

Backend Process Simulation Including Plasma Etch



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Introduction

- Elite as Part of ATHENA
- Processes Simulated by Elite
- Interaction of String and Gridding Algorithms
- Features of Elite include: Plasma Etching and Void Formation
- Step-by-Step Demonstration of Complex Trench Example



ELITE as Part of ATHENA

- ATHENA simulates all types of semiconductor technology processes
 - Inside wafer processes: Implant, diffusion, oxidation, defect generation, etc.
 - Topography processes: Deposition, Etching, Reflow, CMP, etc.
 - Photolithography processes: Imaging, Exposure, Photoresist Development
- In modern technologies these processes take place in any order
- Likewise ATHENA can simulate any sequence of processes



ELITE as Part of ATHENA (con't)

- ATHENA invokes specific modules to simulate each process step
- In-wafer Processes are simulated by SSuprem4 or Flash Module
- Simple topography processes are also handled by SSuprem4
 - Geometrical or vertical etch
 - Conformal deposition



ELITE as Part of ATHENA (con't)

- Elite simulates more sophisticated deposition and etch processes
- Elite takes into account
 - Geometrical and rate characteristics of etch or deposition machine
 - Geometrical and material characteristics of the structure
- Photolithography is simulated by Optolith



Processes Simulated by Elite

- Topography processes are modeled by
 - Defining a machine in the `RATE.DEPO` or `RATE.ETCH` statement
 - Running the machine for a specified period of time
- Wet (Isotropic) Etching
 - `WET` and `ISOTROPIC` parameters in the `RATE.ETCH` statement
- Reactive Ion Etching (RIE)
 - `RIE` flag and combination of `ISOTROPIC`, `DIRECTIONAL`, `CHEMICAL` and `DIVERGENCE` parameters in the `RATE.ETCH` Statements



Processes Simulated by ELITE (con't)

- Chemical Vapor Deposition (CVD)
 - CVD and STEP.COV parameters in the `RATE.DEPO` statement
- Deposition with different geometry of material sources
 - Unidirectional, Dual Directional, Hemispheric, Planetary, Conical
 - `ANGLE1[ANGLE,ANGLE3]`, `DEP.RATE`, `SIGMA.DEP` parameters



Processes Simulated by ELITE (con't)

- Monte Carlo Deposition
 - To estimate step coverage and film density
 - MONTE1/2, ANGLE, SIGMA.DEP, Sticking Coeff. parameters
- Chemical Mechanical Polishing (CMP)
 - Parameters in the RATE.POLISH statement
- REFLOW of glassy silica (oxide, BPSG, etc.)
 - Takes place simultaneously with impurity diffusion
 - When REFLOW flag set on the DIFFUSE and MATERIAL statements



Plasma Etching in Elite

- Monte Carlo based plasma etching model
- Calculates energy-angular distribution of ions emitted from the plasma of RIE etchers
- Etch rates in each point of complex topography are calculated
 - shadowing effects are take into account
 - etch rates could depend on local physical characteristics of the substrate (e.g. doping or stress level)



Plasma Etching in Elite (con't)

- Characteristics of plasma etching machine are specified as follows:

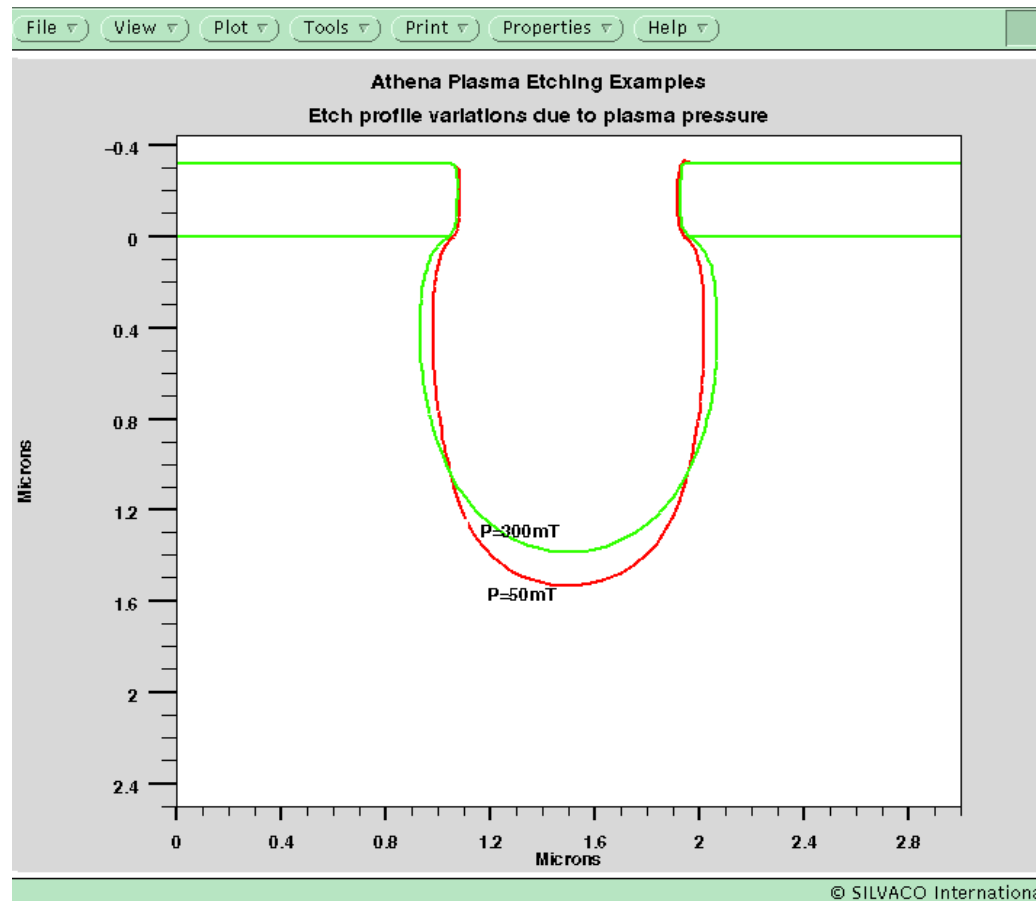
```
RATE.ETCH MACHINE=PETCH PLASMA \  
  PRESSURE = 100 \      pressure           [mTorr]  
  TGAS = 300\  
    gas temperature     [K]  
  VPDC = 32.5\  
    DC bias             [V]  
  VPAC = 32.5\  
    AC voltage in the sheath-  
    bulk interface     [V]  
  LSHDC = 0.005\  
    mean sheath thickness [mm]  
  etc
```

- Relative etch rate coefficient for each material in the structure should be specified:

```
RATE.ETCH MACHINE=PETCH PLASMA MATERIAL=SILICON K.I=1.1
```



ATHENA Plasma Etching Examples – Etch profile Variations Due to Plasma Pressure





Dopant/Stress Dependent Etching

- Dopant/stress dependent etching rate can be specified for any type of etching machine, e.g.:

```
Rate.Depo Machine=RIE MATERIAL=SILICON\  
Impurity=Phos Enh.Max=2 Enh.Scale=5.0 Enh.minC=17
```

