Differences in the accumulation of ion-beam damage in Ni and NiFe explained by atomistic simulations

Laurent Karim Béland*, German D. Samolyuk*, Roger E. Stoller*

Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6138, USA

Abstract

Following low-dose irradiation with a 3 MeV beam of Au ions, i.e. less than one displacement per atom, a lower number of defects were experimentally observed in NiFe than in pure Ni. At higher doses, more damage is observed in NiFe than in pure Ni. Also, at these high doses, defect structures are observed deep in the material, far from the region where ions are implanted, more so in Ni than in NiFe. In this study, these experimental results are explained using atomistic modeling. Sequences of overlapping displacement cascades with intervening defect aging are simulated. Evidence is provided that nanosecond aging at 900K can be used as a surrogate for long-time, room-temperature aging. Then, using this procedure, it is shown that the low defect diffusivity of NiFe leads to less aggregation and recombination events between each displacement cascade in a given volume than in Ni. Variations in the local defect chemistry in NiFe produces a broad spectrum of defect formation energy, leading to the trapping of defects at energetically favorable sites: this explains the low defect diffusivity. Also, this low diffusivity explains why, at high dose, defects in NiFe do not propagate as deeply in the material than in pure Ni.

Keywords: Atomistic modelling, Radiation damage, Concentrated alloy, Nickel, Iron

---

Copyright notice: This manuscript has been authored by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725 with the U.S. Department of Energy. The United States Government retains and the publisher, by accepting the article for publication, acknowledges that the United States Government retains a non-exclusive, paid-up, irrevocable, world-wide license to publish or reproduce the published form of this manuscript, or allow others to do so, for United States Government purposes. The Department of Energy will provide public access to these results of federally sponsored research in accordance with the DOE Public Access Plan (<http://energy.gov/downloads/doe-public-access-plan>).

1. Introduction

Molecular dynamics is routinely used to model primary-damage production in metals and alloys under ion and neutron irradiation [1]. It provides powerful insights into the basic microstructural changes induced by such high-energy irradiation. However, obtaining atomistic information about the kinetic evolution of these defects and their subsequent accumulation as the material undergoes continuous irradiation is still a challenge.

In this study, the behavior of Ni and NiFe is showcased. Ni 50 at.% is a face-centered cubic (fcc) concentrated solid solution. Both elements are crucial subcomponents of many so-called fcc high-entropy alloys, which have recently been proposed and explored as candidate structural materials for nuclear power generation [2]. A

better understanding of the mechanisms by which alloying Ni with Fe modifies the kinetic properties of defects is an important step in that development.

In low-dose ion-beam experiments, with ion energies of a few MeV, NiFe was shown to generate fewer microstructural defects than pure Ni, as measured by Rutherford backscattering (RBS) and TEM [3]. This is in agreement with MD simulations, that predict substantial (of the order of 50 %) reduction of Frenkel Pair yield of displacement cascades in NiFe, relative to Ni [3, 4]. These experiments generated roughly 0.01 displacements per atom (dpa).

As ion fluence and dose is increased, one observes two main trends. First, defect clusters appear deeper and deeper into the sample, well below the expected range predicted by SRIM simulations [5]. Indeed, while SRIM accurately predicts the damage range at low dose, post-cascade defect diffusivity seems to play an important role at higher doses. This effect is much more pronounced in Ni than in NiFe. Second, the integrated defect yield in Ni grows more slowly than in NiFe [5, 6]. In other words, while NiFe seems more radiation-tolerant than Ni at low ion-dose, it accumulates damage at a faster rate than Ni. At 1 dpa, similar integrated damage levels are observed in Ni and NiFe. The RBS measurements concord with recent diffuse X-ray scattering in NiCo irradiated at 1 dpa [7]. At higher doses, RBS suggests that the integrated damage level continues to steadily grow in NiFe, while it saturates and even declines in Ni [6].

