Variability-aware Topography Simulation

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Outline

- Introduction
 - Goals and strategy
 - Project context
- Software integration
- Simulation models
- Simulation examples
- Conclusions and outlook





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Introduction – Goals and Strategy Approach

- For nanometer-scale devices, effects due to topography variations are important to consider, therefore the work on topography simulation within SUPERAID7 aims at:
 - Tight integration of the etching and deposition modules (DEP3D, ANETCH of Fraunhofer and ViennaTS of TU Wien) with background work on lithography simulation (using Dr.LiTHO of Fraunhofer) providing a unified frontend for topography simulation
 - Development of physical models for etching and deposition processes relevant for device and interconnect fabrication
 - Interfacing of feature-scale simulation with external equipment simulation modules
 - Integration of the topography modules with further process steps and device and interconnect simulation
 - Model calibration, verification, and benchmark support



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Introduction – Goals and Strategy State-of-the-art

- Individual modules for simulation of topography steps (lithography, etching, deposition) are available from academia and commercial vendors
 - The physical modeling level of the SUPERAID7 modules is comparable or ahead (the latter in particular for lithography simulation)
- The possibility to run the SUPERAID7 topography modules in an integrated environment and to provide the structures to device and interconnect simulation is – to our knowledge – beyond state-of-the-art

This allows the end-user

- to address advanced topography processes
- to use the results in the context of various applications by running device and interconnect simulations







Introduction – Project Context



Software Integration

Topography Simulation Modules and their Interaction



Software Integration

Example: Integration of DEP3D from IISB with ViennaTS



Simulation Models **Deposition and Etching Models**

- Deposition models are available for
 - general non-linear multiple-species deposition, model is able to reproduce a plenum of processes driven by multiple species by adjusting a few parameters
 - sputter deposition, chemical vapor deposition (CVD), ionized metal plasma deposition, plasma-enhanced CVD, and superconformal deposition
 - transient simulation of atomic layer deposition (ALD) and plasma-enhanced ALD (PEALD)
- Etching models are available for etching of different materials
 - such as (poly)silicon, silicon oxide, TiN, HfO₂
 - with different chemistries, such as Cl₂, HBr, SF₆, CH₂F₂, C_xH_y, CF_x, BCl₃





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Simulation Models Example: Modeling of Non-conformal Oxide Deposition

- Reactive molecules arrive from the reactor and hit the structure surface. The following can happen:
 - Reaction → contribution to layer growth or
 - Re-emission \rightarrow molecule can reach other positions
- Simulation approach:
 - Quasi steady-state with slowly varying local fluxes
 - Solving for local rates R_i, using surface discretization

$$\pi R_i - \sum_{i \neq j} T_{ij} R_j = \pi - \frac{1}{1 - s_c} \sum_{i \neq j} T_{ij} \quad i = 1 \dots N \quad \leftarrow \text{System of N linear equations}$$

Layer profile depends on reaction probability s_c and the geometry, e.g., the aspect ratio of a contact hole



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Simulation Models Example: Physical Etching Simulation

Simple model (view-angle dependent etching), can be applied, e.g., to sputter etching:

- Rate-determining species, e.g., ion, with given angular distribution and etching law $r(\theta_{loc})$
- Local rate $r(\mathbf{x})$ is determined by integrating the flux $\phi(\theta, \varphi)$, taking into account shadowing by the structure leading to a restriction of the solid angle to Ω_{free} :

$$r(\vec{x}) \sim \int_{\Omega_{free}} r(\theta_{loc}) \, \phi(\theta, \varphi) \, d\Omega$$

Complex etching models consider multiple species and laws for interaction with the structure, e.g., for reactive ion etching



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Simulation Models

Example: Reactive Ion Etching of Silicon or Polysilicon

Etching process in a plasma based on Cl₂, HBr, CF₄ chemistry



Simulation Examples Low-temperature Oxide Deposition with Void Formation



Simulation Examples Plasma-enhanced Atomic Layer Deposition (PEALD)



Simulation Examples Plasma-enhanced Atomic Layer Deposition (PEALD)

- We used the experimental data from literature to find the best fitting values for the model parameters
- Adjusting the fitting parameters results in a PEALD model, which fits well with the measurements





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Simulation Examples Simulation of Fin Etching

- Fin etching is carried out using a dry etching process with HBr, Cl₂, and oxygen chemistry
- Using the corresponding model in ANETCH, the profiles can be reproduced using typical values for the fluxes of ions and neutrals and model parameters from literature
- Extension of the model includes the link to equipment simulation for obtaining boundary conditions for fluxes of ions and neutrals





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Simulation Examples Simulation of Fin Etching with Coupling to Equipment Data (1)

Equipment simulation results (Hoekstra et al., 1997)

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Simulation Examples

Simulation of Fin Etching with Coupling to Equipment Data (2)



Simulation Examples Simulation of Gate Stack Patterning (1)

Sample simulation of poly-silicon etching in a SF₆/CH₂F₂ plasma with a bias power set to 75 W and a SF₆ to CH₂F₂ ratio of 0.45:



Sample simulation of titanium nitride etching in a Cl_2/CH_4 plasma:



Simulation Examples Simulation of Gate Stack Patterning (2)

Result of the simulation sequence used to etch through the gate stack of HfO₂ (1.9 nm), TiN (5 nm), and poly-Si (50 nm) with a 10 nm mask:



Simulation Examples Self-aligned Double Patterning (1)

- Carbon lines are created using CD values from a lithography model (1)
- CVD oxide is deposited (2)
- and etched back to form the spacers after carbon line removal (3)





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Conclusions and Outlook

- The topography modules allow the integrated simulation of lithography, etching, and deposition
 - The software provides integration routines for the Fraunhofer and TU Wien tools, based on a Python frontend and a rate-based interface between ANETCH, DEP3D and the ViennaTS level set module
 - The integration is extended by a Geometry Engine Python Package which provides additional functions
- The data exchange with electrical simulation of devices and interconnects is possible via file exchange
- The modules provide a large variety of physical models and capabilities for structure emulation
 - They have been applied to the SUPERAID7 benchmarks cases
 - This will be extended, particularly including equipment simulation, and using further experimental data, e.g., from the Industrial and Scientific Advisory Board







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