Authors:
Ville Jansson
Department of Physics
P.O. Box 43 (Pehr Kalms gata 2)
ville.b.c.jansson@gmail.com
FI-00014 UNIVERSITY OF HELSINKI, FINLAND
Flyura Djurabekova
Department of Physics
P.O. Box 43 (Pehr Kalms gata 2)
FI-00014 UNIVERSITY OF HELSINKI, FINLAND
Monica Chiapetto
Institute of Nuclear Materials, SCK-CEN
2400 MOL, BELGIUM
Lorenzo Malerba
Institute of Nuclear Materials, SCK-CEN
2400 MOL, BELGIUM

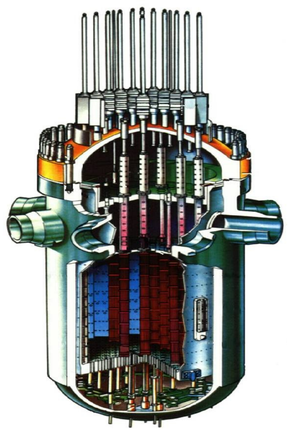
Object Kinetic Monte Carlo

Radiation-induced nanostructure evolution in FeC alloys

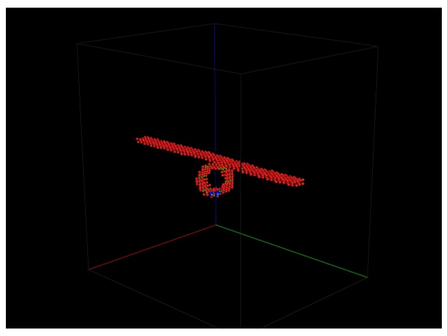
Introduction

Neutron irradiation induces populations of point defects and defect clusters in steels that in the long term cause degradation of the mechanical properties of the materials. These processes are important to understand to e.g. ensure the integrity of the steel wall of the reactor pressure vessel (RPV) during the operational life-time of a nuclear power plant.

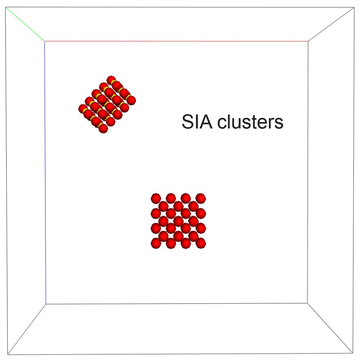
In this work we show how the Object Kinetic Monte Carlo simulation method have been used to build a model of the evolution of the radiation-induced defect cluster populations in Fe-C, the basic model alloy for any steel. The results of the model can be used by higher order simulation models, such as Dislocation Dynamics, to understand the mechanical properties of the materials.



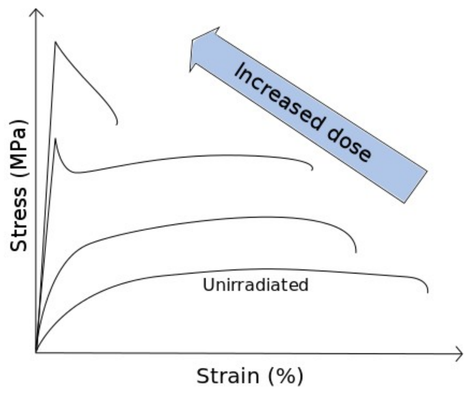
Reactor pressure vessel (RPV)

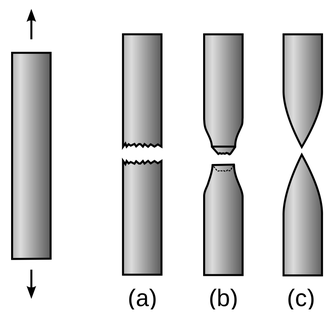


Small C-V clusters are able to trap large dislocation loops (SIA clusters), that in turn are able tor trap dislocations. [N. Anento, A. Serra]



