Damage accumulation in ion-irradiated Ni-based concentrated solid-solution alloys

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Abstract

Irradiation-induced damage accumulation in $\text{Ni}_{0.8}\text{Fe}_{0.2}$ and $\text{Ni}_{0.8}\text{Cr}_{0.2}$ alloys are investigated using molecular dynamics (MD) simulations to assess possible enhanced radiation-resistance in these face-centered cubic (fcc), single-phase, concentrated solid-solution alloys, as compared with pure fcc Ni. The $\text{Ni}_{0.8}\text{Cr}_{0.2}$ and $\text{Ni}_{0.8}\text{Fe}_{0.2}$ alloys demonstrate higher radiation resistance compared to Ni. The total number of point defects produced in $\text{Ni}_{0.8}\text{Cr}_{0.2}$ and $\text{Ni}_{0.8}\text{Fe}_{0.2}$ is approximately 2.5 and 1.4 times lower than in Ni, respectively, due to efficient defect recombination in the chemically disordered alloys. Both interstitial and vacancy clusters are formed in all three materials. In Ni, large interstitial clusters are produced; whereas in $\text{Ni}_{0.8}\text{Cr}_{0.2}$, smaller interstitial clusters are produced but with a higher number. This indicates a higher mobility of interstitials in Ni compared to $\text{Ni}_{0.8}\text{Cr}_{0.2}$. Moreover, $\text{Ni}_{0.8}\text{Cr}_{0.2}$ shows better radiation resistance than $\text{Ni}_{0.8}\text{Fe}_{0.2}$. Larger interstitial clusters and 1.7 times higher numbers of accumulated point defects are observed in $\text{Ni}_{0.8}\text{Fe}_{0.2}$, in comparison with $\text{Ni}_{0.8}\text{Cr}_{0.2}$. Due to the low mobility of vacancies on the MD time scales, they are found primarily as single point defects and small clusters in all materials. While performance improvement is observed in the alloys, the difference in irradiation response between $\text{Ni}_{0.8}\text{Cr}_{0.2}$ and $\text{Ni}_{0.8}\text{Fe}_{0.2}$ indicates the importance of element choice to achieve the desired property.

Keywords: Molecular dynamics simulations, Ion irradiation, Concentrated solid-solution alloys, Ni-based alloys, Defect cluster, Frenkel pair

1. Introduction

Structural materials play an important role in safe, sustainable and economical operation of nuclear power systems. The core of a nuclear reactor experiences extreme environments of high temperature, high stress, chemical reactivity and intense radiation flux. In particular, the structural materials for Generation IV concept fission reactors and tokamak-like fusion power plants will be subjected to unprecedented fluxes of high-energy neutrons and extreme operating temperature [1–4]. Besides nuclear application, materials with high radiation resistance are also needed for high-energy accelerators, such as the next generation high-power rare isotope beam facilities [5]. Highly-focused, high-energy ion pulses create high energy deposition densities in target materials and other accelerator components, leading to changes in structure, thermo-mechanical properties and reduced life-times [6,7]. The development of new high-performance

materials that can withstand such hostile conditions is, therefore, critical for advanced fission and fusion reactor systems, as well as for high-energy physics.

In the search for new materials, a new class of single-phase, concentrated solid-solution alloys (SP-CSAs), which includes high entropy alloys (HEAs), show remarkable mechanical, chemical and magnetic properties, including high yield strength (CoCrCuFeNiTi_x and AlCoCrFeNiTi_x systems), fracture toughness (CrMnFeCoNi alloy), wear resistance (Co_{1.5}CrFeNi_{1.5}Ti and Al_{0.2}Co_{1.5}CrFeNi_{1.5}Ti systems), corrosion resistance (Al_{0.5}CoCrCuFeNi alloy) compared to conventional alloys [8–14]. The main difference between traditional solid-solutions and the SP-CSAs is the existence of multiple principle elements instead of one principle element.

