2D and 3D Computational Model of Plasma-Surface Interactions

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Plasma-surface interaction is a very important topic, especially for plasma applications in materials processing. Numerical modeling of plasma interactions with various solid materials (including such processes as plasma etching, deposition, and implantation) was a subject of numerous efforts in the past, leading to development of a number of simulation codes. Still it is a long way to go to the final goal of reliable and predictive simulations that could be applied to processing in various conditions used in nanotechnology and semiconductor industry.

Low level atomic, molecular, chemical, and physical processes are responsible for complexity of a model realistically describing plasma-surface interactions. The models used in the past were ranging from quantum chemistry models (where single atoms were described at the quantum mechanical level), to molecular dynamics approaches (where targets consisting of atoms and molecules were described through inter-atomic potentials), to cellular models (where solid materials were divided into cells, each cell typically containing many molecules of specified properties), to surface models utilizing differential equations where reaction rates and yields were used to advance solid material boundaries as a result of plasma-surface interactions.

Here, we discuss a computational model of plasma-surface interactions implemented in the FPS-3D feature profile code [1]. The code uses cellular model for solid materials and is capable of treating etching, deposition, and ion implantation, both in 2D and 3D. It allows modeling of materials processing at very different scales, ranging from a few nanometers to a few micrometers. As input parameters, FPS-3D requires that the fluxes of all reactive species to the surface be provided. Those fluxes, and their energy-angle distributions, can be generated by the corresponding plasma codes. Incoming fluxes are represented by particles. Each particle is characterized by the kind of species, as well as by the energy and direction of flight. The Monte Carlo launcher generates those species in correspondence with specified fluxes, so when many particles are launched the result closely corresponds to the specified distribution of fluxes on energy and angle. A size of a Monte Carlo particle (how many molecules it contains) is typically significantly smaller than the size of a material cell, so numerical statistical artifacts could be reduced. All material properties and all reaction mechanisms are specified in the chemistry file. The Monte Carlo treatment of gas and ion reactions is defined by the reaction probability (or by reaction yield), which might depend on particle energy and the angle of incidence to the cell's normal, as well as on the surface temperature. Finite penetration depth of ions into solid materials is included in FPS-3D, which allows treatment of more complex situations such, for example, as etching through the deposited polymer layers.

[1] P. Moroz, "Numerical Simulation of Feature Profile Evolution Using FPS-3D", to be published in November 2011 issue of IEEE Transactions on Plasma Science.