

Modeling surface interactions on the atomic scale: present status and future directions

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Gas-surface interactions in general and plasma-surface interactions in specific allow us to alter and modify surface properties. Processes relying on these interactions include the deposition of thin films, growth of nanomaterials, chemical etching and physical sputtering, catalysis, and so on. Clearly, these processes have found widespread application in many fields, ranging from micro-electronics to medical applications.

Of fundamental importance is a clear and thorough understanding of the underlying mechanisms of these processes on the atomic scale. For instance, single walled carbon nanotubes (SWNTs) have been fabricated since over 15 years by a gas-surface process, but precise control over the SWNT chirality has still not been achieved, due to an incomplete understanding of the formation process on the atomic level.

In PLASMANT at the University of Antwerp, we try to obtain this fundamental understanding through the development and use of atomic scale simulations. In this lecture, I will first present an introduction to our simulation technique and methodology, followed by a discussion of the simulated growth of nanoscopic materials. Specifically, I will address both the successes as well as the issues in our modeling of both thermal and PECVD growth of SWNTs, and the oxidation of silicon. Finally, I will also present some of our future plans regarding modeling of plasma catalysis.