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Evolution of irradiation-induced strain in an equiatomic NiFe alloy☆

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ABSTRACT

The evolution of irradiation-induced atomic strain in an equiatomic NiFe concentrated solid-solution alloy is investigated using both atomistic simulations and x-ray diffraction analysis. The irradiations are performed using 1.5 MeV Ni ions to fluences ranging from 1×10^{13} to 1×10^{14} cm^{-2}. The irradiation simulations are carried out by overlapping 5 keV Ni recoils cascades up to a total of 300 recoils. An increase of volumetric strain is observed at low dose, which is associated with production of point defects and small clusters. Relaxation of strain occurs at higher doses, when large defect clusters, e.g., dislocation loops, dominate.

The study of irradiation-induced defect production and evolution in materials has been an active field of research for more than half a century [1]. In crystalline materials, irradiation with energetic particles changes the material's structure and properties due to the introduction of atomic defects. The defects evolve by diffusion and act as the source of many microscopic and macroscopic damage-induced effects, such as defect clusters, void swelling, and hardening [2,3]. Ion-irradiation-induced defects can also give rise to local deformation of the crystal structure that causes elastic strain. X-ray diffraction (XRD) measurements of irradiated yttria-stabilized cubic zirconia (YSZ) and strontium titanate (STO) have shown that defect-induced strain increases with ion fluence, and STO is more sensitive to irradiation than YSZ [4]. Lacroix et al. has reported a highly-strained region due to point defect clustering in 300 keV Eu-implanted GaN [5]. There are several studies of irradiation-induced defects and associated local strain in ceramics and semiconductors [6–9]. While it is expected that, there will be differences in the evolution of irradiation-induced strains in ceramics, semiconductors, metals and alloys, some correlation may exist, especially for radiation-resistant ceramics (such as ZrO_2 and MgO) and alloys (such as NiFe in this work) where crystallinity is retained.

Austenitic steels and Ni-based alloys are promising candidate materials for nuclear applications in future fission and fusion reactors. Recently, face-centered cubic (fcc) single-phase concentrated solid-solution alloys (SP-CSAs) are also proposed due to their promising radiation-resistance [10]. Ni and Fe are the dominant components of these alloys. To begin understanding the irradiation response of SP-CSAs, our initial efforts focus on investigating the properties of simple binary alloys containing Ni and Fe under irradiation. In this paper, we present the results of a computational and experimental study on irradiation-induced atomic strain in a concentrated NiFe alloy.

In this study, classical molecular dynamics (MD) simulations were used to model the irradiation-induced damage formation and the correlation with atomic-level strain in a fcc NiFe alloy. We used the embedded atom method (EAM) potential by Bonny et al. to describe the atomic interactions for the equiatomic NiFe alloy [11]. To study the irradiation-induced strain, overlapping cascade simulations were performed using the PARCAS MD code [12–14]. The cubic simulation cell with a random mixture of Ni and Fe contained approximately 132,000 atoms and 32 unit cells ($11.5 \times 11.5 \times 11.5$ nm^3). Periodic boundary conditions were applied to all directions to mimic a bulk system. The simulations were run at 300 K, and the heat was extracted from the system by applying a Berendsen temperature control at the outer most three atomic layers of the cell during the cascade events [15]. The simulation cell was shifted by a vector of random length (between zero

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and the cell size) and in a random direction before each recoil event to ensure homogeneous irradiation. A center Ni atom was given 5 keV of kinetic energy to generate the first recoil collision cascade. The SRIM calculated projected range of a 5 keV Ni recoil is 31 Å [16], so the recoil stayed well inside the cell and is not affected by periodic boundary condition and boundary cooling algorithm. While the present simulations do not take into account the heat transfer to the electronic system, recent simulations of single cascades in NiFe employing the two-temperature MD model [17,18], which does account for heat transfer to the electronic system, suggest that the cooling rate of the cascade is not significantly affected by heat transfer to the electrons at these recoil energies. The energy of 5 keV was chosen since more than 90% of SRIM predicted primary recoils from 1.5 MeV Ni ions (experimental irradiation energy) in NiFe are less than 5 keV. The low energy recoils also substantially decrease the simulation time due to the use of small simulation cell, thus allows us to reach the high doses, comparable to experiments. The simulation time for the recoil event was 30 ps to ensure that the system cooled down to 300 K and no energetic interactions remained in the system. In a similar way, and after each shift of the simulation cell, subsequent recoils were generated from the center of the cell. A total of 300 overlapping recoil simulations were performed to achieve a damage dose equivalent to 0.1 dpa, according to NRT equation, which yielded good statistics for characterization of the final damage state [19]. The details of the simulation procedure can be found elsewhere [20].

The damage was analyzed at the end of the simulation for each recoil event using Voronoi polyhedral centered on the initial atom positions. Polyhedra with no atoms were labeled vacancies, and polyhedra with 2 or more atoms were defined as interstitials [13,20]. Defect cluster formation analysis was performed by calculating the distance from each defect relative to all other defects. All defects that were within a fixed cut-off radius (second nearest-neighbor distance 3.65 Å) were interpreted to be a part of the same defect cluster [21,22]. Defects were visualized with the program OVITO [23].

