New method for the precise flux calculation of neutrals for arbitrary surfaces in profile etch simulations

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A precise and efficient model of transport of neutral species is essential for exact profile etch simulations.

Neutral species in plasma etching
- Neutral species contribute to chemical and ion enhanced etching and deposition
- Shadowing, re-emission, physical and chemical properties of surface cause local variations of neutral flux
- Undercut and aspect ratio dependent etching attributed to neutral transport phenomena
- Local flux determine etch and deposition rate

Transport of neutral species essential in plasma etch simulations

Flux calculation of diffuse reflected neutral species
- Local flux of neutral species at surface affected by
  - Direct flux from visible plasma
  - Re-emitted flux from other visible parts of surface
  - Re-emission probability
  - Geometrical setup
- Directional reflection probabilities of neutrals follow cosine law (Lambertian)

Finite element method (FEM) approximates flux $\Phi(x)$ for discrete elements

Complicated calculation of geometrical form factors and visibility of elements

Simplification of form factor integral by definition of small elements

Precise and fast calculation of neutral flux by FEM method, BSP and clip trees.

Utilization of hemisphere algorithm and Nusselt analogon
- Form factor of small area $dA_i$ to element $A_j$
- Projection on hemisphere around $A_i$
- Second projection to unit circle equals form factor

Visibility calculation most CPU intensive
- Significant effort by using binary space partition (BSP) and clip trees

Comparison of simulation with experiments for isotropic etching of silicon in fluorine
- Parameter study of isotropic etching
  - F-radical etching only, neglect ion flux
  - Etch experiments
    - STS Multiplex ICP
    - ICP power 600W, RF power 0, 20°C sample temp., 90sccm SF$_6$, 20 mTorr pressure
    - Etch time 90s, 180s, 540s
    - Mask openings 1.5, 5, 10, 20µm
- Comparison with experiments

Parameter study reveals significant dependency of profile shape on sticking coefficients of mask and Si
- Fair agreement between simulated and experimental result but
- Undercut is overestimated
- Ion bombardment is not negligible at floating potential

Simulation allows efficient studies of process parameters and conforms to experiments.

Conclusion
- Precise and fast calculation for arbitrary profiles and neutral species with diffuse re-emission
- Applicable for trenches with varying mask openings and process setups
- Experiments show influence of ions at floating potential in profile shape
- Undercut is overestimated in case of neglected ion bombardment
- Simulation using new method of neutral transport consistent with experimental results

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