2D and 3D Computational Model of Plasma-Surface Interactions

Paul Moroz
Tokyo Electron US Holdings, Inc.
37 Manning Rd., Billerica, MA 01821

22nd International Conference on Numerical Simulation of Plasmas

September 7 - 9, 2011,
Long Branch, New Jersey, USA

Abstract

We discuss a computational model of plasma-surface interactions implemented in the FPS-3D feature profile code. The code uses cellular model for solid materials and is capable of treating etching, deposition, and ion implantation, both in 2D and 3D. It allows modeling of materials processing at very different scales, ranging from nanometers to micrometers. As input parameters, FPS-3D requires that the fluxes of all reactive species to the surface be provided. Incoming fluxes are computationally represented by particles. Each particle is characterized by the kind of species, and by the energy and direction of flight. The Monte Carlo launcher generates those species in correspondence with specified fluxes, so when many particles are launched the result closely corresponds to the specified distribution of fluxes on energy and angle. A size of a Monte Carlo particle (how many molecules it contains) is typically significantly smaller than the size of a material cell, so numerical statistical artifacts could be reduced. All material properties and all reaction mechanisms are specified in the chemistry file. The Monte Carlo treatment of gas and ion reactions is defined by the reaction probability (or by yield), which might depend on particle energy and the angle of incidence to the cell's normal, as well as on the surface temperature. Finite penetration depth of ions into solid materials is included in FPS-3D, which allows treatment of ion implantation as well as complex situations such, for example, as etching through the deposited polymer layers.

Outline

- Main Characteristics of FPS-3D.
- Main Simulation Steps.
- Cellular Model for Solid Materials.
- Particles in FPS-3D.
- Chemical Reactions.
- Surface Normals.
- Particle Fluxes.
- 2D and 3D Etch Examples.
- Tuning the Reaction Mechanisms.
- Calculating Reaction Yields.
- Defining Reaction Mechanisms and Reaction Rates by Fitting Experiments.
- Conclusions.

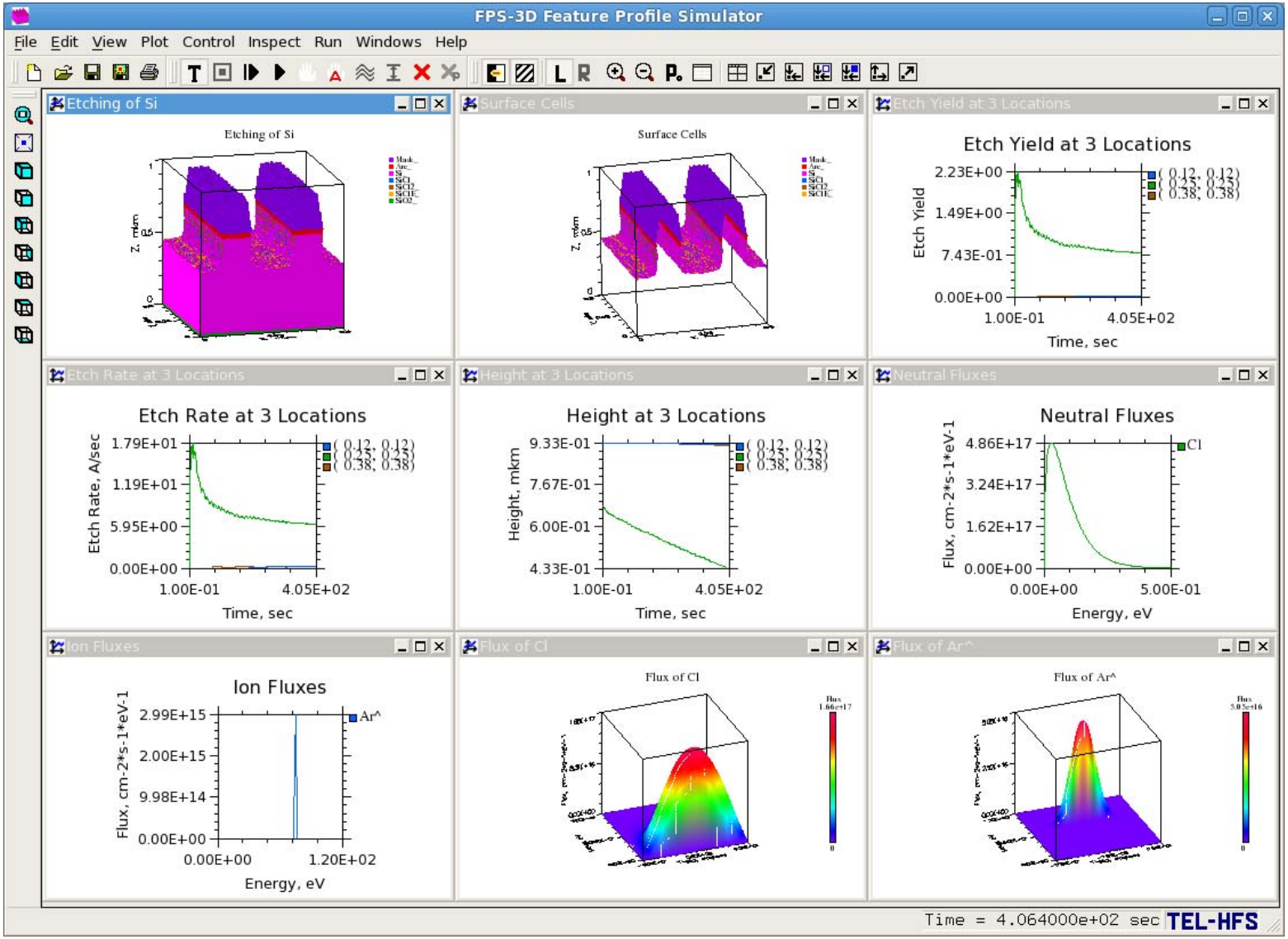
Main Characteristics of FPS-3D.

- FPS-3D is an advanced and general 2D and 3D Monte Carlo feature profile simulator. It uses 2D/3D cellular models for solid materials. It runs all simulations in real processing time.
- FPS-3D is based on an optimized C++ code coupled with advanced MDI GUI and advanced visualization options including fast concurrent graphics constantly updated during the run.
- Main ideology behind the chemistry model, to make FPS-3D more general, was not to hardcode any chemical properties, or any angular or energy dependencies for reactions.
- All the material properties and all chemical reactions are fully specified by the chemistry file. Reactions are presented by separate groups: gas-surface reactions, ion-surface reactions, and deposition reactions.
- Even the most difficult cases of ion reactions, when angular dependencies of yields vary with ion energy, can be conveniently described.
- FPS-3D uses multi-dimensional splines, which makes it work faster and allows consideration of complex chemistry and complex 2D and 3D geometries.
- FPS-3D is fast even on a standard desktop/laptop PC. It can be used for large-scale 3D models with over a million cells while maintaining full concurrent graphics capability. The code includes convenient 2D and 3D geometry reader which simplifies creation of complex-geometry features.

