

Séminaire du SRMP

**Mardi 30 Août
Salle 109, Bâtiment 520
CEA Saclay
10h30**

Object kinetic Monte Carlo calculations of damage accumulation in irradiated Fe and FeCr alloys

**Prof. Maria José Caturla
Universidad de Alicante, Spain**

In this talk we will describe our latest object kinetic Monte Carlo (OKMC) calculations in Fe and FeCr alloys. Regarding Fe, we will describe our work on the nucleation and growth of voids and bubbles at grain boundaries in the presence of He. All parameters describing defect mobilities and defect stabilities have been calculated using DFT by the CEA group at Saclay. Simulations show how, as expected, grain boundaries enhance the formation of voids, but they also allow us to study in detail the different mechanisms for growth and, therefore, the nature of these defects, at different temperatures.

The results obtained in an OKMC simulation will, in most cases, depend on the initial conditions considered. In collaboration with Carolina Björkas and Kai Nordlund, we have studied the influence of the cascade damage obtained from different interatomic potentials on the accumulation of damage during irradiation of Fe. Simulations show that the initial cluster distribution will influence the rate of damage accumulation, something that could be directly compared to experiments. This also means that when validating models with experiments performed in thin films a special care must be taken with the initial damage distribution. We will present our preliminary molecular dynamics results of cascade damage in Fe thin films by Fe ions of energies between 100 and 150keV.

Finally, our OKMC simulations of the resistivity recovery of diluted FeCr alloys will be presented, as well as our latest developments in trying to study concentrated FeCr alloys with an OKMC model.