

Abstract Submitted
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MD Modeling of the Plasma Irradiation of the Hydrogenated Carbon Surface PREDRAG S. KRSTIC, Physics Division, Oak Ridge National Laboratory — Usual approach to the molecular dynamics (MD) simulations of the plasma-surface interactions (PSI) is to average results of irradiation of the surface by a particle beam of a fixed energy and impact angle. However, we have found [1] that most of the PSI processes have a strong dependence on the instantaneous target surface microstructure (including hybridization content, in case of carbon), which is determined by the irradiation history, in particular of energy and type of the impacting particles that created the surface. Therefore, the effect of the various initial parameters that create a surface is not necessarily linearly additive: In order to improve the MD results for the experiments with plasma irradiation of the surfaces, randomization of the impact energies and angles is preferred. We use this approach to simulate sputtering and reflection of the hydrogenated carbon surfaces by hydrogen plasma, in range of temperatures 10,000-200,000 K. Isotopic effects of deuterium and tritium plasmas are also considered.

[1] P. S. Krstic, C. O. Reinhold, and S. J. Stuart, *New J. of Phys.* **9**, 219 (2007).

Predrag Krstic
Oak Ridge National Laboratory

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