Linking reactor-scale plasma modelling with feature-scale profile simulation

Sebastian Mohr[1], Anna Dzarasova[1], Dimitrios Tsamados[2], Vaibhav Deshpande[2], Mohamed Oulmane[2], Giovanni Bozza[2] , Jonathan Tennyson[3]
[1] *Quantemol Ltd., London, United Kingdom;* [2] *Synopsys LLC, Zurich, Switzerland;* [3] *University College London, London, United Kingdom*
E-Mail: s.mohr@quantemol.com

Introduction

- Optimizing the plasma process in the manufacturing of semiconductors gives a great competitive advantage.
- The resulting surface profiles depend on externally set parameters such as power, pressure, or gas mixture. However, this dependence is highly complex.
- Simulations provide an alternative to time and resource intensive trial and error experimental approaches.
- We introduce a joint solution combining reactor scale modelling of the plasma with a feature profile model on the micro scale.

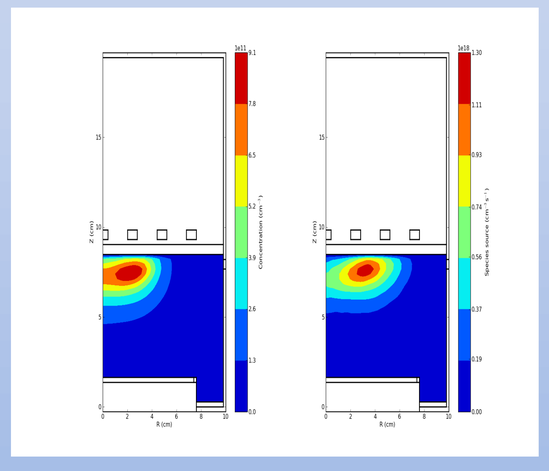

Figure 1. Electron density (left) and atomic flourine production rate (right) in an SF_6 discharge at 75 mTorr and 800 W.

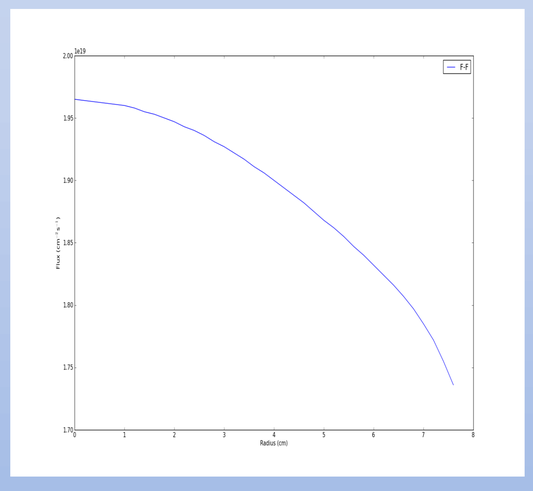

Figure 2. Flux of atomic flourine to the silicon wafer in an SF_6 discharge at 75 mTorr and 800 W. The experimental value is $1.2x10^{18}$ $cm^{-2}s^{-1}$ [3].

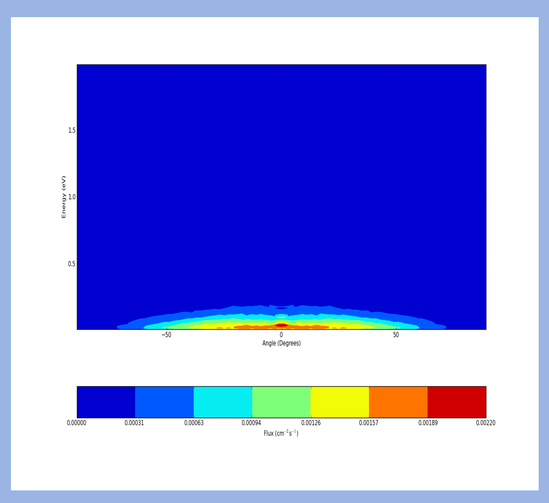

Figure 3. Energy and angular distribution functions of atomic F at the wafer in an SF_6 discharge at 75 mTorr and 800 W.

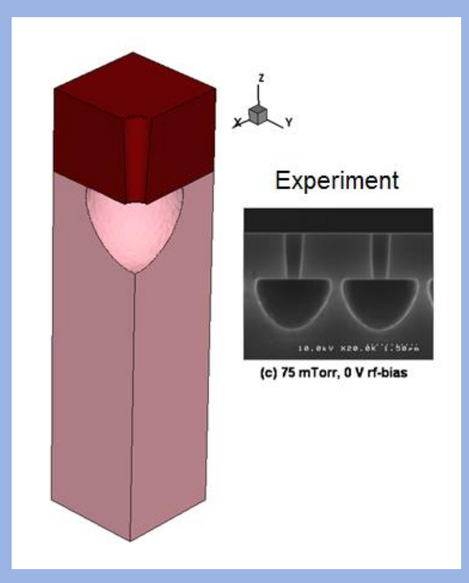

Figure 4. Resulting etch profile of silicon by chemical etching and comparison to experimental results [3].

References:
[1] M J Kushner, *J. Phys. D: Appl. Phys* **42**, 194013 (2009)
[2] Synopsys Inc., *Sentaurus Topography 3D User Guide* (2015)
[3] R J Belen, S Gomez, M Kiehlbauch, D Cooperberg, and E S Aydil, *J. Vac. Sci. Technol. A* ***23****, 99 (2005)*

Quantemol – VT: Plasma Reactor Scale Simulation

Quantemol-VT is a 2D – plasma simulation software especially designed to model industrial reactors. It is based on the Hybrid Plasma Equipment Model (HPEM) by Mark Kushner [1]. The HPEM is fundamentally a fluid simulation, solving the fluid transport equations (continuity, impulse balance, and energy balance equation) to calculate particle densities, fluxes, and temperatures. Additionally, the fluid model can be combined with kinetic simulation techniques such as a Monte Carlo model to calculate particle distribution functions in the plasma volume, essentially substituting the energy balance equation, as well as on surface such as a wafer. In combination with as wide range of optional modules dealing with different phenomena such as surface reactions, electromagnetic effects, or radiation transport, the HPEM is capable of simulating different discharge types (ICP, CCP, Microwave etc.) under a wide range of settings for parameters such as pressure or power. Quantemol-VT provides a user friendly interface to simplify the simulation setup and results visualisation.

Sentaurus Topography 3D: Feature Profile Model

Sentaurus Topography 3D [2] is a three-dimensional feature profile model designed to calculate surface profiles resulting from the interaction between reactive species from a gas discharge and the processed surface. It utilizes a Monte Carlo approach, tracking individual particles and their interaction with the surface. Possible reactions of the particles with the surface include etching, deposition, adsorption, re-emission and reflection, allowing the user to create a comprehensive set of surface reactions for a particular plasma/surface combination. As a result, three-dimensional surface profiles and coverages are produced. In the collaboration between Quantemol and Synopsys, a direct link between Q-VT and Sentaurus Topography 3D was created, which translates the particle distribution functions from Q-VT to the input format for Sentaurus Topography 3D.

Results

- A direct link between the Quantemol-VT industrial plasma simulation and the Sentaurus Topography 3D feature profile model was created.
- This allows to use information on fluxes of reactive species from the reactor scale simulation in the feature profile model.
- As a first example, experimentally obtained etch profiles [3] of silicon by means of an SF_6 discharge were recreated with great agreement.
- Thus, the combined software allows to study the influence of set parameters such as power, pressure, and gas mixture on the resulting etch/deposition profiles without the need for time and resources consuming experiments and subsequent measurements of the profiles.

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