Point defect evolution in Ni, NiFe and NiCr alloys from atomistic simulations and irradiation experiments

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Abstract

Using molecular dynamics simulations, we elucidate irradiation-induced point defect evolution in fcc pure Ni, Ni_{0.5}Fe_{0.5}, and Ni_{0.8}Cr_{0.2} solid solution alloys. We find that irradiation-induced interstitials form dislocation loops that are of 1/3 $\langle 111 \rangle \{111\}$ -type, consistent with our experimental results. While the loops are formed in all the three materials, the kinetics of formation is considerably slower in NiFe and NiCr than in pure Ni, indicating that defect migration barriers and extended defect formation energies could be higher in the alloys than pure Ni. As a result, while larger size clusters are formed in pure Ni, smaller and more clusters are observed in the alloys. Vacancy diffusion occurs at relatively higher temperatures than interstitials, and their clustering leads to the formation of stacking fault tetrahedra, consistent with our experiments. The results also show that the surviving Frenkel pairs are composition dependent and are largely Ni dominated.

Keywords

Ion irradiation, single-phase concentrated solid-solution alloys, molecular dynamics simulations, dislocation loop, face-centered cubic crystals

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1. Introduction

In contrast to conventional alloys that contain one principal element with minor alloying elements, single-phase concentrated solid-solution alloys (SP-CSAs), including high entropy alloys (HEAs), contain multiple principal elements present in almost equal proportions. Thermodynamically such compositions could be readily rendered uninteresting due to intuitive phase separation; however, their high mixing entropies facilitate formation of random solid solutions with rather simple crystal structures. Interestingly, these alloys also possess exceptional mechanical properties such as high strength-weight ratio, wear resistance, high-temperature strength and structural stability, fracture resistance, etc. that are significantly improved over conventional alloys.[1-5] In the addition, these alloys have attracted interest in physical properties such as electrical, magnetic and thermal, thus opening a new research field in metallic materials.[6]

These alloys could be exciting new candidate materials for nuclear power applications, particularly if the enhanced mechanical properties could be coupled with high radiation tolerance for their use as structural materials in nuclear reactors. The inherent disorder (or random arrangement of different elements) could actually help in mitigating damage by annihilation of Frenkel pairs at very early stages of cascade events. With this proposition in view, Ni-based fcc SP-CSAs are the key alloys of interest where understanding radiation response of different compositions in order to design inherently radiation tolerant materials is currently the main focus. [7, 8]

These SP-CSAs are however new, and even the most fundamental radiation damage studies, such as point-defect evolution processes are lacking. Therefore, given the alloy complexity and the lack of literature, here we focus on simpler, binary NiFe and NiCr random alloys. In this work, using molecular dynamics (MD) simulations, we elucidate clustering mechanisms and kinetics of point defects in NiFe and NiCr, and compare them to that in pure Ni. We show that radiation induced point defects lead to formation of interstitial dislocation loops and stacking fault tetrahedra (SFT) in both pure Ni and the two alloys in good agreement with our experimental observations. We find that point defect diffusion is significantly slower in the alloys than in pure Ni. We also show that the sizes of defect clusters are significantly different between pure Ni and the alloys.

2. Methodology

The interaction of electrons, ions and neutrons with materials results in radiation damage primarily due to the displacement of atoms by elastic collisions, which can result in widely separated singular displacement events (e.g., electrons, protons, slow neutrons) and highly localized collision cascades (e.g., heavy ions and fast neutrons). Both processes result in the accumulation, diffusion and interaction of radiation-induced defects. These atomic level radiation damage production processes are conventionally modeled by giving a primary knock-on atom (PKA) kinetic energy that is dissipated in single or multiple elastic collision events, depending on energy, with higher PKA energies leading to a cascade of elastic scattering collisions. The evolution of such radiation-induced defects is the result of the accumulation and diffusion of the defects over time. This process can be broken down primarily into two stages, i.e., ballistic (e.g., collision) stage and kinetic (e.g., relaxation) stage. During the ballistic stage, a large number of atoms can be displaced in collision cascades, as shown by the peak in Figure 1

by a heavy ion, or isolated Frenkel pairs are created in the case of light particles (e.g., electrons or protons). Overtime, many of these radiation-induced defects, whether produced in isolation or in cascades, recombine and annihilate during the kinetic stage leaving only a few surviving defects behind.