This evidence suggests that inter-cascade behavior in

---

*Corresponding author

Email address: belandlk@ornl.gov (Laurent Karim Béland)

NiFe is different than that of Ni. This article presents the results of a computationally-driven investigation of this behavior. The timescales involved are a challenge. Indeed, considering that typical ion-beam experiments generate 0.001 dpa s^{-1} and that, at a level of 0.01 dpa , all atoms in a given volume were involved in an event, inter-cascade annealing takes place over 10 seconds or so. This is clearly out of the reach of traditional MD, which is typically limited to a few nanoseconds.

In principle, on-the-fly kinetic Monte Carlo (kMC) can reach the desired timescales. This method was used to model post-cascade annealing in semi-conductors [8, 9] and metals [10, 11]. It was also shown to be able to capture complex defect reactions in Fe-10%Cr [12]. However, even at this concentration, ripples in the potential energy landscape, caused by the overlap of several pair-interactions, push methods based on following the lowest-curvature and the residence-time algorithm to their limit (c.f. Ref. [13] for more details). The annealing of cascade debris in more concentrated alloys, which possess an even rougher potential energy landscape if modeled using the embedded-atom method, is still out of reach of on-the-fly kMC.

The experiments at hand were performed at room temperature. A common way to proceed is to use short-time, high-temperature MD as a surrogate for long-time, room-temperature simulations. While this approach might be appropriate in many circumstances, its validity is rarely, if ever, tested. In this article, such an approach is validated for Ni cascade debris by comparing it to on-the-fly kMC, and then extended to NiFe in order to shed light on the kinetic processes at hand.

On-the-fly kMC were performed using the kinetic Activation Relaxation Technique (k-ART)[14, 15, 16]. This algorithm combines ART saddle searches [17, 18, 19], the residence-time algorithm [20], graph analysis [21] and the basin auto-constructing mean-rate method [22, 15] to simulate the time-evolution of systems in a fully atomistic way, handling all elastic interactions. In this particular implementation, the active volume concept [23, 24] was added to handle system sizes of 256000 atoms.

2. Assessing the validity of high-temperature MD aging

Our methodology to introduce damage to the system and age it is illustrated in Fig. 1. Initially, individual 10 keV collision cascades were generated using MD in four separate perfect 256000 atoms Ni crystals, using the LAMMPS package [25] with the Bonny 2013 potential [26], at 300K. The MD simulation lasted about 25 ps. These four systems were then used as inputs for k-ART and aged at 300K either until the simulations reached 10 seconds or until the systems became trapped in super-basins too large for k-ART to handle [15, 13]. These four aged and defect-containing systems were reused for subsequent 10 keV MD cascades. The process was repeated either until 4 successful cascades per sample were simulated or if k-ART failed

Figure 1: (a) Simplified schematics of the procedure to simulate and age metals used in this study. (b) The damage remaining after annealing twelve cascade-damaged systems, generated by 4 independent runs following the scheme in (a). 300K k-ART ranging from 3 microseconds to 18 seconds are compared to 500 ps, 900K MD runs. The abscissa and ordinate are equal at the black straight line.

to age the system for at least a few microseconds. Each k-ART aging takes one to three weeks of wall-time, using 12 cpu-cores. In total, we have aged 12 initial configurations with k-ART. We then reused these 12 initial configurations and aged them 500 ps at 900K in MD. A process requiring a waiting time of 0.01 s at 300K, assuming a constant 10 THz attempt frequency and harmonic transition state theory (i.e. a 0.7eV potential energy barrier), should take roughly 500 ps at 900K. By comparing the defects after aging using either k-ART or MD, the validity of the high-temperature MD approach can be assessed.

This assessment is illustrated in Figure 1(b). We see a very clear correlation between the result of the MD and k-ART. Also, on average, both methods yielded an 80 % defect survival rate.

Supplementary runs were performed on one of these initial configurations, for further investigation. Three conditions were simulated: (1) long 300K k-ART simulations, (2) 500ps, 900K k-ART simulations, and (3) 500 ps, 900K MD simulations. Three kART runs were performed at each temperature, as well as six MD runs. See supplementary material at [URL will be inserted by Elsevier] for movies of typical runs[27]. All three methods led to statistically insignificant differences in average survival rates and their standard deviation. Visual inspection also confirms that the stability of defect clusters was consistent within the two approaches.

