

# Simulation Standard

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## Using VICTORY Process for Plasma Etching Simulations

### Introduction

VICTORY Process, the 3D process simulator now includes a module for plasma etching. The module is designed to simulate plasma etching processes at the feature-scale size. The simulation in the reactor-scale region is out of the scope of VICTORY Process. All transport characteristics data (as functions of reactor parameters needed for the feature-scale simulation) are modeled by user definable C-functions and are supplied to the module. The plasma etching simulator shares many elements with the standard physical etching /deposition module such as:

- The topology of a given feature, defined by its layers of various materials, as described by level set functions given on Cartesian meshes
- All fine details of the structure are captured on imbedded finer meshes, and automatic and/or manual adaptive mesh refinement is available
- Particles fluxes, etch rates for different materials and types of particles involved in the process are modeled by appropriate functions, which are implemented in the user accessible C-Interpreter model library
- All feature topological changes caused by the plasma etching process during a given time are captured by the solution of the corresponding partial differential equations acting on the level set functions
- A feature's structure is automatically updated after the simulation time has expired

However, there are some important differences:

Plasma reactor generates two different types of particles: ions and neutrals, characterized by different flux distribution functions. The immediate consequences are:

- Each plasma species has its own etching rates, sticking efficiencies and other parameters, given as single values or functions, for every material present in the simulated structure

- At a given surface point, all plasma particles react with material in a complex way, and the resulting etching rate has to be properly modeled

All of these differences are reflected in the syntax of input deck commands.

The plasma etching module is capable of simulating plasma etching processes by giving the user access to various models of plasma particles' fluxes, etching rates and reactions. This paper shows the most important details and the relevant input deck commands.

### Define the Plasma Etching Process Characteristics

Two different etching agents are recognized and implemented in the plasma etching module: ion and neutral particles, representing all ions and all neutrals produced in a plasma reactor, respectively. Distinguishing ions and neutrals is important in implementing and defining etching rates, sticking efficiencies, fluxes and other parameters. Note that in the current version of the plasma etching module all ions (as well as all neutrals) in the plasma are represented by a single type of ion / neutral particle.

In order to run simulations, a user issues a list of commands to initialize various parameters and access algorithms. One such command defines how a single plasma particle (ion or neutral) reacts with materials in a given

*Continued on page 2 ...*

### INSIDE

<i>How to Mesh in 2D TCAD .....</i>	<i>5</i>
<i>Hints, Tips and Solutions .....</i>	<i>14</i>

structure. It is similar to the chemical definition in the physical etching/deposition module, but with extended capabilities. The command is PLASMAETCHPROPERTIES, and is typically used as follows:

```
PlasmaEtchProperties plasmaname="my_ions" \  
  particles="ions" \  
  material="silicon" rate=0.45 sticking=1.0 \  
  material="photoresist" rate=0.0005 \  
  sticking=1.0 density=1.
```

for ions and similarly for neutrals. The command line defines the rate and the sticking efficiency for all materials in a structure, related to a single active particle acting on a flat horizontal wafer surface, and the the particle density in the reactor ambient.

The `particles` parameter is mandatory. It specifies the type of plasma particle (ion/neutral) related to the list of material properties defined by this command. Any plasma etching simulation must have two PLASMAETCHPROPERTIES commands, one for each type of plasma particle.

A typical example of syntax to define the particles' flux distributions in space is:

```
PlasmaFlux name="my_ionflux" \  
  particles="ions" pri_c \  
  function="plasmaEtchIons" pridep1="theta" \  
  pridep2="surfacematerial" pripar1=2.0
```

for ions, and similarly for neutrals. Again, the `particles` parameter is mandatory and it defines the type of plasma particle the flux distribution definition refers to. In any simulation two such PLASMAFLUX commands must be issued for the two types of plasma particles. The most frequently used distribution functions, namely cosine for neutrals and cosine-to-power for ions, are implemented in the C-Interpreter model library and have been used for the simulations shown in this paper, but any others distribution function can be defined by the user.

