Computational study of α-α' separation behavior of thermal aging neutron-irradiated Fe-Cr alloy using the phase-field method

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1. Introduction

Fe-Cr binary system has been intensively investigated as an important prototype of the stainless steel, which is widely used for the structural material of the nuclear power plants [1-8]. At 563K, the spinodal decomposition takes place due to the presence of the miscibility gap in Fe-Cr system [2] under the neutron irradiation. We compared the three-dimensional phase-field modeling results with the preexisting experimental observation [2]. After we examined the exactness of our developed phase-field code, we tried to predict a role of the temperature in determining phase decomposition behavior between α-phase (Fe-rich) and α'-phase (Cr-rich). So far, the phase-field method has been used to predict the spinodal decomposition behavior in Fe-Cr phase [2, 6-8]. All of studies were performed in a two-dimensional system and adopted the non-dimensional normalized thermodynamic parameters [2, 6-8]. In order to compare the simulation results with the experimental measurements quantitatively, we used the physical dimensional values without any normalization in a three-dimensional space.

2. Methods and Results

In this section some of the techniques used to model the microstructural evolution of Fe-Cr system is explained. Also, the obtained simulation results will be compared with the experimental observations and the effect of the temperature is predicted.

2.1 Model description and Simulation details

We adopted the free energy functional of Fe-Cr system from the reference [9]. The molar Gibbs free energy functional $f(c,T)$ is given as follows:

$$f(c,T) = (1-c)F_{Fe}^0 + cF_{Cr}^0 + RT[c\ln(c) + (1-c)\ln(1-c)] + L_{FeCr}c(1-c) + f_{mo} \quad (1)$$

Where c is the composition of Cr and F_{Fe}^0 and F_{Cr}^0 are the free energies of the pure element Fe and Cr. We used the formulas in ref. [10] in unit of J/mol as follows:

$$F_{Fe}^0 = 1225.7 + 124.134T - 23.5143T\ln(T) - 0.00439752T^2 - 5.89269\times10^{-8}T^3 + 77358.5/T \quad (2)$$

$$F_{Cr}^0 = -8856.94 + 157.48T - 26.908T\ln(T) - 0.00189435T^2 - 1.47721\times10^{-6}T^3 + 139250/T \quad (3)$$

$L_{FeCr} = 20500 - 9.68T$ [9] and the free energy functional from the magnetic ordering is given by,

$$f_{mo} = RT\ln(\beta+1)f(\tau) \quad (4)$$

Where the gas constant $R = 8.3144621\ (J/mol\cdot K)$. β in Eq. 4 is the magnetic moment per atom in Bohr magneton [9] and is

$$\beta = 2.22c(1-c) - 0.008c - 0.85c(1-c) \quad (5)$$

More details about $f(\tau)$ in Eq. 4 is written in ref. [9]. We plotted the free energy functional of Eq. 4 in Fig. 1 and their first derivative in Fig. 2. The free energy curve is smooth curve in Fig. 1, however, we observed the abrupt change when $c \approx 0.66$ in Fig. 2. The magnetic transition from ferromagnetic ↔ paramagnetic takes place at this point, therefore, it gives the dramatically sharp transition in Fig. 2.

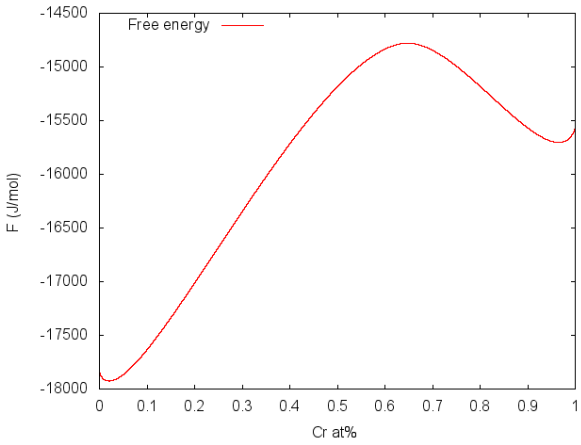


Figure 1: Plot of Eq. 1, total free energy of Fe-Cr binary system at T=563K.

$$\frac{\partial c(\vec{r},t)}{\partial t} = \nabla\cdot\left[M(c)\nabla\left(\frac{\delta f(c,T)}{\delta c}\right)\right] \quad (6)$$

