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Molecular dynamics simulations of plasma-surface and plasma chemistry processes

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Due to the atomic/molecular nature of the plasma surface interactions and the reactivity of the plasma core, molecular dynamics simulations are suitable for understanding the associated basic mechanisms. This is mainly due to availability of interaction potentials of high quality, especially many body and /or reactive potentials. A wide variety of processes can be thus rigorously investigated: Atomic and molecular collisions in the gas phase, nano cluster/soot growth in the gas phase, Plasma wall interactions and surface and subsurface (nano) structuration, plasma (nano) cluster and thin-film growth on materials, Direct treatment of materials surface: nitridation, carbidization, oxidation, plasma grafting, functionalization, plasma reactivity on surfaces including supported nano catalysts. Beside the availability of the interaction potentials, careful modelling of the initial conditions for simulations, hopefully closed to experiments, is required. Moreover, there now exist strategies for including process long time dynamics in molecular dynamics simulations. Due to the high fluxes encountered in molecular dynamics simulations, caution should be paid to the treatment of energy release during bond formation, unphysical collisions, heating. The present lecture will illustrate the different methodological approaches in considering various contexts, in line with experiments, as: plasma (reactive) sputtering and deposition, plasma – catalysis, plasma chemistry, including involving biological media and radicals and plasma irradiation of materials.

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