The results largely indicate that high-temperature MD is an appropriate surrogate for long-time, room temperatures k-ART runs in this case. However, there are two important discrepancies. First, while the diffusion of single interstitials, vacancy clusters and interstitial clusters was well separated in three phases in the 300K simulations, all three processes take place simultaneously in the 900K simulations. Second, in the 900K MD, interstitial cluster diffusivity, relative to vacancy cluster diffusivity, is faster than in the k-ART simulations at 300K and 900K. This suggests that vibrational entropic contributions are significant at 900K. Nonetheless, while these discrepancies indi-

Figure 2: (a) The average number of Frenkel pairs (FP) observed after a sequence of room-temperature cascades and high-temperature aging, in Ni and NiFe. The number of FP calculated by linearly adding the average number of FP generated by 10 keV cascades is given by the dashed lines. (b) The average number of additional Frenkel pairs (FP) produced by displacement cascades. This is the difference between the number of FP observed at the beginning and the end of each cascade, which are separated by 30 ps.

cate one should be careful about drawing detailed conclusions from the 900K MD and generalizing them to room-temperature phenomena, our assessment suggests that it is a valid tool to estimate long-time aging in this particular context.

3. Damage accumulation in NiFe

The high-temperature surrogate method validated in Sec. 2 was used in the scheme illustrated in Fig. 1, with 10 keV cascades. A total of 8 cycles were run in Ni and NiFe. We tried two annealing times at 900K: 0.5 ns and 1.5 ns; in both cases, similar migration barriers are probed, but the longer waiting time allows each defect to execute 3 times more jumps, which is a way to control for kinetic limitations. Results were averaged over 8 runs with different random seeds for each case. See supplemental material at [URL will be inserted by Elsevier] for a movie of a typical simulation [27].

The defect yield in each case is plotted in Fig. 2(a). After each cascade, the number of Frenkel Pairs steadily increases in all systems. If annealing is performed for 1.5 ns, defects accumulate at a slower rate in pure Ni, compared to the simulations where it is annealed for 0.5 ns

Figure 3: (a) The mean square displacement of a single interstitial in Ni and NiFe, computed from MD simulations. The Ni simulation and three NiFe simulations, at 800, 850 and 900 K use the Bonny 2013 potential, while one simulation at 800 K uses the Bonny 2009 potential. (b) A histogram of the formation energy of a single [100] dumbbell interstitial in NiFe.

between cascades. The defect yield in NiFe is independent of the annealing time. After 3 cascades, a similar number of defects is observed in Ni (1.5 ns annealing) and NiFe. In all cases, defects accumulate more slowly than linearly extrapolating the average number of defects produced by single 10 keV cascades; this effect is more pronounced in Ni than in NiFe.

The number of additional defects generated by collision cascades in the pre-damaged sample is plotted in Fig. 2(b). There is a downward trend in damage production as a function of dose. There is no significant difference between simulations were 0.5 ns and 1.5 ns aging were performed. The trend is similar for Ni and NiFe, although cascades in NiFe produce less defects than those in Ni. Preexisting defects seem to limit the ability of cascades to produce primary damage.

Alloying Ni with Fe initially reduces defect production, compared to the pure Ni case. However, the alloy's ability to anneal damage between cascades is limited. Increasing the annealing time from 0.5 ns or 1.5 ns does not lead to more recombination of defects in the alloy, while it significantly increased recombination in pure Ni. This indicates that defect diffusion is more sluggish in NiFe than Ni, inhibiting inter-cascade recombination. This is in good agreement with experiments, where damage accumulates more rapidly in NiFe than in Ni as dose increases.

4. Explaining low defect diffusivity in NiFe

In the previous section, it was shown that kinetic limitations to defect diffusion explain why NiFe accumulates damage more rapidly than Ni under ion-irradiation. What explains this low diffusivity?

