High throughput DFT calculations in metals: synergy of irradiation defects and solutes and combinatorial configurations

C. Domain[1,3], C.S. Becquart[2,3]

[1] EDF R&D, Dpt Matériaux & Mécanique des Composants Les Renardieres, Moret sur Loing, France
[2] Univ. Lille, CNRS, INRA, ENSCL, UMR 8207 - UMET - Unité Matériaux et Transformations, F-59000 Lille, France
[3] EM2VM, Joint laboratory Study and Modeling of the Microstructure for Ageing of Materials

In a classical nuclear power plant, the components near the reactor, such as the cladding (made out of Zr alloys) or the internal structures (austenitic steels) and to a lesser extent the pressure vessel (bainitic / ferritic steels), are subjected to neutron bombardment. In a fusion reactor, high energy particles (H isotopes and He) as well as 14 MeV neutrons bombard the walls (ferritic martensitic steels) and the divertor (tungsten alloys).

In order to predict and understand the ageing of structural materials, a multiscale modelling approach is developed to simulate the microstructure evolution under irradiation. It is based on the key physical phenomena the material experiences. In this approach, there are two main inputs with a strong impact on the microstructure obtained: (i) the source term constituted by the formation of point defects and displacement cascades and (ii) the properties of the defect clusters and solute-defect clusters formed. The key properties of defects and defect clusters are their stability and mobility, e.g. binding energies and migration energies (the material evolution is described in terms of elementary physical mechanisms), which are the inputs of kinetic Monte Carlo models for the modelling of the microstructure evolution.

Industrial alloys are multi-component alloys and the number of possible interactions between solute and defect clusters increases rapidly with the number of solute present. A typical example is the reactor pressure vessel steels, where the main elements observed in the clusters formed under irradiation contain Cu, Ni, Mn, Si as well as P. In order to characterize all the possible interactions between these solutes and the point defects, to build cohesive models, a large number of DFT calculations are necessary, that represent thousands to tens of thousands calculations and billions of CPU hours.