Main Simulation Steps

- Read geometry and parameters from the input file. Inform the user if there is error or incompatibility of parameters that should be corrected.
- Read energy-angle distributions of fluxes from the flux file, or generate fluxes independently based on input parameters.
- Make all requested plots based on input parameters including geometry of the feature, particle fluxes, reactions, etc.
- Run the code. Update geometry and materials (including new materials such as solid reaction products) during the run, and track height, etch rate, and etch yield at specified locations.
- During the simulation, different materials are presented via different colors and via the legends.
- If requested, collect statistics on fluxes at specified locations.
- If requested, record changing geometry in a compact format. This recording could be played back with the full capability of mouse operations, zooming, rotation, shifting, etc. This recording could also be later converted to movies.

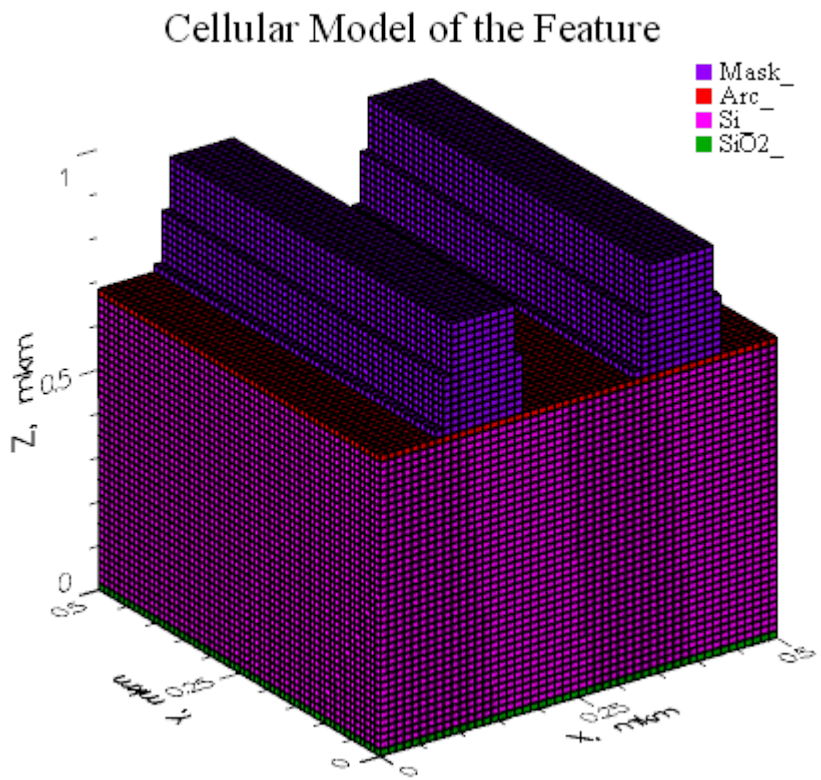
GUI of FPS-3D

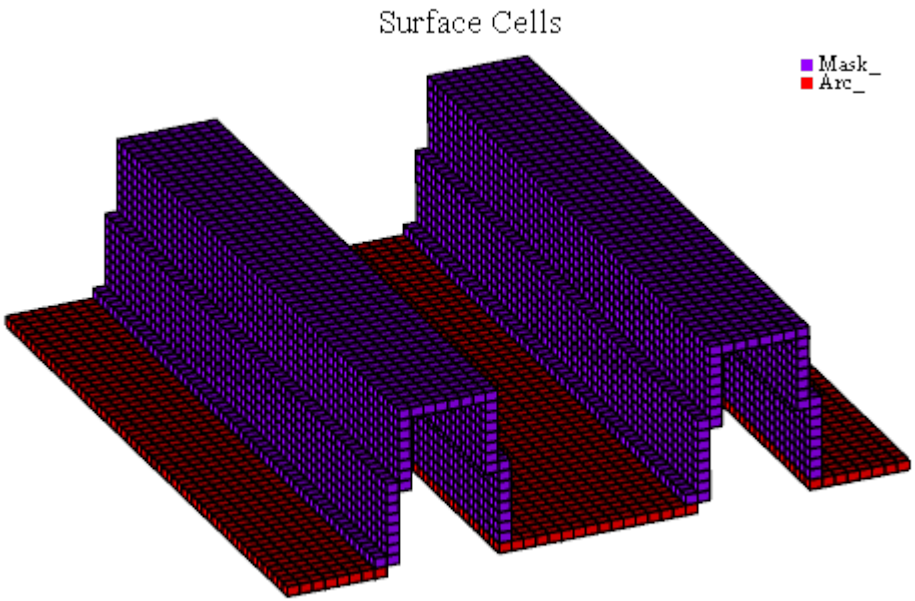

FPS-3D Feature Profile Simulator
File Edit View Plot Control Inspect Run Windows Help
Etching of Si
Surface Cells
Etch Yield at 3 Locations
Etch Yield
2.23E+00
1.49E+00
7.43E-01
0.00E+00
1.00E-01
4.05E+02
Time, sec
Etch Rate at 3 Locations
Etch Rate, A/sec
1.79E+01
1.19E+01
5.95E+00
0.00E+00
Height at 3 Locations
Height, mkm
9.33E-01
7.67E-01
6.00E-01
4.33E-01
Neutral Fluxes
Flux, cm-2*s-1*eV-1
4.86E+17
3.24E+17
1.62E+17
0.00E+00
5.00E-01
Energy, eV
Cl
Ion Fluxes
2.99E+15
2.00E+15
9.98E+14
0.00E+00
1.20E+02
Ar^
Flux of Cl
Flux of Ar^
Time = 4.064000e+02 sec
TEL-HFS

Cellular Model for Solid Materials

- All solid materials of the feature are presented as a combination of cells of equal volume.
- Because density of materials differ, the number of molecules per cell is also varies depending on material.
- Each cell is a complex object. It consists of its body as well as of a deposition layer.
- Each cell knows which elements (materials) it contains and how much molecules each element has.
- When the deposition layer is full, the cell converts it to a new nearby cell. When the cell becomes empty, it is deleted.

Cellular Model Examples





Particles in FPS-3D

- All gaseous species are launched by the Launcher as particles.
- Each particle consists of one type of molecules. It is the role of the Launcher to decide which particle and how big to launch.
- Each particle has particular speed, energy, and direction of flight. The Monte Carlo Launcher makes those decisions based on requested energy-angle distributions for fluxes.
- For better accuracy, the size of the particle (number of its molecules) should be significantly smaller than the size of the cell. There is an input parameter which states the maximum size of the particle relative to that of the cell.

Chemical Reactions

- **Chemical reactions in FPS-3D divided into types:**
  - Gas reactions
  - Ion reactions
  - Implant reactions
- **Gas and implant reactions include temperature dependencies.**
- **Ion reactions are much more complex. They also include angular and energy dependences, and take into account the finite penetration depth.**
- **Example of a gas reaction:**