To answer this question, simulations of the diffusion of single interstitials in NiFe were performed, using both MD and k-ART. In Fig. 3(b), the mean square displacement (MSD) of the interstitial dumbbell is plotted, based on MD runs at 800, 850 and 900 K, using the Bonny (2013) potential. An 800K run using an alternative NiFe potential [28] was also performed, to ensure that the sluggish

diffusion in NiFe is not an artifact of the 2013 Bonny potential. We observe plateaus in the MSD, indicating the dumbbell is trapped. The k-ART simulations also indicate the the dumbbell becomes trapped after a few jumps, with escape barriers of 0.7 to 1.0 eV. In pure Ni, the migration barrier is on the order of 0.15 eV. The effect of alloying on interstitial diffusion is very strong.

How is the interstitial trapped? The answer lies in the broad distribution of interstitial formation energies, which depend on the exact chemistry of the local environment of each site. This distribution is illustrated in Fig. 3(c), a histogram of the formation energy of 100 randomly chosen sites in an NiFe solid solution, after a conjugate-gradient minimization of the structure. The formation energy of the interstitial varies by nearly 2 eV, depending on which site is chosen. Ni-Ni, Ni-Fe and Fe-Fe dumbbell interstitials all exhibit similar breadth in formation energy, of the order of 1.5 eV (not shown). Ni-Ni and Ni-Fe are more energetically favorable, on average, than Fe-Fe interstitials, by a margin of 0.5 eV.

Thus, the slow diffusion of interstitials in NiFe can be understood by the broadness of this distribution. The interstitials will migrate until they find energetically favorable sites, where they will be trapped if they are not connected to other sites with comparable energies. This explains why our NiFe samples are able to anneal out 20 % of the cascade-induced defects in the first 500 ps of high-temperature aging, the same proportion as in pure Ni, but are unable to anneal out more damage when submitted to 1500 ps aging. In contrast, pure Ni can anneal out an extra 10 % of the cascade-induced defects in this additional nanosecond of aging.

One should note that the alloying effect on vacancy diffusivity is much less pronounced. This can be explained by the much narrower distribution of vacancy formation energies, which ranges from 1.2 to 2.15 eV. Also, single vacancies have a large migration barrier in pure Ni (1.2 eV). Therefore, decreasing their diffusivity has much less importance than decreasing the diffusivity of interstitials.

5. Defect clusters

5.1. Interstitial clusters

The cluster distribution of interstitials is plotted in Fig. 4 (a). There are many more interstitials in large clusters in Ni than in NiFe. There are many more single interstitials and clusters of size lesser than 4 in NiFe, compared to Ni. We also see that, in pure Ni, longer waiting times reduce the number of defects in large part by annihilating point defects and tri-interstitial clusters. The annihilation of large clusters plays a smaller role.

Details about the distribution of large interstitial clusters in the final state of the simulations are given in Table 1. There are many more interstitial clusters in Ni than in NiFe. Also, the clusters in Ni are larger than the clusters in NiFe. Finally, the choice of intercascade aging time

Figure 4: The number of (a) interstitials and (b) vacancies contained in clusters of a given size at the end of the 8 cascade-and-aging cycles. The results are aggregated over all 8 simulations for each composition and aging time.

did not have a noticeable effect on these distributions, although there is one less large cluster in the 1.5 ns aged Ni than in the 0.5 ns aged Ni.

The average interstitial cluster size as a function of dose is plotted in Fig. 5 (a). Ni interstitial clusters are larger than NiFe interstitial clusters. Aging time had no systematic effect on the average interstitial cluster size. There is a slight upward trend in the average cluster size as a function of dose for Ni; the effect is ambiguous in NiFe.

The proportion of interstitial defects in clusters as a function of dose is plotted in Fig. 5(c). Ni interstitial are more likely to be found in clusters than NiFe interstitial defects. Aging for 1.5 ns rather than 0.5 ns increases the proportion of interstitials found in clusters. There is an upward trend in this proportion both in Ni and NiFe.

The presence of larger interstitial clusters in Ni than in NiFe is in general agreement with TEM observations [5].