Ideally both stages can be computationally captured via MD simulations, however, to accurately capture atomic forces during the ballistic stage when the atoms come very close to each other, the iterative time step needs to be decreased significantly. As a result, the ballistic stage alone is computationally expensive, and most of the simulations cannot reach the longer time associated with defect diffusion and the kinetic processes that lead to addition defect clustering and evolution. This expense is exceedingly noticeable while modeling multi-component systems. Hence, traditionally MD simulations have largely remained limited to the ballistic stage, and the clustering and diffusion events occurring from surviving isolated defects or small clusters over longer time scales have commonly been captured using additional methods such as kinetic Monte Carlo (KMC) or temperature accelerated dynamics (TAD).[10, 11] Although these methods can model up to experimental time scales, they remain fundamentally limited by the diffusion events that are defined by input parameters, thus making these methods highly probabilistic in nature.

Recently, another approach, a defect-driven method, has been tested that bypasses the ballistic stage, and focuses only on the kinetic stage.[12-14] Under this method, the focus is largely on capturing the evolution of the single point defects that are created by low-energy ballistic events (e.g., electrons and protons) or those that survive single or multiple cascade events. In this approach, instead of creating Frenkel pairs via time-consuming ballistic recoil events, they are randomly distributed at the start of the simulation. The disadvantage is that the processes inherent to more energetic ballistic events, such as the effects of shock waves, high displacement densities, and thermal spike on defect production, are not captured. Also not captured are the dependences of phase transformations, such as amorphization in ordered intermetallic compounds[15] on Frenkel pair concentrations or dose. However, such conventional cascade approaches that adding Frenkel pairs with more PKA events are often limited to smaller simulation cell sizes and are unable to capture the slow evolution of microstructure when Frenkel pairs are added over long simulation time. In the current approach, microstructure evolution is accelerated or driven by the larger Frenkel pair concentration, and the results from this approach have been fruitful in reproducing experimentally observed clusters and in revealing the underlying clustering mechanisms.[16] Similarly, radiation-induced grain growth has been captured in CeO_2 while elucidating the fast kinetics of grain growth observed experimentally.[17, 18] Such interstitial clustering and irradiation induced grain growth had not been captured previously from the conventional cascade methods. This method has also captured defect clusters in other ceramic oxides, such as MgO , UO_2 and ZrO_2 , and has replicated defect evolution observed from the conventional approach, thus validating the idea to bypass the ballistic stage for defect-driven processes.[12, 13, 19] Additionally, this approach is also devoid of the interatomic potential artifacts that may originate from the by Ziegler, Biersack, and Littmark (ZBL) scheme used to model forces of atoms that may come very close to each other during the ballistic stage.[20] It should be noted that this approach is not a surrogate to the traditional energetic cascade approach; it models the interaction and evolution of surviving defects from collision

cascades, as well as the isolated defects that accumulate under irradiation with electrons and protons.