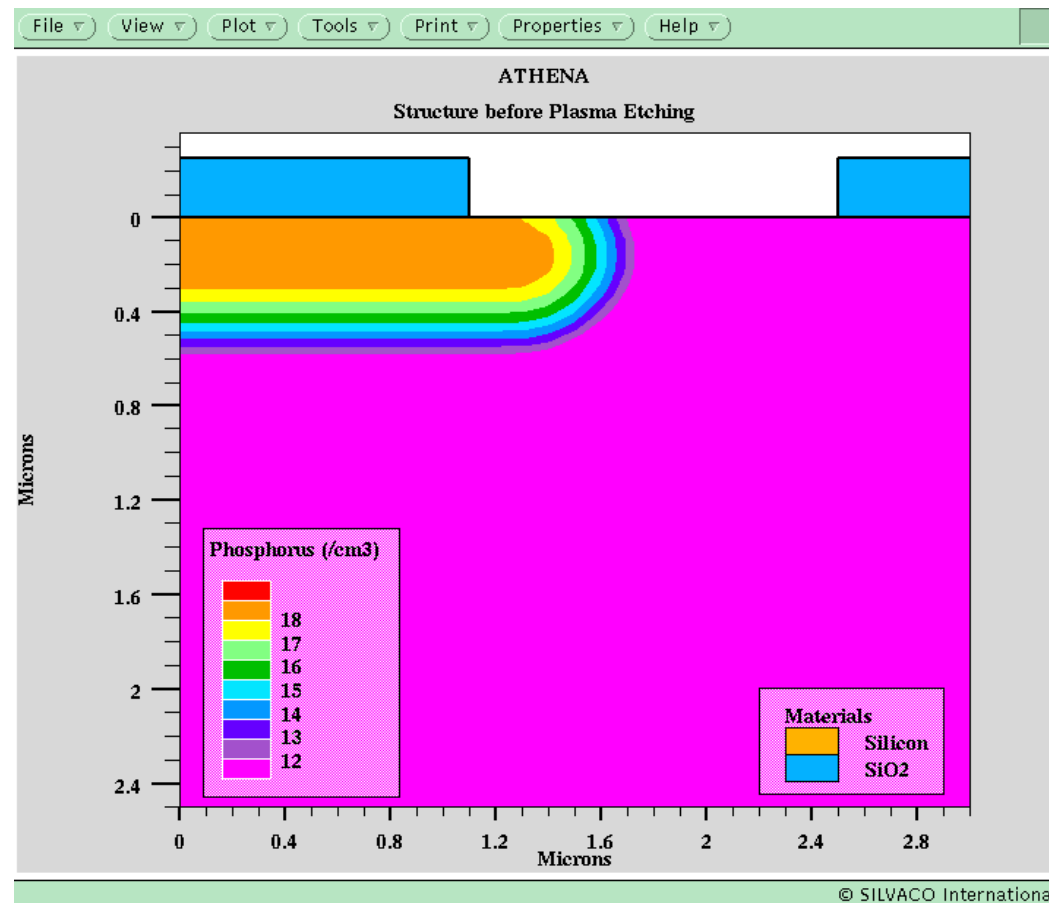
- The enhanced etching rate is defined by the equation:

$$Er_{enh} = ER[1 + 0.5 * Enh.Max * (\tanh(Enh.Scale(C - Enh.MinC)) + 1)]$$

- C is a solution (dopant concentration, stress, etc.)
- Enh.Max defines the maximum enhancement factor
- Enh.MinC is the value of concentration below which enhancement decays
- Enh.Scale is enhancement scaling factor
- For exponentially varying solutions both C and Enh.MinC are used in logarithmic form

