



Atomistic dynamical observation of grain boundary structural changes under electron irradiation

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Abstract

We investigated the structural changes in two grain boundaries with different grain boundary nature during electron irradiation using an atomic-resolution high-voltage electron microscope. It was found that the morphology of one type of grain boundary changed due to boundary movement during the irradiation, whereas another type of grain boundary did not show such structural change. On the other hand, solute segregation was induced in the vicinity of both grain boundaries. It was found that differences between the two grain boundaries, particularly the difference between grain boundary interfacial planes prior to irradiation, caused the different grain boundary migration behavior.

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1. Introduction

The processes of recrystallization and grain growth (by grain boundary migration) during thermal annealing at high temperatures are important processes. These phenomena are generally caused by diffusion of vacancies, and diffusion-induced grain boundary migration and have been investigated in various alloy systems [1–5]. Moreover, grain boundary migration under irradiation has often been observed at even lower temperatures where boundary migration is not caused by thermal annealing [6–10]. The most important difference between these migrations is that the latter one causes simultaneous solute redistribution around the grain boundaries [11,12]. For this reason, the dynamics of grain boundary migration caused by irradiation is quite different from that under pure thermal conditions. Investigations are therefore needed to examine the retardation of radiation-induced grain boundary migration (RIGM) and concurrently induced radiation-induced segregation (RIS) near the grain boundaries.

We have recently examined the RIGM behavior in an Fe–Cr–Ni ternary alloy during electron irradiation using an atomic-resolution high-voltage electron microscope (AR-HVEM) and observed atomistic rearrangements at the grain boundary interface [13]. The aim of this study was to determine the effect of the nature of the grain boundary, especially the initial grain boundary interfacial planes on the grain boundary migration induced by electron irradiation in an Fe–Cr–Ni alloy.

2. Experimental procedure

Specimens of the Fe–Cr–Ni austenitic ternary alloy, each containing (in wt%) 20.1 nickel, 15.2 chromium, and 0.003 carbon and 0.0011 nitrogen as impurities, were used. After solid solution treatment at 1323 K for 30 min and electro-polishing, thin foil specimens (less than 100 nm in thickness) were irradiated with 1.25 MV electrons in an AR-HVEM (JEOL JEM-ARM-1300). Two different grain boundaries were exposed to the irradiation. A field-emission gun (FEG) TEM (JEOL JEM-2010F) was used to measure the average grain boundary geometrical parameters, that is, the misorientation angle θ around [110], the angular deviation $\Delta\theta$ from the coincidence relationship, and the grain boundary planes $(hkl)_1 \parallel (hkl)_2$. Although it is not easy

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Table 1
Some GB parameters of each grain boundary

	[1 1 0] tilt component of misorientation angle	Corresponding Σ value (deviation angle)	Boundary interfacial planes
GB-1 [13]	59°	33 (2°)	$(113)_1 \parallel (771)_2$
GB-2	55°	33 (4°)	$(002)_1 \parallel (111)_2, (111)_1 \parallel (002)_2$

to determine the exact grain boundary planes with TEM, the grain boundary plane orientation could be determined with an accuracy of only 4°. Both grain boundaries had similar misorientation angles and deviation angles from the coincidence relationship but different boundary interfacial planes as shown in Table 1. The angular deviation $\Delta\theta$ exhibit 2–4° angular departure from the coincidence, indicating that both grain boundaries were general or ‘random’ grain boundaries by Palumbo–Aust criterion [14]. The mean displacement rate, irradiation temperature and maximum dose were 4.0×10^{-3} dpa/s, 623 K and 14.4 dpa, respectively. During the irradiation, the dynamics of grain boundary structural changes was recorded on a digital video by a CCD camera attached to the AR-HVEM. The chemical composition near the grain boundary was analyzed using an FEG-TEM equipped with an energy-dispersive X-ray spectroscopy (Noran Inc., VOYAGER-system).

3. Results and discussion

3.1. Grain boundary-1

First, we will present typical results for RIGM behavior obtained in our previous study (Ref. [13]). Fig. 1 shows HREM images of GB-1 (a) before and (b) after

electron irradiation to 14.4 dpa at 623 K [13]. On the TEM scale, the grain boundary was determined by $(113)_1 \parallel (771)_2$ planes prior to irradiation. Due to irradiation, the morphology of the boundary changed to a facet structure by RIGM. One of the pairs of grain boundary planes seemed to be close to $(002)_1 \parallel (111)_2$ planes, although $(002)_1$ planes slightly tilted from $(111)_2$ planes (about 4°). Fig. 2 shows the dynamical behavior of the grain boundary movement during irradiation [13]. At the given time, the grain boundary had already moved and the shape of the boundary had already become a facet-like structure. It is clearly shown that some lattice fringes in the grain on the right side changed into lattice images with an increase in irradiation dose, and the converted lattice images are the same as the images obtained from the grain on the left side.