In this work, we apply this approach to metallic materials, and show that the nature of defect clusters reminiscent of fcc metals can be also be captured via this approach. We mainly model pure Ni, $\text{Ni}_{0.5}\text{Fe}_{0.5}$ and $\text{Ni}_{0.80}\text{Cr}_{0.20}$ materials using a $20 \times 20 \times 20$ fcc unit cell system consisting of 32,000 atoms. In alloys, the atoms are randomly placed to replicate the random nature of SP-CSAs. In most of the simulations, 1 at.% Frenkel pairs (i.e., 320 interstitials and vacancies) are randomly created, and the simulations are run for 5 ns at 300 K, unless mentioned otherwise. This concentration of defects is only slightly lower (factor of four) than that produced in MD simulations by the overlapping of 5 keV cascades in fcc $\text{Ni}_{0.5}\text{Fe}_{0.5}$.^[21] In this work, the interstitials are created by placing lattice atoms at octahedral site leaving behind vacant lattice sites. Thus, equal number of interstitials and vacancies are always created. We use the embedded atom method (EAM) based Bonny 2013 interatomic potential.^[22] This potential is a modified version of the Bonny 2011 potential,^[23] and predicts defect properties such as migration and binding energies in very good agreement with *ab initio* calculations. The details of the potentials can be found elsewhere.^[22] The simulations are carried out using the LAMMPS code.^[24] Periodic boundary conditions are applied in all three directions, and a time step of 2 fs ensures good energy conservation.

Ion-radiation experiments were carried out at room temperature in pure Ni and NiFe samples irradiated using 3 MeV Au to a fluence of $2 \times 10^{13} \text{ cm}^{-2}$. High-resolution scanning transmission electron microscopy (STEM) images were taken at the damage peak with the foil oriented in [011] direction. Double Cs-Corrected STEM (JEOL 3100R05) was employed for STEM imaging with an inner angle of 59 mrad and camera length of 15 cm. The image pixels and exposure time/pixel for imaging in the experiment was 1024×1024 and 30 μs . The STEM samples were prepared by focused ion beam (FIB) by using FEI Helios Nanolab Dualbeam workstation. A flash polishing technique was also adopted to remove FIB-induced damage.

3. Results

3.1 Frenkel pair evolution in pure Ni

We start with Frenkel pair evolution in pure Ni. Figure 2a shows a snapshot of the simulation box containing randomly distributed interstitials (in green) and vacancies (in orange). The time evolution snapshots of the system at $t = 1 \text{ ns}$ and $t = 5 \text{ ns}$ are shown in Figure 2b and 2c, respectively. We find that, at this temperature of 300 K, vacancies remain immobile during the simulation run. This is due to high vacancy migration energy of $\sim 1.09 \text{ eV}$.^[22] In contrast, interstitials diffuse – some of the interstitials annihilate by recombination with vacancies, whereas the surviving ones form interstitial clusters. Figures 2b and 2c show formation of interstitial clusters. Characterization of the clusters reveals that they are interstitial dislocation loops formed on $\{111\}$ planes.

A snapshot of the system revealing the $\{111\}$ planar nature of three dislocation loops is shown in Figure 3a. Figure 3b shows the Ni atoms forming the characteristic ...ABCABC... type fcc stacking of planes in the $\langle 111 \rangle$ direction. The dislocation loop formation introduces an extra 'B' plane breaking the ...ABCABC... pattern, thus creating a stacking fault. The character of the dislocation loops is schematically shown in Figure 3c. We find that the loop has a $1/3\langle 111 \rangle$ Burgers vector, and hence the loop is of

$1/3\langle 111 \rangle \{111\}$ type. The $\{111\}$ planar loop is a characteristic nature of fcc materials; their formation has been widely observed experimentally.

It is important to mention here that such $\{111\}$ loops have been previously captured from MD simulation in fcc Cu using the conventional PKA approach.[25, 26] Here, the observation of loops captured by circumventing the ballistic stage validates that the new approach, requiring much lower computation time, could be used in metallic materials to understand point defect evolution processes.

Interstitial dislocation loops of the same character, and of about 1-8 nm diameter have also been observed under TEM in our ion-radiation experiments. Figure 4 is an inversed fast Fourier transform of a high resolution STEM image showing one interstitial loop. The loops lie on (111) planes thus showing a very good agreement with our MD simulations.

