MD Simulations of Plasma-Surface Interactions of Deuterated Carbon

P.S. KRSTIC, C.O. REINHOLD, Oak Ridge National Laboratory, S.J. STUART, Clemson University — We study plasma-surface interactions (PSI) in the first few nanometers of carbon walls, at fluences of $\sim 10^{20}$ D m$^{-2}$ and impact energies in range of tens of eV. Using an atomistic classical molecular dynamics (MD) approach we are able to take into account the full configuration space of impact plasma particles (atoms, molecules), including their rovibrational states, as well as to describe with the same level of detail the PSI outcome, i.e. of particles ejected by chemical sputtering and reflection. Understanding of the relevant PSI processes, reflecting the deuterated surface microstructure is obtained [New J. Phys. 9, 209 (2007), Europhys. Lett. 77, 33002 (2007)], as well as a good agreement with recent in-house beam-surface experiments. This increases confidence in our MD calculations for impact of plasma particles distributed at a given temperature. Our results show that the products of the PSI of deuterated carbon are significantly different from those of “pure” carbon, highlighting the importance of accounting for the hydrogen content in the walls.

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