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# STABILITY AND MOBILITY OF SELF-INTERSTITIAL ATOMS AND THEIR CLUSTERS IN Fe-Cr ALLOYS: AN ATOMIC-LEVEL STUDY

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## ABSTRACT

We used DFT calculations and a recently developed empirical potential for FeCr to study in detail the stability and mobility of single-SIA and SIA clusters in FeCr alloys of different concentrations, up to 15%Cr. We show that the presence of Cr creates local trapping configurations that can significantly reduce the mobility of single SIA and SIA clusters, thereby explaining a number of experimental observations. The obtained results provide quantitative estimates of this effect for different FeCr compositions.

*Key Words*: Fe-Cr alloys, interstitial, interstitial clusters, mobility, atomistic computer simulation

## 1. INTRODUCTION

High-Cr ferritic/martensitic steels are being considered as structural materials for a large number of future nuclear applications, from fusion to accelerator-driven systems and GenIV reactors. Fe-Cr alloys can be used as model materials to investigate some of the mechanisms governing their microstructural evolution under irradiation and its correlation to changes in their macroscopic properties.

Both ab-initio calculations and experimental evidence show that Cr has a strong interaction with self-interstitial atoms (SIA) and SIA clusters in bcc-Fe. Not only is the mixed dumbbell deduced to be stable from resistivity recovery experiments [1], but stage I (free migration and correlated recombination of single SIA) appears to be strongly suppressed in concentrated FeCr alloys [2] and the presence of Cr is seen to increase radiation-induced hardening [3], slow down loop

mobility [4] and segregate at loop edges [5]. Density functional theory (DFT) calculations show that the mixed dumbbell is indeed stable and that an even stronger attraction exists between crowdions and Cr atoms [6]. They also show that single dumbbells are trapped by specific local Cr configurations, whose existence has also been postulated on the basis of experimental observations [7]. Allowing in a quantitative way for these effects is important in order to develop models capable of describing the microstructure evolution in irradiated FeCr model alloys and high-Cr steels, because SIA and SIA cluster stability and mobility have a fundamental impact on it. For this reason, effort has been recently put to produce an empirical interatomic potential [8] that correctly reflects the SIA-Cr interaction, as well as the sign-changing mixing enthalpy [9].

In the present paper the existing DFT data base of Cr trapping configurations for single SIA is extended and used to validate the reliability of the developed interatomic potential. Next, the potential is used to study the effect of Cr on the stability and mobility of single SIA and SIA clusters, by means of both static and dynamic atomistic calculations. These findings are used to provide explanations to a number of experimental observations concerning irradiated FeCr alloys.

## 2. SOME RESULTS

The results are presented in three sections: DFT results, empirical potential (EP) results for single SIA and small clusters, EP results for one-dimensionally migrating SIA clusters.

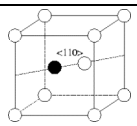
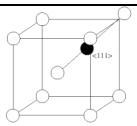
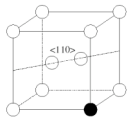
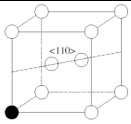
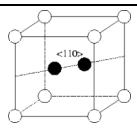
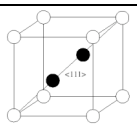
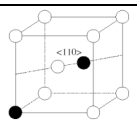
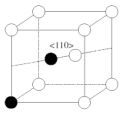
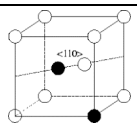
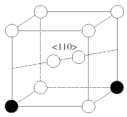
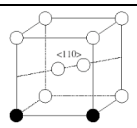
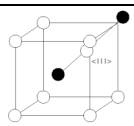
### 2.1. DFT and EP Results

Table I shows a few examples of SIA-Cr configurations in an Fe matrix and provides the corresponding binding energy as calculated by DFT and using the EP. Clearly, the results of the EP are in line with those obtained by DFT in most cases and the configurations can be either strongly binding or repulsive. It should be noted that the calculations shown in the table have been performed in an otherwise pure Fe matrix. The presence of other Cr atoms is expected to change the energy of these configurations. For example, in the presence of 12 extra monatomically dispersed Cr atoms far away from the interstitial, the binding energy of configuration 10 is 0.29 eV according to DFT, i.e. it changes not only value, but also sign, becoming attractive. A full study of all possible Cr configurations, however, can only be performed using the EP.

### 2.2. EP results for single SIA and SIA clusters

Fig. 1 shows the distribution of formation energies for changing Cr configurations around an Fe-Fe dumbbell, as calculated statically using the EP, for different Cr concentrations. It is seen that the energy state distribution becomes broader with increasing Cr concentration and that the most frequent energy state shifts to lower energy, thereby increasing the corresponding average trapping energy. Similar results are obtained for other small clusters characterised by three-dimensional migration.

