Interstitial loop transformations in FeCr

Laurent Karim Béland, Yuri N. Osetsky, Roger E. Stoller

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

Haixuan Xu*

Department of Materials Science, University of Tennessee, Knoxville, TN, USA

Abstract

We improve the Self-Evolving Atomistic Kinetic Monte Carlo (SEAKMC) algorithm by integrating the Activation Relaxation Technique *nouveau* (ARTn), a powerful open-ended saddle-point search method, into the algorithm. We use it to investigate the reaction of 37-interstitial $1/2[111]$ and $1/2[\bar{1}\bar{1}\bar{1}]$ loops in FeCr at 10 at.% Cr. They transform into $1/2[111]$, $1/2[\bar{1}\bar{1}\bar{1}]$, $[100]$ and $[010]$ 74-interstitial clusters with an overall barrier of 0.85 eV. We find that Cr decoration locally inhibits the rotation of crowdions, which dictates the final loop orientation. The final loop orientation depends on the details of the Cr decoration. Generally, a region of a given orientation is favored if Cr near its interface with a region of another orientation is able to inhibit reorientation at this interface more than the Cr present at the other interfaces.

We also find that substitutional Cr atoms can diffuse from energetically unfavorable to energetically favorable sites within the interlocked 37-interstitial loops conformation with barriers of less than 0.35 eV.

Keywords: off-lattice kinetic Monte Carlo, Iron, radiation damage, Chrome, interstitial-loop

1. Introduction

Interstitial loop formation is characteristic of radiation damage and is a main driver of property change in materials in nuclear energy environments. Notably, the stability of interstitial clusters, their mobility and their pinning of dislocation lines are thought to be closely related to swelling, hardening and yield strength for these materials [1, 2, 3, 4, 5].

Interstitial loops with both $1/2\langle 111 \rangle$ and $\langle 100 \rangle$ Burgers vectors are found in irradiated Fe and Fe alloys, including FeCr alloys [6, 7, 8, 9, 10]. However, cascade simulations based on molecular dynamics (MD) lead to the formation of $1/2\langle 111 \rangle$ clusters, but not $\langle 100 \rangle$ clusters; the latter are formed after longer timescales than that generally simulated by MD. Recently, Xu *et al.* numerically showed that $\langle 100 \rangle$ loops can be created in bcc-Fe by the merger of two equal-sized $1/2[111]$ and $1/2[\bar{1}\bar{1}\bar{1}]$ loops [11]. The merger of the loops lead to $\langle 100 \rangle$ formation in roughly half of the simulations and to $1/2[111]$ or $1/2[\bar{1}\bar{1}\bar{1}]$ in the other half. While one would expect the creation process of $\langle 100 \rangle$ loops to be similar in FeCr, there is, to our knowledge, no evidence to this effect in the literature.

Transmission electron microscopy (TEM) experiments suggest that the addition of Cr to Fe changes the relative population of $\langle 111 \rangle$ loops to $\langle 100 \rangle$ loops after

irradiation. There is conflicting evidence as to the sign of the change which might depend upon the exact conditions at which the irradiation and measurements were made [12, 13, 6, 7, 9, 10].

On the theory side, several studies have characterized the effects of substituting Cr in bcc-Fe in a radiation damage context, and more precisely concerning interstitial clusters. Increasing concentrations of Cr in Fe were found to have a non-monotonic effect on the diffusivity of small (less than 100 interstitials) $1/2\langle 111 \rangle$ interstitial-clusters, which reaches a minimum at about 10 at.% Cr, which is related to the interactions between Cr atoms and clusters/loops [1, 14]. This observation is supported by data based on both classical potentials and *ab initio* calculations. This decreased cluster mobility is thought to increase vacancy-interstitial recombination rates and decrease swelling [1]. The effect is generally weaker in larger clusters than in small clusters. Also, for large clusters, the concentration dependence changes, which is related to interactions with Cr-Cr atom-pairs. These findings were in agreement with experimentally measured Cr-concentration profiles of interstitial-clusters [14]. Furthermore, by combining lattice metropolis Monte Carlo with molecular dynamics of dislocation loops interacting with an edge dislocation, it was shown that Cr segregates to the loop tensile strain region and that this decoration increases the stress to move a dislocation through it. This mechanism was proposed as the origin for the Cr-concentration dependent increase in yield stress [15, 3]. Other molecular