5.2. Vacancy clusters

The cluster distribution of vacancies is plotted in Fig. 4(b). The distribution is similar in Ni and in NiFe, although there are more single vacancies in pure Ni than in NiFe and that there are more large vacancy clusters in Ni, using 500 ps aging, compared to NiFe. We also see that, in pure Ni, longer waiting times reduce the number of defects contained in large vacancy clusters.

Details about the distribution of large vacancy clusters in the final state of the simulations are given in Table 1.

Table 1: All large clusters ($N \geq 10$) observed at the end of the eight cascade-and-aging cycles. Each number represents a cluster of that size. For each composition and aging time, the results are aggregated from eight independent runs.

	Ni		NiFe	
	0.5 ns	1.5 ns	0.5 ns	1.5 ns
Large vacancy clusters	12,12,15,15,15,16,17,20,25	14,25,27,27	13,17,19,19,22,24	11,11,12,18,20,22
Large interstitial clusters	11,11,12,14,17,18,22,25,29	11,12,14,15,18,21,24,24	12	12

Figure 5: The average size of (a) interstitial and (b) vacancy clusters. Single interstitials are excluded from the average. The average proportion of (c) interstitial and (d) vacancy defects found in clusters.

This distribution is similar in Ni and NiFe. The choice of inter-cascade aging time had little effect in NiFe. In pure Ni, the longer aging time lead to larger and fewer vacancy clusters.

The average vacancy cluster size as a function of dose is plotted in Fig. 5(b). Ni vacancy clusters are about the same size as NiFe vacancy clusters. Aging time had no systematic effect on the average vacancy cluster size. There is a upward trend in the average cluster size as a function of dose for Ni and NiFe.

The proportion of vacancy defects in clusters as a function of dose is plotted in Fig. 5(d). Ni interstitial are just as likely to be found in clusters than NiFe interstitial defects. Aging for 1.5 ns rather than 0.5 ns increases the proportion of vacancies found in clusters in Ni in the three first overlapping cascades, but it has no significant effect at higher doses or in NiFe. For 0.5 ns aged Ni, 0.5 ns aged NiFe and 1.5 ns aged NiFe, the proportion initially increases with dose and then saturates.

Overall, the statistical sample of large vacancy clusters is too small to discern what effect alloying Ni to Fe has on their distribution. Further study is necessary to clarify this issue.

5.3. Diffusion of defects out of the cascade zone

In our k-ART and MD simulations, we applied periodic boundary conditions. A more realistic simulation would consider boundaries where defects are absorbed and created, since debris from other cells will eventually enter

Table 2: The defects clusters (including point defects) that reached the periodic boundary. The results of 8 runs for each set-up are aggregated. Each run contains 8 cascades. Each number, separated by a comma, represents a cluster (or point defect) that crossed the periodic boundary; its value is the cluster size (1 for point defects). The line number (the outermost left column) corresponds to the number of cascades that have been simulated in the system up to the moment the cluster or point defect first reached the periodic boundary. In the Ni system, some divacancies reached the boundary if 1.5 ns annealing was performed between cascades.

	Ni			NiFe	
	0.5 ns	1.5 ns		0.5 ns	1.5 ns
	Interstitials	Interstitials	Vacancies	Interstitials	Interstitials
1	1,1,1,1,1,2	1,1,1,1,1,1,1,1,2			1,1,1,1,1
2	1,1,1,2,4,12	1,1,1,2,2,3,10,16,18	2	1,1	1,1,1,1
3	1,2,2,2,4,11,15,16	1,1,1,1,2,2,3,8,11,23		1,1,1	1,1,1,2,3
4	1,3,5,11	1,1,1	2	1,1,1,1	1,1,1,2
5	2,3	1,2,3,5,11,12	2	1,1,1,1,1,1	1,1,1,2
6	3	3,5,7,12			1,2,2,3,3
7	3	1,1,2	2		1
8	2,4,4	2,2,8		1,1	1,2,4

the simulation box. While such a set-up is beyond of the scope of this article, it is interesting to track the number and the nature of defects that reached the simulation box boundary.