Within the code the calculation of a total particle's flux at a given surface point is carried out by integrating the flux distribution function along all directions from the point to all points in space at infinity (reactor domain). Any direction which is obstructed by the structure is ignored. This means that its contribution to the total flux is zero. The calculated flux is normalized with a value of a flux at the highest surface point of the structure where all directions toward the space are unobstructed. Thus the flux value for a surface point can be interpreted as a probability for active particles to reach the surface point. Since there are ions and neutrals in the plasma, the probability is multiplied with normalized densities:

- $N_{ion} / (N_{ion} + N_{neut})$  for ions and
- $N_{neut} / (N_{ion} + N_{neut})$  for neutrals, respectively.

Here  $N_{ion}$  and  $N_{neut}$  represent ion and neutral particles' average densities in the plasma. These parameters are provided by the command PLASMAETCHPROPERTIES by means of the parameter `density` as shown above.

Neutral particles play an important role in surface chemistry in plasma etching processes. The sticking efficiency for such particles is usually  $< 1$  or even  $\ll 1$ , which has to be reflected in the flux calculation. Therefore, VICTORY Process calculates secondary flux values for surface points for any type of plasma particles. For any surface point the algorithm takes into account the flux contribution (reflection and re-emission) from all other surface points, provided that the line connecting a given point and any other surface point is not obstructed by the structure. All surface points thereby serve as micro-sources of bounced off plasma particle(s). Those micro-sources are taken into account together with the ambient (plasma reactor) source. The syntax of how to switch on this optional modeling feature will be shown later in this paper.

Besides the particle fluxes, the total etching rate at a surface point, which describes a complex surface chemistry, must be calculated. This rate is modeled as a function of various plasma particles' parameters, such as

- Flux
- Sticking coefficient
- Rate and other values

Various models found in literature are implemented in the open C-Interpreter model library. The command to be issued to select a specific surface reaction model for the plasma etching simulation is PLASMAETCHREACTION. The syntax for examples presented in this paper reads:

```
PlasmaEtchReaction name="my_plasma_etch" \  
  c_function="plasmaetch_hauguthetal" \  
  dep1="Flux" dep2="Rate" dep3="Sticking" \  
  dep4="Surfacematerial" \  
  par1=4.0 par2=20000.0 par3=0.075 par4=5.0
```

In this example the rate model defined by the C-Interpreter model library function "plasmaetch\_hauguthetal" is chosen. Here the dependencies (`dep1`, `dep2`, `dep3` and `dep4`) are properties at the local surface point position, while the parameters (`par1`, `par2`, `par3`, `par4`) are global modifiable surface reaction model parameters. Note that the dependencies "Flux", "Rate" and "sticking" refer to both ions and neutrals. Therefore any of these dependencies in the function's definition must have two entries. In other words two values are passed to the surface reaction model function for each of the dependencies. The simulator automatically supplies the appropriate values whenever the surface reaction model function is called.

The flux models and the etch rate calculation models described above are linked by the command PLASMAETCHTOPOGRAPHYMODEL. For the examples in this paper we link the previously defined models by:

```
PlasmaEtchTopographyModel
  name="my_plasma_etch_model" \
  reactionmodel="my_plasma_etch" \
  fluxmodel1="my_ionflux" \
  fluxmodel2="my_neutralflux"
```

Note that both ion and neutral flux models must be selected by this command to setup an appropriate plasma etching model.

Once all the process models and characteristics are defined as shown above, one can issue the command PLASMAETCH to run the actual plasma etching simulation. In the cases presented here, one example reads:

```
PlasmaEtch model="my_plasma_etch_model" \
  ionname="my_ions" \
  neutralname="my_neutrals" \
  time=10. autoref \
  NeutralSecSource="CONST"
```

By this command all above defined models and parameters are put together. As shown in the example, it is possible to switch on the secondary flux calculation, both for ion and/or neutral particles, by the parameter NeutralSecSource, followed by the name of micro-sources shape function. In the case of ions, the parameter IonSecSource should be used. It only makes sense to switch on the secondary flux calculation if the sticking efficiency for a chosen particle is not equal to 1, because the existence of bounced-off particles can be simulated. It follows from the fact that for any surface point the amount of flux available for re-emission is proportional to  $(1 - \text{sticking efficiency})$ .