*Corresponding author

Email address: xhx@utk.edu (Haixuan Xu)

dynamics results also confirm that Cr influences the interaction between dislocations and dislocation loops [4]. This interaction is dependent on the loop orientation and can lead to an increased resistance to loop absorption by dislocations, which is the opposite of loop absorption in pure-Fe. At high concentration, Cr precipitate formation increases dislocation pinning, leading to increased strengthening. Concerning the effect of Cr on interstitials and very small interstitial clusters (2 or 3 interstitials), calculations based on *ab initio* and classical potentials indicate that addition of Cr to these structures can either accelerate or decelerate diffusion, depending on the exact local atomic configuration [5]. For a more general perspective on the subject, we refer the reader to Ref. [5], that presents a review of the results of atomistic simulations in Fe-Cr alloys in the context of radiation damage.

In this work, we explore the transformation from $1/2 \langle 111 \rangle$ interstitial cluster configurations to the $\langle 100 \rangle$ interstitial cluster configuration in bcc-FeCr using the Self-evolving atomistic kinetic Monte Carlo (SEAKMC)[16]. We organize the paper as follows. We give the details of our simulation set-up in the methodological section. We present the time-evolution of two interlocked 37-atom $1/2 \langle 111 \rangle$ interstitial clusters with various local Cr compositions and show how the local concentrations of Cr control the final outcome. These results are discussed in Section 4. Finally, we draw our conclusions.

2. Methods

A previous study of interstitial cluster transformations in pure Fe showed that they are activated processes with a barrier of 0.73 ± 0.11 eV [11]. It also showed that entropic contributions to this transformation, which become important at temperatures larger than 600K, inhibit the transformation to $\langle 100 \rangle$ configurations. Thus, it is expected that simulating such systems in FeCr will necessitate a method capable of crossing high-energy barriers at low temperatures. For this purpose, we chose the SEAKMC, an off-lattice on-the-fly kinetic Monte Carlo algorithm [16, 17, 18]. While classical molecular dynamics advances in time at a constant rate, the residence time algorithm advances at a pace that increases exponentially with the lowest activation barrier height. Furthermore, SEAKMC explores the potential energy landscape (PEL), which means that it can capture transformations that high-temperature MD would inhibit.

To model the Fe-Cr interatomic interactions, we use the two-band potential developed by Olsson *et al.* [19]. This potential is based on the Fe potential developed by Ackland *et al.* [20], which accurately captures the loop transformation mechanism in pure Fe[11]. Its thermodynamic properties are rather good at the Cr concentrations under study (10 %) [5].

SEAKMC is a variation of the adaptive Monte Carlo algorithm [21], computing transitions states on-the-fly at

each kMC step. By introducing the concept of active volumes, it can handle large-scale systems with atomistic precision at a tractable computational cost. SEAKMC uses minimum-mode following methods to find transition states which are afterwards added to the kMC catalog. While the original version of SEAKMC used the dimer method [22], with small displacement of the all atoms in the active volume during saddle-search initialization, the present study is performed using the Activation-Relaxation Technique *nouveau* (ARTn) [23, 24, 25, 26], which requires displacing only a subset of the atoms in the first few steps of the saddle-search. As we showed in Ref. [27], for the particular problem of interstitial loops in FeCr, ARTn performs much better than the dimer method. Standard dimer searches in this system lead to large transition states (more than 2 eV) that, in turn, lead to unphysical kinetics, while ARTn searches were able to find paths that lead to loop transformation with much lower barriers (less than one eV). ARTn was shown to model the kinetics and thermodynamics of several classes of materials with success, including crystalline [28, 29, 30, 31, 32] and amorphous semiconductors [28, 33, 34], metals [28, 29, 35], alloys [32, 33], metallic glasses [36] and biological systems [37]. We use a version of ARTn based on the improvements presented in Refs. [38, 39, 25]. To minimize flickering motions, we require that events displace the atomic positions by at least 2 Å rmsd for them to be placed in the catalog, as suggested in Refs [40, 41].

