Molecular modelling of plasma-surface interactions

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Plasma-surface interactions are highly complex processes, in which the various plasma factors such as the presence of ions, metastable species, electrons, photons, electric fields etc. may play a role [1, 2]. In the first part of my talk, I will show our most recent insights derived from simulating the interactions of plasmas with nano-materials employing molecular dynamics simulations, in particular in the plasma processing of carbon nanotubes.

In many cases, however, regular molecular dynamics simulations suffer from the short time scales they can cover. Indeed, plasma-surface interactions encompass mechanisms typically extending over time and length scales ranging from the nano-regime to the macroscopic regime. Modelling these interactions is in general highly challenging. In the second part of my presentation, I will therefore focus on our most recent advances in modelling and simulating plasma-surface interactions at the molecular level. In particular, we recently developed a new technique, so-called collective variable-driven hyperdynamics (CVHD), which is capable of reaching time scales up to 10^9 longer than achievable in regular molecular dynamics simulations [3, 4]. A number of example applications will be presented, including fuel pyrolysis and combustion, H-etching of graphite surfaces, and plasma-catalytic conversion of methanol on vanadia surfaces, demonstrating how such CVHD simulations may reveal new insights in plasma-surface interactions, and increase our understanding of the operative mechanisms at the molecular level.

[1] E. C. Neyts, K. Ostrikov, M. K. Sunkara, A. Bogaerts, Chem. Rev. **115**, 13408 (2015)
[2] E. C. Neyts, Plasma Chem. Plasma Processing **36**, 185 (2016)
[3] K. M. Bal, E. C. Neyts, J. Chem. Theory Comput. **11**, 4545 (2015)
[4] K. M. Bal, E. C. Neyts, Chem. Sci. **DOI**: 10.1039/C6SC00498A (2016)