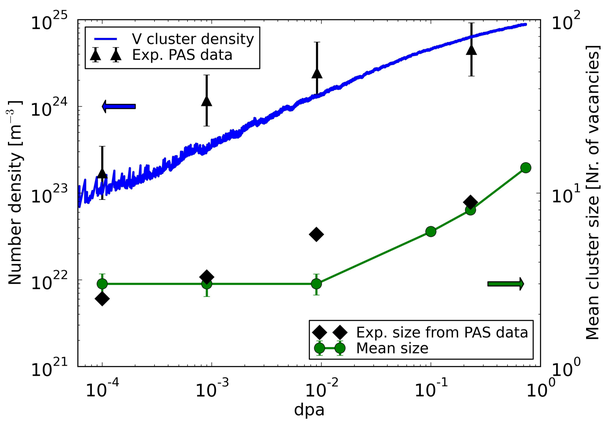
Self-interstitial atom (SIA) clusters are formed like platelets. In Fe, two families of clusters can be distinguished, depending on how the SIA dumbbels are oriented in the cluster: In the 1/2<111> or <100> direction. The 1/2<111> SIA clusters are much more mobile than the <100> type. Large SIA clusters (>150 SIA) become loop-shaped.

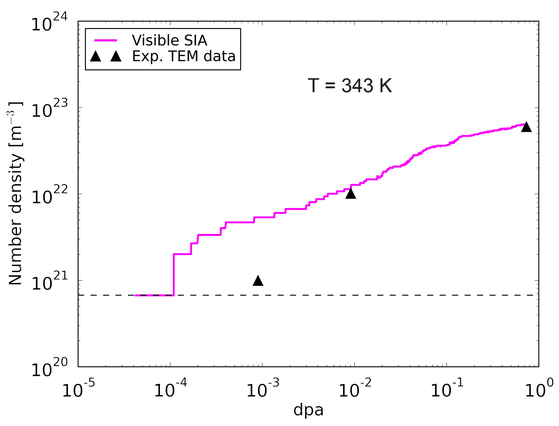




Irradiation induces populations of vacancy (V) and SIA clusters into the material. These cluster populations will hinder the mobility of dislocations, which makes the material brittle over time, as can be obeserved in tensile tests (a).

Results





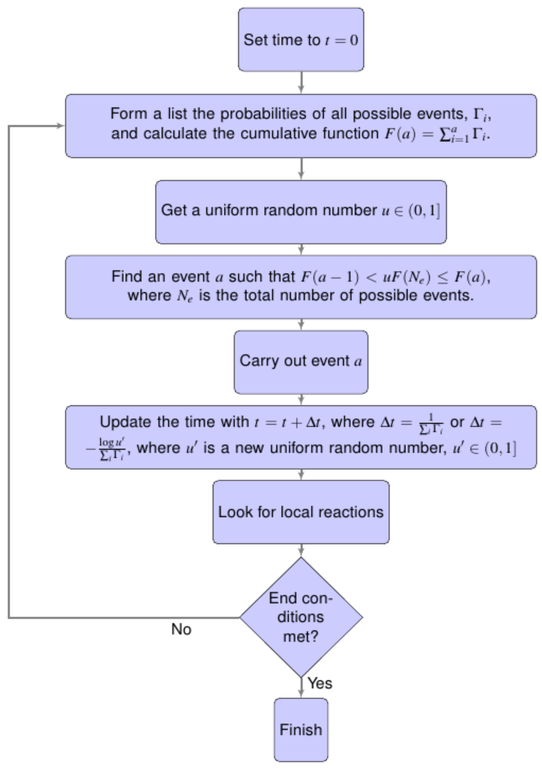
Examples of results from the Fe-C model: Vacancy cluster density and mean size vs displacement per atom (dpa), a measure of accumulated irradiation damage in the material (0.2 dpa ~ 60 years in the RPV of a typical reactor). The data is compared with experimental Positron Annihilation Spectroscopy (PAS) data. To the right is the cluster density evolution for SIA clusters. Only SIA clusters large enough to be obeserved in a Transmission Electron Microsope (TEM) are considered in the figure.

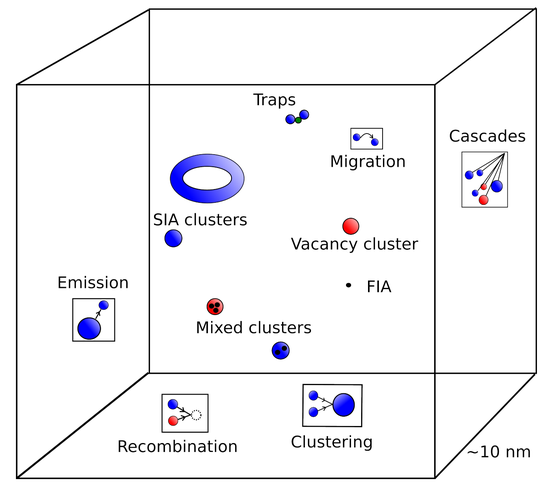
Simulation of the nanostructure evolution under irradiation in Fe-C alloys, V. Jansson and L. Malerba, Journal of Nuclear Materials 443 (2013) 274--285.

