

Kinetic Monte Carlo for irradiated Fe: Impact of Carbon and dislocation loops, and Cr segregation

Dr. Ignacio Martin Bragado (IMDEA Materials Institute Madrid)

In this talk, we will introduce two recent advances on the modeling of Fe using Object Kinetic Monte Carlo (OKMC) modeling will be reviewed: a) the evolution of dislocation loops in iron under irradiation, and the importance of the impact of carbon, will be shown. b) A quasi-atomistic extension of such models to the FeCr binary alloy will be explained.

In particular, we have studied for a) the impact of carbon content on the evolution of nanosized Dislocation Loops (DL) in bcc Fe with dissolved interstitial C atoms and introduced the direct diffusion and explicit interactions of C in an OKMC model. The DL population is demonstrated to vary strongly with the carbon matrix concentration and irradiation temperature/flux, reproducing accurately in-situ TEM observations. The model reveals the physical origin for several temperature regimes, linked to a dominant mechanism of carbon loop trapping.

We will also present in b) a quasi-atomistic OKMC model for α/α' decomposition in FeCr. The model describes atomistically the defects driving diffusion, while following the alloy concentration evolution. We are able to reproduce both phase nucleation in the metastable composition region, and the spontaneous phase decomposition and coarsening within the spinodal decomposition region, together with the time evolution of such processes.