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Multi-scale modeling of ageing and radiation damage of structural materials starting from ab initio calculations

Structural metallic materials used in nuclear facilities are, in addition to thermal ageing, submitted to irradiation which induces the creation of large amounts of point defects. These defects interact with each other as well as with the different elements constituting the alloys, e.g. industrial steels. This, in turn leads to modifications of the microstructure and the mechanical properties. The principal materials concerned are ferritic steels, FeCr alloys and austenitic steels as well as zirconium alloys.

In the framework of multiscale modelling of materials, both the microstructure and the plasticity is simulated. Ab initio DFT calculations are carried out to characterise the elementary mechanisms involved in the ageing of the materials under sollicitation. The resulting quantities on these mechanisms, such as interaction energies or migration energies, are used in larger scale simulation methods in order to predict the microstructure evolution: in molecular dynamics to fit or assess the potentials, in atomic and object kinetic Monte Carlo models as well as in rate theory calculations.

Ab initio methods have been for instance used to determine the properties of point defect clusters as well as those of extended defects such as dislocations in pure metals. The next step towards steels properties, is to take into account the effect of the chemical composition and extensive atomic study of the effect of solute and carbon in Fe ferritic based alloys have been performed. These ab initio data have been used to model the evolution under irradiation of the microstructure of dilute Fe alloys (Fe-CuNiMnSiP-C), representative of the dilute ferritic steels of pressure vessels, using kinetic Monte Carlo (KMC). For this purpose, a Kinetic Monte Carlo model has been developed to investigate the evolution of solute atoms such as Cu, Ni, Mn, Si and P in the presence of point defects (both vacancies and self interstitials). These ab initio data are also used to parameterise object kinetic Monte Carlo to model the long term evolution of the microstructure under irradiation.

The study and atomic modelling of concentrated alloys, e.g. austenitic model alloys, is also underway and first results will also be presented. Furthermore, the recent progress in computation speed renders ab initio molecular dynamics feasible, with system size and simulation time sufficient to study dynamical properties. Some results on the mobility of defects as well as the threshold displacement energies to create defects will also be presented.