

Background

Irradiation with high-energy particles, such as neutrons, ions and electrons, produces microstructural changes in materials. This happens because point defects, i.e. SIA (self-interstitial atoms) and vacancies, are generated in quantities well above the thermodynamic equilibrium concentration and aggregate to form clusters (dislocation loops and small cavities) and then more complex structures (dislocation networks, ...) or interact with impurities and solute atoms, thereby enhancing or inducing phenomena such as precipitation and phase segregation. These microstructural changes will in turn affect the macroscopic properties of the material. It is therefore of fundamental importance, in order to understand and possibly predict the behaviour of materials under irradiation, to be able to model the corresponding microstructural evolution. This evolution is driven mainly by processes taking place at the atomic level, thus at the scale of nanometers and pico- or nanoseconds, and in many cases it is experimentally impossible to obtain detailed information about them. For the study of these processes atomistic computer simulation is therefore a powerful tool and in fact often the only one that can be used.

The most important class of structural materials for nuclear applications are iron alloys and for this reason atomistic computer simulation has been extensively applied to the study of radiation damage in these materials. Yet, there are still features of their microstructural evolution under irradiation that are not fully understood. As a matter of fact, TEM (transmission electron microscopy) studies of irradiated iron, both pure and alloyed, revealed already 40 years ago that two types of dislocation loops can be created in these materials, namely $\frac{1}{2}a\langle 111 \rangle$ and $a\langle 100 \rangle$, whose effect on the macroscopic properties can be drastically different. Atomistic simulations in iron clearly show the formation of $\frac{1}{2}a\langle 111 \rangle$ loops, but these are invariably found to be energetically more favourable than $a\langle 100 \rangle$ loops and despite the number of proposed possible mechanisms to form $a\langle 100 \rangle$, no definitive conclusion has yet been drawn to explain their existence.

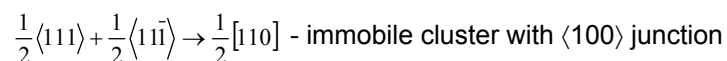
Objectives

In this work we have performed molecular dynamics (MD) studies of SIA cluster properties and interactions between them in iron, with the purpose of finding an explanation for the formation of $a\langle 100 \rangle$ loops under irradiation. These studies have been performed using a recent interatomic potential, capable of reproducing more closely than previous ones the energetics of interstitial configurations in iron. The ultimate aim of the work is to be able to parameterise more correctly larger scale models, such as those based on the use of rate equations and numerical Monte Carlo techniques, capable of actually describing the microstructural evolution in irradiated materials and to provide results comparable with the experimental ones.

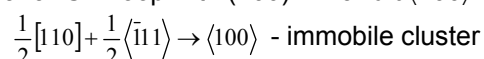
Principal results

We have considered interactions between fast gliding $\frac{1}{2}a\langle 111 \rangle$ SIA loops and observed several types of reaction products, depending on the angle of interaction between clusters, cluster sizes and also temperature. Only the most relevant interaction found is described in what follows and illustrated by snapshots in the figure.