3.2. Grain boundary-2

Fig. 3 shows HREM images of GB-2 (a) before and (b) after electron irradiation under the same conditions as those used for irradiation of GB-1. We could not find any structural change in this boundary. Initially this boundary consisted of low-index planes and had some facet structures. It was therefore thought that the boundary remained stable during the irradiation and that no structural change occurred.

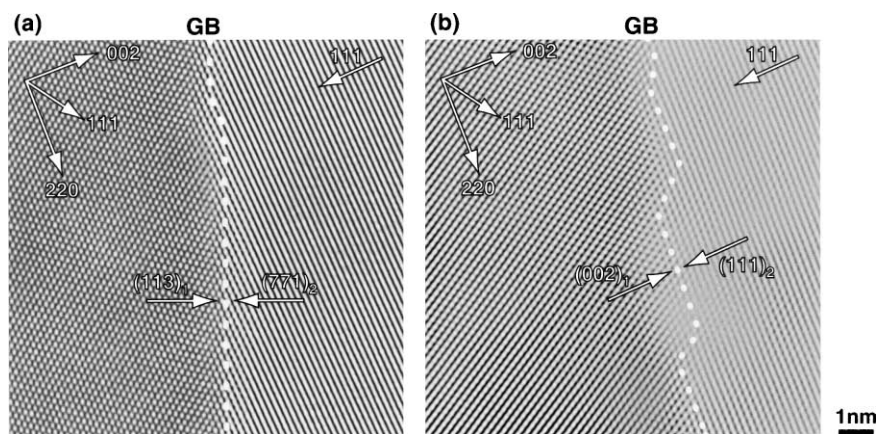


Fig. 1. HREM images of GB-1 (a) before and (b) after electron irradiation to 14.4 dpa at 623 K [13].

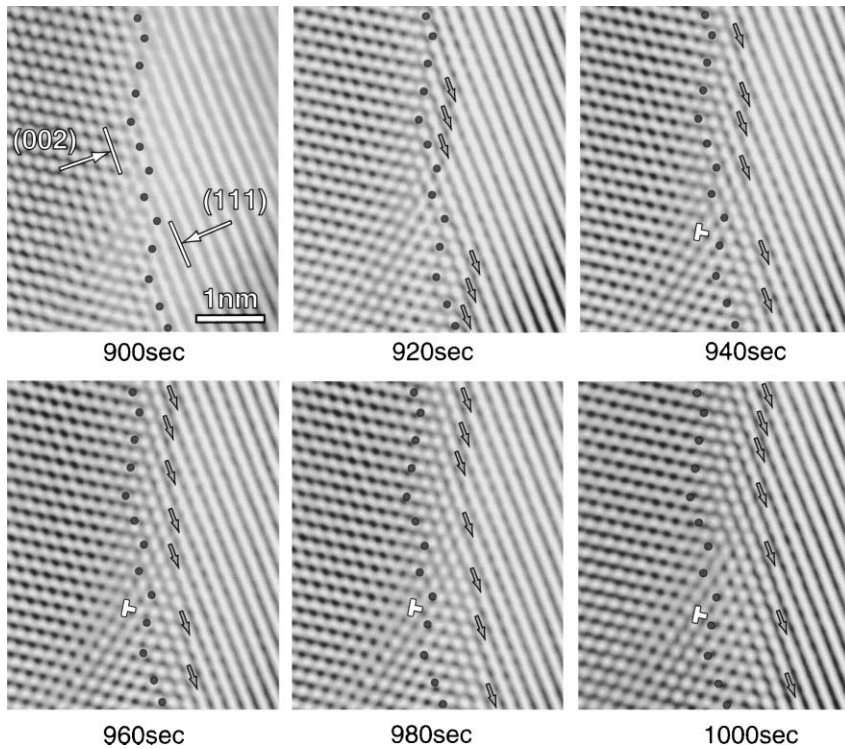


Fig. 2. Dynamical behavior of RIGM on GB-1 during the irradiation [13].