## Examples

The properties of the new VICTORY Process module for plasma etching simulation are demonstrated in the examples shown further in the text. They are based on results published in a paper by Hauguth et al, Microelectronic Engineering 86 (2009) 976-978. Not all parameters required for setting up the plasma etching simulation could be obtained from the publication directly, but could be adjusted by means of calibration. Several parameters were varied in ranges reported in literature, and their effects are presented in the simulation results shown here. In all these cases, some parameters were kept constant, such as:

- Etching rates for materials and single plasma particles
- Sticking efficiency and density for ions
- Global parameters defining flux and rate functions
- Total simulation time

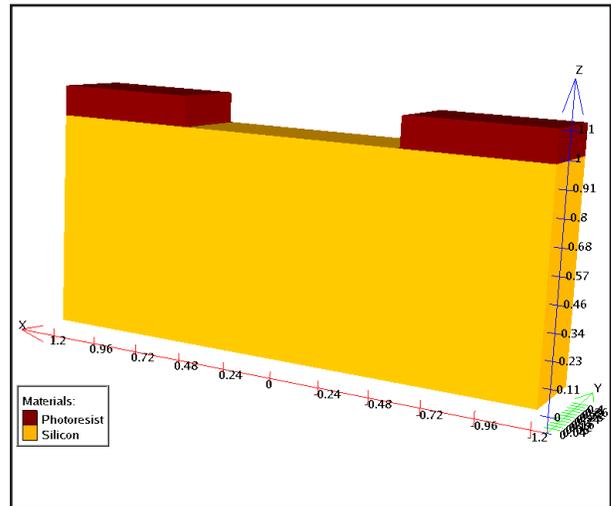


Figure 1. Initial structure before starting the plasma etching simulation.

Note that the etch rates for the mask material are very small in comparison with the silicon ones.

The parameters which were varied are sticking efficiency and density for neutrals.

The common initial structure for all cases is shown in Figure 1.

The structures after performing plasma etching simulation with various parameter combinations are shown in Figures. 2-5.

The densities of ion and neutrals particles are the same for the case shown in Figure 2. Although in real experiments usually  $N_{neut} \gg N_{ion}$ , this case is used for comparison with cases which are much closer to realistic situations.

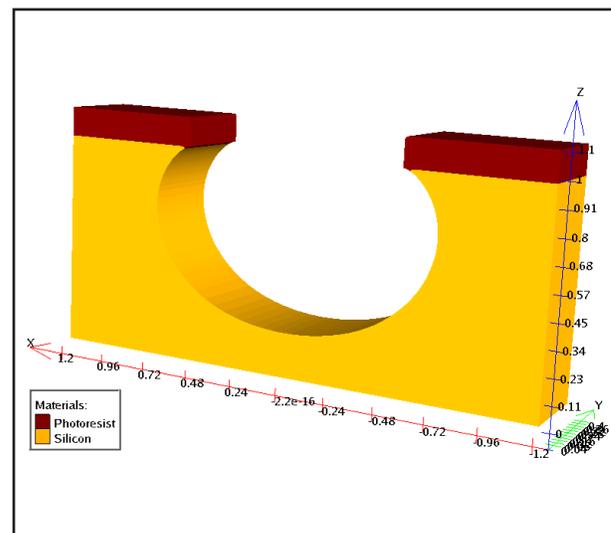


Figure 2. Structure after performing the plasma etching simulation by assuming  $N_{neut} = N_{ion}$ .

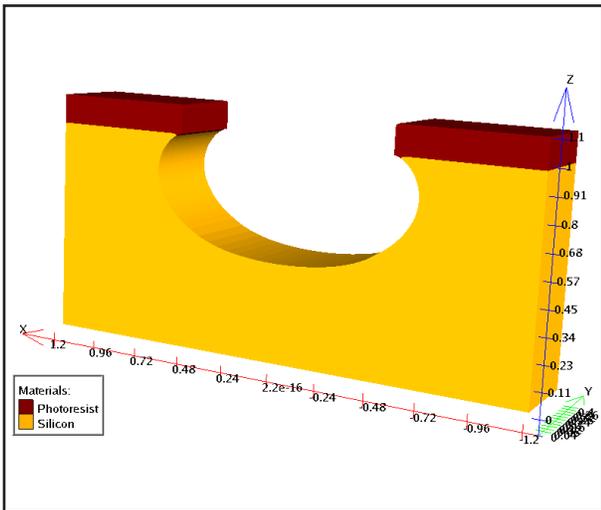


Figure 3. Structure after performing the plasma etching simulation by assuming weakly ionized plasma ( $N_{net}/N_{ion}=10000$ ) and a neutral sticking efficiency of 1.0.