  Si_ + Cl > SiCl_ : 0.5 T1
- **Example of an ion reaction:**

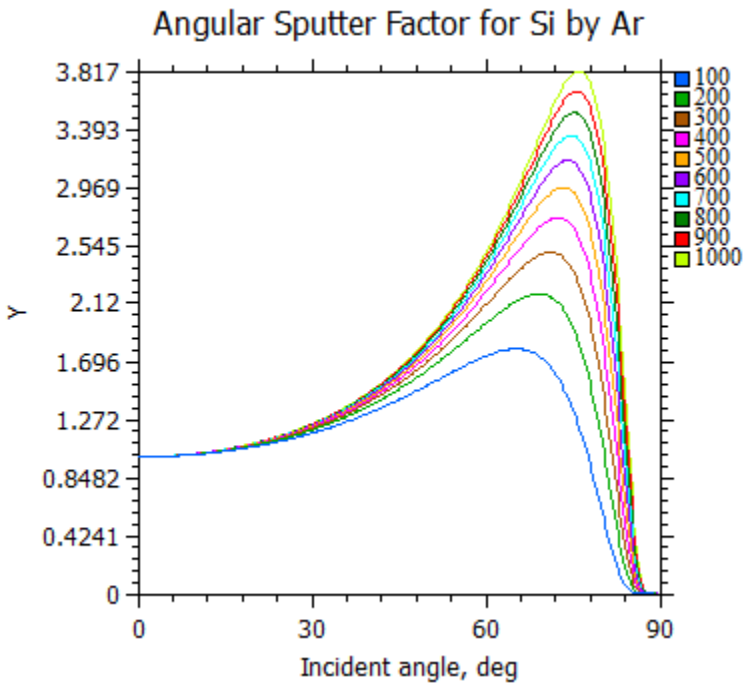
  Solid + Ion > Products : ID Yr m Er,eV Et,eV A1 A2 A3

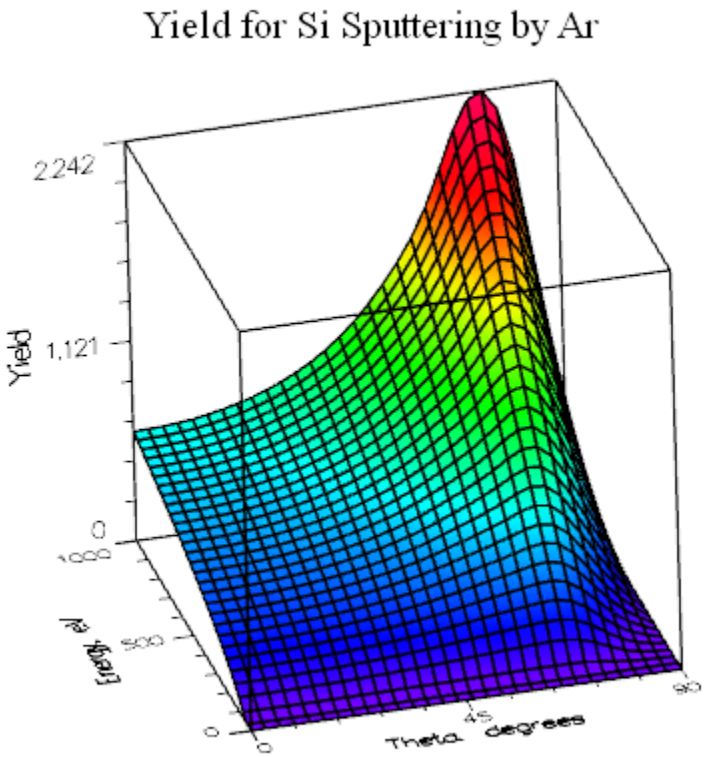
  Si_ + Ar^ > "Si" + Ar : 1 0.20 0.5 100 45 A1 A2 A3

PEOPLE. TECHNOLOGY. COMMITMENT.™

Reaction Dependence on Energy-Angle

- **Reaction yield might strongly depend on energy and angle of incidence. Here is an example how FPS-3D treats sputtering.**



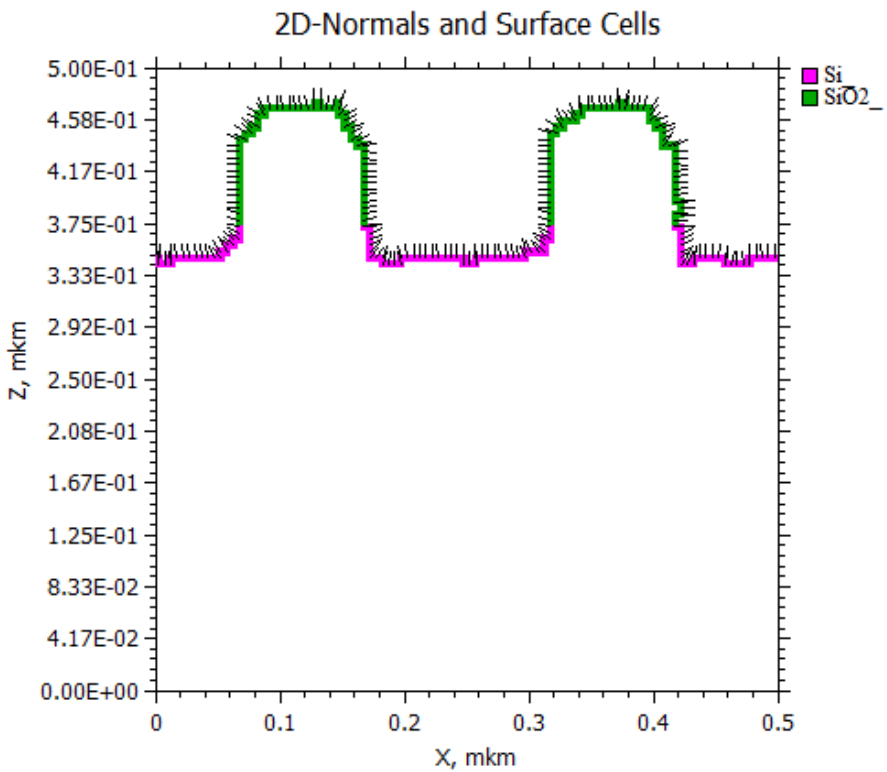


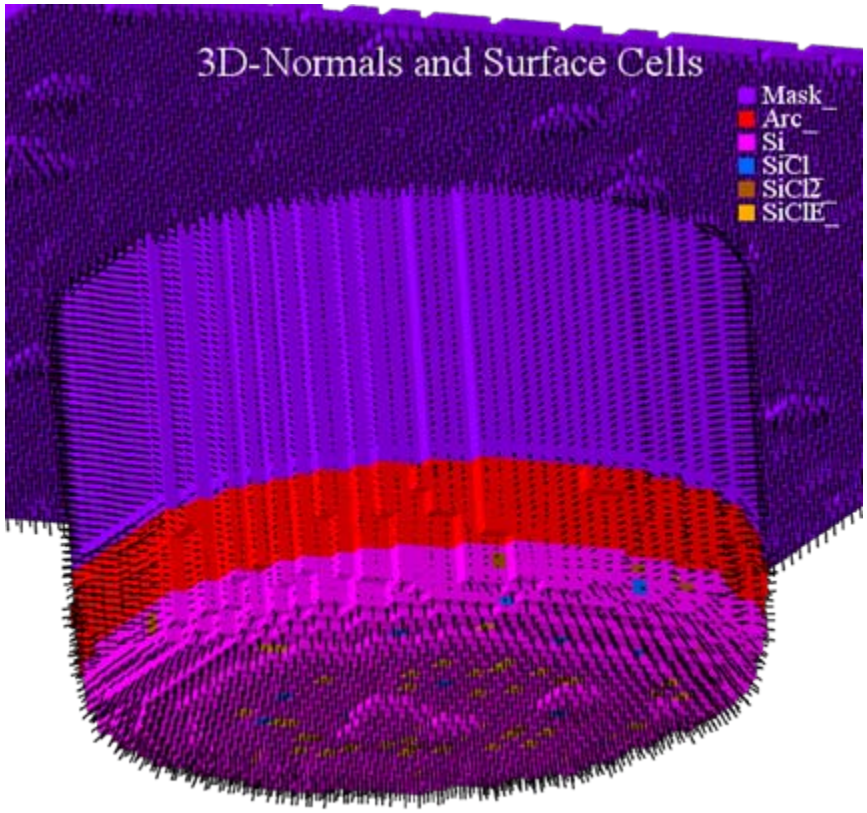
Surface Normals

- Ion reactions might depend on the angle to the surface normal for the cell.
- Surface normals are calculated for all surface cells.
- There is an input parameter that specifies the radius within which neighboring cells are participating in calculation of normals.
- If requested, the normals are continuously plotted during the run, so the user can be sure that they are calculated correctly.