SEAKMC was optimized to perform efficient kinetics simulation of radiation damage in bcc-metals. It has been used with success to model such processes in pure Fe and W-He [18, 42]. A complete review of SEAKMC and detailed implementation details can be found in Ref [43].

All our SEAKMC simulation have a similar initial configuration. This corresponds to a $[111]$ interstitial cluster symmetrically interlocked with a $[\bar{1}\bar{1}\bar{1}]$ cluster, at an acute angle, as defined in Ref. [11], which forms when the two individual clusters collide. The system contains 16074 atoms, including two 37-interstitial clusters. We run the SEAKMC at 500K.

Before running the simulations, we characterized the energetics of Cr substitution within the interstitial cluster. To do so, we ran 360 minimizations with 16073 Fe atoms and 1 Cr atom substitutionally placed at each site within the interlocked clusters.

We perform simulations for several important cases, which are illustrated in Fig. 1. Forty simulations were performed in a system with 10 at.% Cr, randomly distributed across the system (system A). Fifteen simulations were performed with 0 % Cr in the top part of the system and 10 at.% in the bottom part of the system (system B). Ten simulations were performed with no Cr in the middle section of the interstitial cluster, but with 10 at.% Cr elsewhere in the simulation box (system C). Thirty-five simulations were performed with 5 to 15 Cr atoms in the middle section of the interstitial cluster, but none elsewhere in simulation box (systems D). As a subset of

system D, 10 configurations were set with 5 substitutional atoms in the most energetically unfavorable atomic sites within the interstitial cluster.

For visualization and Voronoi polyhedra (VP) computations, we use the OVITO package [44].

3. Results

3.1. Energetics of Cr substitution

The results of the minimizations are illustrated in Fig. 2. We see that the best sites for Cr decoration are on the exterior of the clusters and in some atomic sites near the so called "anchor" at the intersection of the clusters (i.e. the center-left part of Fig 2). This is coherent with computations that predict Cr decoration of individual $\langle 111 \rangle$ interstitial loops. The most unfavorable sites for Cr decoration are also near the "anchor". Interestingly, there was no correlation between the energetics of Cr substitution and VP volumes. The differences between the potential energy of substitution for each site is sizable: at 600K, a 0.13 eV difference implies that the occupation ratio of the most favorable site to the most unfavorable is roughly 24 to 1. In order to completely capture the Cr distribution in these systems, one should perform metropolis Monte Carlo runs, as performed in Ref. [15]. This, however, is out of the scope of our work. Our results, however, show that Cr is distributed non-uniformly in this system. Our SEAKMC simulations evaluated the effect of diverse distributions of Cr decoration on the loop transformation process.

	[111]	$\bar{1}\bar{1}\bar{1}$	[100]	[010]	Incomplete
System A	16	2	1	7	14
System B	0	6	3	5	1
System C	4	6	0	0	0
System D	7	5	8	8	7
Pure Fe	41		31		40

Table 1: The final orientation of the interstitial-cluster after transformation. The numbers indicate the number of SEAKMC runs that led to each orientation.

	Can we reject that ...		
	$P(\langle 111 \rangle) = P(\langle 100 \rangle)$	$P([100]) = P([010])$	$P([111]) = P(N[\bar{1}\bar{1}\bar{1}])$
System A	$\alpha = 0.0755$	$\alpha = 0.125$	$\alpha = 0.0013$
System B	no	no	$\alpha = 0.0313$
System C	$\alpha = 0.002$	no	no
System D	no	no	no
Pure Fe	no	N/A	N/A

Table 2: The statistical significance of the SEAKMC results. We indicate the probability that an equiprobable binomial model can be rejected.

3.2. System A

The results for system A through D are summarized in Tables 1, 2, 3 & 4. 65 % of the SEAKMC simulations led to a transformation to $\langle 111 \rangle$ or $\langle 100 \rangle$, which is similar to results of the simulations in pure Fe. The other 35 % of

Figure 1: The initial configuration for the SEAKMC runs. Grey atoms are Fe atoms not sitting on bcc lattice-sites, orange atoms are Cr atoms not sitting on bcc lattice-sites and yellow atoms are empty bcc lattice-site. The clusters are rotated to emphasize where Cr was placed in each system. The slightly different cluster shapes for each case are due to the effect of Cr atoms on the equilibrium atomic positions after minimization.

