

AB INITIO DEFECT PROPERTIES FOR MODELING RADIATION-INDUCED SEGREGATION IN FE-NI-CR ALLOYS

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Abstract

Radiation-induced segregation (RIS) has been studied with experimental and theoretical methods for over 30 years and many models have been built in an attempt to understand the mechanisms involved. Input parameters for these models are often not available experimentally, limiting the model's predictive capabilities. In an effort to obtain more accurate input parameters we have calculated formation and migration energies for both vacancies and interstitials using *ab initio* methods in face-centered cubic (fcc) Fe-Ni-Cr alloys, with an emphasis on Ni-based alloys with dilute concentrations of Cr and Fe. The data gives new insight into a number of properties including species dependence of migration barriers and binding energies for both vacancies and interstitials. We predict species dependent vacancy migration barriers for Cr (0.82 eV), Fe (0.95 eV), and Ni (1.08 eV) and interstitial migration barriers for Cr (0.08 eV), Fe (0.11 eV), and Ni (0.14 eV) in a Ni matrix. Significant binding between Cr and the <100> interstitial dumbbell was also observed. Further work will build on this data to create a rate theory models for RIS.

1. Introduction

Radiation induced segregation (RIS), the process by which the local composition of an alloy is altered near point defect sinks, is a concern in the nuclear industry. RIS has been linked to intergranular failure in light water reactors as well as enhanced void swelling in fast reactors. There is a need to understand the fundamental mechanisms which drive RIS in order to better predict component lifetimes in existing reactors as well as aid in the design and selection process of candidate materials for the next generations of nuclear reactors.

Numerous experiments have been conducted in high purity alloys in order to gain understanding of the key parameters which influence RIS [1-3]. These experiments show that RIS is affected by alloy composition, radiation dose, dose rate, temperature and materials processing. It is also known that the type and energy of the irradiating particle can affect RIS. While a large body of experimental RIS and related thermokinetic data exists, there is not enough to accurately determine the complex relationships between all the key variables. For example, diffusion data in Fe-Ni-Cr alloys is plentiful but only provides insight into vacancy diffusion, not interstitial transport. Diffusion data is also generally taken at high temperature and uncertain extrapolations are required to predict diffusion at reactor temperatures. Experiments are also somewhat limited in constraining the possible atomic level mechanisms that are driving RIS, such as the role of interstitial migration. Nonetheless, models have been created to help develop an understanding of the mechanism associated with RIS and to attempt to predict the amount of segregation in various alloys under a number of different environmental conditions.

The possible atomistic mechanism leading to RIS are generally thought to include the "inverse Kirkendall" effect, potentially consisting of vacancy and/or interstitial components, and defect-solute complexes [4]. Despite many years of study, the dominant RIS

mechanisms in austenitic Fe-Cr-Ni are still not known for certain. RIS at grain boundaries in fcc steels is generally strong Cr depletion, milder Fe depletion, if any at all, and compensating Ni enrichment. Due to the lack of kinetic data, RIS models include assumptions about which mechanism is dominant and underlies the experimental observations. The most common assumption is that RIS is dominated by a vacancy mediated inverse Kirkendall effect, which is the foundation of the influential model of Perks, *et al.* [5, 6], the similar model of Watanabe, *et al.* [7], and the more atomistic based model of Allen, *et al.* [8]. In these models Cr exchanges preferentially with the vacancy flux, depleting it near the grain boundary. Other models explain the experimental data by proposing significant interstitial contributions and defect-solute complexes. Defect-solute complexes refer to the case when a species binds strongly to a defect, either an interstitial or a vacancy, and is therefore dragged along to the sink with the defect. Lam, *et al.* [9, 10] invoked Ni interstitial binding as a key mechanism of RIS in Fe-Cr-Ni alloys. Faulkner [11, 12] concludes that repulsive interactions between interstitials and oversized Cr drive Cr from the boundary. A vacancy-Cr complex has been proposed to explain cases of Cr enrichment at grain boundaries for thermal non-equilibrium segregation (TNES) in Austenitic stainless steels and more recently in Ni-based alloys [13, 14]. TNES is similar to RIS but occurs via thermally created vacancies, with no interstitials present, and building consistent RIS and TNES models based on the inverse Kirkendall effect requires that vacancies are strongly bound to Cr solutes. At present one cannot be certain about the mechanisms dominating segregation in Austenitic Fe-Cr-Ni. Diffusion data provides some insight into solute transport via vacancy mechanisms but the role of interstitials and defect-solute binding is still largely undetermined, even at a qualitative level.