The SP-CSAs may be candidates as structural material for nuclear applications where high radiation tolerance is a primary concern [15]. The random nature of the elements in SP-CSAs, without solvent and solute elements, might facilitate the recovery of radiation damage by efficient dynamic annealing at very early stages of the energy deposition [16]. Understanding the complex electronic correlations and non-equilibrium atomic interactions is a grand challenge [17]. Recent work has shown that chemical disorder in SP-CSAs can lead to reduction in electron mean free path and both electrical and thermal conductivities, which can significantly impact energy dissipation and, consequentially, defect evolution during ion irradiation [16]. While improved understanding of the radiation response in chemically disordered concentrated alloys is highly desirable, very few experimental and simulation studies have been performed on such alloys [18–21]. The life-time of the thermal phase of a collision cascade can be tuned by the choice of elements in a multicomponent alloy. Caro *et al.* have studied the thermal conductivity of equiatomic binary and quaternary alloys by varying mass, atomic size and cohesive energy, and they speculated that the radiation resistance of HEAs can be improved by tailoring alloy complexity to lower the thermal conductivity [18]. Recent studies have showed that the CoCrCuFeNi nano-crystalline HEA exhibit high phase stability under 2 MeV electron irradiation over a wide temperature range from 298 to 773 K [19]. Aidhy *et al.* have studied the slow evolution of Frenkel pairs (FPs) in equiatomic NiFe and NiCr alloys, and they observed the formation of dislocation loops and stacking fault tetrahedral [20]. In spite of these efforts, the radiation response of SP-CSAs, particularly the dependence on the non-equiatomic concentration and elemental composition, remains vastly unexplored.

In the current work, molecular dynamics (MD) simulations are applied to compare the irradiation-induced defect production between elemental face-centered cubic (fcc) Ni and the two binary alloys, Ni_{0.8}Fe_{0.2} and Ni_{0.8}Cr_{0.2}, both of which are single-phase, concentrated solid-solutions with the fcc structure. While the fcc Ni_{0.5}Fe_{0.5} is stable, fcc Ni_{0.5}Cr_{0.5} is not a stable solid solution. The reason for choosing the composition of 80% versus 20% is due to the limitation of Cr solubility, since above 22% the fcc structure is not stable. The focus is to study the effects of chemical disorder, in alloys with the same composition, on the accumulation and evolution of point defects due to overlapping cascades produced by ion irradiation. We focus on these random binary alloys due to the lack of suitable interatomic potentials for other more complex multicomponent systems. We validate the stability of the potentials employed in a system far from equilibrium by comparing our results with previous simulations and experiments. Understanding the effects of chemical disorder on defect evolution in these simple binary alloys reveals the impact of solid-solution alloying on defect dynamics, which may provide a pathway to prevent material degradation in extreme radiation environments by controlling alloy complexity.

2. Methodology

2.1. Simulation

We used the embedded atom method (EAM) based, the Bonny potential to model pure Ni, Ni_{0.8}Fe_{0.2} and Ni_{0.8}Cr_{0.2} fcc SP-CSAs [22]. This potential was developed to study the production and evolution of radiation defects, particularly, point defects. Since it is not possible to capture long-term effects of radiation on reactor structural materials by investigating single cascades, we simulate the effect of prolonged radiation damage by cumulative irradiation, i.e. overlapping of single cascades. The MD simulation code LAMMPS was used to create the random mixture of elements to mimic the SP-CSAs fabricated for experimental studies [23]. An adaptive time step MD code PARCAS was used for the cascade simulations [24–26]. The simulation cell size was 115×115×115 Å³ containing 132,000 atoms. The cell was relaxed at 300 K. Periodic boundary conditions were applied to all directions to replicate an infinitely large bulk system. The Berendsen temperature control was applied to the periodic boundaries to remove the excess heat produced by the cascades [27]. In PARCAS, the electronic stopping is modeled as a friction force for atoms with kinetic energies higher than 1 eV and calculated using the SRIM code version 2013 [26,28,29].

In recent experimental irradiation studies of Ni and similar Ni alloys [Ref. 16], 1.5 MeV Ni ions and 3 MeV Au ions were used; we have calculated the recoil spectra for these ions in NiFe using SRIM and found that 88.5% of the recoils are less than 5 keV. Thus, the simulations in this study are based on the overlap of 5 keV cascades. At the beginning of the simulation, a recoil energy of 5 keV was given to a central atom in a random direction. The simulation was run at 300K for 30 ps. The simulation time was chosen so that the system cooled down to 300K, and there were no energetic interactions remaining in the system. After each cascade, the damaged simulation cell was shifted by a random displacement vector between zero and the cell size. Then a second recoil was initiated from the center of the cell and so on. This allowed a uniform distribution of damage and avoided cascades interacting with the cell borders. The details of the simulation procedure can be found elsewhere [30]. It is known that the dose rate in displacements per atom per second (dpa/s) in the MD simulations is orders of magnitude higher than in a reactor environment. While the limited simulation time between overlapping cascades is insufficient to allow significant migration and recombination, which may overestimate the actual damage accumulation rate, the relative difference in defect production, cluster formation and damage accumulation behavior attributed to the chemical effects (20% Ni, 20% Fe, or 20% Cr in Ni) should be valid using this accelerated MD approach. A total of 400 recoil simulations were performed to achieve a damage dose equivalent to 0.133 dpa (displacements per atom), which yielded good statistics for the final damage state.