These results are summarized in Table 2. In all simulations, only single interstitials or interstitial clusters reached the boundary, except in the Ni system annealed for 1.5 ns between cascades, where a few divacancies escaped as well (k-ART indicates that the divacancy migration energy in pure Ni is 0.46 eV, compared to 1.10 eV for a single vacancy). This suggests that defect evolution takes place mostly by interstitial migration, although it seems small vacancy clusters also contribute to defect evolution in Ni. It also seems that large interstitial defects, while very mobile in Ni, are largely immobile in NiFe. Many more defects reached the boundary in Ni than in NiFe, no matter the duration of annealing. Also, defect clusters reaching the boundary were much larger in Ni than in NiFe. Longer annealing times lead to larger and more numerous defects reaching the periodic boundary.

These results are consistent with a larger diffusivity of defects in Ni than in NiFe. Aggregation and escape from the cascade regions are more important in Ni than in NiFe. Also, this is consistent with high-dose experiments, where damage is observed further beyond the implanted region in pure Ni than in NiFe [5, 6].

6. Further discussion

In the previous sections, our simulations were shown to qualitatively capture a number of experimental trends. Ni

exhibits more defects at low dose than NiFe, but the latter accumulates damage more rapidly. Interstitial clusters are larger in Ni than in NiFe. Defect clusters diffuse more deeply in Ni than in NiFe. Quantitatively, however, our simulations likely do no concord with the experiments.

Take, for instance, the dose-dependance of accumulated damage. As dose is increased, a similar number of defects in Ni and NiFe is observed after 3 cascades if a long (1500 ps) annealing time is chosen in our simulations. In the experiments, this crossover happens at 1 dpa. [6] It is difficult to precisely estimate the effective dose involved in a collision cascade. Nonetheless, it is likely that our simulations underestimate the dose required to reach the crossover, compared to the experiments, even though they qualitatively capture this crossover.

This discrepancy can be explained by many factors. First, our simulations only consider a sequence of 10 keV cascades. In the ion irradiations, a broad distribution with much higher energies is involved, which would probably considerably change the results. Second, waiting 1.5 ns at 900K is not a perfect surrogate to quantitatively capture the experimental inter-cascade aging conditions (although it seems to be adequate to give a qualitative assessment of the process). Third, as we mentioned in Sec. 5.3, applying periodic boundary conditions is not realistic. It might overestimate the recombination of fast glissile interstitial clusters with vacancy clusters, due to the re-entry of escaping clusters.

More generally, experimental measurements take place well after ion-implantation is performed; important defect dynamics takes place during this period. Also, ion-beam experiments involve vastly more cascades events than our MD modeling, and involve spacial fluctuations and gradients of energy deposition. Furthermore, our simulations generated a relatively limited number of extended defect structures, while experiments generate a very large number of them. Hence, a direct comparison of our simulations to these experiments is not possible.

One way to make better quantitative predictions would be to characterize the diffusivity of all defect clusters in Ni and its alloy, and the primary damage production of cascades in a pre-disordered medium, and include this information in mean-field rate theory [29], or object KMC [30] schemes. Also, the development of potentials tailor-made to study such diffusion would help. Replacing the high-temperature framework used in this study with another accelerated method, such as temperature-accelerated dynamics [31] or hyperdynamics [32], might also lead to more quantitatively accurate results. A grand canonical framework (absorbing and emitting boundary conditions) could also lead to improved accuracy.

7. Conclusion

In order to simulate inter-cascade annealing, short-time high-temperature MD was shown to lead to outcomes similar to those produced by long-time, room temperature

k-ART simulations. Thus, a comparison of damage accumulation in Ni and NiFe under ion-irradiation could be performed, taking inter-cascade annealing into account.

