energy balance Δg^D is expressed as follows[8]:

$$\Delta g^D = -(\Delta G / V)(\Delta\sigma / \sigma_E^{I/II})\pi (r^D)^3 + 3\Delta\sigma \cdot \pi (r^D)^2 \qquad (6)$$

, where the ΔG is free energy change due to phase transformation, V is the mole volume, $\Delta\sigma$ is the total energy balance of interface, the $\sigma_E^{I/II}$ is the side-interface energy and r^D is the radius of nucleus. If the Δg^D becomes negative at the interface, the second phase is

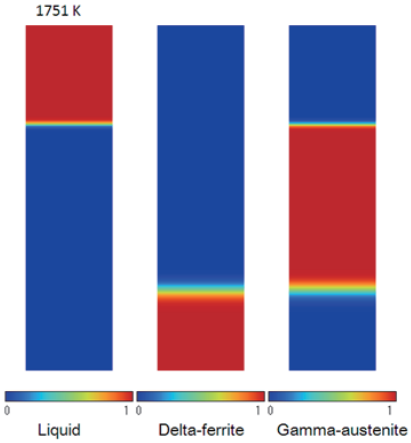

Fig. 3 The phase fields and carbon density of delta-ferrite and liquid phase at 1776 and 1766 K.

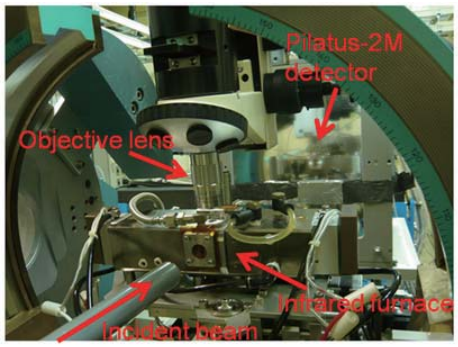

Fig. 4 Photo of Hybrid TRXRD/LSCM system.

artificially put at the interface. During the calculation, it became negative below the peritectic temperature, and austenite phase was set into the calculation domain. **Figure 3** shows the phase field of delta-ferrite, liquid phase and austenite phase at 1751 K. The austenites grew and eroded the delta-ferrite phase. In other method, it is a candidate the application of Neumann rejection method to generate the nucleation probability. For instance, if the driving force of phase transformation is defined as ΔF, the distribution probability of nucleated austenite is given as following expression: $\exp(-\Delta F / k_B T)$.

The next discussion is the about the setting parameter and evaluation of calculation results. In the calculation, the interface mobility was set to 5.0D-10 m^4/J/sec. However, the setting parameter was not based on the theory in the model and it is from the literature. Furthermore, in the case of welding, the cooling rate is high and complex change of interface mobility is predicted. Then, the calculation results should be checked. Furthermore, if there is no data about interface mobility in the considered system, it should be acquired with experiments. For these purpose, the application of hybrid in-situ observation system[7] is suggested. The system was developed by our research group and the appearance of the system is shown in **Fig. 4**. The infrared furnace and laser scanning confocal microscopy are set on a multi-axis goniometer in

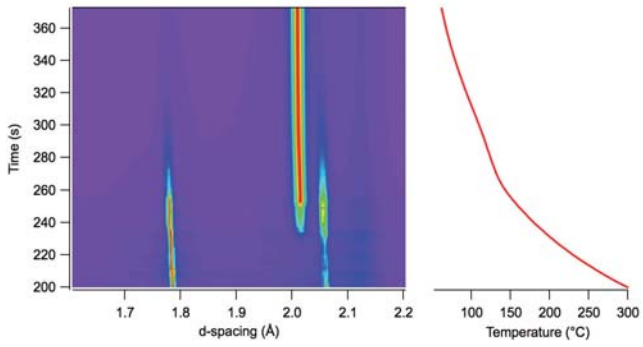

Fig. 6 Temperature-time-d-spacing and intensity diagram during the martensitic transformation of Cr-Ni steel.

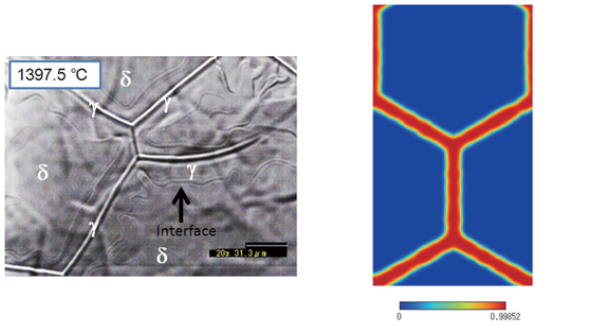

Fig. 5 A snap shot of LSCM image and the phase field for the austentite precipitation from delta-ferrite at high in low-carbon steel.

the synchrotron radiation source (SPring-8, Hyogo, Japan). Then the confocal microscopy gives a morphological change of microstructure during phase transformation in real space [8] and the bright X-ray enables in-situ observation in reciprocal lattice space, at the same time. For instance, **Fig. 5** shows comparison between confocal microscopy image and phase field at the 1670 K. The same morphology of microstructure was observed using interface-mobility parameter of 5.0D-10 m^4/J/sec. That means the parameter is in the reasonable range.

Furthermore, the hybrid system could be used for in-situ observation of microstructural change in reciprocal lattice space. For instance, the **Fig. 6** the time, temperature, d-spacing and intensity diagram during the martensitc transformation of Cr-Ni steel (111fcc, 110bcc and 200bcc reflection in descending order of d-spacing). The data were analyzed using the method described in Ref.9. Of course, the phase evolution can be identified. Figure 6 shows martenistic transformation. The behaviour of element partitioning[9-11] also can be traced from the change of lattice parameter. Furtheremore, the movement of crystal during phase transformation is also tracked. That information is useful to assess the phase-field and element concentration evolution in the phase-field model. Although the microstructural change at high temperature is hard to trace, the hybrid in-situ observation technique enables in-situ observation to assess the calculation results of phase-field model.

4. Conclusions

Two problems applying the phase-field technique to the welding research were discussed. For the second-phase nucleation in the peritectic or eutectic reaction, some rule should be applied to rationalize the second-phase putting in the calculation domain. In the present work, the energy balance of heterogeneous nucleation for the nucleus of cylindrical shape was used to judge the generation of second phase in solidification processes. Furthermore, it was suggested that hybrid in-situ observation technique is useful to assess the setting parameter such as interface mobility and to check the calculation results.

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