PEOPLE. TECHNOLOGY. COMMITMENT.™

Examples of Surface Normals

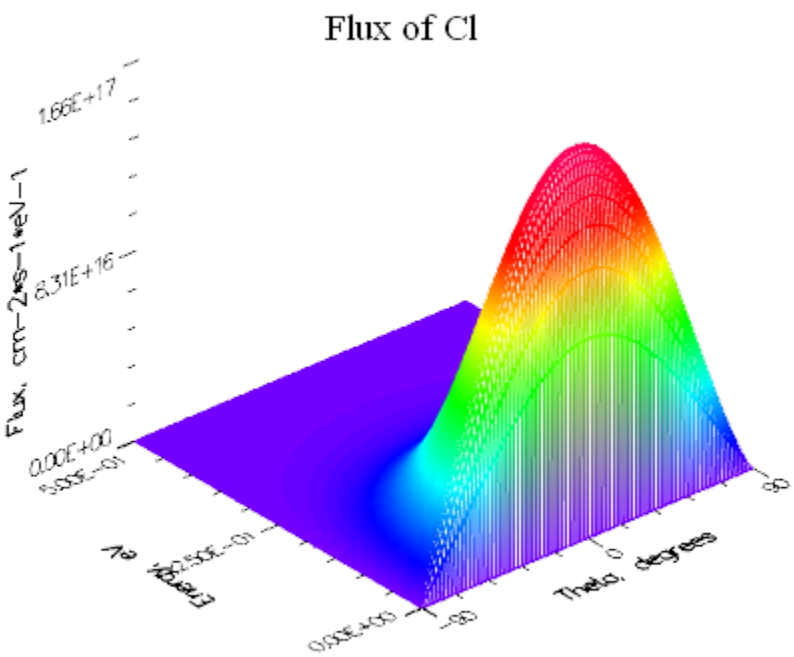


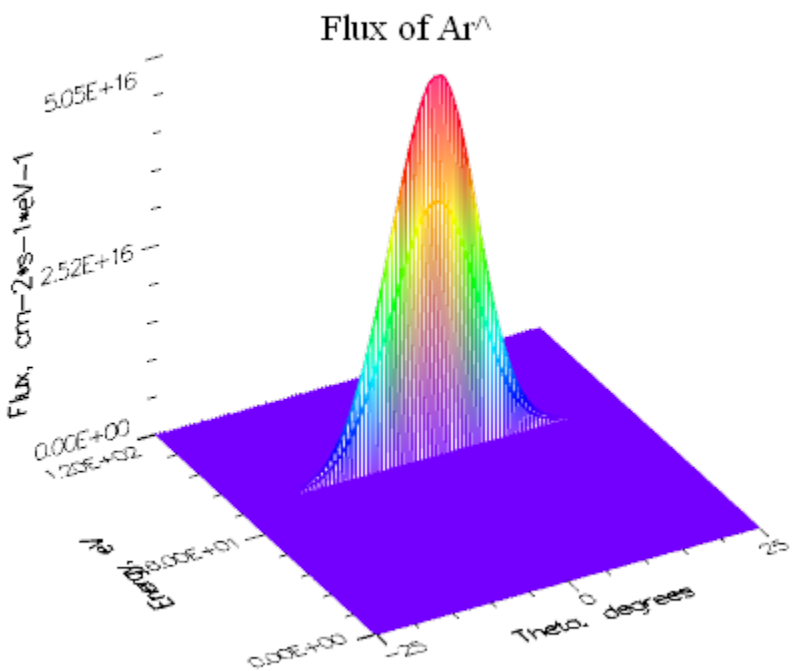


Particle Fluxes

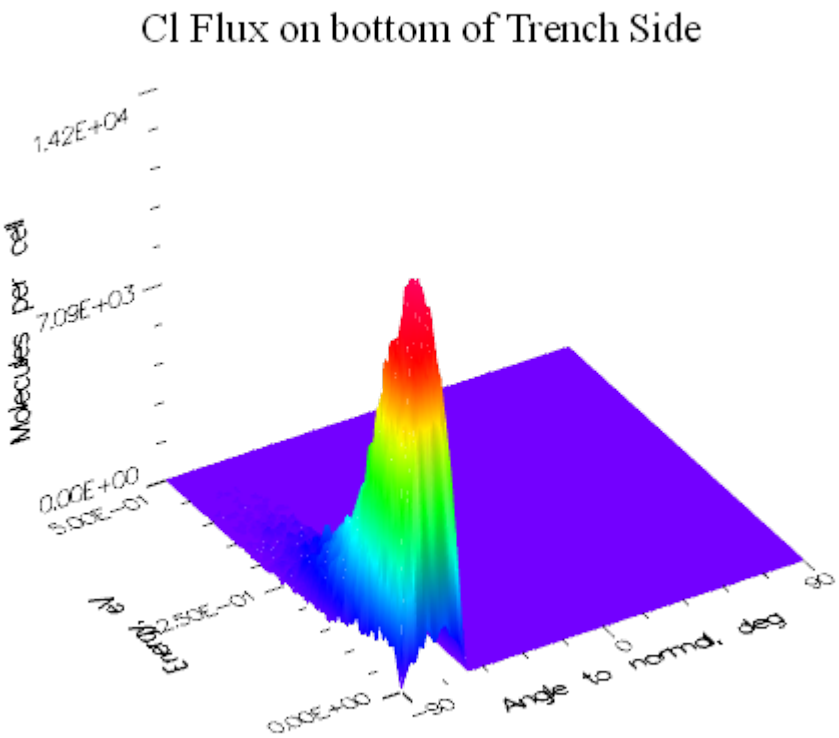
- **FPS-3D can calculate and show particle fluxes at any specified location on the feature surface.**
- **Fluxes are different locations on the feature could vary very significantly. For example, if one place is shaded from the flux then the flux there could be very small.**
- **Local fluxes are calculated relative to the local normals.**
- **A cell, selected for flux statistics, counts all particles that come to its surface, as well as the particle type, energy and direction.**
- **Those fluxes are plotted.**

