EXMONAN

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Atomistic Modelling of Segregation and Precipitation under irradiation in Fe-Cr and Fe-Cr-C alloys

F. Soisson

DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette, France.

Kinetics of segregation and precipitation under irradiation result from a balance between several competing mechanisms: the acceleration of diffusion due to high supersaturations of vacancies and self-interstitials, the annihilation of these point defects at sinks, such as grain boundaries, dislocations or clusters, the coupling between fluxes of solute and point defects, the ballistic mixing within displacements cascades.

We present a review of a recent atomic scale modelling of Fe-Cr and Fe-Cr-C alloys under irradiation, using ab initio calculations, cluster dynamics and kinetic Monte Carlo simulations, which takes into account these different mechanisms. Fe-Cr and Fe-Cr-C alloys are the base of ferritic steels, used in a wide range of nuclear applications. Below 600°C, they undergo a coherent decomposition between Fe-rich (α) and Cr-rich (α') phases [1]. The simulations show, that depending on the irradiation conditions, the α-α' phase separation can be accelerated by orders of magnitude or completely suppressed [2]. They also show that irradiation may lead to a radiation-induced segregation of Cr at grain boundaries, which can enhance or oppose equilibrium [3]. Finally, we consider the possible effects of carbon atoms (and other interstitial impurities) on the α' precipitation, which result from the strong vacancy-carbon interaction in Fe-based alloys.

[1] O. Senninger, E. Martínez, F. Soisson, M. Nastar, Y. Bréchet, Acta Mater. 73, 97-106 (2014).

[2] F. Soisson, T. Jourdan, Acta Mater. 103, 870-881 (2016)

[3] O. Senninger, F. Soisson, E. Martinez, M. Nastar, C.-C. Fu, Y. Bréchet, Acta Mater. 103, 1-11 (2016).