Multicomponent Modeling of Radiation-Induced Segregation Behavior in Ion-irradiated Stainless Steel 316

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1. Introduction

Radiation-induced segregation (RIS) is a phenomenon of the compositional change of an alloy at sinks under irradiation at a moderated temperature [1]. Because of its potential relevance to irradiation assisted stress corrosion cracking (IASCC) of stainless steels, a main material for reactor internals, a lot of basic research on austenitic stainless steels has been carried out in recent years. Stainless steel is basically composed of three major elements; Fe, Cr, and Ni. There are also minor elements such as Si, P and Mo. Various models have been proposed to estimate RIS in a binary and ternary model alloy containing major elements of SS. However, multicomponent modeling above quaternary system is necessary for a real system to estimate RIS of the SS.

In this work, we extended the basic ternary modeling which was reported last KNS annual meeting to the quaternary system. The RIS behavior of Si in SS 316 during the ion irradiation was calculated, and compared with the experimental results.

2. Methods and Results

2.1 Modeling methodology

Fe-Cr-Ni-Si quaternary system was basically used to simulate RIS in SS316. We extend the ternary model implemented by Perks *et al*. [2] to our system. The model was based on the inverse Kirkendall effect, in other words, vacancy mechanism. Si is rather smaller species than Fe, and we consider the coupling parameter provides the fraction of each solute forming the mixed dumbbell. Differential rate equations for point defects and solutes are basically described below.

$$\frac{\partial C_k}{\partial t} = -\nabla J_k$$

$$J_k = -D_k \alpha \nabla C_k + d_{kv} C_k \nabla C_v - d_{ki} C_k \nabla C_i$$

$$\frac{\partial C_v}{\partial t} = -\nabla J_v + \eta G_{dpa} - K_{vi}(D_v + D_i) C_v C_i - S_v D_v (C_v - C_v^{eq})$$

$$\frac{\partial C_i}{\partial t} = -\nabla J_i + \eta G_{dpa} - K_{vi}(D_v + D_i) C_v C_i - S_i D_i (C_i - C_i^{eq})$$

The detailed equations are described elsewhere [2]. The most important term is d_{kv} which represents diffusivity correlation factor of atom-defect relationship. As the factor increase, atoms move easily with vacancies.

The coupling parameter β_k is described as [3]:

$$\beta_k = \frac{\exp(E_{ki}^b/kt)}{\sum_k C_k \exp(E_{ki}^b/kt)}$$

To consider grain boundary effect, grain boundary sink strength (S^{GB}) was introduced [4]. There were one or two boundaries with S^{GB} at the center region of the grain. The both end of the boundary of the system were fixed as deep boundary conditions which represented an infinite large grain. The calculated composition was convoluted with X-ray generation profile having the standard deviation of 1 nm [5].

2.2 Experiment

The test material was a solution annealed plate of SS 316. A small disk specimen like a TEM sample, 3 mm in diameter and 100 μm in thickness was prepared for the irradiation test. The irradiation was carried out using heavy-ion irradiation machine of KIGAM. The ion source was Fe^{4+} with the total energy of 8 MeV. The temperature of the specimen was about 400°C, and the irradiation time was up to 4 hr. The total fluence was estimated about 10 dpa by SRIM/TRIM calculation. After the irradiation test, the orientation of the grain boundaries were identified by EBSD, and a small region was cut by FIB technique to observe the microstructure using TEM. The maximum irradiation depth of the samples was about 2 μm. We observed the region of 0.5 μm depth (~2 dpa) and the region of 1.0 μm depth (4 dpa). The depletion and enrichment of solute atoms were measured using TEM/EDS.

2.3 RIS in SS316

Fig. 1 shows the TEM micrograph of a twin with a width of 6 nm. The dose of the specimen was calculated as 2 dpa. There were black and white spots distributed evenly in the upper and lower boundary. The spots are ledges along the boundary planes which led to a distortion of the lattice. The ledges showed high RIS compared to the coherent region of the twins because they had high sink strength and acted as perfect sinks.

