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Cr segregation on dislocation loops enhances hardening in ferritic Fe–Cr alloys

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Abstract

The effect of chromium on iron hardening via segregation on dislocation loops was studied by atomic scale computer modeling. A combination of Monte Carlo and molecular dynamics techniques together with the recently determined Fe–Cr interatomic potentials fitted to ab initio data was used to investigate Cr segregation on ½⟨1 1 1⟩ interstitial dislocation loops and its impact on the interaction with moving dislocations. The Monte Carlo results reveal that Cr atoms segregate to the loop tensile strain region and dissolve well above the temperature corresponding to the solubility limit. The molecular dynamics results demonstrated that local micro-chemical changes near the loop reduce its mobility and increase the strength. The stress to move a dislocation through the array of Cr "decorated" loops increases due to modification of the dislocation–loop interaction mechanism. A possible explanation for a number of experimental observations being dependent on the radiation dose and for Cr concentration effects on the yield stress is given on the basis of the modeling results.

Keywords: Bcc metals; Dislocation loops; Hardening; Segregation

1. Introduction

High Cr (9–12 wt.%) ferritic/martensitic (F/M) steels are candidates for structural materials in Fusion and GenIV reactors [1], as well as for fuel cladding and as a spallation target in accelerator driven systems [2]. The resistance of F/M steels to radiation effects such as swelling and embrittlement is known to depend on the Cr content (see, for example, Little [3], Kohyama et al. [4], and Garner et al. [5]). Selection of the optimal steel composition for a particular application requires an understanding of the basic mechanisms responsible for the radiation effects and their variation with Cr content. The radiation damage in Fe and Fe–Cr alloys usually visible by transmission electron microscopy (TEM) consists of a mixed population of interstitial dislocation loops with Burgers vectors $b = \langle 1\,0\,0 \rangle$ and ½⟨1 1 1⟩ [6,7]. These loops are taken to be the microstructure responsible for matrix hardening effects due to dislocation pinning. Experiments have shown that the relative population of the two kinds of loops depends on the Cr content, radiation dose and temperature. In general it is accepted that the fraction of ⟨1 0 0⟩ loops, which is dominant in pure Fe [8], decreases with increasing Cr concentration, with a mixed population of ½⟨1 1 1⟩ and ⟨1 0 0⟩ loops present in Fe–Cr alloys containing more than 6 at.% Cr [6,9]. At the same time, the addition of Cr results in a decrease in the mean size of the dislocation loops, observed under the similar radiation conditions (see experimental data for pure Fe [8] and Fe–Cr [9]), from >5 nm in pure Fe down to about 2 nm, which is hardly resolvable by TEM (when dealing with ferromagnetic complex alloys which require complicated remote handling due to activation after neutron irradiation). An attempt to correlate

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the radiation-induced microstructure with the changes in mechanical properties using the dispersed barrier model was made by Matijasevic and Almazouzi [9], who proposed that the change in the yield stress Δ ($\Delta\sigma_{0.2}$) can be expressed as:

$$\Delta = \alpha M \mu b (N \times d)^{1/2} \quad (1)$$

where α is the obstacle strength parameter, *M* is the Taylor coefficient, μ is the shear modulus, *b* is the value of the Burgers vector, and *N* and *d* are the density and mean size of the obstacles [10]. Eq. (1) gives a good fit to the measured change in the yield stress at low irradiation doses up to 0.06 dpa with $\alpha = 0.6$, as shown in Fig. 1a. At higher doses, however, fitting Eq. (1) to the experimental results for Fe–Cr alloys demands an increase in the obstacle strength parameter up to 0.9 at a dose of 0.6 dpa, while $\alpha > 1.0$ must be used to comply with the $\Delta\sigma_{0.2}$ value obtained at 1.5 dpa for Fe–12Cr alloys (see Fig. 1b and c). It is important to note that correlation of $\Delta\sigma_{0.2}$ with the population of dislocation loops in pure Fe irradiated at similar doses [8] requires α to be about 0.5, unlike in Fe–Cr alloys. Several possible explanations can be put forward to explain the increase in hardening of Fe–Cr alloys at low doses compared with higher doses. The most obvious ones are:

1. the appearance of a new radiation damage microstructure not visible by TEM but contributing strongly to dislocation pinning and, hence, to the measured hardening;
2. modification of the observed obstacles, i.e. dislocation loops, as they become significantly stronger than in pure Fe;
3. a combination of 1 and 2.

