Interaction of high flux plasma with Fe and RAFM steels: experimental and computational assessment

A. Bakaeva, D. Terentyev, A. Puype, A. Dubinko

SCK•CEN, Nuclear Materials Science Institute, Boeretang 200, 2400 Mol, Belgium

As a contribution to the CRP on "Plasma–Wall Interaction with Reduced Activation Steel Surfaces in Fusion Devices", over 2017-2018 we have completed the computational assessment at atomic scale to characterize the interaction of hydrogen with dislocation micostructure in BCC Fe, as prototype material for F/M steel. The impact of high flux deuterium plasma on iron and several RAFM steel samples was also studied. In both cases, the analysis was mainly dedicated to understanding of the trapping and retention of D atoms in the matrix, and microstructural changes induced by the high flux plasma.

In brief, the atomic-scale computational analysis was performed to characterize the residence of H atoms in bcc Iron matrix and its self-interaction, interaction with vacancies and dislocations. It has been revealed that H exhibits rather weak self-interaction (binding energy of 0.22 eV), and the formation of multiple hydrogen clusters is not conducted by the release of self-interstitial Fe thus creating the thermally stable Hn-vacancy complex – contrary to the situation with Helium. The interaction energy with screw and edge dislocation was found to be 0.27 and 0.47 eV, respectively. However, the energy landscape of corresponding to the Hn cluster on the dislocation line neither revealed a possibility of the transformation of such complex into the stable cluster accommodated with the emission of kinks. Finally, the binding of H and Hn clusters with a single vacancy was assessed. The binding of a single H amounts to 0.62 eV, and two more H atoms are bound without losing the binding strength. Fourth and fifth atoms can be further added, but the corresponding binding energy goes down to 0.2 eV. The addition of the sixth atom is no longer favourbale. Hence, the growth of Hn cluster on vacancy or dislocation line should occur given the external source of free vacancies, which could be supplied thanks to intensive plastic deformation of the sub-surface region under high flux plasma exposure.

On the experimental side, two sets of exposure were performed, namely: (i) pure Iron in reference and heavily deformed state; (ii) exposure of several RAFM steels including two chemically tailored grades produced specially to improve the mechanical properties and two conventional 9Cr steels – Eurofer97 and T91. Two advanced grades were produced by applying thermo-mechanical-chemical (TMC) treatment. By performing primary mechanical testing it has been revealed that while preserving acceptable yield strength and ultimate tensile strength, the ductile to brittle transition temperature was shifted down to approximately -140 °C. This grade and two standard 9Cr grades (T91 and Eurofer97) have been selected for the preliminary high flux plasma exposures at Pilot-PSI linear plasma generator in Netherlands. The exposure temperature was 450K. The thermal desorption spectroscopy (TDS), scanning electron microscopy (SEM) and transmission electron microscopy (TEM) analysis has been performed on as-exposed materials. The TDS has revealed one major release stage at 450K-500K and several minor release stages in the temperature range 700-1000K. Plastic deformation applied to pure Fe resulted in the increase of the trapping of H released at stage I, but also invoke the appearance of the second release stage around 650K. It has been discussed that this release stage is probably due to the pinning at the sub-grains formed as a result of the heavy plastic deformation. The SEM analysis revealed quite strong surface modifications in a form of slip bands, roughening and rarely observed blister-like surface defects (the nature is still to be confirmed) in pure Fe and conventional RaFM steels. The surface modification was clearly less evident for the advanced TMC grade.