Figure 3: An illustration of loop transformation to $\langle 111 \rangle$ in system A. The red circles indicate the subregion that is changing orientation within the interstitial-cluster. (a)-(e) are in chronological order. The potential energy of the configurations is indicated at the bottom. We chose (a) as the reference state for potential energy calculations.

Figure 2: A color-coded representation of the potential energy involved by substituting a single Cr atom within the interstitial clusters for each of the atomic sites. 0 eV corresponds to the potential energy of the system if placing the single Cr atom in the most energetically favorable position.

	[111]	[111]	[100]	[010]
System A	0.83 ± 0.04 eV	0.83	0.83 eV	0.82 ± 0.04 eV
System B	N/A	0.84 ± 0.03 eV	0.85 ± 0.04 eV	0.88 ± 0.01 eV
System C	0.83 ± 0.08 eV	0.84 ± 0.04 eV	N/A	N/A
System D	0.88 ± 0.06 eV	0.84 ± 0.04 eV	0.87 ± 0.02 eV	0.88 ± 0.06 eV
Pure Fe	0.73 ± 0.11 eV			

Table 3: The highest barrier crossed by the SEAKMC simulations that led to a given orientation of the final configuration. The standard deviation is also reported for final configurations with more than 2 data points.

	[111]	[111]	[100]	[010]
System A	-0.6 ± 0.9 eV	-0.1	1.0 eV	-0.3 ± 1.6 eV
System B	N/A	-0.8 ± 0.6 eV	0.2 ± 1.5 eV	0.6 ± 1.4 eV
System C	-0.3 ± 0.9 eV	0.3 ± 0.3 eV	N/A	N/A
System D	-0.6 ± 0.9 eV	-0.3 ± 0.9 eV	0.1 ± 0.5 eV	0.9 ± 0.8 eV
Pure Fe	0			

Table 4: The potential energy of the final state of each SEAKMC simulations. We report the mean difference between these final potential energies and the average potential energy of the final state for runs that led to successful loop transformation in each system. The standard deviation is also reported for final configurations with more than 2 data points.

runs were stuck performing oscillatory transitions in the interlocked configuration after several thousands of kMC steps and weeks of calculation.

The $\langle 111 \rangle$ orientation is preferred over the $\langle 100 \rangle$ orientation (45 % vs 20%). This difference is significant at the $\alpha = 0.755$ level. In pure Fe, the ratio is 37 % vs 28%, which is not a statistically different result. We note that the [111] orientation is preferred to the [111] ($\alpha = 0.0013$) and that the [010] is preferred over the [100] orientation ($\alpha = 0.125$).

The potential energy of the final states are similar for all orientations. The average potential energy for the different orientations varies by 0.4 eV, while the standard error

for these averages is also of 0.4 eV; the difference is not statistically significant.

The highest activation barrier crossed during the transformation does not correlate with the final outcome. Regardless of the final orientation, we obtain a value of $0.82 \text{ eV} \pm 0.04 \text{ eV}$, which is not statistically different from the value found in pure Fe.

In Fig. 3, we illustrate a typical example of interstitial-clusters evolving toward $\langle 111 \rangle$. Initially, in panel (a), only the lower third of the aggregate is in the $\langle 111 \rangle$ orientation. In panel (b), we see, as emphasized by the red circle, that a subsection of the atoms is aligned with the $\langle 111 \rangle$ direction. One could say the the $\langle 111 \rangle$ "front" progressed. In panels (c), (d), and (e) we see this "front" progressing until the transformation is complete. We see that the energy progressively decreases throughout the process. In Fig. 4, we show an equivalent illustration for the transformation to $\langle 100 \rangle$. In this case, "nucleation" of the $\langle 100 \rangle$ subregion, as emphasized by the red circles, starts in the middle third of the aggregate and progressively transforms the middle and top third of the cluster, before finally transforming the bottom half.

3.3. System B

By removing the Cr from the top part, the results were significantly different than those for system A. Fourteen of the fifteen attempts to transform were successful. Six runs led to the $\bar{1}\bar{1}1$ configuration, three runs led to the $[100]$ orientation and five runs led to the $[010]$ orientation.