Regardless of the mechanisms assumed in RIS models, the availability of accurate input parameters is limited. For example, defect migration energies appear in exponential terms of the diffusion coefficients and have been shown to be of particular importance in modeling RIS data. Allen, *et al.*, [8] showed through sensitivity studies that of all input parameters in his model, only the migration barriers had a significant contribution to explaining the difference between model predictions and data for RIS at grain boundaries. He concluded that differences in migration energies are more important than attempt frequencies in explaining the RIS data. By calculating a species and local environment dependent migration barrier, Allen's model was able to better predict trends and quantitative amounts of segregation than similar models which assumed constant barriers.

While substantial progress has been made in the area of RIS prediction by empirical fitting of kinetic parameters, many questions remain about the mechanisms that facilitate RIS, how these mechanisms are affected by the multi-component nature of steels and nickel-based alloys, and the exact values of key kinetic parameters. Our goal is to use *ab initio* methods to parameterize RIS models for temperatures and compositions where experimental values of important kinetic parameters have not been measured. This approach provides insight to the diffusion mechanisms of vacancies and interstitials in multi-component alloys and brings us closer to the accurate prediction of RIS without additional experimental segregation data. The present paper reports studies of the defect energetics for Ni based Fe-Ni-Cr alloys.

2. Methodology

Vacancy and interstitial migration and formation energies are calculated in the fcc Fe-Ni-Cr system using the Vienna *Ab initio* Simulation Package (VASP) [15, 16], a quantum mechanical density functional theory based *ab initio* code. All defect calculations were run

with a 270 eV energy cutoff, the Perdew-Burke-Ernzerhof [17] parameterization of the generalized gradient approximation, the projector-augmented wave method [18, 19] and a 3x3x3 k-point mesh unless stated otherwise. All calculations were spin-polarized and initiated with a ferromagnetic alignment. Defects were studied in a 108(\pm 1) atom periodic 3x3x3 supercell of the fcc conventional cell, where the cell shape and volume were fixed but ionic relaxations were allowed. The volume of the cell in each simulation was based on the alloy concentration present in the cell. The volume concentration dependence was determined by fitting a quadratic function of X in Ni_{1-x}M_x (M = Cr, Fe) over 30+ *ab initio* calculations, where X ranges from [0, 1]. These calculations allowed ionic relaxation and volume and cell shape changes. They were run with energy cutoffs of 479 eV for Ni-Cr alloys or 500 eV for Ni-Fe alloys and 1728 k-points per reciprocal atom. The quadratic equations for Cr and Fe are listed in equations 1 and 2, respectively, where x denotes the concentration of the solute present in the alloy. Barriers for migration were calculated by comparing the energy of the stable defect configuration to the activated state along the migration path. For the vacancy and interstitial migrations considered in this paper the activated state is a high symmetry point, so no additional constraints were placed on the system to stabilize this configuration. For each barrier the stable and activated state were run at the same volume, providing a substantial cancellation of errors. The barriers are estimated to be converged with respect to k-point mesh and energy cutoff to within about 25 meV based on similar calculations. This error is acceptable for most applications but is of similar size as some of the interstitial migration barrier differences, which will require further calculations if greater precision is needed.