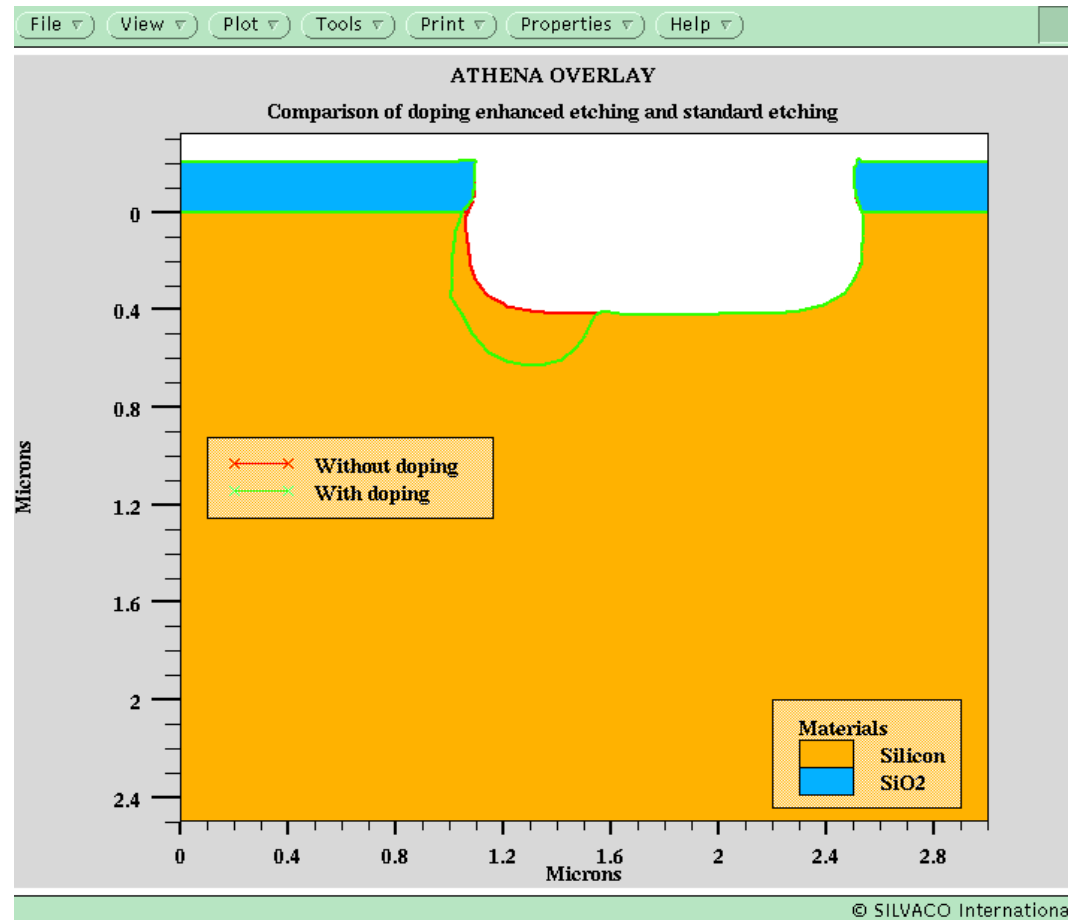


Structure Before Plasma Etching





ATHENA Overlay – Comparison of Doping Enhanced Etching and Standard Etching



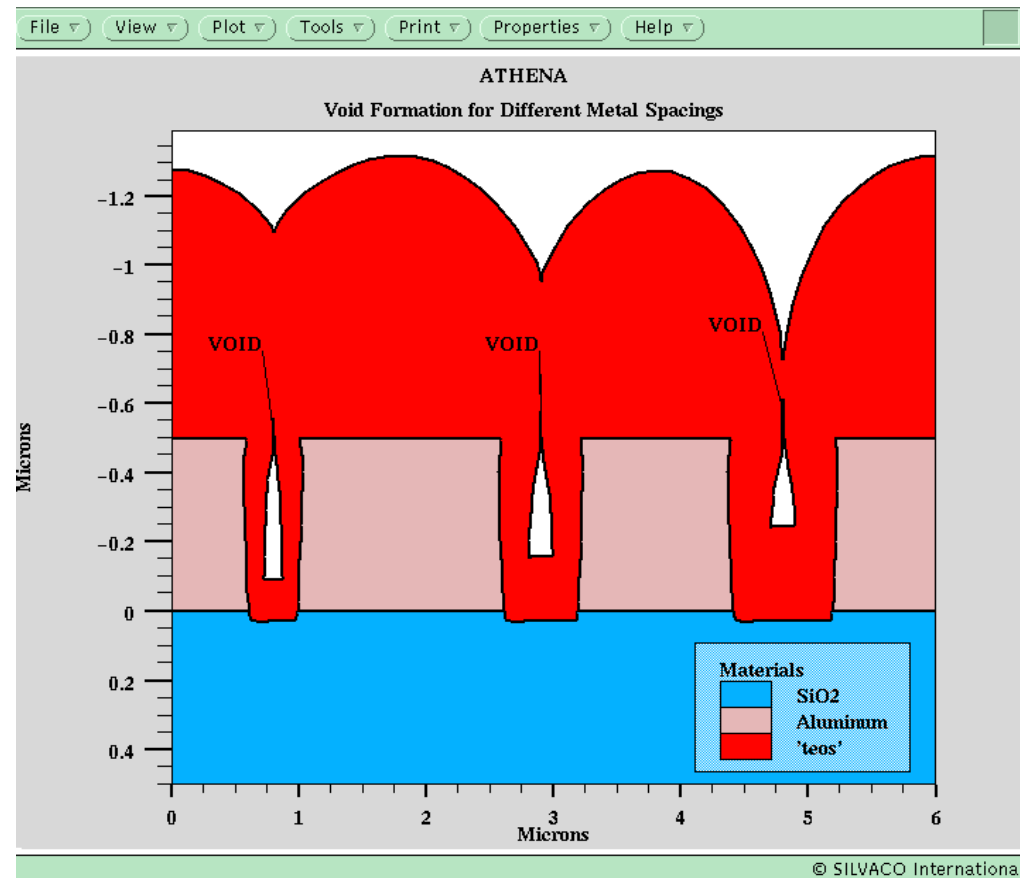


Void Formation in Elite

- Algorithm which allows formation of keyhole voids during material deposition into trenches or vias
- Void boundary condition are set correctly so subsequent deposits do not fill the void
- Void formation can be followed by simulation of viscous reflow of the deposited material to reduce or eliminate the void
- Next figure shows that the position of the void rises with contact width



Void Formation for Different Metal Spacings





Interaction of String and Gridding Algorithms

- In Elite, exposed surface is considered as a string of joined points
- During etching or deposition each point of the string advances
- New positions of each point are defined by local etch/deposition rate
- In contrast to other topography simulators, Elite links the string with a simulation grid



Interaction of String and Gridding Algorithms (con't)

- During etching, the string cuts through into the grid
- Special regridding algorithm is applied to the area under the new surface
- During deposition, the string advances outside the simulation grid
- Special gridding algorithm is applied to cover newly deposited area



Complex Trench Formation Example

- Some of discussed Elite capabilities are demonstrated in the following example
- The example consists of a complex process sequence in order to show that ATHENA allows the easy transition from in-wafer to topography processes and back
- Demonstration is focused on Elite /SSuprem4 interface and on gridding issues

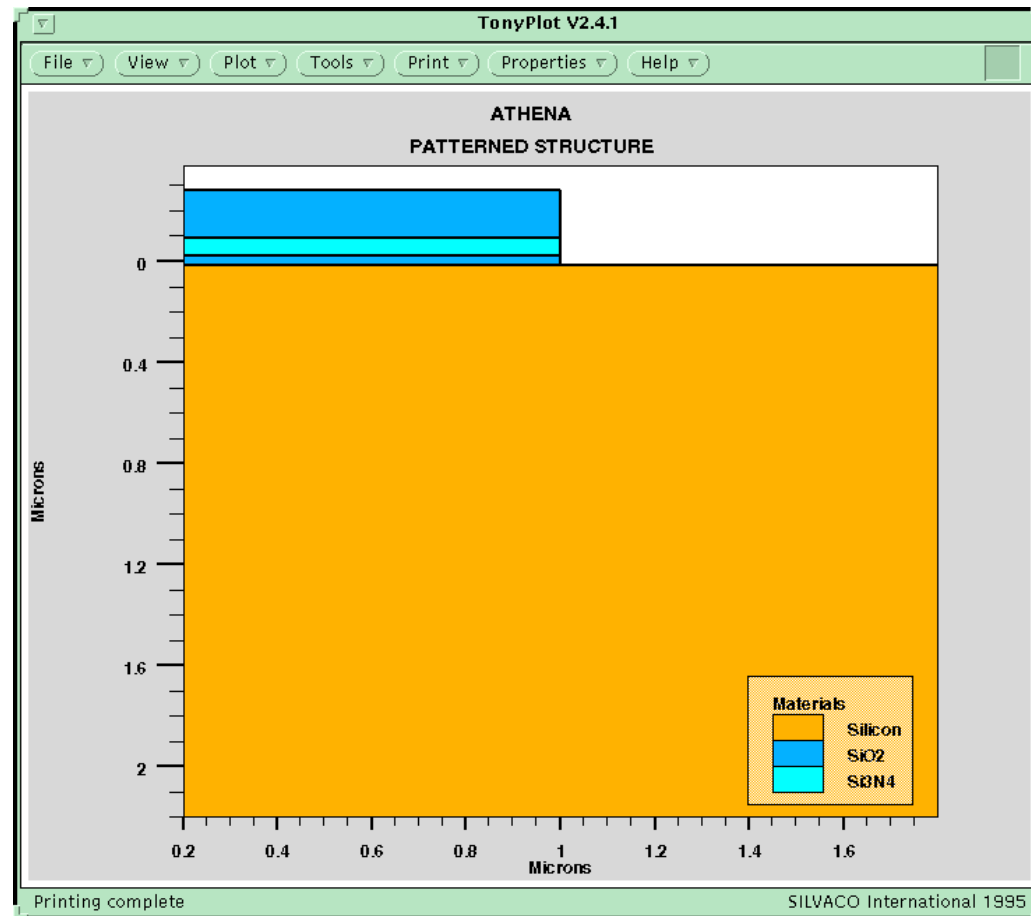


Complex Trench Formation Example (con't)

- First, an oxide/nitride/oxide stack is formed by oxidation and conformal deposition
- Then the stack is patterned using simplified mask process (Figure 5)
- After that a nitride spacer is formed by combination of conformal deposition and etch-back using RIE (Figure 6)
 - ISOTROP and DIRECT parameters are used to control shape and width of the spacer

