Acta Materialia 135 (2017) 54–60

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Full length article

Irradiation-induced damage evolution in concentrated Ni-based alloys[☆]

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ARTICLE INFO

Article history:
Received 25 January 2017
Received in revised form
10 May 2017
Accepted 2 June 2017
Available online 6 June 2017

Keywords:
Concentrated solid-solution alloys
Ferro/antiferromagnetic coupling
Ion irradiation
Damage evolution
Molecular dynamics simulations

ABSTRACT

Understanding the effects of chemical complexity from the number, type and concentration of alloying elements in single-phase concentred solid-solution alloys (SP-CSAs) on defect dynamics and microstructure evolution is pivotal for developing next-generation radiation-tolerant structural alloys. A specially chosen set of SP-CSAs with different chemical complexity ($Ni_{80}Fe_{20}$, $Ni_{80}Cr_{20}$ and $Ni_{40}Fe_{40}Cr_{20}$) are investigated using 1.5 MeV Mn ions over a wide fluence range, from 2×10^{13} to 1×10^{16} ions cm^{-2} at room temperature. Based on an integrated study of Rutherford backscattering spectroscopy in channeling geometry and molecular dynamics simulations, the results demonstrate that $Ni_{40}Fe_{40}Cr_{20}$ is more radiation tolerant than $Ni_{80}Fe_{20}$, $Ni_{80}Cr_{20}$ and elemental Ni in the low fluence regime. While chemical complexity of this set of SP-CSAs is clearly demonstrated to affect defect evolution through suppressed defect production and enhanced recombination at early stages, the effect of the mixed ferro- and antiferromagnetic interactions is not the only controlling factor responsible for the improved radiation performance. The observed strong alloying effect on defect evolution is attributed to the altered defect migration mobilities of defect clusters in these alloys, an intrinsic characteristic of the complex energy landscapes in CSAs.

1. Introduction

Research on the radiation behavior of conventional metallic alloys, based of one principal element and small amount of alloying additions are well documented in recent reviews [1–11]. These review articles concern both the influence of experimental variables (e.g. radiation temperature, dose, ion flux) and microstructural parameters (e.g. grain size, concentration of alloying elements) on radiation damage in metallic alloys. Advances in the development of single-phase concentrated solid solution alloys (SP-CSAs) have attracted increasing attention in material science [12–25]. In sharp contrast to conventional alloys, SP-CSAs consist of two to five principal elements mixed in equiatomic or near equiatomic ratios, or in high concentrations, that form random solid solutions on the simple underlying crystalline lattice, such as the face-centered cubic (fcc) lattice. These SP-CSAs possess extraordinary mechanical properties [12,17] and outstanding physical-chemical properties compared with conventional alloys, such as excellent corrosive and wear resistance [24], and enhanced radiation tolerance [13,17]. It is assumed that the random nature of the elements in SP-CSAs, without solvent and solute elements, is one of the characteristics of SP-CSAs that stimulates the recovery of radiation damage by efficient dynamic annealing at very early stages of defect evolution [13]. Their outstanding physical and chemical properties have triggered study of their potential for nuclear applications [26,27]. Thus, understanding and predicting radiation damage evolution in SP-CSAs is crucial for nuclear applications.

In recent experimental irradiation studies of 1.5 MeV Ni-irradiated SP-CSAs, Zhang et al. [13] have reported that alloying of

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http://dx.doi.org/10.1016/j.actamat.2017.06.002
1359-6454/

Ni with Fe suppresses primary damage production in $Ni_{50}Fe_{50}$ as compared to elemental Ni. They correlated different irradiation performance with increasing localized heat dissipation due to the 4 to 5 times higher residual electrical resistivity of $Ni_{50}Fe_{50}$ compared to elemental Ni [13]. Moreover, Jin et al. [16] have also shown that a significant reduction of electrical and thermal conductivity is expected for the alloys with mixed ferro/antiferromagnetic interactions. Since the highest electrical resistivity and lowest thermal conductivity was identified in the alloys with Cr content [16], the production and migration of defects are expected to be more locally confined in the alloys with a mix of ferromagnetic (e.g., Ni, Fe, Co) and antiferromagnetic elements (e.g., Cr, Mn), as compared with the alloys composed of all ferromagnetic elements, which may contribute to an enhanced defect recombination rate in the alloys with mixed ferro/antiferromagnetic interactions [28].

Elemental Ni and three Ni-based SP-CSA single crystals were selected for study. The SP-CSAs exhibit different magnetic properties: $Ni_{80}Fe_{20}$ is a ferromagnetically coupled alloy; $Ni_{80}Cr_{20}$ is an antiferromagnetically coupled alloy; and $Ni_{40}Fe_{40}Cr_{20}$ is a mixed ferro/antiferromagnetic coupled alloy [28]. Since increased electrical resistivity with increasing chemical disorder, from elemental Ni to binary and to more complex ternary alloys, has been observed (7.2, 15.4, 100, and 105 $\mu\Omega$ cm, for Ni [29], $Ni_{80}Fe_{20}$ [30], $Ni_{80}Cr_{20}$ [29], and $Ni_{40}Fe_{40}Cr_{20}$ [31], respectively), this set of fcc crystals is ideal to investigate the influence of mixed ferro/antiferromagnetic interactions on defect evolution in ion irradiated SP-CSAs. In this article, elemental Ni is compared with non-equiatomic $Ni_{80}Fe_{20}$, $Ni_{80}Cr_{20}$, and $Ni_{40}Fe_{40}Cr_{20}$ alloys regarding defect evolution under 1.5 MeV Mn ion irradiation at room temperature (RT) over a wide fluence range (from 2×10^{13} to 1×10^{16} ions cm^{-2}). The irradiation response was evaluated using Rutherford backscattering spectrometry in channeling conditions (RBS/C). The results unambiguously show that the intrinsic disorder resulting from randomly arranged elemental species in $Ni_{80}Fe_{20}$, $Ni_{80}Cr_{20}$ and the more complex $N_{40}Fe_{40}Cr_{20}$, compared to elemental Ni, leads to a considerable delay of damage accumulation under the ion irradiation conditions used in this study.