**Table I. Binding energies of different Cr-SIA configurations: DFT and EP**

| Configuration | DFT | EP | Configuration | DFT | EP |
|---|---|---|---|---|---|
| 1.  | 0.08 | 0.14 | 7.  | 0.37 | 0.40 |
| 2.  | -0.08 | 0.16 | 8.  | 0.05 | 0.11 |
| 3.  | -0.42 | -0.29 | 9.  | 0.22 | -0.02 |
| 4.  | 0.15 | 0.04 | 10.  | -0.21 | -0.07 |
| 5.  | -0.02 | 0.13 | 11.  | 0.15 | 0.19 |
| 6.  | -0.04 | -0.05 | 12.  | 0.55 | 0.65 |

## 2.3. EP results for one-dimensionally migrating SIA clusters

Fig. 2 shows the result of molecular dynamics studies performed with the EP to obtain the one-dimensionally migrating SIA cluster diffusivity in FeCr and pure Fe. The ratio of the diffusion coefficient in FeCr to that in Fe is plotted versus Cr concentration. It can be seen that this ratio first decreases and then increases and that the minimum ratio shifts to lower Cr concentrations for larger cluster sizes. These results can be rationalized within the model proposed in [10], which allows the experimentally measured Cr concentration dependence of swelling rates in FeCr alloys to be qualitatively explained [11].

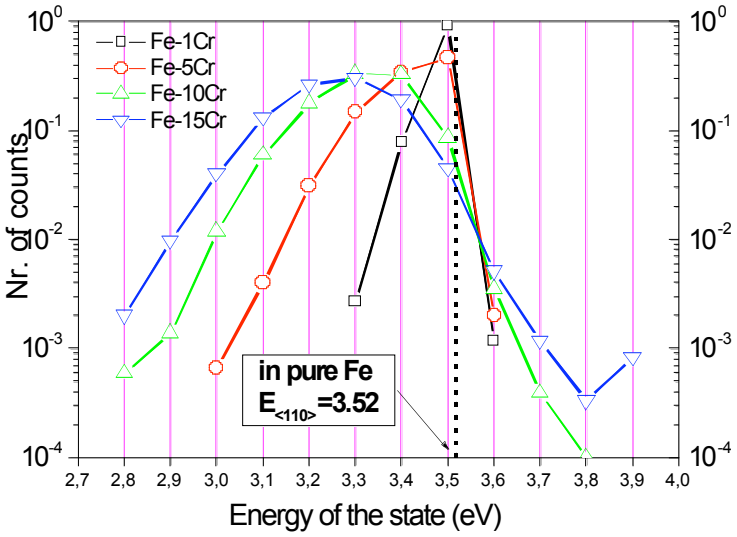



**Figure 1. Energies of state for different Cr-SIA configurations in Fe-Cr alloys of different concentrations. The energy of the Fe-Fe dumbbell in pure Fe is indicated for reference.**

## 3. CONCLUSIONS

The present work shows that modelling radiation-induced microstructure evolution in concentrated alloys where, as in Fe-Cr, solute atoms interact strongly with point-defects and point-defect clusters requires a large amount of calculations in order to be able to assess quantitatively the effect of solutes on, for example, SIA cluster mobility. The existence of a large amount of trapping configurations for single SIA and SIA clusters can be used to explain qualitatively the suppression of recovery stages in FeCr compared to Fe observed in resistivity recovery experiments [1,2,7]. It also provides a key for explaining the increased density of small loops experimentally observed in irradiated FeCr compared to Fe [5]. The results of larger clusters that can only migrate one-dimensionally can be used to explain the swelling decrease and then increase observed when adding Cr to Fe [10-12], as well as the experimentally observed slowing down [4]. More quantitative results can possibly be obtained by introducing our data (energy state distributions, reduction of diffusion coefficient) in specific models describing the evolution of the microstructure as a function of time, dose or temperature.

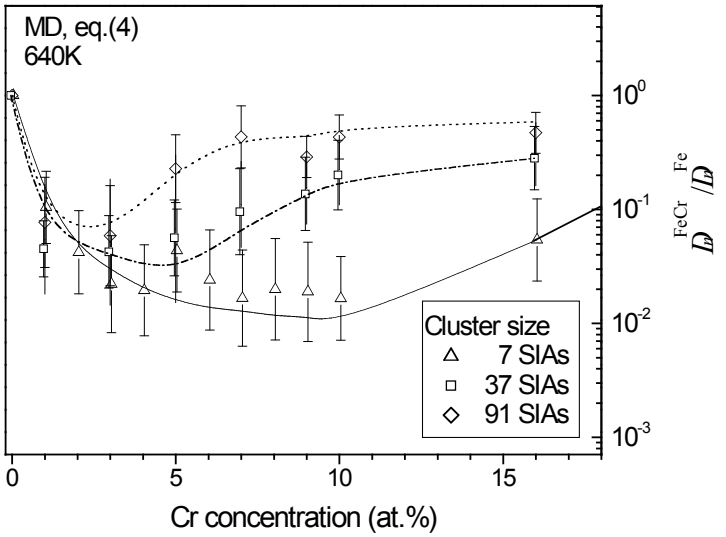



**Figure 2. Ratio between SIA cluster diffusion coefficient in FeCr and in Fe versus Cr concentration for different cluster sizes.**

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