2.2. Defect Analysis

The Voronoi cell method was used to identify vacancies and interstitials. In this method, Voronoi polyhedra were centered on each atom position in the ideal fcc crystal and compared with atoms in the defective crystal. Polyhedra with no atoms were labeled as vacancies and polyhedra with 2 or more atoms were labeled as interstitials [24].

In addition, we also analyzed the formation of clusters and the cluster size distribution for all investigated cases. Interstitial and vacancy clusters were identified separately. Cluster analysis was done by calculating the distance between each defect and all other defects. All defects that were within a fixed cut-off radius from each other were interpreted to be a part of the same defect

cluster. The cut-off radius was set as the second-nearest-neighbor distance (3.65 Å), which is the general cut-off distance used in several previous studies [30,31]. Although the choice of cluster size limit is arbitrary, clusters were divided into three main size categories, (1) small clusters consisting 2-10 point defects, (2) medium clusters consisting 11-50 point defects, and (3) large clusters consisting more than 50 point defects. Defects were visualized with the program OVITO [32].

3. Results

3.1. Accumulation of point defects

In Fig. 1, the accumulation of point defects with increasing number of recoils in pure Ni, $\text{Ni}_{0.8}\text{Fe}_{0.2}$ and $\text{Ni}_{0.8}\text{Cr}_{0.2}$ alloys is presented. It shows that the smallest numbers of point defects are produced in $\text{Ni}_{0.8}\text{Cr}_{0.2}$, followed by $\text{Ni}_{0.8}\text{Fe}_{0.2}$; whereas the highest defect numbers are produced in pure Ni. The overlapping of defect production curves at low dose (less than 20 recoils) is nearly linear, which may indicate non-overlapping recoil events in the simulation cell. For the simulations run at 300K, both interstitials and interstitial clusters are mobile. The observed reduction of defect numbers in the binaries compared to Ni could be due to either higher defect annealing during the displacement cascades or to changes in defect mobility. In addition, we find that in the case of $\text{Ni}_{0.8}\text{Cr}_{0.2}$, defect accumulation exhibits saturation at around 100 recoils, whereas no saturation level is observed for pure Ni and $\text{Ni}_{0.8}\text{Fe}_{0.2}$, even at 400 recoils.

The simulation results clearly show that irradiation-induced damage accumulation is more efficiently suppressed in $\text{Ni}_{0.8}\text{Cr}_{0.2}$ than either $\text{Ni}_{0.8}\text{Fe}_{0.2}$ or pure Ni for the current recoil energy. Furthermore, $\text{Ni}_{0.8}\text{Fe}_{0.2}$ shows much better resistance to irradiation than pure Ni. Similar results have been observed experimentally by Zhang and coworkers in comparing Ni and equiatomic NiCo and NiFe alloys irradiated with either Au or Ni ions [16]. Their work showed that the accumulated damage level in NiCo is about half that in Ni while the damage accumulation level in NiFe is even lower than that in NiCo. On a related note, several works have been done on the radiation response of body centered cubic (bcc) Fe-Cr solid solution alloys containing 5-15% Cr. It was reported that there is no significant effect of Cr on final defect population compared to pure Fe in both single and overlapping cascades up to 50 keV recoil energy [30,33–35]. To elucidate possible chemical effects on defect production and damage accumulation resulting from Fe and Cr, the present work focuses on the two binaries of $\text{Ni}_{0.8}\text{Fe}_{0.2}$ and $\text{Ni}_{0.8}\text{Cr}_{0.2}$ with the same crystalline structure and the same composition.