$$\text{Volume per atom (Ni - Cr)} = 0.72x^2 + 0.07x + 10.94 \quad (1)$$

$$\text{Volume per atom (Ni - Fe)} = 0.27x^2 + 0.79x + 10.93 \quad (2)$$

Calculations are also performed to study how the defects bind to solutes in the matrix. This will affect the ability of the solute to diffuse through that defect flux. The solute-vacancy binding energy was calculated using two methods, direct and indirect. The direct method compares two energies, that of the solute and vacancy sitting on first nearest-neighbor sites and that of the solute and vacancy as far apart as possible in the cell considering the periodic boundary conditions. The farthest separation possible from a vacancy in a cubic 108 atom simulation cell is an eleventh nearest-neighbor, which in the ideal lattice (no relaxation off the fcc positions) gives a separation of $a\sqrt{11/2}$, where a is the lattice constant. The direct method only approximates the binding energy since it is possible that even at the eleventh nearest-neighbor distance the solute and vacancy may still interact with each other. The indirect method accounts for this possible interaction by calculating the binding energy with four different VASP calculations. In this method the energy of the vacancy and solute atom are subtracted separately from the energy of the system where they interact as first nearest-neighbors, and the method is described in detail in Ref. [20]. As the number of atoms in the simulation cell increases the binding energies of these two methods should converge. Equations 3 and 4 are examples of these two methods where Cr is the solute, Ni is the solvent, v is a vacancy present in the system, and E_b is the binding energy. These calculations are run at constant volume, where the volume is determined from the solute composition, as described above. The volume of the defected supercells is set to that of the corresponding undefected supercell with the same composition.

$$E_b^{\text{direct}}(\text{Cr-v}) = E(106\text{Ni}, 1\text{Cr}, v, 1\text{st nn}) - E(106\text{Ni}, 1\text{Cr}, v, 11\text{th nn}) \quad (3)$$

$$E_b^{\text{indirect}}(\text{Cr-v})=E(106\text{Ni}, 1\text{Cr}, \text{v}, 1\text{st nn})-E(107\text{Ni}, 1\text{Cr}) -E(107\text{Ni}, \text{v})+E(108\text{Ni}) \quad (4)$$

The vacancy formation energy, E_{vf} , is calculated in pure Ni by comparing the energy of a cell containing a vacancy to that of an undefected cell (scaled to conserve the appropriate number of atoms). The interstitial formation energy, E_{if} , is calculated in an analogous manner. Equations 5 and 6 provide equations for vacancy and interstitial dumbbell formation in pure Ni. Interstitial calculations are run at constant volume where the volume per atom is based on the solute concentration dependence and then scaled to 109 atoms. The formation energy of a solute interstitial is obtained by adding the binding energy of a solute and an interstitial to the formation energy of a pure Ni interstitial. This is equivalent to forming a Ni interstitial with a solute atom far away and then exchanging the solute atom with the Ni interstitial. Equation 7 is an example for calculating the formation energy of a Ni-Cr mixed interstitial dumbbell. The solute-interstitial binding energy is calculated in an analogous manner as the solute-vacancy binding energy, demonstrated in equations 3 and 4.

$$E_{\text{vf}}(\text{v in Ni})=E(107\text{Ni}, \text{v}) - \frac{107}{108} E(108\text{Ni}) \quad (5)$$

$$E_{\text{if}}(\text{Ni-Ni dumbbell})=E(109\text{Ni}, \text{dumbbell}) - \frac{109}{108} E(108\text{Ni}) \quad (6)$$

$$E_{\text{if}}(\text{Ni-Cr dumbbell})=E_{\text{if}}(\text{Ni-Ni dumbbell})+E_b(\text{Cr-dumbbell}) \quad (7)$$

3. Results and Discussion

This section presents calculated migration and formation energies for vacancies and interstitials in the Fe-Ni-Cr system. The calculations were benchmarked for the pure nickel case where experimental data is available for comparison. Results in the dilute Ni-Cr and Ni-Fe binaries are then discussed.

3.1 Pure Nickel

Using VASP, the formation energies of six different interstitial configurations were calculated in pure fcc Ni. These calculations were performed with a volume of 109 Ni atoms (scaled from an undefected 108 Ni supercell), a 479 eV energy cut off and a 4x4x4 k-point mesh. The six configurations studied were the $\langle 100 \rangle$, $\langle 111 \rangle$ and $\langle 110 \rangle$ dumbbells and the octahedral, tetrahedral and crowdion interstitial sites (see Figure 1).