The accumulation of small defects undetectable by TEM has been confirmed by other techniques. Thus positron annihilation spectroscopy (PAS) studies reported the accumulation of small clusters, <1 nm in size, consisting of a few tens of vacancies in Fe [11,12]. These clusters are stable up to almost 300 °C and their concentration increases with dose, reaching $>10^{24}$ m^3, so they can act as obstacles to dislocation glide [13]. However, these clusters can explain the hardening increase with increasing irradiation dose, but not with Cr concentration, as it was proved that their concentration is significantly lower in Fe–Cr alloys compared with pure Fe [9,12]. Moreover, because the concentration of these clusters decreases in high Cr alloys the contribution to hardening of other unknown sources must be even stronger. Another possible invisible microstructure could be small interstitial clusters/loops accumulating as the dose is increased. The extensive formation of small interstitial clusters in primary damage events (displacement cascades) in pure Fe and Fe–Cr alloys has been proven by atomistic simulations [14,15] and theoretical analysis of the experimental data on the basis of the production bias model [16]. There should be a significant number of small, invisible by TEM, interstitial clusters/loops with a size of ⩽2 nm, and the number of these clusters should increase with increasing radiation dose. However, their fate depends on the alloy composition. Thus the majority of loops produced by cascades are of ½⟨1 1 1⟩ type [17] and because of their high mobility can easily escape from the bulk to grain boundaries and dislocations. This leads to an increase in the population of significantly less mobile ⟨1 0 0⟩ loops in pure Fe. With the addition of Cr the fraction of ½⟨1 1 1⟩ loops starts to increase due to the confinement effect of chromium atoms in solution. The maximum effect appears at Cr concentrations of ~9–12 at.% [18,19]. It is therefore reasonable that the concentration of both visible and invisible ½⟨1 1 1⟩ loops increases with irradiation dose and Cr concentration. On the other hand, the accumulation of small ½⟨1 1 1⟩ loops/clusters alone cannot explain a significant increase in hardening, as these are not obstacles to dislocations, as recently reported [20]. Actually, small ½⟨1 1 1⟩ loops (⩽2 nm) glide towards dislocations and athermally reform into superjogs without any hardening effect.

From the above discussion we could conclude that either new unknown obstacles appear or known obstacles, such as small interstitial loops, become much stronger under prolonged irradiation in high Cr alloys. We suggest that small interstitial clusters/loops formed directly in high energy cascades mostly disappear at dislocations and grain

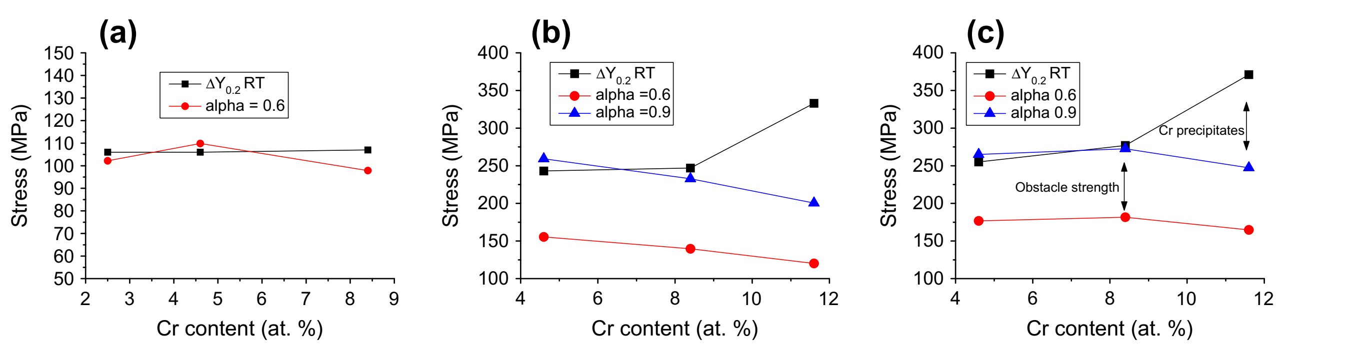

Fig. 1. Hardening measured in Fe–Cr alloys irradiated by neutrons up to (a) 0.06, (b) 0.6 and (c) 1.5 dpa, measured at room temperature (RT) and 300 °C [9]. Prediction of the Orowan dispersed barrier model with loop strength (α) taken as 0.6 and 0.9 is also shown. Hardening using the dispersed model was calculated using Eq. (1) and data for loop size and density were reported in Matijasevic and Almazouzi [9].