3.2. Interstitial diffusion in pure Ni

Fig. 2 provides a visual demonstration of vacancy and interstitial clusters formation and their distribution in pure Ni after 400 recoils. The initial system before any cascade damage is a perfect structure containing no defects. The interstitials are shown in blue and the vacancies in green. The first observation is that a large number of vacancies are individually present and randomly distributed in the system; a few of the vacancies have formed small vacancy clusters. In contrast, there are practically no individual interstitials present. In addition, there are only a few small interstitial clusters, and most of the interstitials have formed a single large cluster. Upon crystallographic analysis, we find that the large interstitial cluster is a dislocation loop lying on a $\{111\}$ plane.

Similar $\{111\}$ planar interstitial loops have also been observed in previous MD simulations of ion irradiated fcc Cu and α -Fe [36,37]. Very recently, Aidhy *et al.* have also reported similar dislocation loops in pure Ni [20]. In these previous studies, small dislocation loops containing only a few interstitial atoms were observed, in contrast to the very large dislocation loop observed here. This difference is due to the large number of recoils in the present study, which leads to progressive clustering of interstitials.

The average cluster size distributions in pure Ni for different numbers of recoil events is shown in Fig. 3. Two different behaviors for the interstitials can be observed in these distributions. First, after 100 recoils, the number of single interstitials is very low and has already saturated. Second, the number of defects in intermediate size clusters (i.e., between 2 and 50) decreases with increasing number recoils; whereas the number of interstitials in large clusters (> 50) increases rapidly with increasing number of recoil events. This quantitative analysis also supports the observations from the cluster snapshot in Fig. 2. This observation can be explained based on recombination and diffusion of point defects. *In this simulation of overlapping cumulative recoil events, two diffusion processes are happening. One is from cascade heating during each cascade event on short time scales (30 ps). The other process occurs on longer time scales; for example after 200 cumulative recoils, the simulation time has reached 6 ns and after 400 recoils the total simulation time is 12 ns.* Due to high diffusivity and the inherent propensity to form clusters, there are very few isolated interstitials at any recoil stage. Most of the interstitials form smaller and medium sized clusters (for cluster sizes 2-10 and 11-30) at an early stage of recoil accumulation (i.e., by 100 recoils, see Fig. 3). As the system is further damaged by the continued overlapping of recoil events, these clusters aggregate to form larger clusters. This process is consistent with the decrease in the numbers of smaller and medium clusters, as well as the simultaneous increase in the number of larger clusters (i.e., 51 and above). In addition, the rate at which the number of defects in the larger clusters increases is much higher than the decreasing rate of intermediate size clusters. This indicates that the newly created point defects contribute directly to the growth of large clusters, instead of forming small clusters. Thus, the large dislocation loop observed in Fig. 2 grows due to the production and diffusion of newly form point defects, as well as at the expense of aggregation of smaller and medium sized clusters (Fig. 3).

3.3. Interstitial diffusion in $\text{Ni}_{0.8}\text{Cr}_{0.2}$

We now turn our attention towards $\text{Ni}_{0.8}\text{Cr}_{0.2}$, which was damaged and analyzed in the same manner as Ni above. Here, we find that point defect diffusion is significantly different from that for pure Ni in Fig. 2. In Fig. 4, we show that vacancies and interstitials mostly remain as single point defects. There are also some small vacancy and interstitial clusters. However, despite 400 recoils, formation of large dislocation loops is not observed. The small dislocation loops observed in Fig. 4, however, maintain their crystallographic character, and they form on $\{111\}$ crystallographic planes, as observed in the pure Ni case above.

The cluster size distribution for $\text{Ni}_{0.8}\text{Cr}_{0.2}$ is quite different than for pure Ni. Interstitials mostly remain as single point defects or form small clusters, as shown in Fig. 5a; the results show no significant variation in the number of interstitials at each size interval, which indicates that the number of interstitials has nearly saturated at 100 recoils for all size intervals. To obtain a better understanding of the saturation level, the size distributions at lower numbers of recoil events

(from 10 to 50) were also analyzed. Fig. 5b shows that in the case of single interstitials, the saturation level is achieved at 20 recoil events. This indicates strong annealing dynamics in $\text{Ni}_{0.8}\text{Cr}_{0.2}$. Also, alloying reduces the mobility of point defects and defect clusters, which in turn inhibits the formation of large dislocation loops as observed in pure Ni.

