Variability-aware Topography Simulation

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Outline

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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

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**

**WP3**

**Software Integration**

**Topography Simulation Modules and their Interaction**

- Dr.LiTHO
- ANETCH
- DEP3D

*Python frontend*

*Rate-based interface*

ViennaTS

- Level set geometry engine
- Physical etching models
- Non-linear deposition model
- (PE)ALD models
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, CₓHᵧ, CFₓ, BCl₃
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 $\rightarrow$ contribution to layer growth
  - 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

$$\pi R_i - \sum_{i \neq j} T_{ij} R_j = \pi - \frac{1}{1 - s_c} \sum_{i \neq j} T_{ij} \quad i = 1 \ldots N$$

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

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 $\Omega_{free}$:

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

Complex etching models consider multiple species and laws for interaction with the structure, e.g., for reactive ion etching
Simulation Models
Example: Reactive Ion Etching of Silicon or Polysilicon

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

- Silicon surface with certain fraction covered by Cl/Br

- Adsorption of Cl/Br radicals

- Ion induced desorption of etch products containing Cl/Br

- Local etch rate

- Change of surface state

- Etching by F radicals

Simulation Examples
Low-temperature Oxide Deposition with Void Formation

- Simulation of low-temperature oxide (LTO) deposition with the LPCVD (low-pressure chemical vapor deposition) model of DEP3D using a sticking coefficient $s_c = 0.2$
Simulation Examples
Plasma-enhanced Atomic Layer Deposition (PEALD)

- TiN PEALD using TDMAT and N_2/H_2 plasma is modeled based on an adaptation of a model for conventional ALD.
- The film growth (deposition of a single layer of TiN) takes place only during the H_2-N_2 plasma step.

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.
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

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

Equipment simulation results (Hoekstra et al., 1997)

Ion flux
Neutral flux

Relative change (center / Radius = 4 cm / Radius = 8 cm)
0 % / +17 % / +6 %
0 % / 0 % / -11 %
Simulation Examples
Simulation of Fin Etching with Coupling to Equipment Data (2)

- Ratio of etch rates center / 4 cm / 8 cm: 52 / 55 / 50 (relative units)
- Due to overetching, the resulting fin profiles are only slightly modified.

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 Cl₂/CH₄ 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)
Simulation Examples
Self-aligned Double Patterning (2)

- Non-conformal deposition followed by perfectly anisotropic etching
- Conformal deposition followed by chemical dry etching
- Non-conformal deposition followed by chemical dry etching

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