Goals of IMPACT’s Plasma Team

- Couple models at various scales to understand plasma-surface interaction and predict profile evolution
- Build even stronger interactions between PIs and sponsors
- Key Projects
  - Develop fast algorithms to determine energy and angular distributions of all plasma species
  - Develop fundamental models for plasma-surface interactions
  - Develop predictable profile simulator for etch and deposition processes
Faculty Presentation: Plasma

Michael A. Lieberman
Emi Kawamura and Ying Wang

Electrical Engineering, UC Berkeley
Current Milestones

- Develop fast algorithms to determine the energy and angular distributions of energetic ions on the wafer surface.
- Validate with particle-in-cell simulations and/or experiments.

1D/2D Fast Models of Energy/Angular Distributions from PIC Simulations

- 2D Ion Density
- 2D Ion Energy Distribution
- 2D Ion Angular Distribution
- Triple Frequency Ion Energy Distribution
- Ion Angular Distribution Versus Pressure
- Fast Neutral Angular Distribution Versus Pressure

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Electromagnetic Effects

- Electromagnetic effects in capacitive discharges (joint with D. Graves)
Nonlinear Power Deposition Effects

- 2D PIC results at 15mT in 13.56MHz argon discharge.
- Observation of current harmonics that peak near series resonance frequency.
Future Milestones

- Develop fast algorithms to determine the energy and angular distributions of energetic ions, fast neutrals, secondary electrons, and photons on the wafer surface.
- Validate with particle-in-cell simulations and/or experiments.
- Provide energy and angular distributions as input to the feature profile simulator.
Faculty Presentation: Plasma
David B. Graves
Joseph Vegh
Chemical Engineering, UC Berkeley
Current Milestones

- Plasma-surface interactions in nanoscale feature shape evolution
- Expose low-k dielectrics and photoresist with beams of ions, radicals and photons under vacuum conditions; measure etch/roughening rates
- Use molecular dynamics simulations to develop insights into how features etch in the presence of depositing and etching precursors

MD Simulated Hole Etched via CF$_3^+$ in Si

- After ~8400 CF$_3^+$ impacts (~2.7x10$^{17}$ cm$^{-2}$)
- C – Red
  F – Green
  Si – White
- Hole contour shown in blue
- Nominal hole depth ~8.4 nm
- Nominal hole width ~2.2-3.2 nm
- Note ‘halo’ of damage around hole ~1 nm thick

Top View

Side View
Beam Studies of PR Roughness

- Expose sample to controlled fluxes of ions, radicals, photons: beam-exposed samples follow roughness observed in plasmas

Ar⁺ & VUV Beam

100° C

200 nm
Reactor Scale Modeling

- Models of chemically active plasmas

- O₂ profile in ICP
Future Milestones

• Plasma-surface interactions in nanoscale feature shape evolution

• Expose low-k dielectrics and photoresist with beams of ions, radicals and photons under vacuum conditions; measure etch/roughening rates

• Use molecular dynamics simulations to develop insights into how features etch in the presence of depositing and etching precursors
Faculty Presentation: Plasma
Jane P. Chang
John Hoang
Chemical and Biomolecular Eng., UCLA
Current Milestones

- Use experimental beam systems to measure the pertinent kinetics parameters, such as sticking and recombination coefficients
- Formulate reaction mechanisms to be incorporated in a Monte Carlo simulator to account for surface evolution, especially with competing etching/deposition processes

Challenges:
- Many spatially-varied variables ($n_n, p, n_i, T_e$ ...) highly coupled
- Complex kinetics and numerically robustness
Monte Carlo Feature Scale Model

- Ions specularly scatter
- Neutrals diffusively scatter
- Surface composition by elemental balance
- Surface reactions with specific probabilities
- Simulation domain:
  - 10-50 Å grid size
  - Transport of species in grid lengths
- Surface reaction:
  - reaction probability based on kinetics
  - elemental balances
  - multiple interactions possible
- Surface advancement:
  - grid cells removed and/or added
- Rigorous incorporation of physics and chemistry
- Computationally robust and straight-forward
Feature Scale Model Calibration

Assumption
- Ion-flux limited regime (grey)
- Yield is relatively constant

Feature Scale Model
- Trench dimension dictates total particles
- Particles sampled at source plane

Controlled Experiment
- No time scale, only particle counts
- Calculated normalized difference in particle flux and compare with model

Verify Experiment with Model
- Yes
- Finished
- Numbers Agree?
- No, repeat

Calibrated model enables predictive modeling of feature profile evolution

- Calibrated model enables predictive modeling of feature profile evolution

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Results from a Hybrid Model

DOE shows general decrease in etch depth from center to edge

DOE shows general increase in SWA from center to edge

• Calibrated hybrid model explains general trends in SWA and etch depth
Challenges in Obtaining Kinetics Data

- Obtain physically-accurate feature profile evolution and its final form based on the direct simulation Monte Carlo (DSMC) method
- Limited kinetic and physical data for various chemistries
Quantification of SiO$_x$Cl$_y$ formation and etch rate in Cl$_2$ plasmas

- Radicals: Cl and O
- Ions: Ar$^+$ and Cl$^+$
- Etch rate (QCM)
- Etch surface (XPS)
- Etch products (QMS)

Use beam system with quartz crystal microbalance (QCM) and quadrupole mass spectrometry (QMS) to obtain kinetics data
Extension of Feature Scale Model into 3D

- 3-D feature scale modeling finds application in predicting LER
- Estimate 3D surface normal for neutrals and using 2D projections of interface cells in x-y plane and x-z plane
Future Milestones

- Use experimental beam systems to measure the pertinent kinetics parameters, such as sticking and recombination coefficients, etch yields, angular etch dependencies to quantify the etching of SiO$_x$Cl$_y$ films

- Formulate reaction mechanisms to be incorporated in a Monte Carlo simulator to account for surface evolution, especially with competing etching/deposition processes

- Extend the model into 3-D and convert the code to run in parallel using MPI

- Integrate inputs from plasma models, reactor models, and MD simulations to further improve the predictive capability of the profile simulator
Plasma, Surface, and Feature Scale Models

- Particle-in-cell, Monte Carlo collision (PIC-MCC)
  - Energy and angle of all species

- Molecular dynamics (MD) simulations and beam experiments
  - Fundamental surface reactions

- Monte Carlo feature scale model coupling with reactor model
  - Origin of surface evolution

- couple models at various scales to understand plasma-surface interaction and predict profile evolution