3.4. Comparison between alloys and pure Ni on defect accumulation

In this section, we compare the accumulation of point defects (vacancies and interstitials) and their evolution in pure Ni, $\text{Ni}_{0.8}\text{Fe}_{0.2}$ and $\text{Ni}_{0.8}\text{Cr}_{0.2}$. The results in Fig. 6 reveal that elemental Ni produces the largest interstitial clusters compared to the binary alloys. There are no large defect clusters in $\text{Ni}_{0.8}\text{Cr}_{0.2}$; instead the fraction of interstitials is comparable between all size intervals. The total number of point defects is much higher (≈ 2.5 times) in pure Ni (532 ± 37) than in $\text{Ni}_{0.8}\text{Cr}_{0.2}$ (230 ± 16), where both Ni and $\text{Ni}_{0.8}\text{Cr}_{0.2}$ are subjected to the same number of recoils and cascade energy (Fig. 1). Surprisingly, the number of single point defects (7 ± 0.3) in Ni is negligible compared to $\text{Ni}_{0.8}\text{Cr}_{0.2}$ (48 ± 1.5). This suggests very high mobility of interstitials in Ni compared to $\text{Ni}_{0.8}\text{Cr}_{0.2}$ that results in high diffusion rates and clustering of point defects, which in turn leaves few isolated interstitials in Ni. In contrast, smaller size and higher numbers of interstitial clusters are produced in $\text{Ni}_{0.8}\text{Cr}_{0.2}$, whereas the number of clusters is lower in pure Ni (Fig. 4 and 2). Aidhy *et al.* also observed a similar relation between size and numbers of clusters for Ni and $\text{Ni}_{0.8}\text{Cr}_{0.2}$ using a different simulation approach [20]. In the case of $\text{Ni}_{0.8}\text{Fe}_{0.2}$, we observe a higher damage level (FPs, 393 ± 29) and larger interstitial cluster formation compared to $\text{Ni}_{0.8}\text{Cr}_{0.2}$. This might be due to less efficient defect recombination and slower interstitial mobility in $\text{Ni}_{0.8}\text{Fe}_{0.2}$. The result suggests that the choice of alloying element is critical for desirable radiation resistance in the SP-CSAs.

The number of vacancies in different size distributions is shown in Fig. 7. Vacancies behave quite differently from interstitials. Although the vacancy yields are higher in Ni compared to the binary alloys, similar to the case for interstitials, the size distributions are very different. Vacancies mostly remain as single point defects and small clusters. There are no large vacancy clusters in any of the materials. The snapshots in Figs. 2 and 4 also supported this quantitative analysis. It has been reported that vacancies are completely immobile until 700 K and start to diffuse around 1000 K in pure Ni on MD timescales [20]. In our simulations, the temperature reaches around 900 K in the cascade core, which might facilitate the formation of a few small vacancy clusters. Due to the low mobility, single vacancies and small clusters do not diffuse to form large dislocation loops at the temperature and recoil energy of the current study.

4. Discussion

The suppression of defect production and radiation resistance by alloying has been studied extensively in steel and conventional alloys [38–40]. It has been previously reported that 80 keV Ni^+ ion irradiation of NiCr alloys, containing 8% and 17% of Cr, produces fewer defects than pure Ni [41], and these authors suggested that the reduction is due to the low probability of dislocation loop nucleation in the cascade core, although the average number of FPs created by each cascade might be comparable for all materials due to very similar masses. Our simulations support this speculation, as the average number of FPs from each cascade are 5 ± 1 , 7 ± 1 and 8 ± 2 for Ni, $\text{Ni}_{0.8}\text{Fe}_{0.2}$ and $\text{Ni}_{0.8}\text{Cr}_{0.2}$, respectively. This indicates that alloying does not have a

significant effect on point defect production in this energy range, when independent cascades are taken into account. So, the main difference is due to cascade overlap.

