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Modelling irradiation effect of EUROFER under Fusion Power Plant-Relevant Conditions

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In fusion power reactor, the properties that controlled the behaviour of materials are affected at the atom scale: (i) the crystalline structure is locally destroyed where a displacement cascade occurs, (ii) the chemical bond is affected by transmutation products such as He and H, (iii) an radiation induced microstructure will take place due the diffusion of these point defects and impurities EFDA has launched a programme since 2002 to develop and validate modelling tools to predict the radiation effects in the reference ferritic martensitic steel Eurofer. Up to now, the effort has been devoted (i) to validate the multi-scale modelling approach based on ab-initio energetics map of point defects and He, (iii) to develop inter-atomic potentials for Molecular Dynamics simulation of displacement cascades and dislocation dynamics.

Formation and migration energies and diffusion mechanisms of small vacancy (n<) and interstitial clusters (n<) were computed with the ab-initio code SIESTA and used to successfully predict via Kinetic Monte Carlo the experimental recovery stages of radiation damage in ultra high purity Fe. A complete He and point defect energetics mapping was ab-initio determined in Fe-C and used to reproduce via Rate Theory He-desorption from pre-implanted specimens. A developed “magnetic” potential is capable of transferring the magnetic properties of Fe due to the 3d-electron correlation to the scale of the Molecular Dynamics. An inter-atomic potential is being developed to reproduce the thermodynamics of the Fe-Cr system.

The program will now be devoted (i) to develop atom-scale reference kinetic methods to predict the phase – stability of the Fe-Cr thermally and under irradiation (ii) to predict at the atom scale the core structure and dynamics of screw dislocation and their collective behaviour at the meso-scale, using Discrete Dislocation Dynamics (iii) to validate at the relevant scale using the multi-beam CEA-CNRS facility JANNUS. JANNUS allows irradiating with double (dpa, He) or triple (dpa, He, H) beam and characterising (TEM, AP-FIM, nano-identation) volume of materials of the same order as the ones that can be simulated. The strategy with materials with increasing complexity of chemical composition and initial microstructure will be presented. The resulting modelling tools and associated data base should be used to correlate exoperimental data from varied irradiation source and to optimize IFMIF testing programme and extrapolate the results with enhanced confidence.