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Effect of thermal and collisional processes on the performance of plasma-facing components in mixed materials environment ^{1*}

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Understanding the performance of plasma facing materials (PFMs) during reactor operation in multi-materials environment depends on several factors such as dynamic evolution of materials composition of plasma facing components (PFCs), presence of gases from chamber environment and from gas injection system, and impurities accompanying the DT flux to PFCs. The interplay of these effects can add significant complexity to understanding the effects of core plasma particles impacts on PFC surfaces, materials lifetime, fuel particle recycling, and overall plasma performance. This is an important area for the successful operation of the tokamaks and requires comprehensive integration of various effects and the interplay of all physical processes involved.

We enhanced our Monte Carlo ITMC-DYN simulation package to include detail descriptions of various processes in self-consistent matter to predict PFCs erosion and composition, formation and build up of impurity layer, and various effects on hydrogen isotopes diffusion and recycling. The package includes simultaneous modeling of multiple ion species, their penetration and mixing, scattering/reflection, physical and chemical sputtering, dynamic surface evolution/modification, and potential compounds formation. Integrated modeling also includes thermal diffusion, segregation processes, and recombination/desorption of species in this multi-component surface composition.

This work summarizes our analysis of both collisional and thermal processes on the surfaces of mixed materials in the application to materials and particles parameters specific for fusion reactor conditions. Effect of carbon impurities, in particular, requires most detailed analysis since small concentrations of carbon can significantly change dynamics of hydrogen isotopes interaction with metallic walls. We showed, for example, that chemical compounds formation on the surface of liquid lithium results in essential decrease in the diffusion of deuterium to the bulk that can lead to the significant increase in hydrogen desorption from the surface and higher recycling of fuel that was found in NSTX experiments. On the other hand, small concentration of carbon on tungsten surface can provide a barrier for deuterium desorption resulting in higher accumulation in the bulk that can lead, e.g., to the blistering in tungsten. We showed that surface segregation combined with particles diffusion, enhanced by radiation damage are the processes responsible for the dramatic changes in tungsten surface evolution during the irradiation by carbon ions. Relatively small change in target temperature can lead to significant changes from carbon build-up layers on the surface resulting in minimum tungsten erosion to the enhanced erosion of tungsten. It was also shown that most important parameters in these interactions are the magnitude of carbon impurity ions influx and target temperature, while the expected range of deuterium energies is found to have small effect in reactor performance. Results of our simulations were benchmarked against several recent experiments with good agreement. This allowed explanation of various mechanisms responsible for the enhanced erosion of high-Z materials as well as expectations to future tokamaks and ITER performance.

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