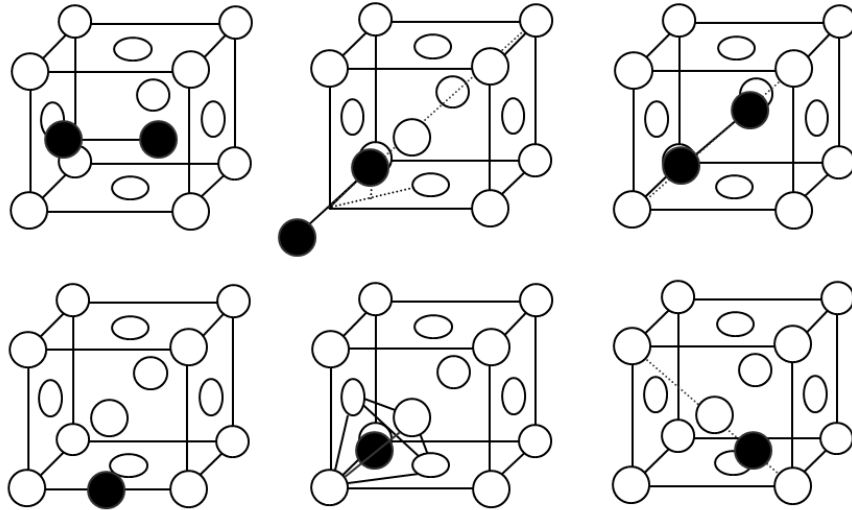


Figure 1 Six possible interstitial sites in the fcc lattice

These calculations confirmed that the $\langle 100 \rangle$ dumbbell was the most stable interstitial configuration, consistent with previous models in other fcc metals [21-24] and experiments in Ni [25]. The $\langle 100 \rangle$ dumbbell formation energy was calculated to be 4.07 eV. The formation energies of the other interstitial configurations are reported relative to the $\langle 100 \rangle$ dumbbell value in Table 1.

Table 1 Formation energies of six possible interstitial sites in the fcc lattice relative to the $\langle 100 \rangle$ dumbbell configuration

Interstitial Configuration	Relative Formation Energies (eV)
$\langle 100 \rangle$ Dumbbell	0.00
Octahedral	0.18
$\langle 111 \rangle$ Dumbbell	0.62
Tetrahedral	0.62
$\langle 110 \rangle$ Dumbbell	0.92
Crowdion	0.92

Two migration paths for the $\langle 100 \rangle$ dumbbell were compared. One path consisted of a linear motion along the $\langle 100 \rangle$ directions with a midpoint at the octahedral site, resulting in a new $\langle 100 \rangle$ dumbbell in the neighboring cell on a second nearest-neighbor site. The other path consists of a shift and rotate mechanism by which a $\langle 100 \rangle$ oriented dumbbell circumvents the octahedral site and becomes a $\langle 001 \rangle$ dumbbell on a nearest-neighbor site, shown in Figure 2. The second-neighbor hop has a migration barrier of at least 0.18 eV, obtained by comparison of the $\langle 100 \rangle$ and octahedral states, whereas the rotation mechanism has a migration barrier of 0.14 eV, which is in excellent agreement with the experimental value of 0.15 ± 0.01 eV [24]. This result supports that the shift and rotation mechanism is the preferred interstitial migration path, as previously reported [24, 25].

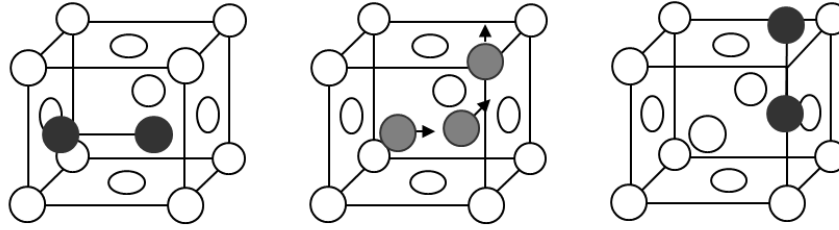


Figure 2 Proposed migration mechanism for the $\langle 100 \rangle$ dumbbell

The vacancy formation energy in pure Ni is calculated to be 1.43 eV. While reported experimental values range from 1.45 to 1.8 eV, the recommended value is 1.79 ± 0.05 eV [24]. The exact source of the error in the calculation is not clear at this point, although there are some known problems associated with the local density approximation and the generalized gradient approximation in defect formation energy calculations [26, 27].