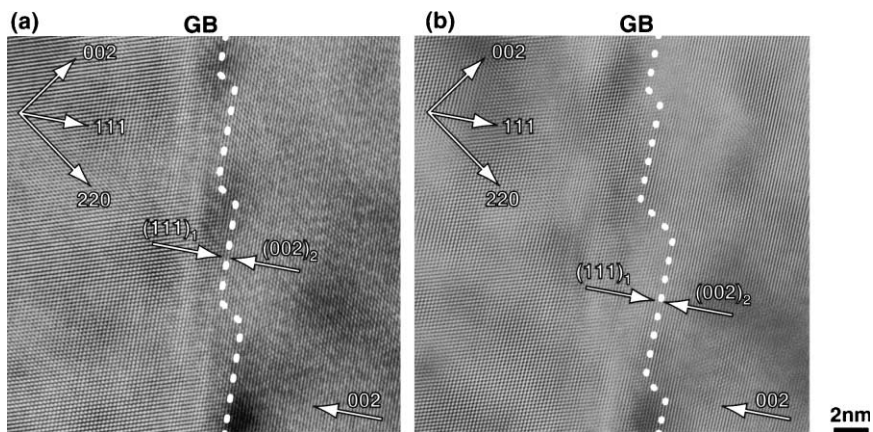


Fig. 3. HREM images of GB-2 (a) before and (b) after electron irradiation to 14.4 dpa at 623 K.

3.3. RIS behavior

The graphs in Fig. 4 show concentration profiles near the boundaries after irradiation on (a) GB-1 and (b) GB-2. Strong nickel enrichment and chromium/iron depletion were induced at both boundaries. This is evidence that both grain boundaries acted as preferential sink sites for excess point defects. However, there is a

difference in the shapes of the concentration profiles near the two grain boundaries. At GB-2, symmetrical concentration profiles were observed whereas the concentration profiles were asymmetrical for GB-1, and RIS was enhanced in the region where the boundary had migrated. The magnitude of the RIS at the boundary interface of GB-1 was also higher than that of GB-2.

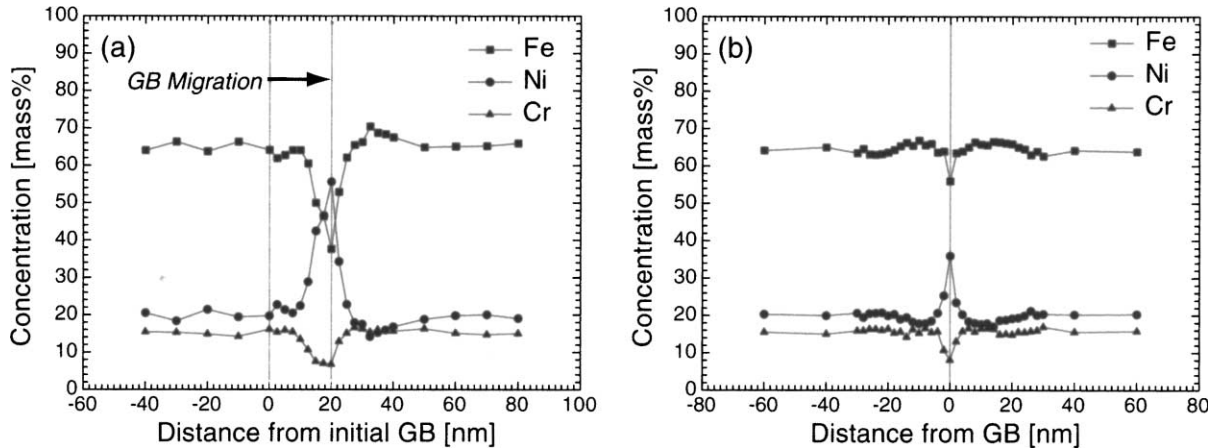


Fig. 4. Concentration profiles around the grain boundaries after the irradiation: (a) GB-1 and (b) GB-2.

4. Discussion

Theoretically, one of the important processes for the RIGM is the diffusion of excess point defects to and their annihilation at grain boundaries. A notable finding in the present study is that both grain boundaries acted as effective sink sites for the point defects because strong RIS apparently occurred there. It is therefore expected that the most effective parameter for grain boundary structural change is the initial grain boundary nature, i.e., the grain boundary plane. In the light of the present results, a grain boundary consisting of high order index planes like GB-1 shows a relatively high grain boundary energy for atomic rearrangements to occur at the boundary during irradiation to form a lower energy boundary like GB-2. Consequently, a driving force for such atomic rearrangement should be the change of the boundary energy between the unirradiated and irradiated structures. The grain boundary structure (such as morphology and interfacial planes) of GB-1 after the irradiation was similar to that of GB-2, although GB-2 did not show any structural change during the irradiation.

5. Conclusions

We investigated structural changes at two different grain boundaries in an austenitic Fe–Cr–Ni alloy induced by electron irradiation. It was found that a grain boundary consisting of high index interfacial planes can move during electron irradiation and adopt a different morphology. On the other hand, another grain boundary consisting of low index interfacial planes did not

show any structural change. In both cases, strong solute redistribution was induced near the grain boundaries by RIS, although the distribution profiles were different from each other. The results of the present study suggest that an atomic rearrangement around the grain boundaries occurs to form a lower energy boundary and that the driving force of RIGM is the difference of the boundary energy before and after grain boundary migration during the irradiation.

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