Development for Fe-Cr-Ni-based Structural Materials on the Molten Salt Reactor

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1. Introduction

The Fe-Cr-Ni alloy has been the main candidate for structural materials of 4th generation reactors because of their excellent corrosion resistance and high-temperature strength [1, 2]. However, the embrittlement phenomenon is widely known as caused by precipitation in the Fe-Cr-based alloy, and there is the radiation-induced segregation phenomenon with irradiation [3]. Therefore, it is important a comprehensive analysis of microstructural evolution behavior considering dislocation caused by irradiation on the Fe-Cr-Ni system.

Recently, the phase-field model is widely used in the material science to analyze the microstructural evolution behavior because of it is possible to simulate with various phenomenon [4]. In addition, we can observe the microstructure morphology using the phase-field model. Therefore, we conduct phase-field modeling to observe the microstructural evolution behavior in the Fe-Cr-Ni system.

We investigate the microstructural evolution behavior including the α, α′, and G-phase precipitation using a multi-component multi-phase-field model with irradiation and elastic effects. To improve the numerical stability and computational cost, we apply the semi-implicit Fourier spectral method [5] and CUDA(Compute Unified Device Architecture) method [6].

2. Methods and Results

In this section some of the techniques used to model the detector channel are described. The channel model includes a SiC detector, cable, preamplifier, amplifier, and discriminator models.

2.1 Phase-field method using WBM model

To investigate the microstructural evolution in Fe-Cr-Ni system, we conduct the CALPHAD based phase-field modeling considering two governing equations, the Cahn-Hilliard equation [7] and the Allen-Cahn equation [8].

$$(1)\quad \frac{\partial c_A(\boldsymbol{r},t)}{\partial t} = V_m^2 \nabla \cdot \left[M_{A,A} \nabla \left(\frac{\delta F}{\delta c_A} \right) + M_{A,B} \nabla \left(\frac{\delta F}{\delta c_B} \right) \right]$$

$$(2)\quad \frac{\partial \phi(\boldsymbol{r},t)}{\partial t} = -M_\phi \left(\frac{\delta F}{\delta \phi} \right)$$

where the $c_A(\boldsymbol{r},t)$ and $c_B(\boldsymbol{r},t)$ are the concentration of A and B(Cr or Ni) component, the $M_{A,B}$ is the chemical mobility of the A, B components, which are pure Cr and Ni, respectively. The $\frac{\delta F}{\delta c_A}$, $\frac{\delta F}{\delta c_B}$, and $\frac{\delta F}{\delta \phi}$ are the variational derivative of A component and of order parameter ϕ. The M_ϕ is the kinetic parameter of FCC phase. The total free energy(F) using WBM(Warren-Boettinger-McFadden) model is given by [9]

$$(3)\quad F = \int_V \left[F_{bulk} + \frac{\kappa_\phi}{2} |\nabla \phi|^2 + \frac{1}{2} \sum_i \kappa_i |\nabla c_i|^2 \right] dV$$

where κ_ϕ, κ_{Cr} $(= \frac{1}{6} L_{FeCr})$, and κ_{Ni} $(= \frac{1}{6} L_{FeNi})$ are the gradient energy coefficients for ϕ, Cr, and Ni. The F_{bulk} is the bulk free energy given by

$$(4)\quad F_{bulk} = (1-h) f_{BCC} + h f_{FCC} + \frac{\omega}{2} \phi^2 (1-\phi)^2$$

where h $(\phi) = \phi^3(6\phi^2 - 15\phi + 10)$ is the interpolation function. The f_{BCC} and f_{FCC} are the free energies of BCC and FCC phases, respectively.

$$(5)\quad f_\varphi = \sum_i c_i G_i^{ref} + RT(\sum_i c_i \ln c_i) + \sum_i \sum_{j>i} c_i c_j L_{ij}^\varphi + c_i c_j c_k L_{ijk}^\varphi$$

i, j, k = Fe, Cr, Ni
φ = BCC, FCC

where G_i^{ref} is the φ phase free energy of pure component i, R (=8.3144 $J/mol \cdot K$) is the gas constant, T is the absolute temperature. L_{ij}^φ is the interaction parameter between i and j components.

2.2 Semi-implicit Fourier spectral method with constant mobilities

Simulating the multi-component multi-phase systems is computationally expensive. Therefore, to improve the computational efficiency, we apply the semi-implicit Fourier spectral method to Cahn-Hilliard equation and Allen-Cahn equation. The explicit Euler Fourier spectral form for governing equations with constant mobilities is given by

$$(6)\quad \frac{\partial c_{Cr}(\boldsymbol{r},t)}{\partial t} = -M_{Cr,Cr} \boldsymbol{k}^2 \left(\frac{\delta F}{\delta c_{Cr}} \right) - M_{Cr,Ni} \boldsymbol{k}^2 \left(\frac{\delta F}{\delta c_{Ni}} \right)$$

$$(7)\ \frac{\partial c_{Al}(\boldsymbol{r},t)}{\partial t} = -M_{Ni,Cr}\boldsymbol{k}^2\left(\frac{\delta F}{\delta c_{Cr}}\right) - M_{Ni,Ni}\boldsymbol{k}^2\left(\frac{\delta F}{\delta c_{Ni}}\right)$$

$$(8)\ \frac{\partial \phi(\boldsymbol{r},t)}{\partial t} = -M_{\phi}\left(-\frac{\partial h}{\partial \phi}f_{BCC} + \frac{\partial h}{\partial \phi}f_{FCC} + \omega\phi(1-2\phi)(1-\phi) + \kappa_{\phi}\boldsymbol{k}^2\phi\right)$$

$$(9)\ \frac{\delta F}{\delta c_A} = (1-h)\frac{\partial f_{BCC}}{\partial c_A} + h\frac{\partial f_{FCC}}{\partial c_A} - \kappa_A\nabla^2 c_A$$

where $\boldsymbol{k}$ is the reciprocal vector and ω is interface barrier term.