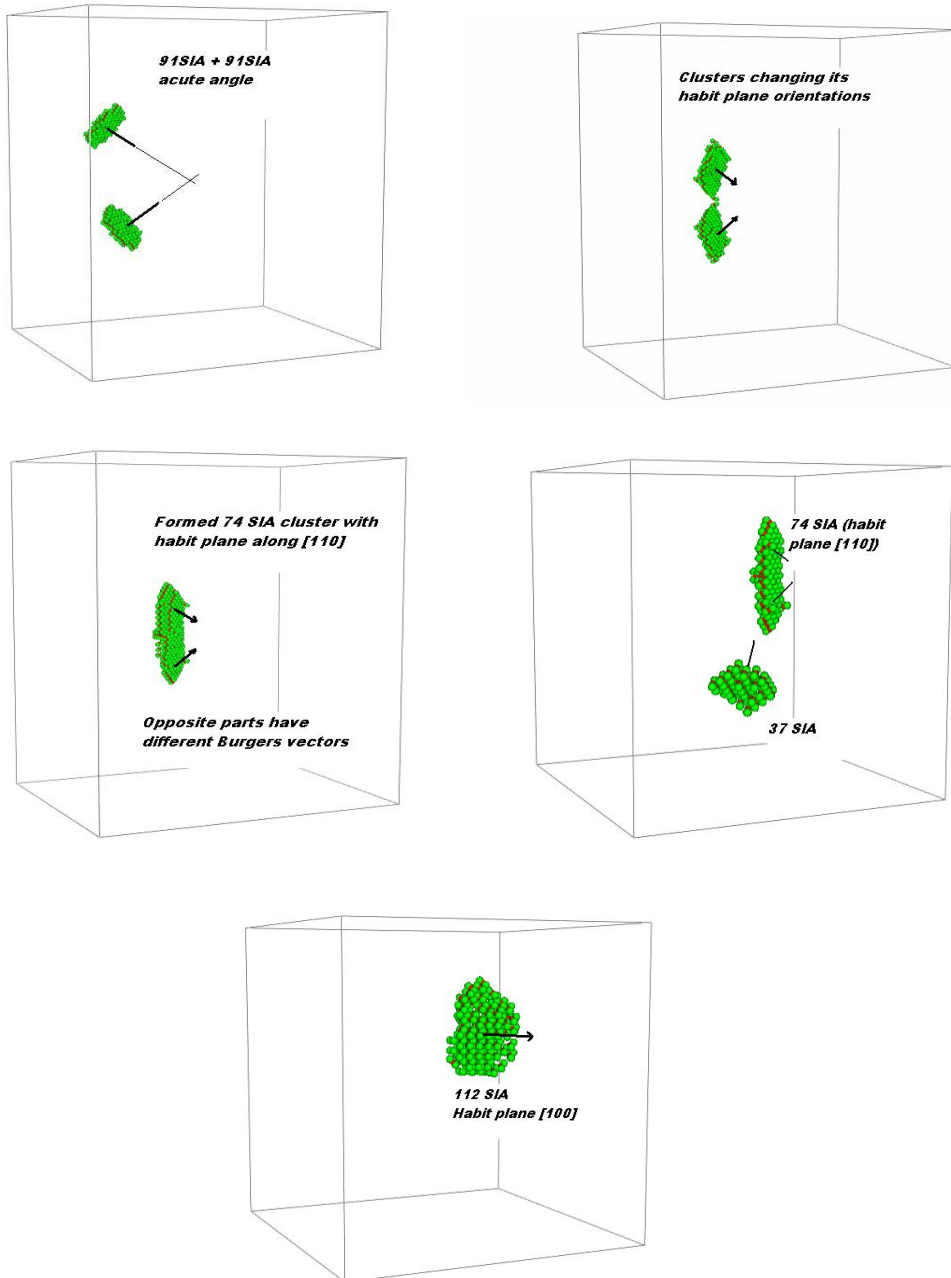
When two $\frac{1}{2}a\langle 111 \rangle$ loops of similar size (~ 4 nm \varnothing) approach each other along directions intersecting at acute angles, they rotate their habit planes (HP) to (110) , while keeping their initial Burgers vector. As soon as they join, they get to share the same (110) plane, creating a junction where the Burgers vector becomes $\langle 100 \rangle$:



If now the product of interaction this reaction, i.e. the immobile planar cluster with (110) HP, interacts with another $\frac{1}{2}a\langle 111 \rangle$ loop, whose Burgers vector must be non-collinear with those of the first two interacting clusters, then the formation of a planar SIA loop with (100) HP and $a\langle 100 \rangle$ Burgers vector is produced.



Both these successive reactions lead to a decrease of the energy of the system, which means that the final products are stable. The binding energies of the formed complexes depend on the sizes of the reacting species and are of the order of tens of eV. Although further studies are needed, this three-loop reaction appears to be a possible mechanism for the formation of $a\langle 100 \rangle$ loops.



Future work

The introduction of the reactions obtained by MD simulation in rate equation and kinetic Monte Carlo models is expected to allow a more correct prediction of the microstructural evolution of iron alloys under irradiation. The following step will be the investigation of the stability of SIA loop configurations and of the above described reactions in iron alloys. In particular, alloys containing up to ~15% Cr (range of composition of high-Cr ferritic/martensitic steels for nuclear applications) will be studied, since it has been already shown that Cr affects the mobility of SIA clusters and may therefore have an effect on their stability and interaction as well, as also suggested by a number of experimental studies.

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