MD simulation study of nanolayer formation by continuous carbon deposition on a silicon (100) surface

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One of the most important aspects in case of particle surface interaction is to observe surface deformation, defects along with reorganization and distribution of matter at the surface in the sub-monolayer range. By using molecular dynamics (MD) simulations and DFT calculations, a better understanding of distribution of atoms on the surface, surface deformation and defects information can be achieved. Level-three force fields capable of simulating the breaking and formation of chemical bonds have recently been conceived for a more realistic simulation of systems involving reactive species. In this presentation, we will use MD simulations coupled to the reactive force field developed by J. Kieffer's group [1-3] to investigate how carbon atoms deposit onto the Si(100) surface and a SiC thin film forms [4]. A (100) silicon surface having size of a 4nm x 4nm was created and continuous carbon deposition at 300K was modeled to study the formation of thin SiC films. 100 carbons were sent to the surface in a continuous manner and in such a way to have a fluence similar to experimental conditions for carbon deposition. Deposition energies ranging from 1 to 30eV were simulated with several incidence angles. The evolution of the sticking coefficient with the progressive coverage of the surface is monitored. It varies in between 0.86 to 0.99 for the variation of the fluence from 1.0×10^{14} to 5.0×10^{14} $atoms/cm^2$. The variation of the sticking coefficient with increasing fluence is not uniform. Implantation of C and distribution of C atoms in the sample as well as the amount of defects caused by the carbon implantation are monitored, showing an amorphization of the top monolayers of the sample. The damaged depth increases to 3 monolayers at 5eV and 4 monolayers at 10eV, compared to 1 monolayer at 1eV. The different properties are compared for the different angles and energies.

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