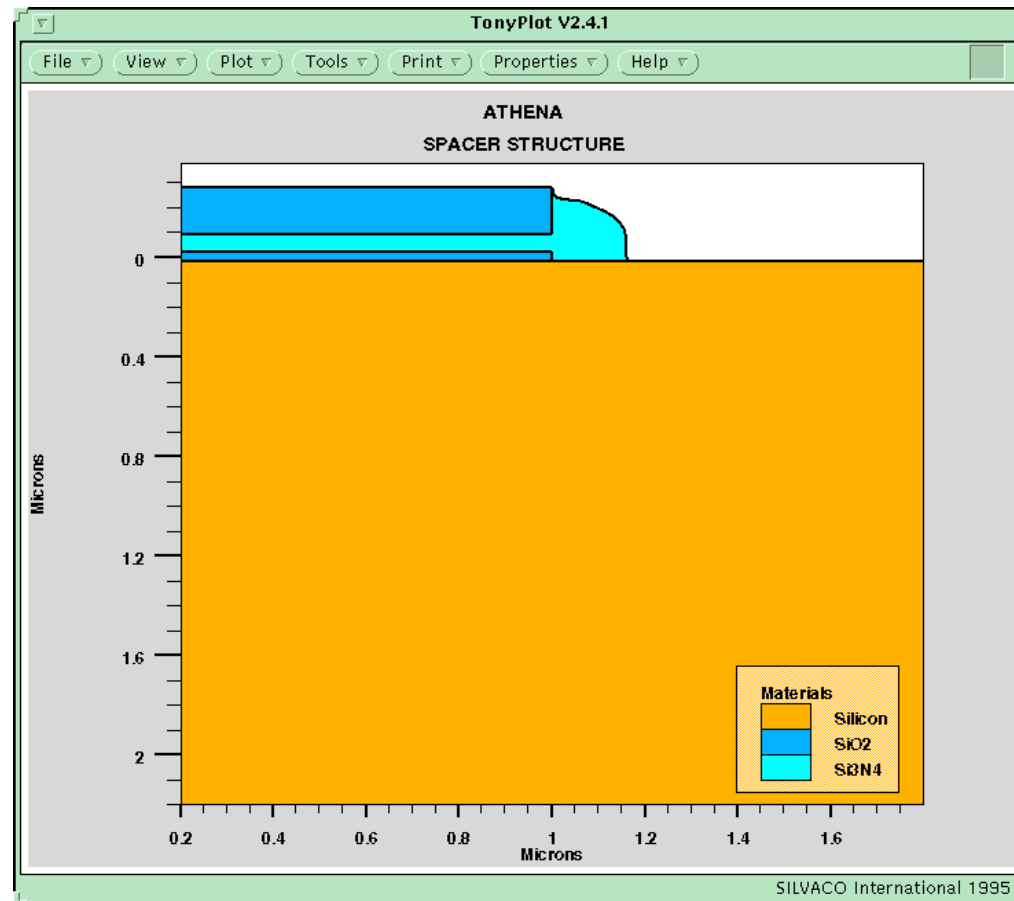


Patterned Structure





Spacer Structure



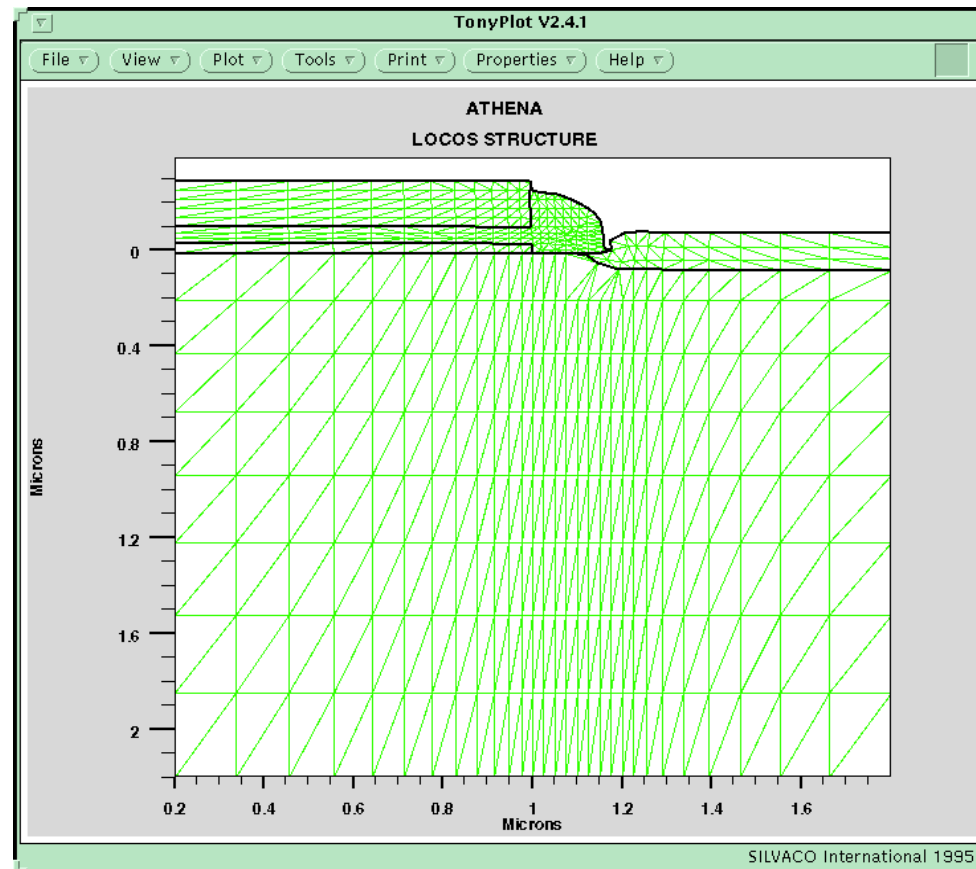


Complex Trench Formation Example (con't)

- The thick spacer is used to reduce length of LOCOS with short Bird's Beak
- Viscous stress-dependent oxidation gives accurate LOCOS (Figure 7)
- The grown LOCOS serves as a mask for subsequent Trench etching
- So far a very coarse grid in substrate was used. This saved a lot of simulation time
- Much finer grid is needed for trench formation and doping. This is achieved by DevEdit remeshing (Figure 8)