We found that interstitial diffusivity in NiFe is low, compared to pure Ni, because they can be trapped at energetically favorable sites, which in turn leads to decreased inter-cascade recombination of defects in the alloy. As a consequence, while fewer defects are present in the alloy than in Ni at low ion dose (i.e. the first few cascades), similar amounts of damage are present in NiFe and Ni at higher dose (i.e. after 4 successive cascades). This is in broad agreement with experimental evidence. Our results also suggest that, as a result of their different diffusivity, more defects escape the cascade region in Ni than in NiFe, which might explain why damage is observed in much deeper regions in Ni than in NiFe at high dose. Our simulations also indicate that larger interstitial clusters are found in Ni than in NiFe.

8. Acknowledgments

Research at the Oak Ridge National Laboratory sponsored by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, "Center for Energy Dissipation to Defect Evolution", an Energy Frontier Research Center. LKB acknowledges additional support from a fellowship awarded by the Fonds Québécois de recherche Nature et Technologies. We thank Alexandre Barachev, Ke Jin, and Raina Olsen for insightful discussions.

- [1] 1.11 - primary radiation damage formation, in: R. J. Konings (Ed.), *Comprehensive Nuclear Materials*, Elsevier, Oxford, 2012, pp. 293 – 332.
- [2] S. J. Zinkle, L. L. Snead, Designing radiation resistance in materials for fusion energy*, *Annual Review of Materials Research* 44 (2014) 241–267.
- [3] Y. Zhang, G. M. Stocks, K. Jin, C. Lu, H. Bei, B. C. Sales, L. Wang, L. K. Béland, R. E. Stoller, G. D. Samolyuk, M. Caro, A. Caro, W. J. Weber, Influence of energy dissipation on defect evolution in nickel and Ni-based fcc alloys, *Nature Communications* 6 (2015).
- [4] L. K. Béland, C. Lu, Y. N. Osetsky, G. D. Samolyuk, A. Caro, L. Wang, R. E. Stoller, Features of primary damage by high energy displacement cascades in concentrated Ni-based alloys, *Journal of Applied Physics* (2015) Submitted.
- [5] C. Lu, K. Jin, L. K. Béland, F. Zhang, T. Yang, Y. Zhang, H. Bei, R. E. Stoller, L. Wang, Direct observation on defect structure, range and evolution in ion irradiated single crystal Ni and Ni binary alloys, *Scientific Reports* (2015) Submitted.
- [6] K. Jin, H. Bei, Y. Zhang, Ion irradiation induced defect evolution in Ni and Ni-based fcc equiatomic binary alloys, *Journal of Nuclear Materials*.
- [7] R. J. Olsen, K. Jin, C. Lu, L. K. Béland, L. Wang, H. Bei, E. D. Specht, B. C. Larson, Investigation of defect clusters in ion-irradiated Ni and NiCo using diffuse x-ray scattering and electron microscopy, *Journal of Nuclear Materials* (2015) Submitted.
- [8] L. K. Béland, Y. Anahory, D. Smeets, M. Guihard, P. Brommer, J.-F. Joly, J.-C. Pothier, L. J. Lewis, N. Mousseau, F. Schietekatte, Replenish and relax: Explaining logarithmic annealing in ion-implanted c-si, *Physical review letters* 111 (10) (2013) 105502.