The vacancy migration path is more straightforward than that of interstitials. It is generally assumed that vacancies exchange with atoms on first nearest-neighbor lattice sites. This exchange in Ni has a calculated migration barrier of 1.08 eV, which agrees well with the reported experimental value of 1.04 ± 0.04 eV [24]. A second nearest-neighbor vacancy exchange was calculated for comparison and was found to be energetically unfavorable, with a barrier of 3.92 eV.

3.2 Cr Impurity in Ni

To study dilute concentrations, a single atom of Cr was added to the pure Ni matrix. Cr migration through vacancy exchange in a Ni environment has a barrier of 0.82 eV, which is significantly lower than that of Ni. A second nearest-neighbor Cr-vacancy exchange was calculated to have a barrier of 3.58 eV, which is lower than that of Ni but still very energetically unfavorable. The lower Cr barrier suggests that Cr would migrate preferentially over Ni through a vacancy flux, although additional barriers are needed to determine the diffusion coefficients [28]. In terms of RIS, faster Cr diffusion would lead to Cr depletion at defect sinks through the inverse Kirkendall effect, assuming no competing mechanisms were present (e.g., strong vacancy drag or interstitial effects).

Another factor which must be considered with regards to preferential Cr migration is the Cr-vacancy binding energy. A vacancy must become a first nearest neighbor to the Cr in order to exchange with it. If this event is favored or suppressed by Cr-vacancy coupling it will affect the ability of Cr atoms to diffuse. The first nearest-neighbor Cr-vacancy binding energy was calculated using the direct and indirect methods to be 0.04 eV, independent of method. A positive binding energy indicates repulsion in this calculation, i.e. the system is more stable when the vacancy is far from the Cr atom. This would hinder the ability of the Cr to diffuse. The small positive binding energy would also argue against a vacancy-Cr drag mechanism for Cr diffusion in Ni rich alloys, which is generally associated with a strong vacancy-solute binding. Simonen, *et al.* [13] created a simple model, which included both inverse Kirkendall vacancy exchange and vacancy-solute complex mechanisms, to predict TNES of Cr in a Fe-Cr-Ni system. He found that the model required a solute-vacancy attractive binding energy of 0.5 eV to observe any significant amount of segregation through this mechanism. Based on the binding energy calculated above a vacancy-Cr drag mechanism induced by Cr-vacancy coupling would not occur in Ni-based alloys.

Interstitial diffusion of Cr in the dilute regime was also considered. One Cr atom as part of a Ni-Cr $\langle 100 \rangle$ mixed dumbbell migrates to form a new $\langle 001 \rangle$ Cr-Ni mixed dumbbell. The migration barrier was calculated to be 0.08 eV, which is less than the 0.14 eV barrier determined for Ni migrating in the same environment. This implies that Cr would migrate preferentially over Ni through an interstitial flux if all other factors were equal. In terms of RIS this would lead to relative Cr enrichment at defect sinks if no competing mechanisms were present. Again the binding energy of Cr to this type of defect will play an important role in determining diffusion through this mechanism. If the formation energy of an interstitial dumbbell containing a Cr atom is greater than that of a pure Ni dumbbell, Cr will be less likely to diffuse through this mechanism. Initially, the interstitials are formed through high energy ballistic events but as they migrate a new atom can be incorporated into the dumbbell at each step and another left on the lattice site. After a few migration steps unstable interstitial combinations could easily exchange for ones that are energetically more favorable. The formation energy of the mixed Ni-Cr dumbbell was calculated to be 3.62 eV, which is much less than that of the pure Ni dumbbell (4.07 eV). This lower formation energy is due to the attractive binding energy of the Cr and the $\langle 100 \rangle$ dumbbell. The binding energy was calculated to be -0.49 eV and -0.45 eV using the direct and indirect methods, respectively. The indirect binding energy calculation was performed with a 479 eV energy cut off and a $4 \times 4 \times 4$ k-point mesh. These energetics indicate preferential formation and migration of Cr in a mixed dumbbell over that of pure Ni. Calculations for Ni migrating as a mixed dumbbell as well as other interstitial configurations (e.g., Cr-Cr dumbbells) also important for understanding interstitial diffusion and are underway.