We solved the time-dependent Cahn-Hilliard equation to simulate temporal and spatial distribution of the Cr

composition as Eq. 6 [11]. The mobility $M(c)$ is given as follows: [12, 13]

$$M(c) = \frac{1}{V_m} c(1-c)\left[cM_{Cr} + (1-c)M_{Fe}\right] \quad (7)$$

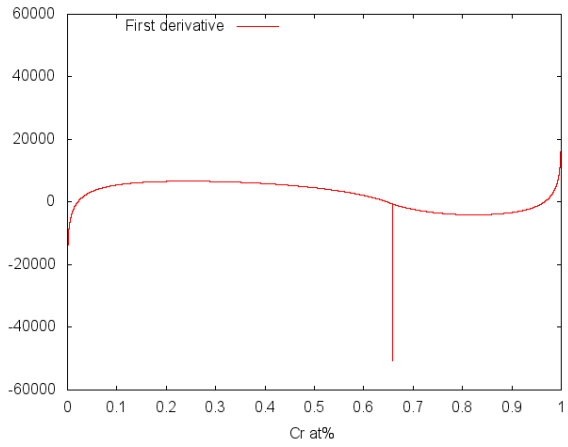
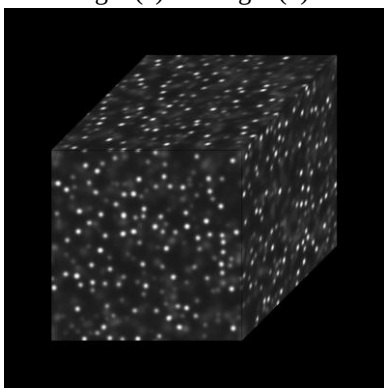


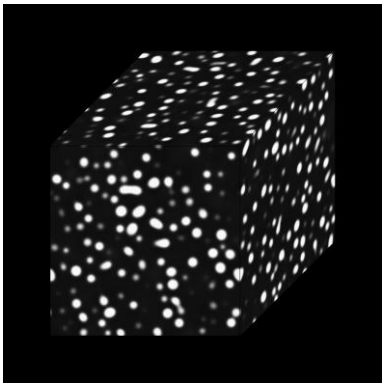
Figure 2: Plot of the first derivative of Eq. 1 with respect to Cr composition at T=563K.

2.2 Simulation results

We plotted the microstructure we obtained from the simulations in Fig. 3(a) and Fig. 3(b).



(a)



(b)

Fig. 3. Plot of Cr composition of Fe-18Cr alloy. The system size is 51.2^3 nm^3 and the periodic boundary condition is applied. (a) 2000Δt (b) 36000Δt

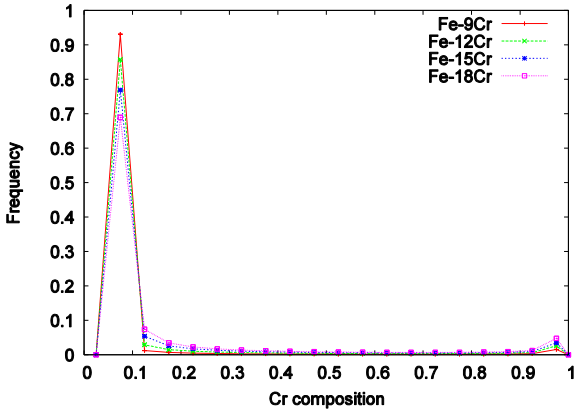


Figure 4: Plot of Cr composition distribution at 36000Δt (T=563K)

In Fig. 4, we clearly found that the left peak (<0.1) gets lower and the right peak (>0.9) gets higher as the averaged Cr composition increases.

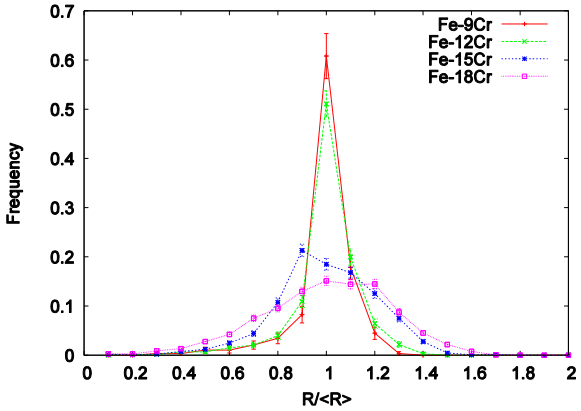


Figure 5: Plot of precipitate (α') size distribution at 36000Δt (T=563K).

We found that the precipitate (α') size distribution alters dramatically according to the Cr composition in Fig. 5.

3. Conclusions

We performed the phase-field simulations of Fe-Cr binary system. We compared obtained results with the experimental observations. We found our simulation framework can describe the experimental results reasonably and we characterized the microstructural characteristics of Fe-Cr system, where the experimental data is not present.

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