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Phase-field modeling of Mn-Ni-Si precipitate behavior on the bcc-Fe matrix

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1. Introduction

The formation of Mn-Ni-Si precipitate (hereafter MNS precipitate) is widely accepted by one of the main reasons of late stage hardening and embrittlement of Reactor Pressure Vessel (RPV) during nuclear power plant (NPP) operation [1, 2]. Since MNS precipitate is not considered in current regulatory model, this late stage hardening can be a limiting factor for life extension of nuclear power plants up to 80 or more years. The stability of the MNS precipitate was investigated from the thermodynamic view point [1] and they concluded that MNS precipitate is a stable phase even with very little Cu contents, and they assessed UW1 thermodynamic database which can predict the thermodynamic stability of MNS precipitate at operating temperature of NPP (~290°C) [1]. Based on the non-classical nucleation theory [3], we performed the phase-field modeling of nucleation and growth of MNS precipitate. The microstructure evolution of Mn-Ni-Cu precipitate has been simulated using the phase-field method [4, 5] and their approaches are focused on a role of the Cu contents. Also, a role of the interstitial loop on the nucleation and growth kinetics of MNS precipitate was analyzed.

2. Methodology

We adopted a set of Cahn-Hilliard equation (Eq. 1) and a set of Ginzburg-Landau equation (Eq. 2) to handle the microstructural evolution of multi-component RPV steel.

$$\frac{\partial c_i(\vec{r},t)}{\partial t} = \nabla \cdot M_i \nabla \frac{\delta F}{\delta c_i(\vec{r},t)} \quad \text{(Eq.1)}$$

Where i is Mn, Ni and Si in this study.

$$\frac{\partial \eta(\vec{r},t)}{\partial t} = -L_i \frac{\delta F}{\delta \eta(\vec{r},t)} \quad \text{(Eq.2)}$$

Where the phase-field variable $\eta = 0$ for $\alpha(BCC)$ and $\eta = 1$ for $\gamma(FCC)$ and $0 < \eta < 1$ at the interface between two phases. Mobility $M_i(\eta, T)$ is given as follows [4, 5]:

$$M_i(\eta, T) = C_{oi}(1 - C_{oi})\left\{(1-\eta)\frac{D_i^{\alpha}(T)}{RT} + \eta\frac{D_i^{\gamma}(T)}{RT}\right\}$$

(Eq.3) where R is the gas constant, T is the temperature and C_{oi} is the nominal composition of the alloying elements.

In order to predict the MNS precipitate behavior on α-Fe matrix, we adopted UW1 thermodynamic database [1] assessed by Xiong et al. The total energy of the system is given as follows [4, 5]:

$$F = \int_V \left\{[1 - h(\eta)]G_C^{\alpha}(c_i, T) + h(\eta)G_C^{\gamma}(c_i, T) + Wg(\eta) + \sum_{i=1}^{4}\frac{1}{2}\kappa_i(\nabla c_i)^2 + \frac{1}{2}\kappa_\eta(\nabla\eta)^2 + \frac{1}{2}C_{ijkl}\left(\varepsilon_{ij} - \varepsilon_{ij}^0\right)\left(\varepsilon_{kl} - \varepsilon_{kl}^0\right)\right\} dV \quad \text{(Eq. 4)}$$

where $G_C^{\alpha}(c_i, T)$ and $G_C^{\gamma}(c_i, T)$ are free energies of each component at each phases (α and γ) which are obtained from UW1 database. $h(\eta)$ is set to $\eta^2(3 - 2\eta)$ and $g(\eta)$ is $\eta^2(1-\eta)^2$ in our calculations. κ_i and κ_η is the gradient coefficient which makes the interface diffuse. $\frac{1}{2}C_{ijkl}\left(\varepsilon_{ij} - \varepsilon_{ij}^0\right)\left(\varepsilon_{kl} - \varepsilon_{kl}^0\right)$ is the free energy contribution from the elastic energy. ε_{ij}^0 will be discussed in Section 4 in detail. We assumed the stiffness tensor is homogeneous as α-Fe value $C_{11} = 243$ GPa, $C_{12} = 145$ GPa and $C_{44} = 116$ GPa.

3. Thermodynamic input

We plotted phase diagram of Mn-Ni-Si system at 290°C using UW1 database [1] in Fig. 1.

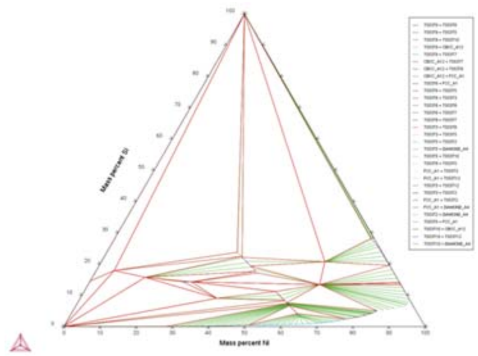

Fig. 1. Phase diagram of Mn-Ni-Si system at 290°C using UW1 database.

We found various types of ordered phase in Fig. 1 and we found that the phase diagram in Fig. 1 is consistent with former works [1, 2].
We choose the composition of LC alloy in reference [1] (Mn-1.16at%, Ni-0.8at%, Si-0.43at%, Fe-97.61at%) and we found that the equilibrium fraction of T6 phase is 1.295 mole% and 98.705 mole% BCC phase.

4. Effect of inhomogeneous elasticity

For the lattice defects, such as dislocation loops, the eigenstrain (stress-free strain) is given as follows [1]:

$\varepsilon_{ij}^0 = b \otimes n = (b_i n_j + b_j n_i)/2d$ (Eq. 5) where b and n are Burgers vector and normal vector of slip plane and d is the inter-planar spacing of the slip planes. We will systemically investigate how the elastic field arose by the lattice defect affects the nucleation and kinetics process of MNS precipitate on α-Fe matrix.

5. Comparison with experimental observations

Recently, atom probe method has been widely used to analyze the microstructure of radiation damaged RPV steel [1, 2]. Our obtained microstructure from the phase-field modeling will be compared with the experimental observation using the atom probe tomography.

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