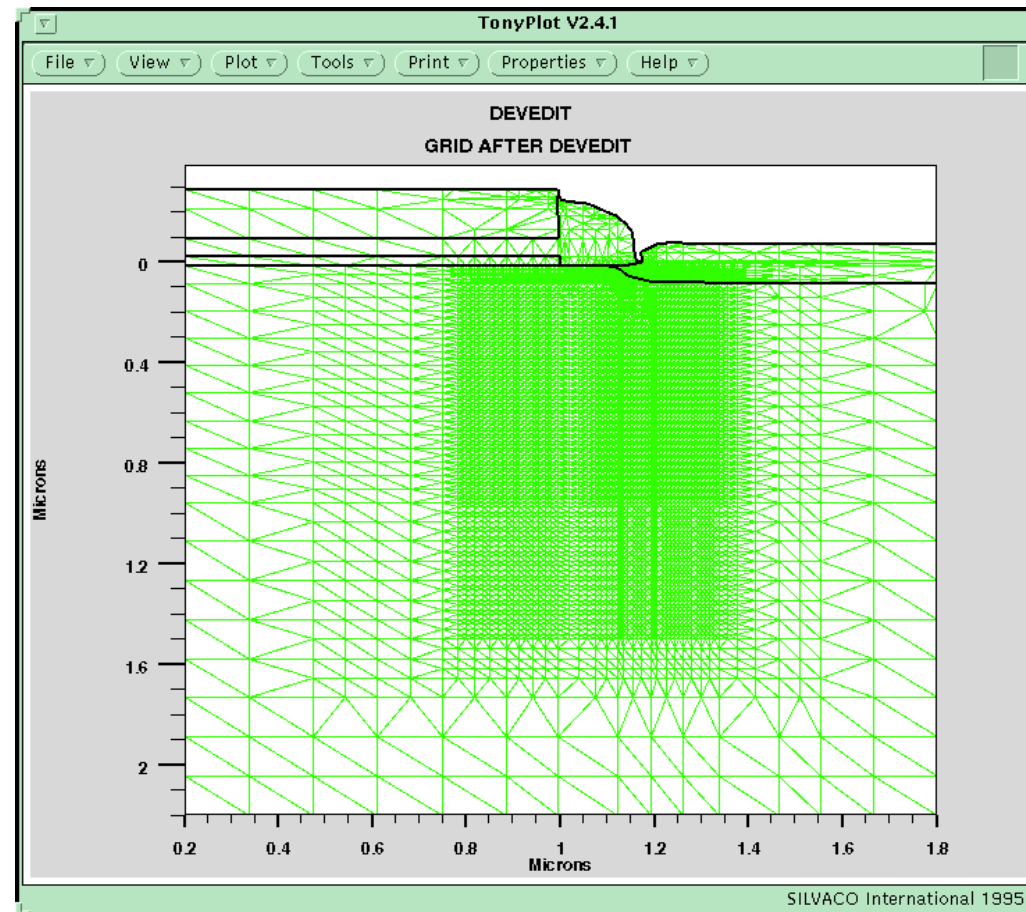


LOCOS Structure





Grid After DevEdit



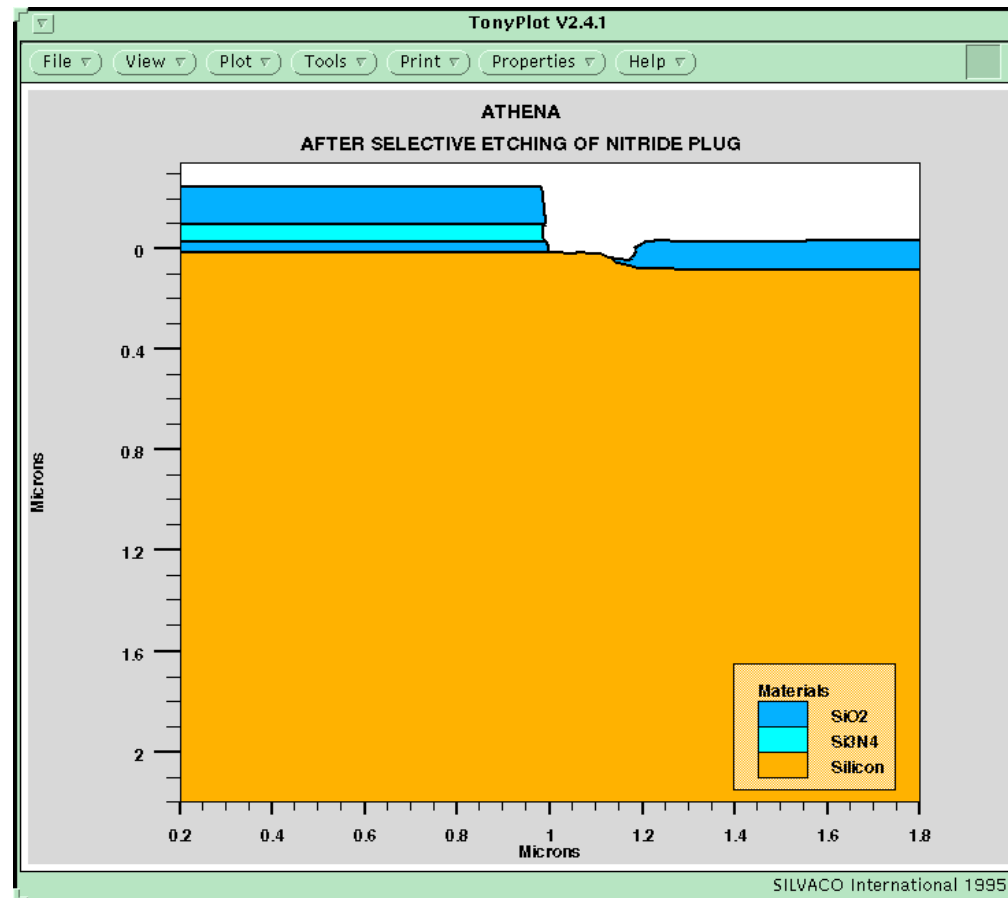


Complex Trench Formation Example (con't)

- Next step opens a window for subsequent trench etching
- It uses a selective nitride etching simulated by RIE model with high directional etch rate for nitride (Figure 9)
- Deep trench is formed using high directional component of silicon etch rate (Figure 10)
- Tuning of the trench shape could be done by varying the isotropic rate

