PO1057

Numerical simulations of the deposition of hexane molecules and fragments on silicon

Lotta Mether[1], Krister Henriksson[1], Kai Nordlund[1], Canan Turgut[2], Patrick Philipp[2]

[1]University of Helsinki, University of Helsinki, Finland [2]Centre de Recherche Public – Gabriel Lippmann, Belvaux, Luxembourg

lotta.mether@helsinki.fi

In the context of plasma surface treatments, a proper understanding of the plasma-surface interaction during the deposition process is of great importance. The structure of the first monolayer of deposited matter largely determines the general properties of the deposited surface, as well as its adhesion properties in the case of reversible adhesion. The initial growth of this monolayer, in turn, is governed by the adhesion of the various molecules present in the plasma.
In order to gain insight into the molecule-surface interaction during the initial stages of the process, we perform numerical studies of the deposition of organic molecules and molecular fragments in the sub-monolayer range. The deposition process is simulated using molecular dynamics (MD), and the sticking of the various species, as well as its dependence on the energy and incidence angle, are determined. In order to minimize computational effects, we repeat the simulations using both classical and ab-initio MD. In addition, the chemical bonds between molecules and substrate are studied using static density functional theory (DFT) calculations.
In our initial work, we study the deposition of hexane molecules and fragments onto a reconstructed (100) silicon surface. We determine the sticking probability of each fragment, while systematically varying the deposition energy and incidence angle. The simulation results show no adhesion of intact hexane molecules, whereas sticking is frequent for molecular fragments, with the probability roughly decreasing for increasing fragment size and angle of incidence. In this presentation the simulation setting and numerical results of our study will be discussed in detail.

Keywords
surface functionalisation
plasma-surface interaction
molecular dynamics
DFT