We need to calculate Cr and Ni concentrations, respectively, and Fe concentration is dependent on Cr, Ni concentrations ($c_{Fe} = 1 - c_{Cr} - c_{Ni}$). Therefore, the semi-implicit Fourier spectral form is following as:

$$(10)\begin{bmatrix} c_{Cr}^{n+1} \\ c_{Ni}^{n+1} \end{bmatrix} = \frac{1}{D}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix}\begin{bmatrix} c_{Cr}^{n} - \Delta t\boldsymbol{k}^2 F_{Cr} \\ c_{Ni}^{n} - \Delta t\boldsymbol{k}^2 F_{Ni} \end{bmatrix}$$

$$(11)\ F_{Cr} = M_{Cr,Cr}\left((1-h)\frac{\partial f_{BCC}}{\partial c_{Cr}} + h\frac{\partial f_G}{\partial c_{Cr}}\right) + M_{Cr,Ni}\left((1-h)\frac{\partial f_{BCC}}{\partial c_{Ni}} + h\frac{\partial f_G}{\partial c_{Ni}}\right)$$

$$(12)\ F_{Ni} = M_{Cr,Ni}\left((1-h)\frac{\partial f_{BCC}}{\partial c_{Cr}} + h\frac{\partial f_G}{\partial c_{Cr}}\right) + M_{Ni,Ni}\left((1-h)\frac{\partial f_{BCC}}{\partial c_{Ni}} + h\frac{\partial f_G}{\partial c_{Ni}}\right)$$

2.3 Simulation results

We observed the microstructural evolution behavior for α, α′, and G-phases at 650K.

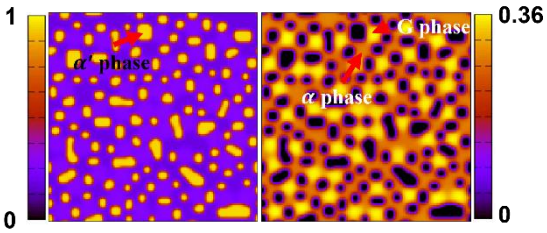

Fig. 1. Cr (left) and Ni(right) concentration fields. The Cr-rich and Ni-depleted phase α′, Cr-depleted and Ni-depleted phase α, and Cr-depleted and Ni-rich phase G-phase.

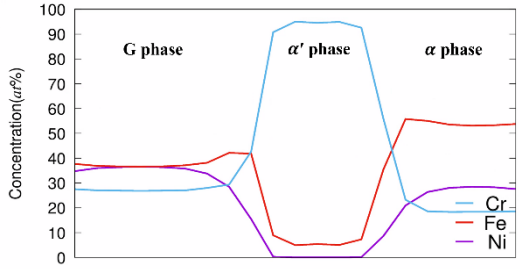

Fig. 2. The concentration distribution in the Fe-Cr-Ni system.

As shown in Fig. 1 and Fig. 2, we observe three phases with different concentration profiles. The α phase is a Cr-depleted phase, while the α′ phase is a Cr-rich phase. So, the Cr concentration distribution is consistent with previous studies for Fe-Cr-based system. Also, both phases (α, α′ phases) are Ni-depleted phases. However, there is a Cr-depleted and Ni-rich phase that G-phase.

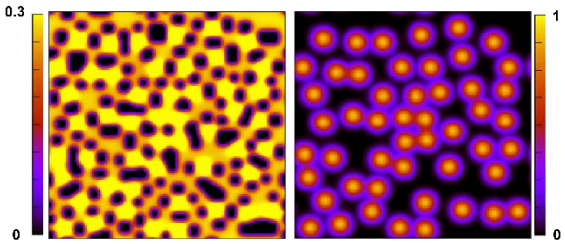

Fig. 3. Ni concentration (left) and structural order parameter (right) fields.

In the Eq. (4), the structural order parameter (ϕ) was 1, then free energy term for BCC phases was zero, only free energy term for FCC was existed. So, we observed the Ni-rich G-phase when structural order parameter was 1 as show in Fig. 3.

The number of α′ precipitate and particle size increased with the nominal Cr concentration, which was consistent with previous study [10]. In addition, the higher the initial Cr concentration, the faster the onset of phase separation.

3. Conclusions and Future Work

We conducted multi-phase multi-component phase-field modeling to analyze the microstructural evolution behavior in the Fe-Cr-Ni system. We observed three phases α (Cr depleted phase), α′ (Cr rich phase), and G-phase (Cr depleted and Ni-rich) and their concentration distributions. Also, our simulation results are consistent with Thermo-Calc thermodynamic software.

We will examine the effect of Ni and Cr compositions on the Fe-Cr-Ni system using the phase-field model. Also, we will determine the optimal composition for the structural material design on the molten salt reactor.

To simulate irradiation effect, we will consider the cascade mixing model and the elastic effect. Also, we will apply the radiation-enhanced diffusion (RED) model to consider the effect of the vacancy concentration under irradiation.

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