3.2 Vacancy diffusion in pure Ni

Now we focus on vacancy diffusion to understand at what temperatures do they start to diffuse in this interatomic potential, and to elucidate their clustering processes. Figure 5a shows a snapshot of the system containing 1 at.% vacancies created by randomly removing atoms from the system. A vacancy-rich region is possible in reality, as the existence of the vacancy-rich and interstitial-rich regions before and after the damage peak is intrinsic from ion implantation or ion irradiation. We perform mean square displacement (MSD) calculations to understand vacancy diffusivity as a function of temperature. MSD is related to diffusivity (D) via the relationship, $MSD = 6Dt$, where t is time. MSD plots for three temperatures at 700 K, 1000 K and 1200 K are shown in Figure 5b. The plots show that vacancies are completely immobile (on these MD timescales) until 700 K, but start to diffuse at 1000 K, and are fully diffusing at 1200 K. Therefore, we use 1200 K as the simulation temperature to capture vacancy evolution.

Using the same system of 1 at.% vacancies, we perform simulation for a prolonged time of 40 ns. Figure 6a and 6b show the system snapshots at $t = 1$ ns and $t = 40$ ns, respectively. Since there are no interstitials present for the vacancies to annihilate, we find that the vacancies diffuse to form vacancy clusters. At $t = 1$ ns, some of the vacancies associate to form clusters, and some are still present individually. However, by 40 ns, all vacancies have aggregated into clusters. Characterization of these clusters reveals that they are SFT commonly observed in irradiated fcc metals. Similar SFT are observed in our ion-radiation experiments. SFT between 2 – 5 nm consisting of $\{111\}$ planes are highlighted with circles, as shown in Figure 6c, in very good agreement with our MD simulations.

A key point emerges here; these simulations confirm that SFT can form even by mere aggregation of vacancies. Over the years, many different mechanisms have been put forward on the formation of SFT under plastic deformation, melt-quench and irradiation conditions.[27, 28] In relation to irradiation processes, three main mechanisms are generally applicable. The first one is by Silcox and Hirsch,[29] and the explanation is based on dissociation of a vacancy-type Frank dislocation loop. This mechanism was later supported by MD simulation in fcc Cu, and the details of the mechanism can be found elsewhere.[30] The second mechanism is based on void collapse, i.e., SFT form by direct collapse of voids. This mechanism was illustrated using TAD-MD simulations by Uberuaga et al.[31] The third mechanism is by mere aggregation of single vacancies.[27,

32-34] Both experiments and MD simulations have supported the first two mechanisms, whereas the dynamical occurrence of the third mechanism has never been captured from MD simulations. It is quite likely that the methodology chosen to carry out MD simulations has allowed operation of only the first two simulations (see Refs[30, 31]); whereas the kinetic evolution of free vacancies required to trigger the third mechanism has remained illusive. Our simulation thus supports the third mechanism and the experimental observation of SFT formation from electron irradiation [35]. In addition, this mechanism could also be responsible for the experimentally observed growth of SFT, and their formation far away from the cascade regions.[36] The atomistic details of SFT formation mechanism will be discussed separately in future work.

3.3 Frenkel pair evolution in NiFe alloy

Now we turn our attention on $\text{Ni}_{0.5}\text{Fe}_{0.5}$ alloy. Figure 7a shows a snapshot of the random alloy containing 0.5 at.% Frenkel pairs each of Ni and Fe at $t = 0$ ns amounting to a total Frenkel pair concentration of 1 at.%. Similar to pure Ni, the vacancies remain immobile at 300 K, and some of the diffusing interstitials annihilate by recombination with vacancies. However, there is a difference in the evolution of surviving interstitials between the alloy and pure Ni.