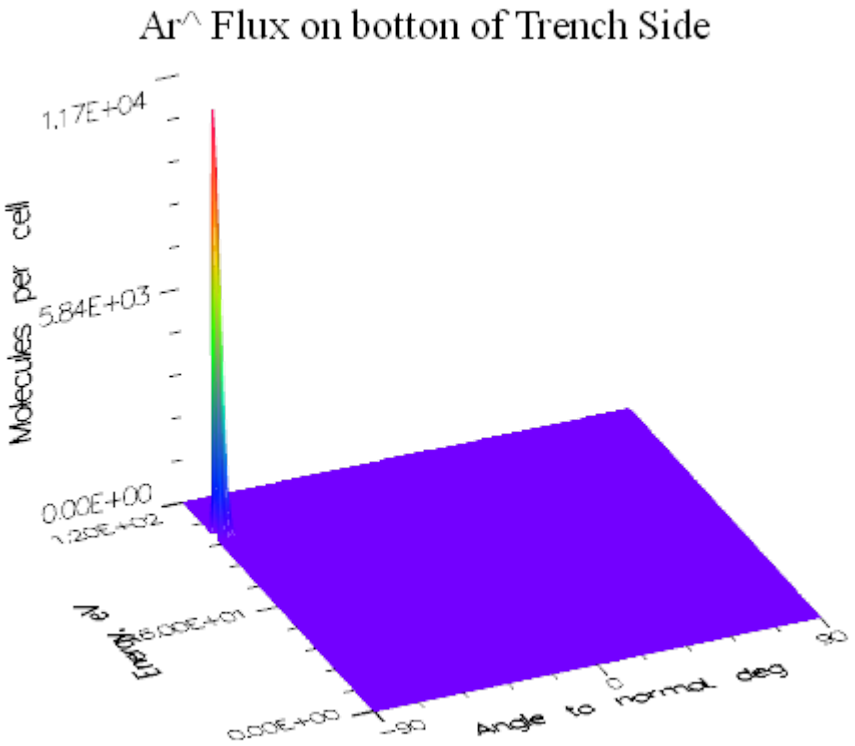
Example of Launcher Fluxes





Example of Local Fluxes





Tuning the Reaction Mechanisms

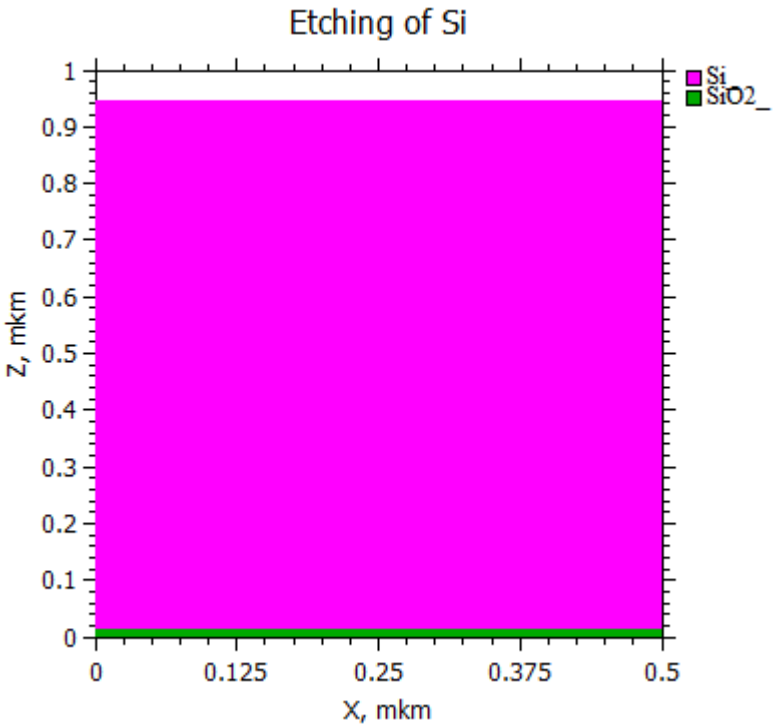
- All reactions in FPS-3D are based on pair interactions of molecules on the surface and on the condition in the cell (the types of molecules it contains).
- In FPS-3D, there is no any assumption on the dependence of reaction yields on external fluxes (or on the ratio of neutral to ion fluxes) or on the surface coverage, contrary to what many other feature profile codes do.
- All reactions in the chemistry file include yield/probability coefficients, which are often not known in advance. Those coefficients can be found by comparing with known experiments.
- Those reaction coefficients can be found by the method of optimization in a multi-dimensional parameter space.
- It is not difficult to satisfy a particular experiment. Often multiple different solutions could be found.
- However, situation significantly complicates when the data is available from different experiments, for example, at different energies, different flux ratios, and for different but related species. Then it really becomes an optimization problem, so the same coefficients satisfy all the different conditions. Then usually the acceptable solution range becomes rather unique.