2. Experimental methodology

2.1. Ion irradiation and ion beam analysis

Elemental Ni and the three SP-CSAs alloys of $Ni_{80}Fe_{20}$, $Ni_{80}Cr_{20}$ and $Ni_{40}Fe_{40}Cr_{20}$ single crystals in fcc structure [28] were used in this study. Prior to ion irradiations, the crystalline quality of the pristine samples was measured and compared using the RBS/C technique. Ion irradiations were performed at RT using 1.5 MeV Mn^+ ions at the Ion Beam Materials Laboratory (ORNL-IBML) at the University of Tennessee in partnership with Oak Ridge National Laboratory [32]. Irradiations were performed in a random direction by tilting the crystals with an angle of 7° relatively to the surface normal. The flux was maintained at 4.1×10^{11} ions $cm^{-2}s^{-1}$ for all ion fluences. The mean projected range of Mn ions has been estimated, based on SRIM calculations [33], where the ion range R_P is ~500 nm with a range straggling ΔR_P ~ 100 nm. For ion fluences ranging from 2×10^{13} to 1×10^{16} ions cm^{-2}, the corresponding conversion factor to displacements per atom (dpa) at the damage peak is ~1.19×10^{-15} dpa cm^2, as determined from SRIM calculations using the Kinchen-Pease model under an assumed threshold displacement energy of 40 eV for all elements [13]. Therefore, the damage dose at the peak ranges from ~0.02 to ~11.85 dpa.

RBS/C experiments, using a 3.5 MeV He^+ beam along both the <100>-axial direction and off-channel (random) direction, were performed on all irradiated crystals to quantify the resulting irradiation-induced damage. A Si detector was placed at a 155° angle with respect to the beam direction. The energy resolution of the experimental setup was about 15 keV [32].

2.2. Simulation

The irradiation simulations were done using molecular dynamics (MD) code PARCAS [34,35]. The interactions between the modeled alloys were described using an EAM based potential developed by Bonny et al. [36]. The recoil simulations were initiated by giving 25 keV energy to a central Ni atom. To achieve a damage dose equivalent to 0.015 dpa (NRT), 150 cumulative recoil simulations were performed. The simulation cell was shifted by a random displacement vector between zero and the cell size in the [100], [010] and [001] directions before each subsequent recoil simulation to replicate the random nature of the overlapping cascade. The simulation cell size was $284 \times 284 \times 284$ Å^3 containing 2,050,000 atoms. Each simulation ran for 100 ps at 300 K. Periodic boundary conditions were applied in all directions to mimic an infinitely large bulk system. The temperature was scaled at the periodic boundaries using Berendsen temperature control. The damage was analyzed at the end of the simulation using Voronoi polyhedra centered on initial atom positions. Polyhedra with no atoms were labeled as vacancies, and polyhedra with 2 or more atoms as interstitials. The details of the simulation procedure can be found elsewhere [37].

3. Experimental results

The RBS/C results of Mn-irradiated $Ni_{40}Fe_{40}Cr_{20}$ are shown in Fig. 1(a). The random and channeling spectra from a pristine sample are also included, which indicate the fully random (amorphous-like) and essentially defect-free levels, respectively. The spectra taken in channeling orientation on the pristine crystals obviously exhibit a much lower yield than the random one. The value of the axial minimum yield, χ_{min} ~0.06, obtained for the Ni sublattice below the surface peak attests to the high quality of the single crystals used for this study. The spectra recorded in the <100>-axial direction on Mn-irradiated crystals exhibit, as compared to those for pristine samples, an increase in the backscattering yield with increasing ion fluence (at least up to 1×10^{15} ions cm^{-2}) due to the accumulation of irradiation damage. With further irradiation to ion fluences from 1×10^{15} to 3×10^{15} ions cm^{-2} and to 1×10^{16} ions cm^{-2}, no further increase in backscattering yield is observed, indicating that the damage level has reached a saturation steady state. At the highest fluence (1×10^{16} ions cm^{-2}), the backscattering yield is much lower than the random level, indicating that a fully amorphous-like state is not reached based on ion-channeling criteria.

Another important feature of the actual RBS/C data is the absence of a damage peak in the Mn-irradiated channeling spectra. In RBS/C measurements [38], interstitials, interstitial clusters and small amorphous-like clusters cause direct backscattering of the probe beam that is normally observed as a damage profile with peak in the backscattering yield [13]. As the backscattering yield does not show a clear damage peak around channel 1152 (i.e. the depth corresponding to this channel is 400 nm). The shape of the spectra suggests that neither amorphous clusters nor a high concentration of interstitials are the dominant defect types [13]. Instead, dislocation loops and stacking fault tetrahedra (SFT) are responsible for the significant dechanneling and, therefore, the increase in backscattering yield [39]. The lack of an apparent damage region has been reported and attributed to extended defects in other studies [13,28], e.g., 1.5 MeV Ni-irradiated Ni, $Ni_{1-x}Fe_x$ (x = 35–60), $Ni_{50}Co_{50}$ and $Ni_{25}Co_{25}Fe_{25}Cr_{25}$. This supposition was further supported by high-resolution transmission electron