In contrast to almost all the interstitials that have aggregated to form clusters in pure Ni, there are significant number that are individually present by the same simulation time of 5 ns in NiFe alloy. In addition, while fewer and larger-sized clusters can be seen in pure Ni (Fig. 2c), smaller-sized and higher numbers of clusters are found in the alloy (Fig. 7b). This quantization of interstitials, and their comparison is shown in Figure 8a. For example, there are 12 single interstitials, 6 clusters of di-interstitials, etc in NiFe. In contrast, there are only 2 clusters of di-interstitials, and the rest of the clusters contain at least 6 interstitials in pure Ni. The interstitial kinetics towards cluster formation appears to be slower in NiFe alloy than in pure Ni. Thus, we find that there is a different dynamics of defect evolution between the two materials, and the interstitial kinetics is slower in the alloy than in pure Ni.

While the kinetics are different, we find that the total number of surviving defects do not differ significantly. This comparison is shown in Figure 8b where the percentage of surviving Frenkel pairs is plotted against the percentage of initially created Frenkel pairs before the start of the simulation. In both cases, we find that there are only slightly lower numbers of surviving Frenkel pairs in NiFe than in pure Ni. Thus, it appears that the addition of Fe to Ni has a larger effect on the cluster sizes due to significant modification of migration energies and extended defect formation energies, but not on the total number of surviving defects illustrating smaller influence on recombination energies during the kinetic stage. It is important to mention here that the defect formation and recombination during the ballistic stage could still be significantly different between the alloy and pure Ni. Recent MD simulation by Beland et al [9] showed that, for the same PKA energy cascade, more Ni Frenkel pairs are created than in NiFe alloy, consequently leading to larger number of surviving Frenkel pairs in pure Ni. Thus, this key result inherent only to PKA methodology is not captured in our simulations. However, they found smaller clusters sizes in the alloy than in pure Ni, consistent with our simulations.

An important feature of the defect-driven method followed here to create Frenkel pairs is that one could create Frenkel pairs of different kinds, i.e., Frenkel pairs of either

only Ni or only Fe or both can be created. This preferential defect creation is not possible via the conventional cascade simulation method. We find that this feature allows better understanding of separate effects on the underlying defect evolution mechanisms. For example, using this feature in CeO_2 , by creating only oxygen defects, it was found that the system heals completely leaving no surviving defects. In contrast, when Ce defects were created, they led to formation of interstitial dislocation loops.[16, 37] In addition, Ce defects created new oxygen defects that were not originally present at the start of the simulation. Thus, it was concluded that the presence of Ce defects leads to radiation damage in the material, whereas presence of only oxygen defects does not.

We use this feature here to further understand radiation damage in NiFe. We perform three simulations, differentiated by the type of Frenkel pairs. Thus, 1 at.% Frenkel pairs are created either of Ni, or Fe or both. Figure 9a shows the percentage of surviving Frenkel pairs of Ni and Fe in the three simulations. In the first simulation, where defects of both Ni and Fe are simultaneously created, we find that there are more (~65%) Ni surviving Frenkel pairs than Fe. More interestingly are the other two simulations where only one type of Frenkel pairs are initially created. We find that even when Fe Frenkel pairs are initially absent in the Ni-only simulation, the system creates new Fe Frenkel pairs. Similarly, new Ni Frenkel pairs are created in the initial Fe-only system. Furthermore, there percentage of surviving Ni and Fe Frenkel pairs is almost same irrespective of the initial defect kind. Thus, the system reacts to alloy chemistry, and is driven to an equilibrium concentration of defects that relate to the principal elements and their concentration in the alloy. The formation of new defects is evident in interstitial dislocation loops. A snapshot of one dislocation loop formed in Fe-only Frenkel pair system is shown in Figure 8b where we find that both Ni (green) and Fe (black) interstitials are simultaneously present.

Similar phenomenon is observed in $\text{Ni}_{0.8}\text{Fe}_{0.2}$ alloy, i.e., new defects are created even if they are not initially present at the start of the simulation (Figure 9c). By comparing Figure 9a and 9c, we also observe that the surviving defect percentage of Ni and Fe is composition dependent, i.e., there are more surviving Ni Frenkel pairs in higher Ni composition $\text{Ni}_{0.8}\text{Fe}_{0.2}$ alloy than there are in lower concentration $\text{Ni}_{0.5}\text{Fe}_{0.5}$ alloy.