There are three overlapping stages in the irradiation-induced defect evolution process [42,43]. In the collision stage (ballistic phase within ~ 1 ps [20]), FPs form and reach a maximum concentration. In the annihilation or relaxation phase, defects recombine to their equilibrium configurations and in-cascade clusters nucleate. Finally, in the cascade-cooling phase, a diffusion phase (kinetic phase, a few ps after the ballistic phase [20]) occurs, where thermally activated defects can migrate to form clusters (such as, dislocation loops) or annihilate by recombination. The third process might play a major role in the reduction of defect yield in $\text{Ni}_{0.8}\text{Cr}_{0.2}$, and the formation of the large interstitial cluster in pure Ni. Thermally activated diffusion can be indirectly affected by transport properties, such as the electron mean free path or electrical thermal conductivity [16]. Zhang *et al.* has reported that $\text{Ni}_{0.5}\text{Fe}_{0.5}$ showed higher defect reduction than pure Ni, which they associated with the 4 to 5 times higher residual electrical resistivity of $\text{Ni}_{0.5}\text{Fe}_{0.5}$ compared to pure Ni [16]. In our simulations, $\text{Ni}_{0.8}\text{Cr}_{0.2}$ exhibits the lowest defect yield compared to $\text{Ni}_{0.8}\text{Fe}_{0.2}$ and Ni. This is consistent with the explanation of Zhang *et al.* as the electrical resistivity of the $\text{Ni}_{0.8}\text{Cr}_{0.2}$ alloy is much higher than $\text{Ni}_{0.8}\text{Fe}_{0.2}$ and pure Ni [44,45]. Recent studies have reported that the disordered electronic system in these alloys can significantly reduce the local heat conduction that might play an important role in defect reduction [16, 46]. Jin *et al.* has also shown that the type of element can have a large influence on the disorder of electronic system. In particular, alloys with Cr content showed the highest electrical resistivity and lowest electronic thermal conductivity [46].

5. Conclusion

Atomistic simulations are utilized to study the accumulation of cascade damage in Ni-based SP-CSAs. The damage level saturates after about 100 recoil events for $\text{Ni}_{0.8}\text{Cr}_{0.2}$; whereas no saturation level is achieved for elemental Ni and $\text{Ni}_{0.8}\text{Fe}_{0.2}$. We have observed the formation of a large interstitial cluster in elemental Ni, which is attributed to the high mobility of Ni interstitials. Larger interstitial clusters are formed in $\text{Ni}_{0.8}\text{Fe}_{0.2}$ compared to $\text{Ni}_{0.8}\text{Cr}_{0.2}$, but smaller than elemental Ni. Vacancies remain immobile at the irradiation temperature and recoil energy for all materials; as a result, large vacancy clusters do not form. We show that the difference in defect production between the solid-solution alloys and pure Ni in the current study is governed by the diffusion of point defects during overlapping cascades. Our simulation results are in agreement with some previous simulation results and experimental findings, which provide some validation of the potentials used to describe these alloys. Finally, this study indicates that the $\text{Ni}_{0.8}\text{Cr}_{0.2}$ alloy possesses the best radiation resistance among the Ni-based fcc binary SP-CSAs studied so far.

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Figure 1

Fig. 1. Accumulation of point defects in pure Ni, Ni_{0.8}Fe_{0.2} and Ni_{0.8}Cr_{0.2} alloys with increasing numbers of cumulative recoils and the corresponding dose in displacements per atom (dpa).

Figure 2

Fig. 2. Snapshot of defect cluster formation in pure Ni after 400 cumulative recoils. Green color shows the vacancies and blue color shows the interstitials.

Figure 3

Fig. 3. Numbers of interstitials in different cluster size distributions after 100 (blue), 200 (red), 300 (green) and 400 (black) cumulative recoils in pure Ni. Distribution is calculated from the average of three sets of recoil simulations.

Figure 4

Fig. 4. Snapshot of point defects in $\text{Ni}_{0.8}\text{Cr}_{0.2}$ alloy after 400 cumulative recoils. Green color shows the vacancies and blue color shows the interstitials. Small interstitial loops are formed unlike a large one in Fig. 2.

Figure 5

Fig. 5. (a) Number of interstitials in different size distributions for $\text{Ni}_{0.8}\text{Cr}_{0.2}$. (b) Similar analysis of the size distribution as in (a) but at lower recoil events. Distribution is calculated from the average of three sets of recoil simulations. Numbers of recoils are indicated in the legend.

Figure 6

Fig. 6. Comparison of interstitial cluster size distribution between pure Ni, Ni_{0.8}Fe_{0.2} and Ni_{0.8}Cr_{0.2} alloys after 400 cumulative recoils. Distribution is calculated from the average of three sets of recoil simulations.

Figure 7

Fig. 7. Comparison of vacancy cluster size distribution between pure Ni, Ni_{0.8}Fe_{0.2} and Ni_{0.8}Cr_{0.2} after 400 cumulative recoils. Distribution is calculated from the average of three sets of recoil simulations.