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Advancements in Feature Scale Simulations

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Main industrial applications of plasmas are for the materials processing, in particular, for the semiconductor industry. Complexities of modern multi-step processes and used chemistries, as well as requirements on accuracy of processing constantly increase, while features become smaller and of higher aspect ratio. As result, searching for optimal experimental parameters becomes more difficult and could benefit significantly from numerical simulations. The corresponding feature-scale (FS) simulation codes are thus become of great importance as no other numerical approach (at least, at present time) is capable of simulating feature profiles resulted from materials processing, be that due to etching, deposition, or both those processes going on at the same time or one after another in cycles. Plasma ion implantation is also often happens during etching processes and it affects the results of etching. Simulation includes a few steps: (1) compute the species coming to the surface from the plasma and their energy and angle distributions, (2) estimate all surface reactions due to incidence of incoming species as well as by-products of surface reactions, and (3) use a FS simulation, such as FPS3D [1-4], to simulate the results of etching or deposition. If simulation does not correspond to experimental results, we have to adjust the parameters, modify a set of incoming species, or their energy and angular distributions, or the surface reactions. If we are sure that the plasma simulations are correct then the surface reactions would be the main culprit. The surface reactions are typically poorly known. Because there is a large set of surface reactions, and each reaction might depend on a few parameters, we typically come to a problem of multi-parameter optimization. In this presentation, we discuss the design of FPS3D as a general FS code applicable to most situations arising in materials processing. Examples of simulations are provided for very different chemistries and scales, including ALE and ALD, as well as the HAR etching. [1] P. Moroz, IEEE Trans. on Plasma Science, 39, 2804 (2011). [2] P. Moroz, D. J. Moroz, ECS Transactions, 50, 61 (2013). [3] P. Moroz, D. J. Moroz, J. Physics: CS 550, 012030 (2014). [4] P. Moroz, D. J. Moroz, Japan. J. Appl. Phys. 56, 06HE07 (2017).