3.4 Frenkel pair evolution in NiCr alloy

We model the NiCr alloy for $\text{Ni}_{0.8}\text{Cr}_{0.2}$ composition, which forms a stable fcc solid solution. Similar to NiFe, we create Frenkel pairs of both Ni and Cr and run the simulation for 5 ns. A final snapshot of system is shown in Figure 10a. Similar defect features are observed in NiCr, i.e., vacancies remain immobile at 300 K, and interstitials diffuse to either annihilate with vacancies or form interstitial dislocation loops on {111} planes. The defect kinetics is slower in NiCr than Ni, as also observed above for the NiFe alloy. Figure 10a also shows that there are larger numbers of single interstitials and smaller-sized clusters compared to that in pure Ni in Figure 2c, which is another common feature with the NiFe alloy. The defect quantization is shown in Figure 10b, where we find that smaller-sized and higher numbers of clusters are found in NiCr compared to pure Ni. We also find that new Frenkel pairs are created when not originally present as shown by the percentage of surviving Frenkel pairs in Figure 10c. In addition, the surviving defect percentage is also composition dependent. We model a hypothetical $\text{Ni}_{0.5}\text{Cr}_{0.5}$ system similar to that in NiFe knowing such composition doesn't form stable

fcc phase; the defect quantization is shown in Figure 10d. We again find that defect concentration is dominated by Ni in both $\text{Ni}_{0.8}\text{Cr}_{0.2}$ and $\text{Ni}_{0.5}\text{Cr}_{0.5}$, and there are more Ni defects in the alloy that has higher Ni composition.

4. Discussion

The simulations reveal that point defect diffusion followed by clustering kinetics is different between the alloys (NiFe and NiCr) and pure Ni. The results presented here indicate that diffusion is slower in alloys leading to slower cluster formation. This is supported by the work of Tsai and Yeh [2], who experimentally showed that the addition of other elements (such as Co, Cr, Fe and Mn) in pure Ni to form HEAs increases migration barriers, thus decreasing overall diffusivity. For example, they showed that Ni migration barrier increased from 2.95 eV in pure Ni to 3.28 eV in NiCoCrFeMn thus decreasing the overall kinetics. This effect is largely attributed to different local atomic environments, i.e., different chemical and elastic effects, even enhancing the possibility of atomic ‘binding’ at certain sites. In the diffusion couple experiments, Tsai and Yeh found that the mean potential energy difference between lattice sites for Ni atoms increased by 60.3 meV from pure Ni to NiCoCrFeMn alloy leading to longer occupation time at low-energy sites, thus contributing to slower diffusion. Similar kinetics effects have also been observed in steels. For example, both experimental and computational modeling illustrated that addition of Cr to Fe (in a Fe-15Cr alloy) reduces dislocation loop formation attributed to suppression of interstitial mobility by Cr atoms.[38, 39] The slower kinetics is also reminiscent in cluster sizes observed in our simulations where clusters of smaller sizes are formed in alloys than in pure Ni.

The methodology to replicate irradiation-induced point defects is applied to elucidate underlying point-defect evolution mechanisms, and captures the experimentally observed cluster types. A key insight that new point defects can be formed during the kinetic stage such that an overall chemical equilibrium of defects is eventually attained irrespective of the initial defect concentration is noteworthy. Unraveling this mechanism becomes largely possible as this method provides a *controlling knob* in preferentially creating point defects.

In conclusion, MD simulations show that interstitial dislocation loop of $1/3\langle 111 \rangle\{111\}$ type are formed in pure Ni and in NiFe and NiCr alloys in agreement with our experimental observations. Vacancy diffusion can lead to the formation of SFT. Out of the three mechanisms presented in literature and discussed above, these simulations show that stacking fault tetrahedron formation can occur by vacancy aggregation mechanism. Finally, we find that the key difference between the alloys and pure Ni is the kinetics of point defect evolution, i.e., point defects diffuse more slowly eventually leading to smaller cluster sizes in the alloys compared to pure Ni.

