Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Challenges in Modeling of the Plasma-Material Interface PREDRAG KRSTIC, Stony Brook University and University of Tennessee — Recent work with lithium coatings deposited on a variety of metallic and graphitic surfaces, in a number of tokamak fusion machines around the world, has provided evidence of the sensitive dependence plasma behavior has on these ultra-thin deposited films. Our computer simulations, validated by recent experiments, have elucidated roles of lithium in carbon walls to the recycling of the plasma hydrogen [1]. We performed quantum-classical atomistic calculations on many thousands of random trajectories to clarify the interplay of lithium and oxygen in amorphous carbon. We show that the presence of oxygen in the surface plays the key role in the increased uptake chemistry and suppression of erosion, while lithium has a decisive role in achieving high concentrations of oxygen in the upper layers of the surface upon bombardment by deuterium. D atoms preferentially bind with O and C-O. The plasma-facing walls of the next-generation fusion reactors will be exposed to high fluxes of neutrons and plasma-particles and will operate at high temperatures for thermodynamic efficiency. To this end we have been studying the evolution dynamics of vacancies and interstitials to high doses of tungsten surfaces bombarded by self-atoms, using classical molecular dynamics. Results show surprising saturation of the defects upon cumulative irradiation of only 1 DPA, as well as the defects clustering at the tungsten surface. These findings are obtaining validation in recent experiments.

Predrag Krstic
Stony Brook University and University of Tennessee

Date submitted: 15 Nov 2013 Electronic form version 1.4