3.3 Fe Impurity in Ni

Similar calculations to those done for the Ni-Cr alloys have been performed for vacancies in Ni-Fe alloys. Fe has a vacancy migration barrier of 0.95 eV in a pure Ni matrix. This is an intermediate value between the barriers for Cr (0.82 eV) and Ni (1.08 eV). The binding energy between and Fe atom and a vacancy in the Ni matrix is slightly repulsive at 0.01 eV and 0.02 eV, calculated by the direct and indirect method, respectively.

Interstitial diffusion of Fe in the dilute regime was also considered. One Fe atom as part of a Ni-Fe $\langle 100 \rangle$ mixed dumbbell migrates to form a new $\langle 001 \rangle$ Fe-Ni mixed dumbbell. The migration barrier was calculated to be 0.11 eV. Similar to the vacancy migration case this interstitial migration barrier is an intermediate value between that for Cr (0.08 eV) and Ni (0.14 eV) migration. It should be noted that the differences of these barriers is small compared to that of vacancy migration and comparable to the estimated error of the calculations. The formation energy of the mixed Ni-Fe dumbbell was calculated to be 4.13 eV, which is more than that of the pure Ni dumbbell (4.07 eV) and the mixed Ni-Cr dumbbell (3.62 eV). This is due to a slightly repulsive binding energy between the Fe solute and the $\langle 100 \rangle$ dumbbell. The binding energy was calculated to be 0.05 eV and 0.06 eV, calculated by the direct and indirect method, respectively. The indirect binding energy calculation was performed with a 479 eV energy cut off and a $4 \times 4 \times 4$ k-point mesh. Although the Fe interstitial migration barrier is lower than that of Ni, the higher Ni-Fe $\langle 100 \rangle$ dumbbell formation energy will hinder the ability of Fe, relative to Ni and Cr, to diffuse through an interstitial mechanism.

4. Conclusion

Ab initio calculations have been used to study point defect formation and migration in Ni rich Ni-Fe-Cr alloys and provide quantitative insight into the mechanisms by which they diffuse. This information will be used in future work to calculate diffusion coefficients and parameterize RIS models where experimental data is lacking. The calculations were benchmarked in pure Ni and showed excellent agreement with experimental data for both interstitial and vacancy migration. The calculations also agreed with previous models and experiments in fcc metals that the $\langle 100 \rangle$ interstitial dumbbell is the most stable configuration and that it migrates through a shift and rotate mechanism.

Through our *ab initio* calculations we demonstrate that Cr has a significantly lower migration barrier than that of Fe or Ni when migrating in a Ni matrix through a vacancy mechanism. These results are summarized in Table 2. While barriers do not translate directly into diffusion coefficients, differences of this magnitude could have a large impact on diffusion, especially at low temperature, since the barriers influence the diffusion constants through an exponential term. The correlation factors and weak repulsive solute-vacancy binding energies will also affect the diffusion coefficients. The vacancy-X binding energies calculated by the indirect method are also presented in Table 2, where X denotes the solute type, Cr or Fe,

Table 2 Species dependence of vacancy and interstitial migration and binding energies in a Ni host

Species	Vacancy Migration Energy (eV)	Interstitial Migration Energy (eV)	Vacancy-X Binding Energy (eV)	Ni-X $\langle 100 \rangle$ Binding Energy (eV)
Cr	0.82	0.08	0.04	-0.45
Fe	0.95	0.11	0.02	0.06
Ni	1.08	0.14	N/A	N/A

Interstitial migration barriers in Ni with dilute concentrations of Cr and Fe as part of the $\langle 100 \rangle$ mixed dumbbell have the same ordering as vacancy migration, with Cr < Fe < Ni. These results are also summarized in Table 2. The species dependence of these barriers is small in magnitude compared to that for vacancy migration, but larger as a percentage of the total barriers. Based on the differences in barriers alone, one might expect more RIS to occur via the vacancy flux in a Ni rich system. However, the significant species dependence in the dumbbell-solute binding energies may increase the species diffusion bias and the contribution of interstitials to RIS. These binding energies are listed in Table 2 for Ni-X $\langle 100 \rangle$ dumbbells, where X denotes the solute type, Cr or Fe. Other factors, such as different types of interstitial hops, dumbbell rotation and the effects of local environment on dumbbell formation and migration energies may play a significant role in the diffusion of each species and work on an interstitial diffusion model is ongoing.

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