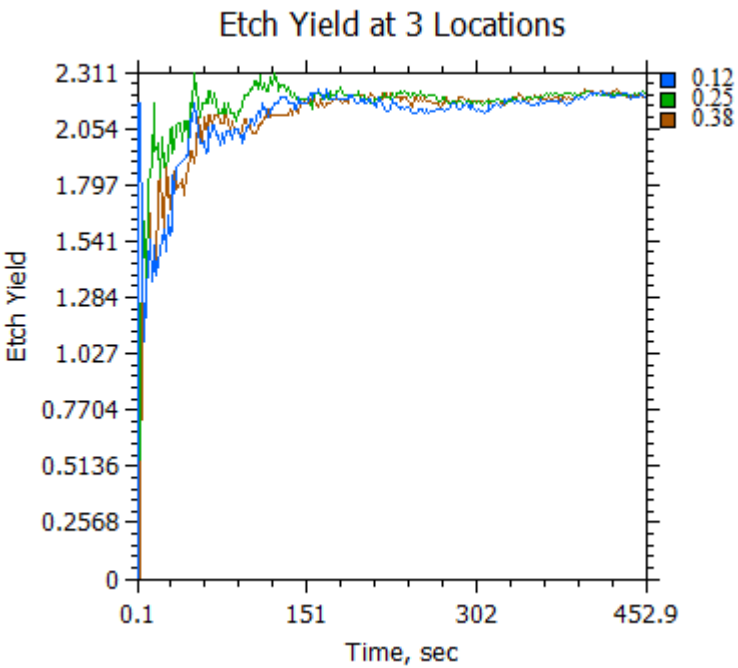
PEOPLE. TECHNOLOGY. COMMITMENT.™

Calculating Reaction Yields

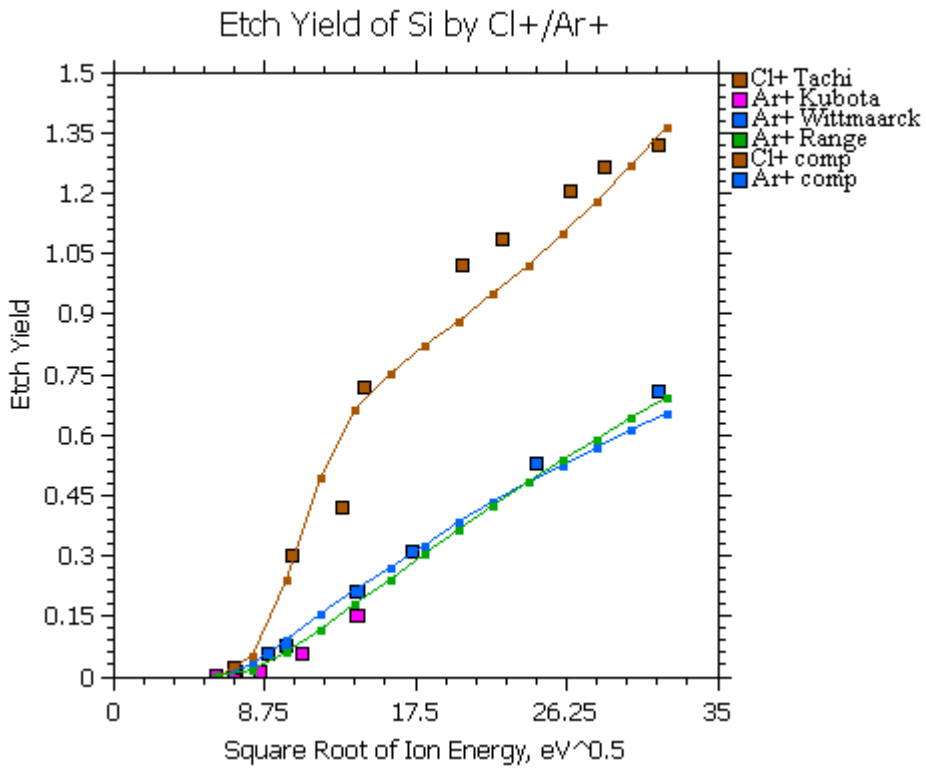
- **Reaction yields data are usually available from beam experiments, when the energy, the angle, and the flux ratios could be precisely controlled.**
- **For those tasks, the FPS-3D's geometrical model is very simple – just a flat surface of a particular material.**
- **The etch rate and the etch yield are then computed and compared with the experimental data. When there is a discrepancy, the reactions are changed and/or the reaction coefficients vary until there is a satisfactory agreement.**

Example of Calculating Reaction Yields

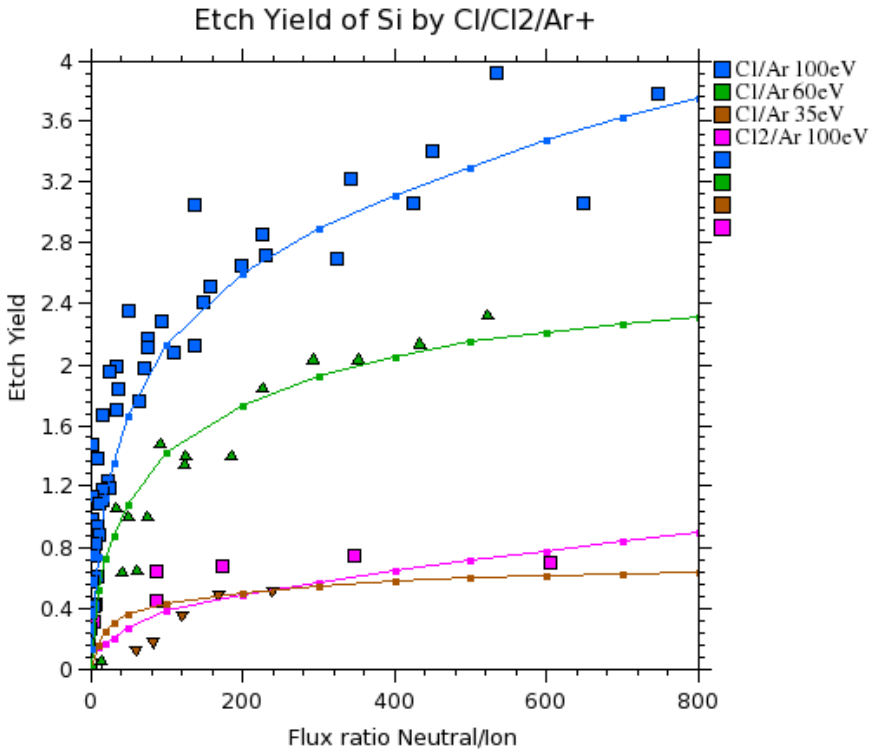


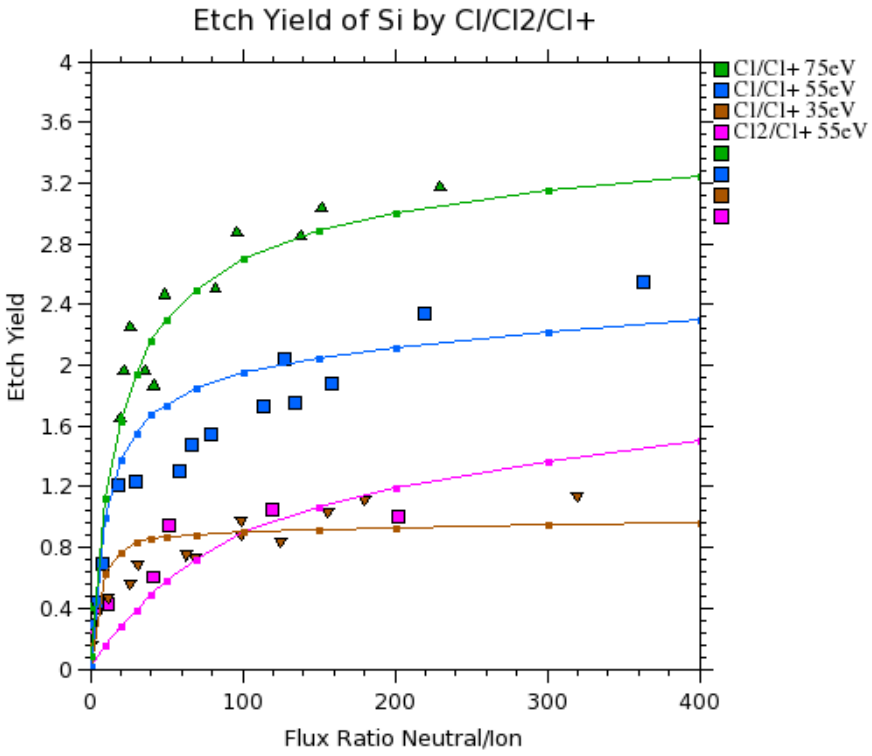


Defining Reaction Mechanisms. Sputtering of Si by Ar+ and Cl+ Ions.