No runs led to the $[111]$ orientation, in stark contrast with System A, where this orientation was favored. The highest activation barrier crossed during transformation is $0.85 \text{ eV} \pm 0.04 \text{ eV}$. The potential energy of the final state does not depend on loop orientation.

3.4. System C

By removing the Cr from the center part of the interstitial-cluster, $\langle 100 \rangle$ orientation is completely suppressed. Five runs led to a $[111]$ cluster and five runs led to a $\bar{1}\bar{1}1$ cluster.

The highest activation barrier crossed during transformation is $0.84 \text{ eV} \pm 0.05 \text{ eV}$. The potential energy of the final state does not depend on loop orientation.

3.5. System D

35 simulations were made with Cr in the middle part of the interlocked cluster (system D). The $[100]$ and $[010]$ final orientations are in equal number (8 each) and more numerous than the $[111]$ and $\bar{1}\bar{1}1$ final orientations (7 and 5, respectively).

The highest activation barrier crossed during transformation is $0.87 \text{ eV} \pm 0.05 \text{ eV}$. The potential energy of the final state does not depend on loop orientation.

When placing Cr atoms in the unfavorable sites (as identified in section 3.1), they first diffused to more favorable sites. This happens with a barrier of less than 0.35 eV,

which is significantly lower than the barrier required for loop transformation. In other words, it is kinetically feasible for Cr to segregate towards the thermodynamic equilibrium distribution before loop transformation.

4. Discussion

The mechanism that permits loop transformation in FeCr is very similar to the mechanism in pure Fe. This transformation happens through a sequence of local reorientation of the crowdions. The overall limiting potential energy barrier to this transformation in FeCr, as computed through our SEAKMC runs, is not statistically different from the barrier in pure Fe.

As reported in Table 1, the outcome of the interstitial loop transformation can be controlled by Cr decoration. By placing the Cr atoms at various position in the system, we have been able to inhibit certain final cluster orientations, sometimes partly, sometimes completely. Our runs show that regardless of Cr decoration, the overall activation barrier limiting the transformation is identical for all final orientations. The relative potential energies of the final states is also independent of Cr decoration. Thus, we must exclude that the depth of the potential energy basins and that the height of the activation barriers crossed during the loop transformation are responsible for the effects of Cr decoration.

This leads us to conclude that Cr content changes the multiplicity of paths that lead to each final orientation. Loop transformation takes place by changing the orientation of small group of atoms near the $\langle 111 \rangle / \langle 100 \rangle$ boundaries within the cluster, which involves the rotation of a few tens of crowdions. The presence of Cr locally inhibits this rotation. Once a sufficiently large subsection of the cluster has rotated towards the $\langle 111 \rangle$ or $\langle 100 \rangle$ orientation, decreasing the potential energy of the system, the remainder of the loop will also rotate in that direction, crossing low-energy barriers, irrespective of Cr decoration or not. We note that previous studies have shown that Cr decoration increases the difficulty of unpinning interstitial loops to dislocations, which involves a rotation of the interstitial cluster. The effect we observe here is similar, albeit very localized.

The fact that System A exhibited a strong asymmetry, preferring the $[111]$ orientation over the $\bar{1}\bar{1}1$ orientation, shows that this effect depends on the exact local arrangement of Cr decoration. Indeed, Cr was randomly placed in the system at 10 % at. concentration throughout the whole system, which indicates the asymmetry was caused by random fluctuations of its spacial distribution.

Our results in System A suggest that the $[111]$ and $\bar{1}\bar{1}1$ orientations are favored by the addition of Cr. However, our results in the other systems indicate that this conclusion depends greatly on the exact spacial distribution of Cr atoms. It is interesting to note that we have not found a way to place Cr atoms so to completely inhibit the transformation to $[111]$ and $\bar{1}\bar{1}1$ and favor

Figure 4: An illustration of loop transformation to $\langle 100 \rangle$ in system A. The red circles indicate the subregion that in changing orientation within the interstitial-cluster. (a)-(f) are in chronological order. The potential energy of the configurations is indicated at the bottom.

the $[100]$ and $[010]$ orientations. While such atomistic configuration might exist, our results suggest that Cr decoration most probably favors a greater concentration of $[111]$ and $[\bar{1}\bar{1}1]$ interstitial loops.