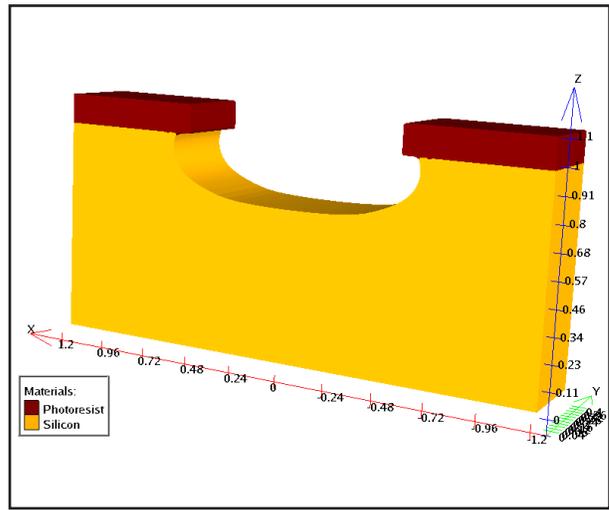


Figure 4. Structure after performing the plasma etching simulation by assuming weakly ionized plasma ( $N_{net}/N_{ion}=10000$ ) and a neutral sticking efficiency of 0.5.

In the cases shown in Figures 3, 4 and 5 a high ratio between the neutral and ion flux was applied ( $N_{net}/N_{ion} = 10000$ ). This corresponds to typical plasma etching conditions of low ionization degree. The sticking efficiency for the neutral particles was varied for these cases:

- Figure 3 - neutral sticking efficiency : 1.0
- Figure 4 - neutral sticking efficiency : 0.5
- Figure 5 - neutral sticking efficiency : 0.2

There is a significant qualitative difference in the cases shown in Figures 4 and 5, where the sticking efficiency  $< 1$ , in comparison to the case shown in Figure 3. Only these two cases show the experimentally observed un-

der-etching below the mask. Because these domains are invisible for the main source (reactor domain) of active particles, their appearance is only due to bounced-off active particles from the rest of the structure.

## Conclusion

The plasma etching module in VICTORY Process is capable of simulating complex processes within a feature scale for three-dimensional structures. The technological parameters from the reactor scale can be included by means of transport characteristics (plasma particles' distribution functions, etching rates etc.) via user's definable C-functions stored in an open model library. The distinction between plasma ion and neutral particles is fully implemented into the code, which allows complex models to be applied. One of the main results of the example presented in this paper is the module's ability to predict the etching of domains covered by the mask, which is caused by bounced-off active particles.

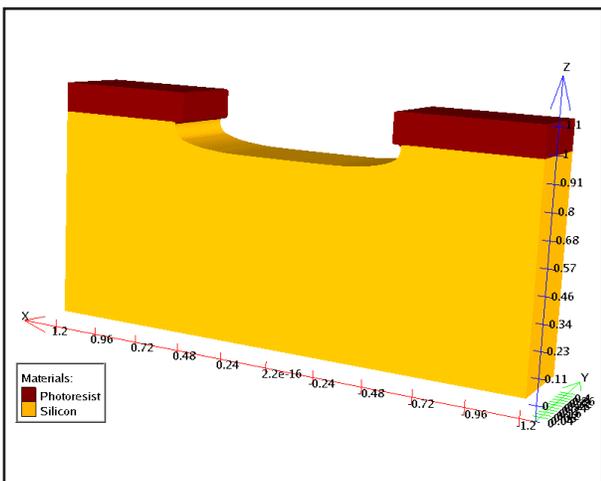


Figure 5. Structure after performing the plasma etching simulation by assuming weakly ionized plasma ( $N_{net}/N_{ion}=10000$ ) and a neutral sticking efficiency of 0.2.