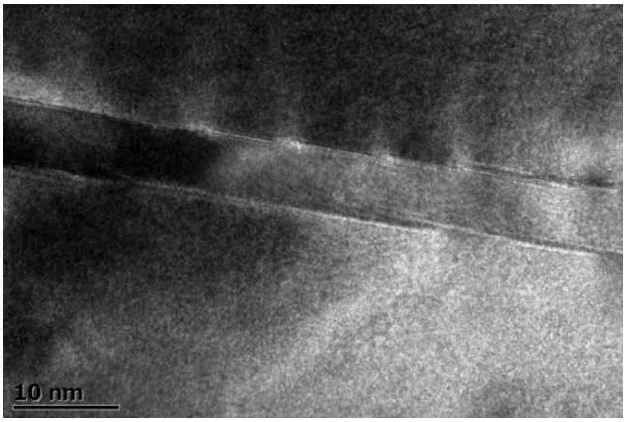

Fig. 1. TEM image of closely spaced twins in SS 316. The upper twin plane shows many ledges located periodically.

(a)

(b)

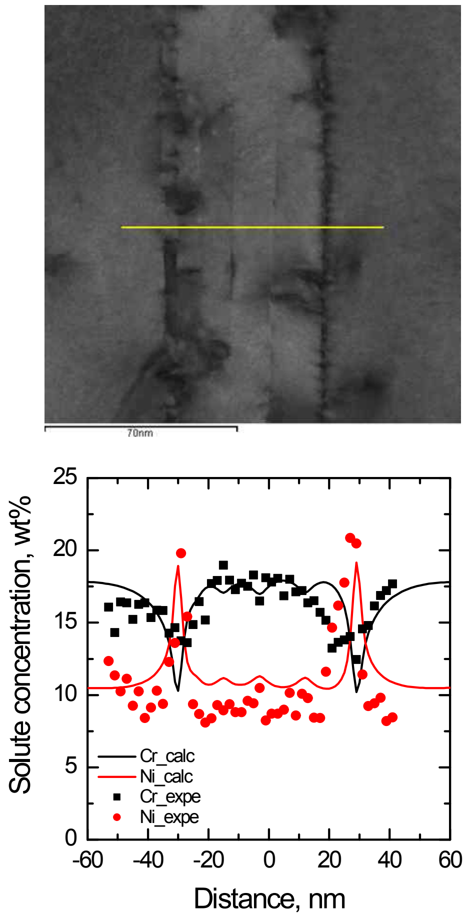

Fig. 2. (a) TEM image of twins with the spacing of 57 nm, and (b) solute concentration of the measured and calculated RIS.

Fig. 2 shows the measured and calculated results of multi-twin boundaries. There were six boundaries and five regions, and the total spacing was measured to be 57 nm. As shown in the TEM image, the outer boundaries had many black spots with high sink strength. In contrast, the inner boundaries showed a rather clear boundary plane with low sink density. It is believed that the inner boundary was more coherent than the outer boundaries, as expected from the observation. The EDS results revealed that there was reduced RIS in the inner boundaries, as shown in the line-scanning and point-analysis results. In our calculations, the sink strength of the inner boundaries was set at 1/500 times that of the outer boundaries. The calculated profile was in good agreement with the experimental measurements. There were tiny deviations in the EDS points on the inner boundaries, which were expected for small peaks of depletion or enrichment. The reduced RIS behavior of the inner boundaries could be attributed to the high coherency of and the reduced defect concentration in the small volume between the twinned regions.

3. Summary

A theoretical evaluation of RIS in SS316 was implemented by multicomponent modeling. The calculated results were compared to the measured values, and these results were sensitive to model parameters. However, the calculated amount of depletion/enrichment shows a fair agreement with the measured one with the uncertainties of the parameters. This modeling could be useful to estimate the RIS behavior of SS 316.

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