- [9] L. K. Béland, N. Mousseau, Long-time relaxation of ion-bombarded silicon studied with the kinetic activation-relaxation technique: Microscopic description of slow aging in a disordered system, *Physical Review B* 88 (21) (2013) 214201.
- [10] H. Xu, R. E. Stoller, Y. N. Osetsky, Cascade defect evolution processes: Comparison of atomistic methods, *Journal of Nuclear Materials* 443 (1) (2013) 66–70.
- [11] L. K. Béland, Y. N. Osetsky, R. E. Stoller, H. Xu, Slow relaxation of cascade-induced defects in Fe, *Physical Review B* 91 (5) (2015) 054108.
- [12] L. K. Béland, Y. N. Osetsky, R. E. Stoller, H. Xu, Interstitial loop transformations in FeCr, *Journal of Alloys and Compounds* 640 (2015) 219–225.
- [13] L. K. Béland, Y. N. Osetsky, R. E. Stoller, H. Xu, Kinetic activation-relaxation technique and self-evolving atomistic kinetic monte carlo: Comparison of on-the-fly kinetic monte carlo algorithms, *Computational Materials Science* 100 (2015) 124–134.
- [14] F. El-Mellouhi, N. Mousseau, L. J. Lewis, Kinetic activation-relaxation technique: An off-lattice self-learning kinetic monte carlo algorithm, *Physical Review B* 78 (15) (2008) 153202.
- [15] L. K. Béland, P. Brommer, F. El-Mellouhi, J.-F. Joly, N. Mousseau, Kinetic activation-relaxation technique, *Physical Review E* 84 (4) (2011) 046704.
- [16] N. Mousseau, L. K. Béland, P. Brommer, F. El-Mellouhi, J.-F. Joly, G. K. NTsouaglo, O. Restrepo, M. Trochet, Following atomistic kinetics on experimental timescales with the kinetic activation-relaxation technique, *Computational Materials Science* 100 (2015) 111–123.
- [17] N. Mousseau, G. Barkema, Traveling through potential energy landscapes of disordered materials: The activation-relaxation technique, *Physical Review E* 57 (2) (1998) 2419.
- [18] R. Malek, N. Mousseau, Dynamics of lennard-jones clusters: A characterization of the activation-relaxation technique, *Physical Review E* 62 (6) (2000) 7723.
- [19] N. Mousseau, L. K. Béland, P. Brommer, J.-F. Joly, F. El-Mellouhi, E. Machado-Charry, M.-C. Marinica, P. Pochet, The activation-relaxation technique: Art nouveau and kinetic art, *Journal of Atomic, Molecular, and Optical Physics* 2012.
- [20] A. B. Bortz, M. H. Kalos, J. L. Lebowitz, A new algorithm for monte carlo simulation of ising spin systems, *Journal of Computational Physics* 17 (1) (1975) 10–18.
- [21] B. D. McKay, Nauty user’s guide (version 2.4), Computer Science Dept., Australian National University (2007) 225–239.
- [22] B. Puchala, M. L. Falk, K. Garikipati, An energy basin finding algorithm for kinetic monte carlo acceleration, *The Journal of chemical physics* 132 (13) (2010) 134104.
- [23] H. Xu, Y. N. Osetsky, R. E. Stoller, Self-evolving atomistic kinetic monte carlo: fundamentals and applications, *Journal of Physics: Condensed Matter* 24 (37) (2012) 375402.
- [24] H. Xu, R. E. Stoller, L. K. Béland, Y. N. Osetsky, Self-evolving atomistic kinetic monte carlo simulations of defects in materials, *Computational Materials Science* 100 (2015) 135–143.
- [25] S. Plimpton, Fast parallel algorithms for short-range molecular dynamics, *Journal of computational physics* 117 (1) (1995) 1–19.
- [26] G. Bonny, N. Castin, D. Terentyev, Interatomic potential for studying ageing under irradiation in stainless steels: the FeNiCr model alloy, *Modelling and Simulation in Materials Science and Engineering* 21 (8) (2013) 085004.
- [27] See supplemental material at [URL will be inserted by Elsevier] for movies.
- [28] G. Bonny, R. Pasianot, L. Malerba, FeNi many-body potential for metallurgical applications, *Modelling and Simulation in Materials Science and Engineering* 17 (2) (2009) 025010.
- [29] S. I. Golubov, A. Barashev, R. E. Stoller, Radiation damage theory, Tech. rep., Oak Ridge National Laboratory (ORNL) (2012).
- [30] C. Domain, C. Becquart, L. Malerba, Simulation of radiation damage in Fe alloys: an object kinetic monte carlo approach, *Journal of Nuclear Materials* 335 (1) (2004) 121–145.
- [31] M. R. So, A. F. Voter, et al., Temperature-accelerated dynamics for simulation of infrequent events, *The Journal of Chemical Physics* 112 (21) (2000) 9599–9606.
- [32] A. F. Voter, Hyperdynamics: Accelerated molecular dynamics of infrequent events, *Physical Review Letters* 78 (20) (1997) 3908.