ABSTRACT ICTP-2014-SMR-2614

2014 Joint ICTP-IAEA Conference on Models and Data for Plasma-Material Interaction in Fusion Devices, 3–7 November 2014, International Centre for Theoretical Physics (ICTP), Trieste, Italy.

The atomistic phenomena at the plasma-surface interfaces[1*]

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Plasma-Material Interface (PMI) is one of the largest technical challenges to the advancement of thermonuclear magnetic fusion energy due to the wall erosion lifetime, thermo-mechanical and neutron damage of the reactor containment walls exposed to the fusion plasma.

Our basic hypothesis is that much of understanding on the fundamental phenomena and much information on the interactions at the plasma-material interface can be obtained by the atomistic approach, i.e. at the time scale of sub-fs to 10 ns and at the spatial scale up to few tens of nm. We have tested this hypothesis so far on several plasma-material interfaces, amorphous carbon irradiated by hydrogen plasma, lithiated and oxidized carbon irradiated by hydrogen plasma, tungsten surface irradiated by the self-atoms and deuterium, all well integrated and in agreement with experimental validation.

How to build a theoretical approach integrated with experiment? It is worth noting that, for example, a flux of 10^{25} particles/m^{2}s at the hot gas-material interface means that, statistically, one particle is impinging on a surface of 10 nm^2 every 10 ns. This gives to the system enough time to evolve freely from the external influx of energy and particles, still staying far from equilibrium. With an impact particle energy of 100 eV this would result in heat flux of ~160 MW/m^2. However, a typical chemistry-based process, like is chemical sputtering, at impact energies $\leq$100 eV, fully evolves at the interface for less than 50 ps, implying that each impact is independent, uncorrelated, and discrete. However, each impact changes the surface, functionalizing it for the subsequent collision, i.e. building a dynamic surface with memory, and depositing energy.

By cumulative irradiation of both pre-damaged and virgin surfaces of monocrystal tungsten by deuterium atoms of impact energy of few tens of eV, we simulate by classical molecular dynamics (CMD) the creation of a deuterium "protective layer", discussing also the competing diffusive outgoing flux. The depth and width of the layer depend on the deuterium impact energy and the diffusion rate of deuterium in tungsten, the latter being influenced by the tungsten temperature and damage. Found simulation results resonate with the recent DIFFER experimental results.

It has been known that defects in tungsten, in particular at the grain boundaries and in vacancies, are preferable sites for deuterium and helium retention. We study by CMD the dynamics of the defects creation, in particular their number saturation as function of fluence. We also study the cumulative retention of deuterium at impact energies below 100 eV as functions of tungsten temperature at models of the dislocation boundaries. We obtain a strong preference of the retention of the impact particles at the boundaries at high temperature of 1000K.

The recent unexpected finding concerning carbon wall conditioning by lithium in NSTX and in a number of other fusion machines, was resolved by quantum-classical atomistic computer simulations, showing that the presence of oxygen in the surface plays the key role in the increased uptake chemistry and suppression of erosion, while lithium is decisive factor in achieving high concentrations of oxygen.

[*]This work was supported in part by the Institute of Advanced Computational Science at SUNY Stony Brook, and by the LDRD programs of Princeton Physics National Laboratory and of Oak Ridge National Laboratory.