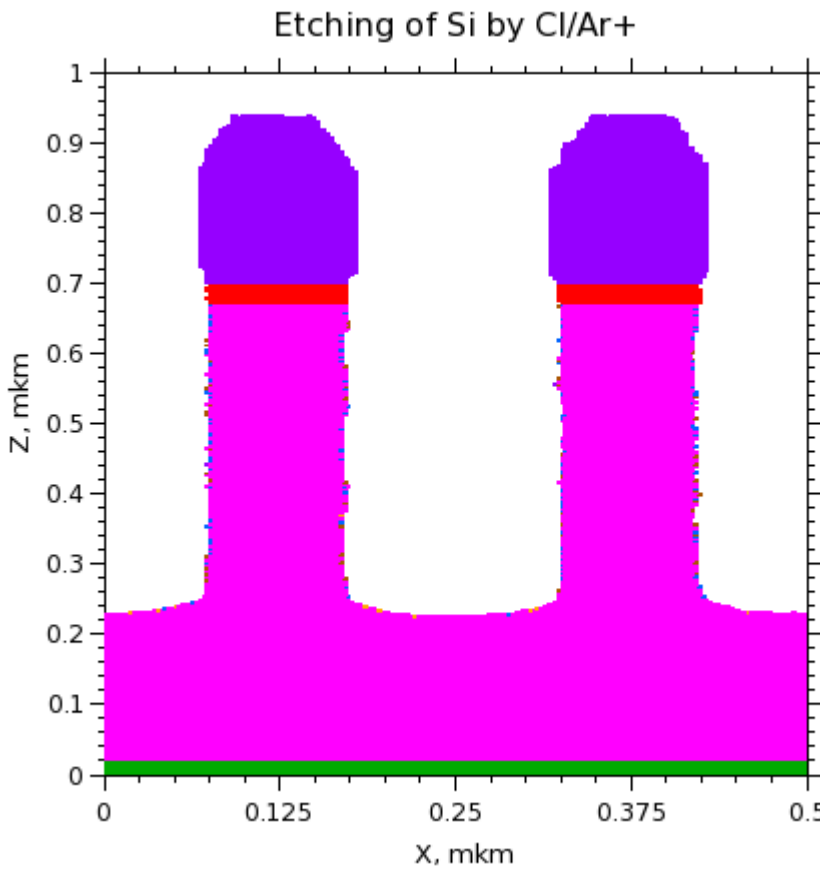


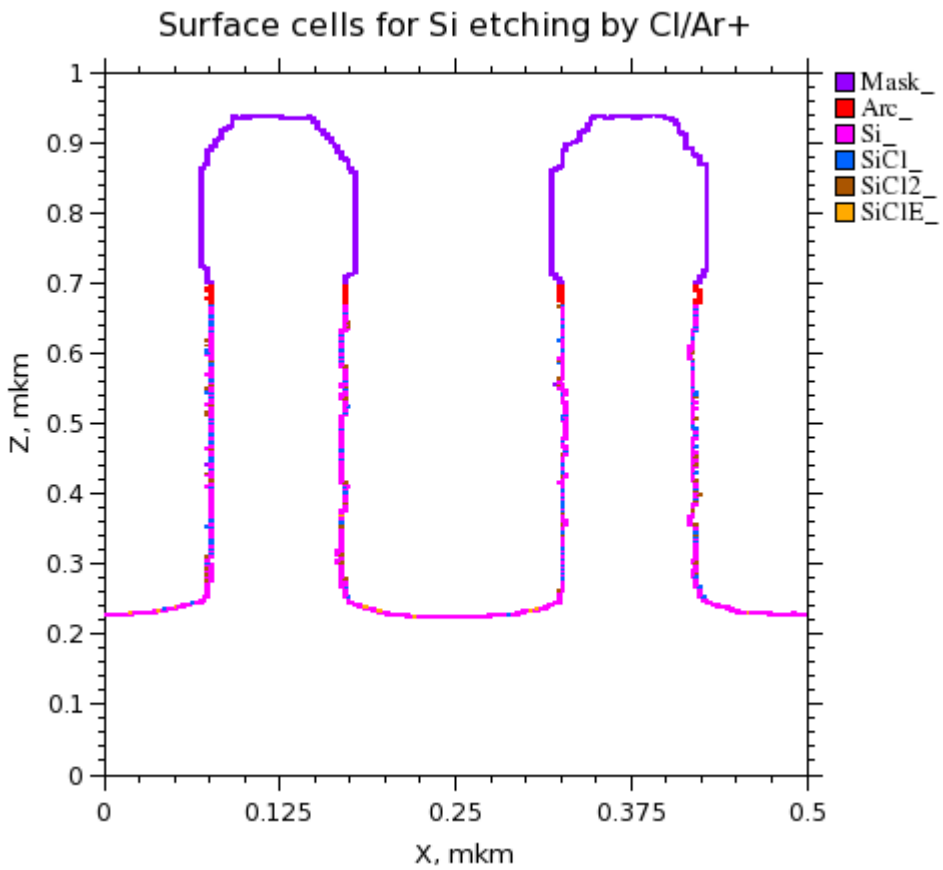
Defining Reaction Mechanisms and Reaction Rates by Fitting Experiments