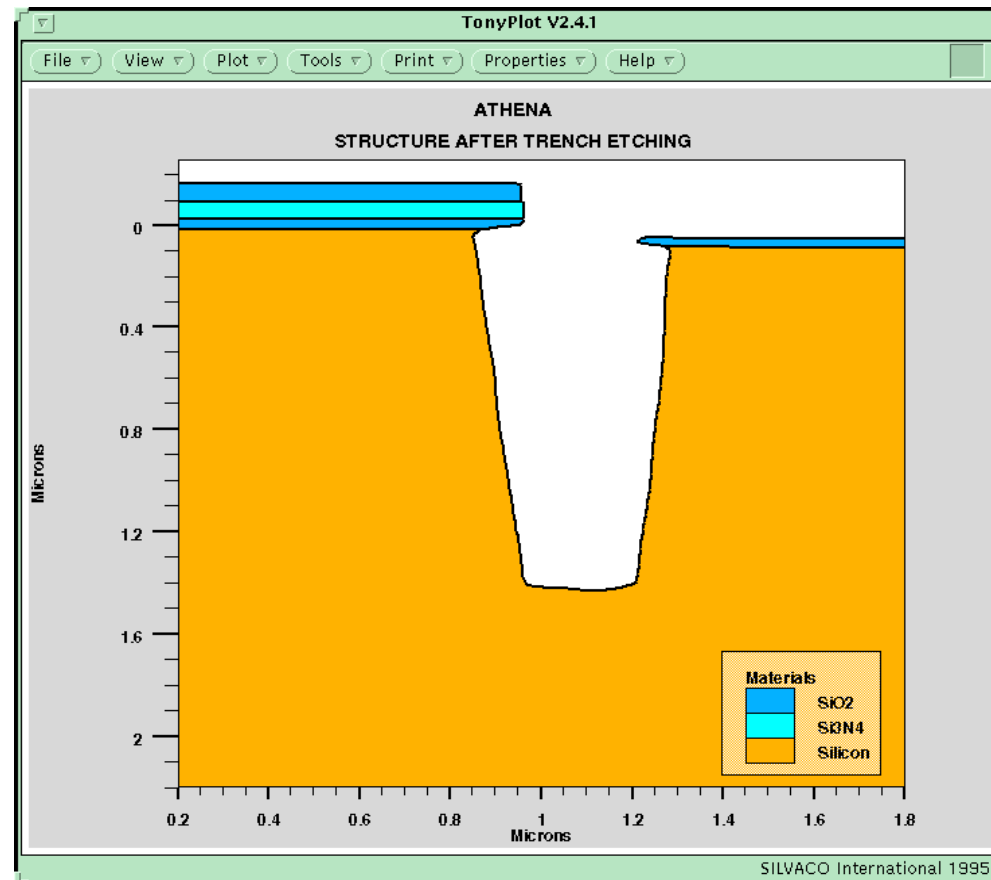


After Selective Etching of Nitride Plug





Structure After Trench Etching



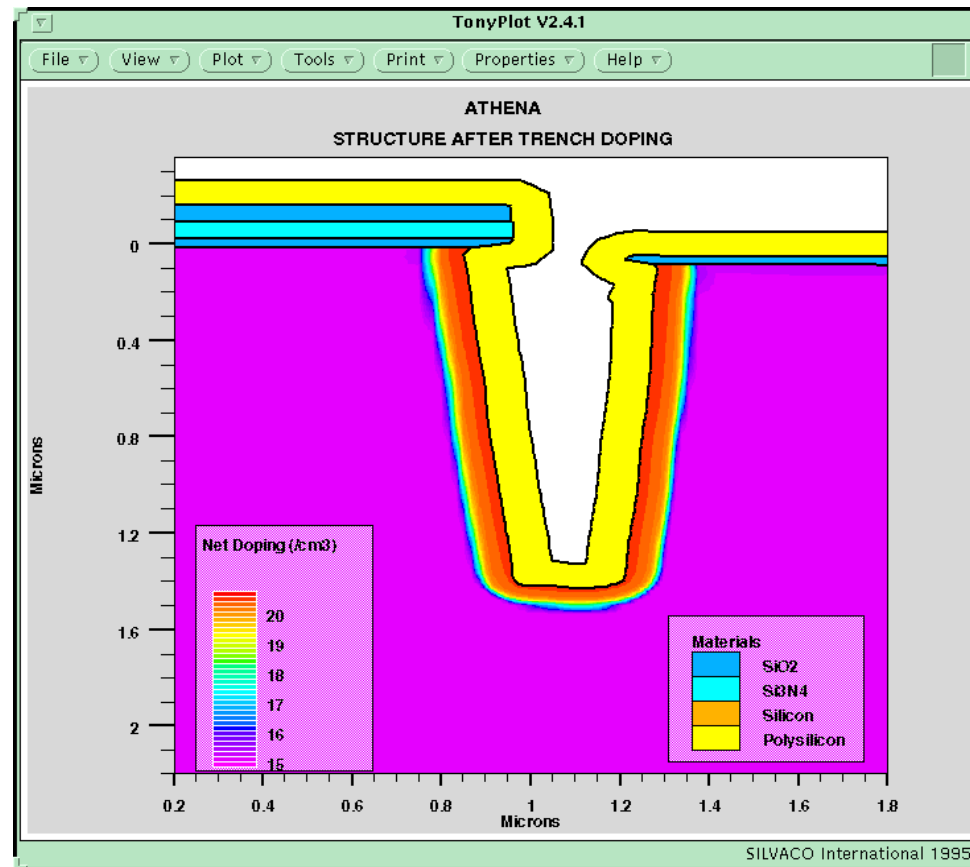


Complex Trench Formation Example (con't)

- Next step is to dope walls and bottom of the trench
- This is done by CVD deposition of phosphorus doped poly-layer and subsequent diffusion (Figure 11)
- It should be mentioned that substrate is not doped because thin oxide layer is left after trench etching
- Then polysilicon is etched completely (Figure 12)

