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Effect of silicon substrate crystallinity on single atom plasma deposition/implantation

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The sticking and reorganization of atoms at the surface and in the sub-monolayer range is of great importance in the field of plasma surface treatments. Although the sputtering and deposition of matter is mainly governed by the species in the plasma as well as their distributions of impact energies and incidence angle on the substrate, the local structure of the substrate may also play an important role.
Molecular dynamics simulations (MD) allow us to gain important insights into those deposition mechanisms: they enable the user to control precisely the trajectory of the incident atoms as well as the surface upon which they are being deposited. By using a level-three force field capable of modelling the breaking and formation of chemical bonds, we investigate how carbon and titanium atoms interact with different types of silicon surfaces. Two types of surfaces are considered: a crystalline (100) surface and an amorphous surface. The impact angle and/or the energy of the incident atom are varied in order to determine the condition for adhesion and the extent of atom implantation in conditions similar to plasma deposition.
While carbon implantation on crystalline surfaces is influenced by a channelling effect at incidence angles close to 45° and results in deeper implantation depths, the carbon implantation on amorphous surfaces is maximal at normal incidence. Titanium deposition, on the other hand, is much less influenced by the crystallinity of the substrate.

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