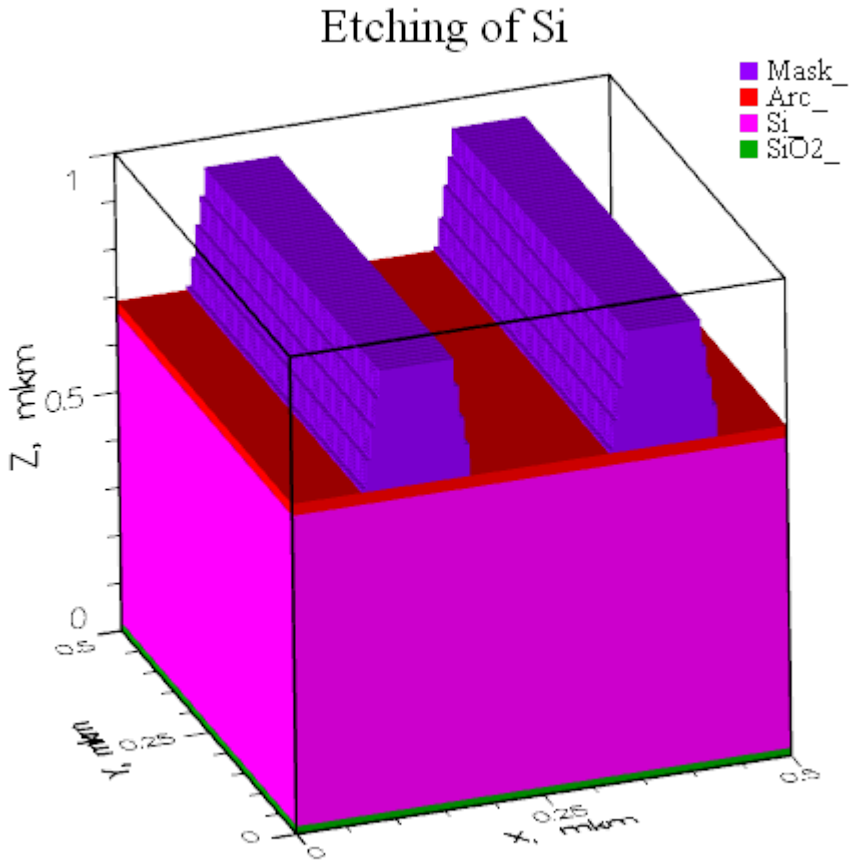


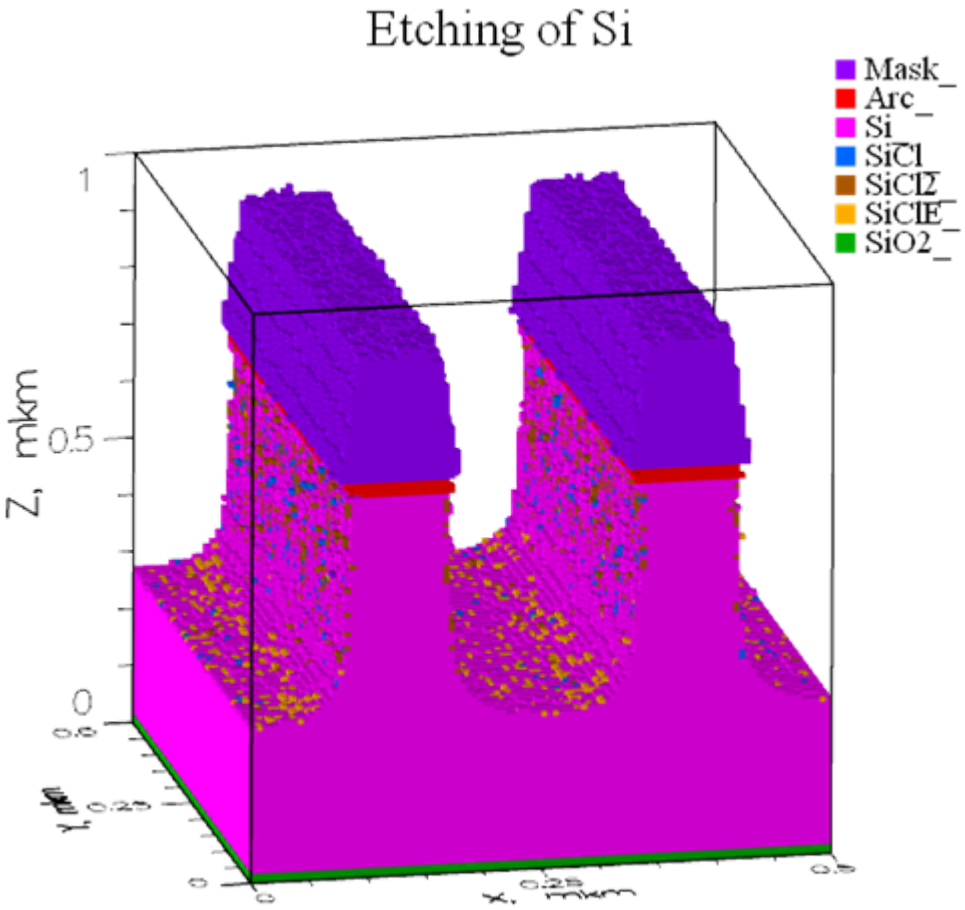
2D Etch Example



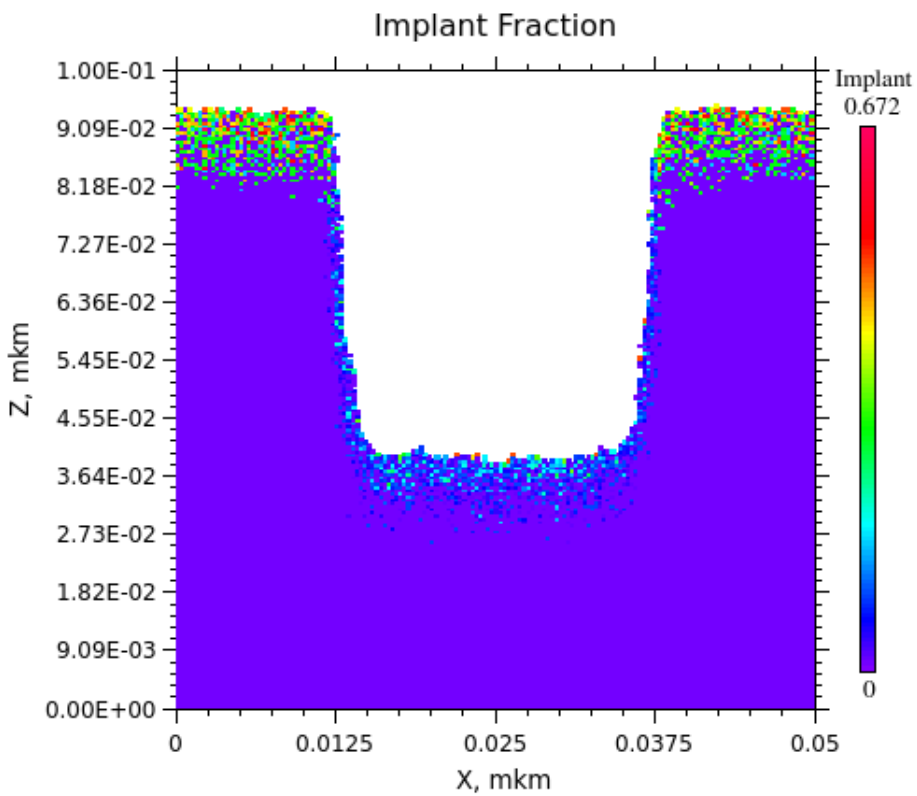


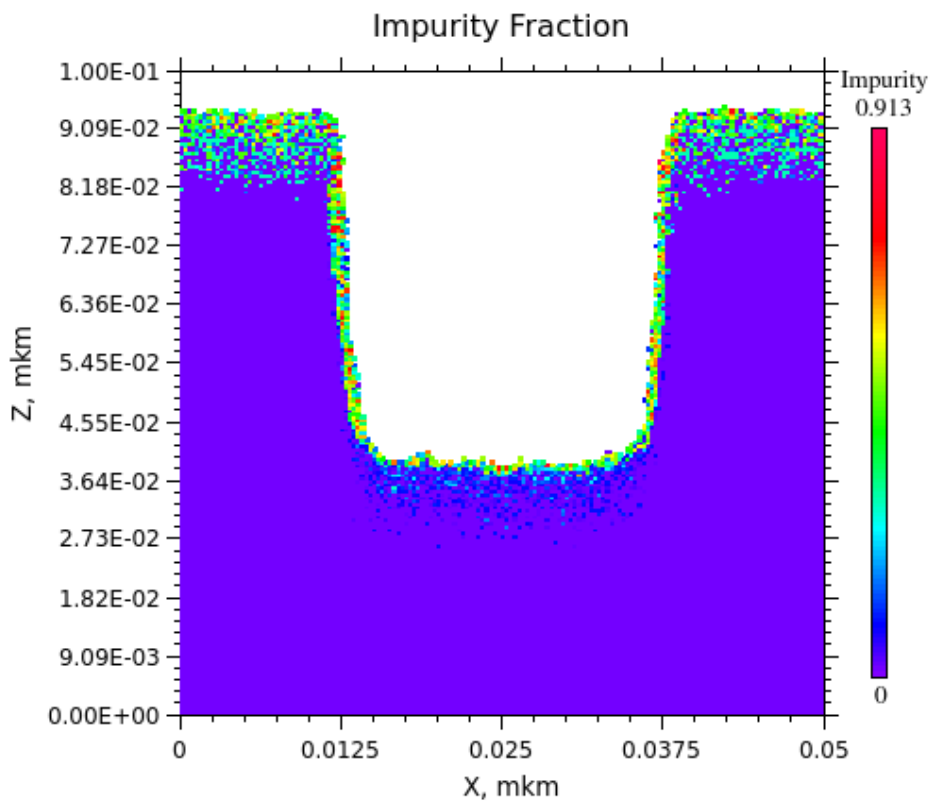
3D Etch Example





Implant and Impurity Distributions during Etching of Small Features





Conclusions

- **FPS-3D is a Monte Carlo particle code that uses cellular representation of solid materials. All cells have the same volume, but might contain different number of molecules depending of the densities of corresponding materials.**
- **FPS-3D has 2D and 3D modes, producing similar results when distribution in 3rd coordinate is uniform.**
- **FPS-3D is a user-friendly and convenient code. It is fast, and possesses GUI and graphics capabilities.**
- **FPS-3D produces results for etch or deposition rates which mainly depend on the particular physical conditions and not on the selected computational parameters such, for example, as the size of the cells or the size of the Monte Carlo particles, although details such as the roughness or accuracy might be different.**
- **FPS-3D can be applied to models of very different scales, from a few Angstroms to a few micrometers.**
- **FPS-3D can treat etching, deposition, and implantation cases.**