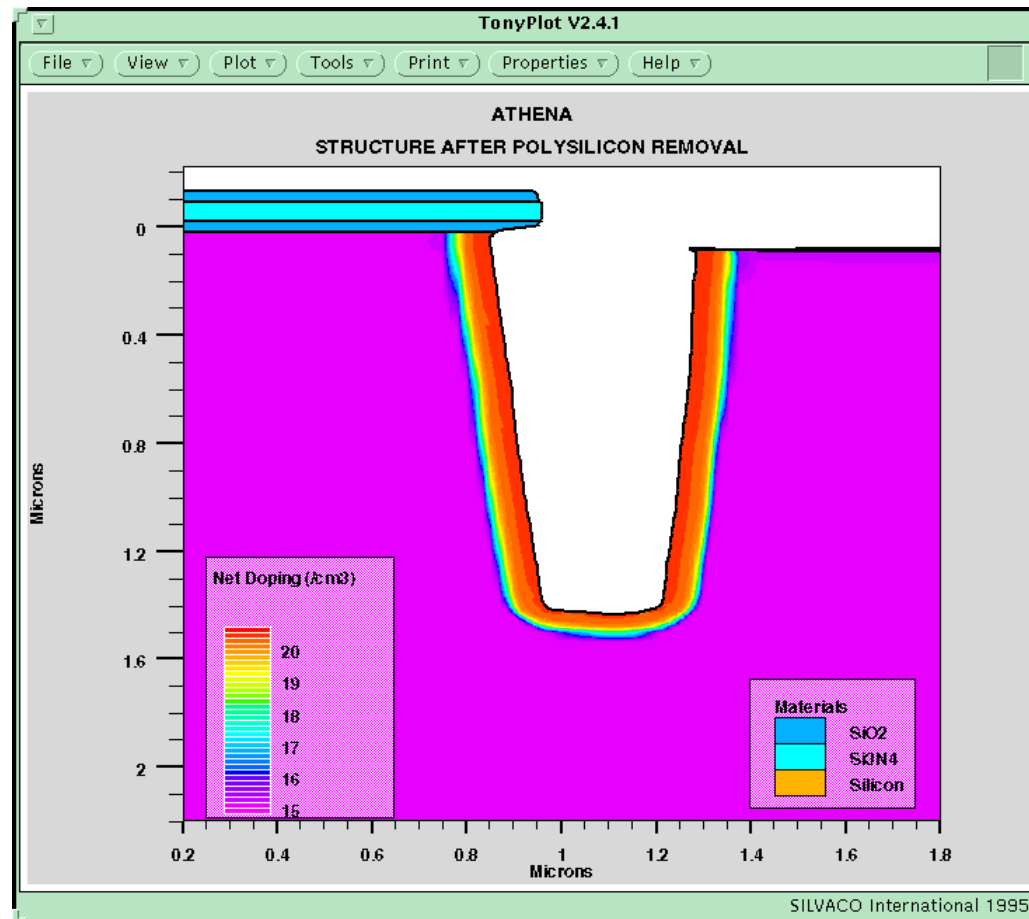


Structure After Trench Doping





Structure After Polysilicon Removal



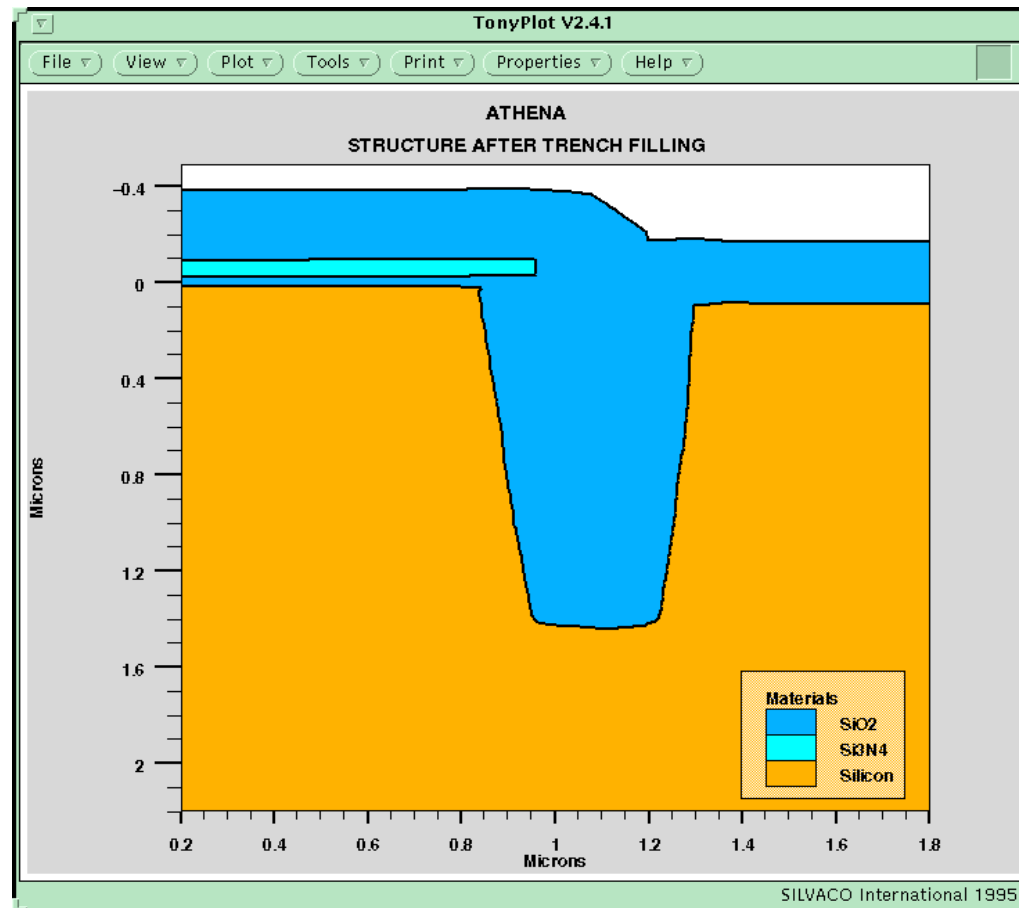


Complex Trench Formation Example (con't)

- However, some residual polysilicon islands could remain after etching
- Slight reoxidation is used to consume these residuals (shown in figure on page 33)
- After that the trench is filled using oxide CVD deposition (shown in figure on page 34)
- A void could be formed in the process



Structure After Trench Filling



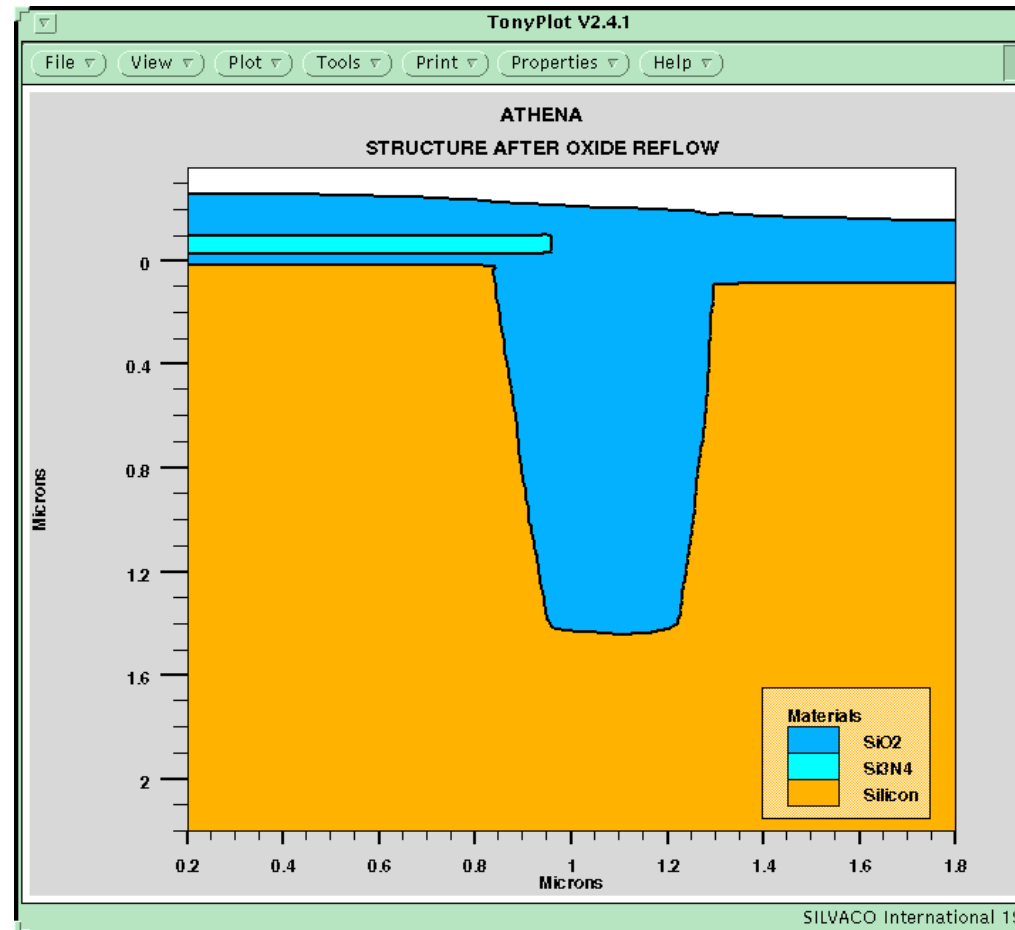


Complex Trench Formation Example (con't)

- After the trench is filled the outer oxide surface is always non-planar
- There are several methods of surface planarization
- One of them is viscous reflow which removes the step formed previously (Figure 15)
 - Impurity redistribution takes place simultaneously with reflow
- The final step of the process etches all excessive material layers and leaves only filled trench (Figure 16)