To determine the effect of cluster size on the evolution of strain, we separately analyzed the strain induced by four different configurations of defect clusters. The size and number of clusters are given in Table 1. The defect configurations were created by a random distribution of interstitials in different sections of a simulation cell containing 16,500 atoms. To understand the effect of cluster size and configuration, the total number of interstitials was kept constant (30) for each configuration cell. For example, six clusters containing five interstitials each were created by the random distribution of 5 interstitials (total 30 interstitials) in a way that the clusters that formed did not interact with each other. The interstitials were placed within one to two lattice parameters of each other, and no vacancy was created in order to accelerate cluster formation and avoid recombination. The simulations were carried out using the LAMMPS code at 300 K for 1 ns [24]. The details of the procedure can be found elsewhere [25]. The Dislocation Extraction Algorithm (DXA) implemented in the OVITO software package, was used for dislocation analysis [26]."

Before the strain calculation, thermal noise was removed by minimizing the potential energy of the system using the conjugate gradient method. The elastic lattice deformation was determined by comparing the atomic positions of irradiated system with a pristine reference configuration based on the ideal crystal structure. The strain tensor was calculated for atoms that have been identified as crystalline atoms through common neighbor analysis [27]. The elastic strain calculation modifier implemented in OVITO was used for the strain calculation. For every central atom in an elastically deformed FCC lattice, OVITO calculates the 12 vectors from the center atom to its 12 nearest neighbors. The program then maps each of these neighbor vectors to a corresponding ideal FCC reference lattice. The details of the method and the implementation of the algorithm can be found elsewhere [23,28].

Table 1
The configurations of the simulated interstitial clusters. The first column gives the cluster size in number of interstitials, the second column provides the number of clusters of each size and the third column shows total number of interstitials in the cell.

Cluster size	Number of clusters	Total number of interstitials
5	6	30
10	3	30
15	2	30
30	1	30

Experimentally, high-quality NiFe single crystals were grown in an optical floating zone furnace [29]. The NiFe samples, cut into 1 mm thick disks perpendicular to the ⟨100⟩ crystallographic direction, were electrochemically polished in order to remove the damage introduced by the machine cutting process. The single crystals of the binary equiatomic alloys were irradiated using the tandem accelerator at the University of Tennessee [30]. The samples, tilted 7° off the surface normal, were irradiated at room temperature with 1.5 MeV Ni ions at fluences ranging from 1×10^{13} to 1×10^{14} cm^{-2}. The depth profiles for vacancy production and implanted ions for the Ni ion irradiations were simulated using the Stopping and Range of Ions in Matter (SRIM-2013) [16]. The "Kinchin-Pease" mode was used, assuming 40 eV as the threshold displacement energy for Ni and Fe, and 8.232 g cm^{-3} as the density of the NiFe alloy [31–34]. The depth profile of the local damage dose (displacements per atom or dpa) was determined from the SRIM-predicted vacancy production profile, atomic density of the target material and the ion fluence. The XRD analysis was performed with an X'Pert Pro MRD PANalytical diffractometer in the Bragg reflection geometry using a Cu Kα anticathode at the Center for Nanophase Materials Science (CNMS) in Oak Ridge National Laboratory. For strain measurements, Symmetric θ-2θ scans were recorded in the vicinity of the (200) reflection using a (220) Ge monochromator and a 0.03 mm primary slit, which provided a monochromatic incident X-Ray beam, as well as a 0.03 mm detector slit that provided 2θ resolution of 0.01°.

MD simulations are performed to understand point defect accumulation in NiFe alloy. The damage accumulation behavior in the fcc NiFe alloy is shown in Fig. 1(a) by the increase in number of interstitials as a function of overlapping recoil cascades. The number of interstitials increases almost linearly up to about 50 recoils, which may indicate non-overlapping of the recoil events. Defect accumulation reaches saturation at around 250 recoils, although there is still a slight increase of defects at 300 recoils. Similar behavior has been reported recently for damage accumulation in other alloys [20]. The effect of irradiation damage on the volumetric strain is illustrated in the Fig. 1(b), where a rapid increase of the volumetric strain is followed by a gradual decrease. There is a clear relation between defect production and overall strain induced in the system. The strain is highest at a dose corresponding to about 80 overlapping recoils, and there is a significant decrease in defect accumulation rate at about the same dose. From closer inspection of the two sets of data, one can see that at almost every instance of a sudden increase in defect numbers, there is a corresponding peak in the strain curve.

To understand the relationship between strain and defects, the size distribution of defect clusters is analyzed at different stages of the simulation. As expected, the number of interstitials in large clusters increases with increasing number of recoils (Fig. 2). Fig. 2a shows that, at lower numbers of recoils, small defect clusters (2–4 interstitials) are dominant. Although the total number of isolated interstitials increases (Fig. 2a) with increasing number of recoil events, their fraction decreases compared to the overall size distribution (Fig. 2a–inset). Only a few medium and large sized defect clusters are created for less than 80 recoil events. The cluster size distributions at higher numbers of recoils are shown in Fig. 2b. The number of defects present in isolated and small clusters remains roughly constant as shown in Fig. 2b, but their fraction decreases slightly (Fig. 2b-inset). In contrast, the fraction of interstitials in large clusters increases, and clusters containing 11–30 interstitials are the dominant size distribution.