OKMC simulations of Fe-C systems under irradiation: sensitivity studies, V. Jansson and L. Malerba. Submitted to Journal of Nuclear Materials.

The nanostructure evolution in Fe-C systems under irradiation at 560 K, V. Jansson, M. Chiapetto and L. Malerba. Journal of Nuclear Materials 442 (2013) 341--349.

Method: OKMC





Objects and events in OKMC

In Object Kinetic Monte Carlo (OKMC), clusters and defects are defined as ”objects” with pre-definded characteristics, such as how they migrate and how they interact with each other. Possible events in this model are migration jumps, defect emissions from objects, and cascades. The two former events are thermally activated and their probability frequency are given by the formula:

$$\Gamma = \nu \exp \frac{-E_a}{k_B T}$$

Where ν is the attempt frequency, E_a the activation energy, T the temperature and k_B the Boltzmann's constant. $E_a = E_m$ (the migration energy) for migration events and $E_a = E_m + E_b$ (migration + binding enenrgy) for emission events. **All probabilities for all possible events in the system need to be pre-defined in OKMC.**

OKMC does not consider the bulk atoms, but only the defect clusters. In Atomistic KMC, which considers every atom in the sysytem (and not clusters as special objects), the bulk atoms are taken into account. The main challenge of AKMC is to tabulate all energy barriers for all possible atom jumps in the lattice. These tables tends to be very large and memory-consuming and other methods, like artificial intelligence, have successfully been deplyed to speed up the simulations.

The time step is inverse proportional to the sum of all event probabilities in the system, as given by the Resident Time formula:

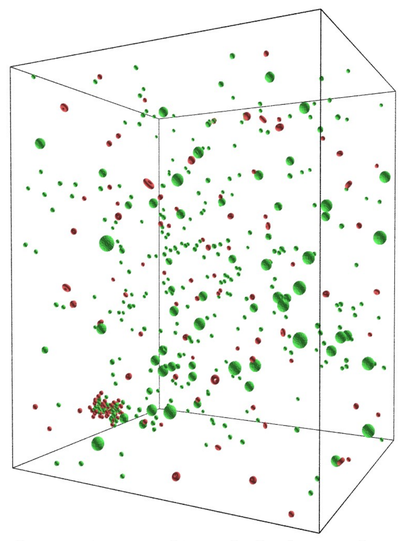
$$\Delta t = \frac{1}{\sum_i \Gamma_i}$$

The time step will be small when only fast-moving objects are present in the system and large with only slow-moving objects present. This allows for simulation of processes that may take femtoseconds to years – even decades.

Discussion

The Object Kinetic Monte Carlo (OKMC) method has been used to build a model for the radiation-induced nanostructure evolution in Fe-C. The model correctly reproduces experimental data in terms of vacancy and self-interstitial atom (SIA) cluster densities and mean size evolutions at both low (<470 K) and high (560 K) irradiation temperature. The model is also able to reproduce a post-irradiation annealing experiment. The model shows the importance of the presense of carbon and carbon-vacancy complexes for the nanostructure evolution, as these complexes are able to trap the mobile SIA clusters and allow these clusters to grow large.

OKMC is a good method for simulating processes too slow to be simulated by Molecular Dynamics. The method is well suitable to simulate defects in solids, as long as the probabilites of the preocesses, such as diffusion and emission are known. The system does not need to be three-dimensional, but can also be a surface. If needed, instead of considering only the clusters, every single atom in the system might be considered (Atomistic KMC). The precision of the simulation is then increased, but the simulation will be computationally more expensive. The proper choice between AKMC and OKMC depends on the nature of the research problem.



Fe-C system after 0.2 dpa of irradiation at 563 K. Green defects are V clusters and red SIA clusters.

Simulation videos:

343 K 563 K

HELSINGIN YLIOPISTO
HELSINGFORS UNIVERSITET
UNIVERSITY OF HELSINKI
MATEMAATTIS-LUONNONTIETEELLINEN TIEDEKUNTA
MATEMATISK-NATURVETENSKAPLIGA FAKULTETEN
FACULTY OF SCIENCE