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Point defect evolution in FCC Ni, NiFe and NiCr alloys from atomistic simulations and irradiation experiments

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Figures

Figure 1. Schematic showing generation of point defects forming a peak during the ballistic phase followed by vacancy-interstitial recombination during the kinetic phase leaving behind few surviving defects.

Figure 2. Frenkel pair evolution in pure Ni. Snapshots at (a) $t = 0$ ns, (b) $t = 1$ ns, and (c) $t = 5$ ns. Randomly distributed interstitials in (a) aggregate to form clusters in (b) and (c). Vacancies remain immobile throughout the simulation. Color scheme: vacancies in orange and interstitials in green.

Figure 3. (a) Three interstitial dislocation loops highlighted in $\{111\}$ planes. (b) A stacking fault created by a dislocation loop breaking the ...ABCABC... stacking sequence in fcc. (c) Crystallographic schematic of the dislocation loop.

Figure 4. An inversed fast fourier transform of a high resolution STEM image showing an irradiation induced interstitial dislocation loop in pure Ni. The loop is about 3 nm in size.

Figure 5. Vacancy diffusion in pure Ni. (a) 1 at.% randomly distributed at $t = 0$ ns. (b) Mean square displacement of vacancies at 700 K, 1000 K and 1200 K showing the vacancies start to diffuse at 1000 K, and are mobile at 1200 K.

Figure 6. Formation of SFTs in MD simulation using 1 at. % vacancies as the initial structure as shown in Figure 5a. (a) system at $t = 1$ ns, (b) $t = 40$ ns. SFTs have nucleated in (a) by vacancy aggregation, and have fully formed by 40 ns in (b). (c) TEM observation of SFTs as open triangles consisting of $\{111\}$ planes, marked in the white circles in an irradiated sample.

Figure 7. Point defect evolution in $\text{Ni}_{0.5}\text{Fe}_{0.5}$ alloy. (a) Randomly distributed 0.5 at.% Frenkel pairs each of Ni and Fe at (a) $t = 0$ ns and (b) $t = 5$ ns.

Figure 8. (a) Cluster size: number of clusters containing different number of atoms. $\text{Ni}_{0.5}\text{Fe}_{0.5}$ alloy has large number of small clusters compared to pure Ni. (b) Comparison between percentage of surviving Frenkel pairs as a function of initial Frenkel pair concentration in Ni and $\text{Ni}_{0.5}\text{Fe}_{0.5}$ in 5 different systems. Surviving Frenkel pairs are almost similar in the two materials.

Figure 9. Percentage of surviving Frenkel pairs after 5 ns in three different systems initially containing Ni & Fe, Ni-only and Fe-only defects in (a) $\text{Ni}_{0.5}\text{Fe}_{0.5}$ alloys, and (c) $\text{Ni}_{0.8}\text{Fe}_{0.2}$ alloy. (b) Dislocation loops containing both Ni and Fe interstitials even though system initially contained Fe-only defects. Color scheme: Ni interstitials in green and Fe interstitials in black.

Figure 10. (a) Snapshot of $\text{Ni}_{0.8}\text{Cr}_{0.2}$ system at $t = 5$ ns. (b) Cluster size: number of clusters containing different number of atoms. $\text{Ni}_{0.8}\text{Cr}_{0.2}$ alloy has large number of small clusters compared to pure Ni (c) Percentage of surviving Frenkel pairs after 5 ns in three different systems initially containing Ni & Fe, Ni-only and Fe-only defects in (a) $\text{Ni}_{0.8}\text{Cr}_{0.2}$ alloys, and (d) hypothetical $\text{Ni}_{0.5}\text{Cr}_{0.5}$ alloy.

Graphical abstract

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