However, our simulations indicate that this effect of Cr decoration on the outcome of the loop transformations is modest. Indeed, except for system C, which is a physically very unlikely configuration, the ratio of $\langle 111 \rangle$ to $\langle 100 \rangle$ orientations varies from 3:4 to 9:4. Considering that loop transformation is only one among many factors leading to radiation damage defect evolution, such as defect creation in displacement cascades, defect cluster aggregation, cluster migration, and interaction of these defects with various structures (grain boundaries, surfaces, dislocations, etc.), such changes in the outcome of loop transformations might not play a critical role. The decrease of $\langle 111 \rangle$ cluster mobility caused by Cr might have a stronger overall effect in reducing the proportion of $\langle 100 \rangle$ outcomes by significantly diminishing the total number of reactions between $\langle 111 \rangle$ clusters.

We also note that since the kinetics described here depend on the precise emplacement of Cr atoms, the results of these simulations crucially depend upon which atomic sites the classical potential favors Cr decoration. While our results do not give a definitive answer as to which orientation will be preferred by adding Cr to Fe, they do provide great insight into how Cr affects the loop-transformation mechanism.

A more thorough statistical analysis of different loops might give a more definitive answer. Ideally, one would want to generate the initial decoration of Cr through a Metropolis Monte Carlo scheme, or even better, use loops created by time-evolving MD-generated displacement cascade debris. However, this is out of the scope of the present study for two reasons. First, because of computational costs. The search for saddle-point is much more time-consuming, notably because the potential-energy surface (PES) of FeCr is much rougher than that of pure Fe. Thus, saddle-point searches fail more often in FeCr. Also, such a rough PES leads to oscillations between states con-

nected by small forward and inverse barriers, i.e. flickers, which wastes CPU time. Overall, reactions that take a day to simulate in Fe, using 12 CPU cores, typically take a week in FeCr. Second, our results suggest that the outcome of dislocation loop reactions depends very subtly on the spatial arrangement of Cr decoration. Thus, to ensure physical meaning, such a study would need to compare diverse interatomic potentials and also perform *ab initio* validations.

What our results do suggest is that the conflicts in the experimental literature concerning the effect of Cr decoration on the distribution of dislocation loop orientations [12, 13, 6, 7, 9, 10] may be explained by the fact that the different experimental conditions have favored different Cr arrangements within the interstitial clusters, leading to dissimilar outcomes.

Finally, we note that an alternative mechanism was recently proposed to explain the presence of $\langle 100 \rangle$ loops in pure Fe, in which they are formed by the growth and destabilization of C15 interstitial-clusters [45]. It would be interesting to verify if such a mechanism exists in FeCr.

5. Conclusion

We have performed adaptive Monte Carlo simulations, using an implementation of SEAKMC that uses the ARTn, to investigate the transformation of two glissile interstitial cluster loops into $\langle 100 \rangle$ and $\langle 111 \rangle$ interstitial cluster loops in FeCr at 10 % at. concentration.

We found that the mechanism that leads to loop transformation is very similar in both pure Fe and FeCr. The relative energies of the final states after transformation are identical and the activation barriers are not statistically different in Fe and FeCr, either for transformations to $\langle 100 \rangle$ or to $\langle 111 \rangle$. In both cases, the process takes place as a series of local rotation of a few $\langle 111 \rangle$ crowdions within the interlocked clusters.

We found that Cr decoration is not uniform across the interlocked clusters. Cr substitutional atoms can diffuse from unfavorable site to favorable sites with activation

barriers well below the overall activation barrier for loop transformation.

We also showed that the outcome of the transformation is controlled by the spacial distribution of the Cr atoms. Cr locally inhibits reorientation of the crowdions, thus blocking some of the kinetic paths that lead to one final configuration or another.

Our investigation suggests that the transformation to the $\langle 111 \rangle$ configuration is probably favored over the $\langle 100 \rangle$, but more extensive statistics, notably using more interatomic potentials, will be needed to give a definitive answer to this problem.

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SEAKMC is available upon request to the authors.

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