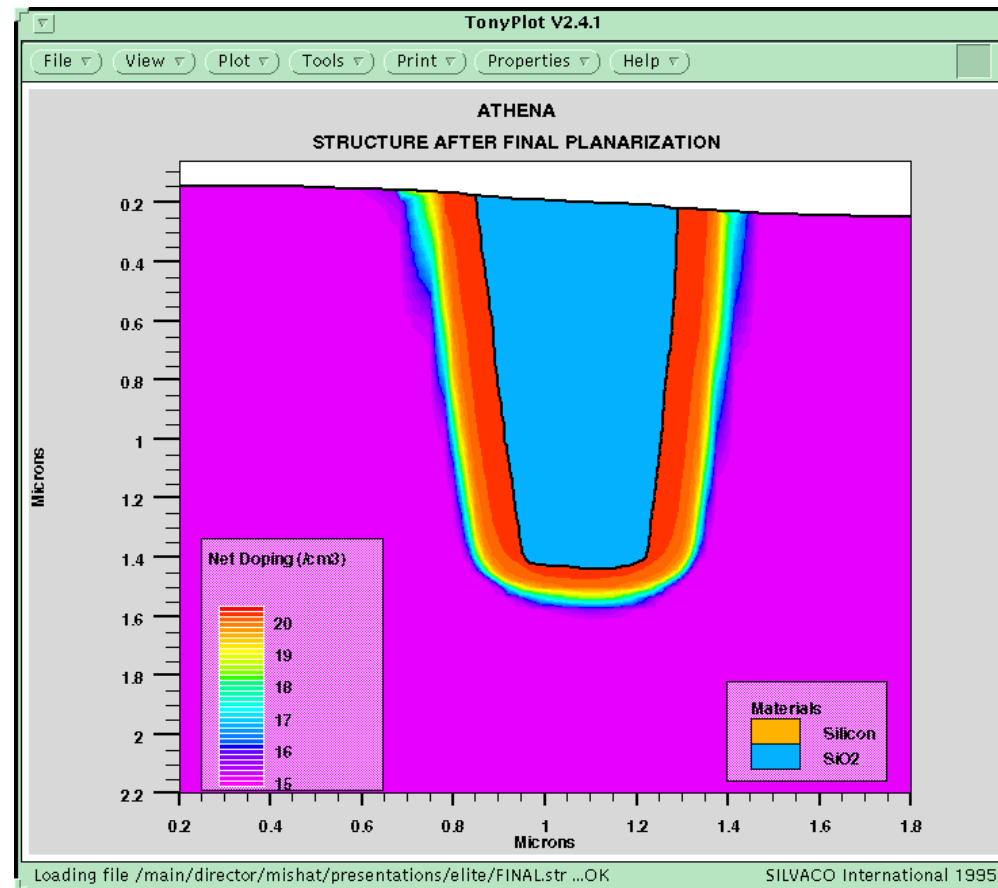


Structure After Oxide Reflow



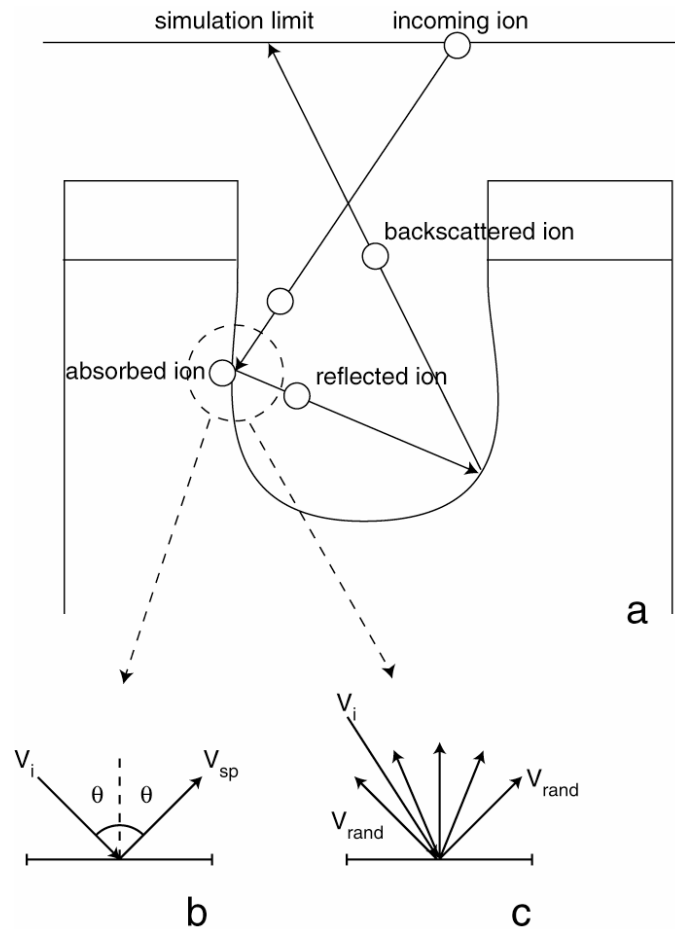


Structure After Final Planarization





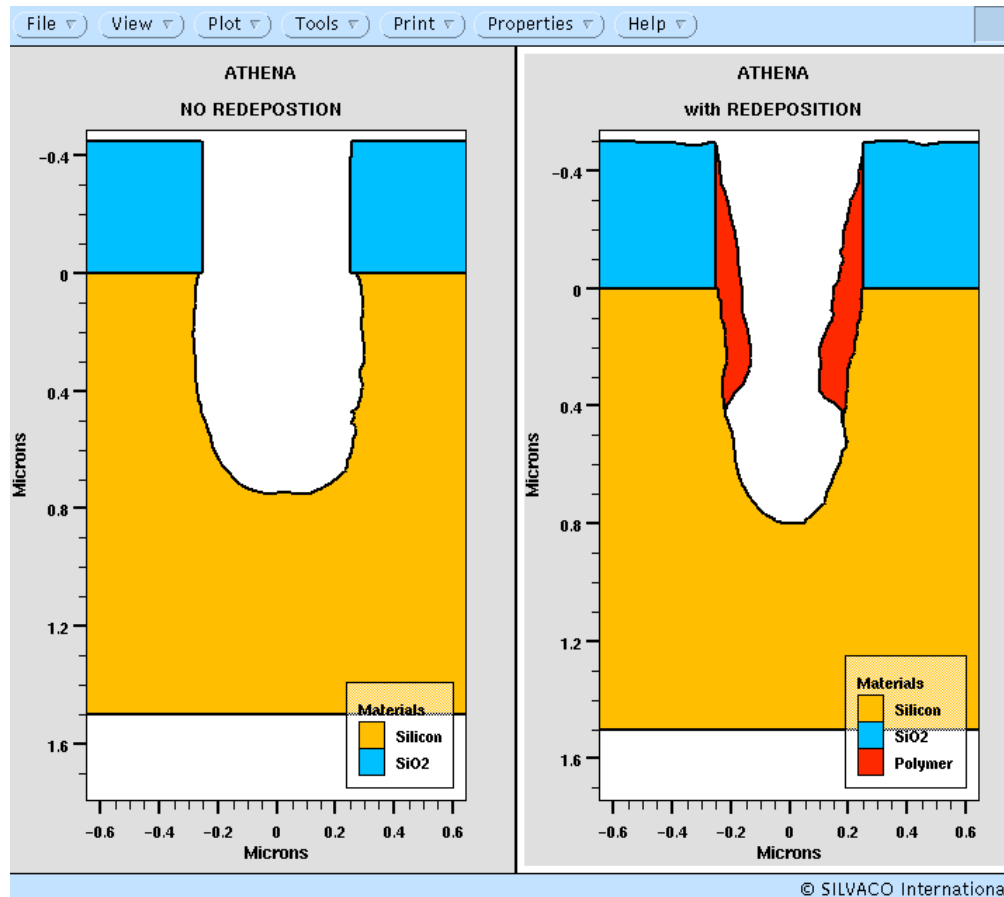
Schematic of Monte Carlo Etch



- Diagram of Plasma Flux algorithm (a) including zoom-in of ion reflection models (b and c)



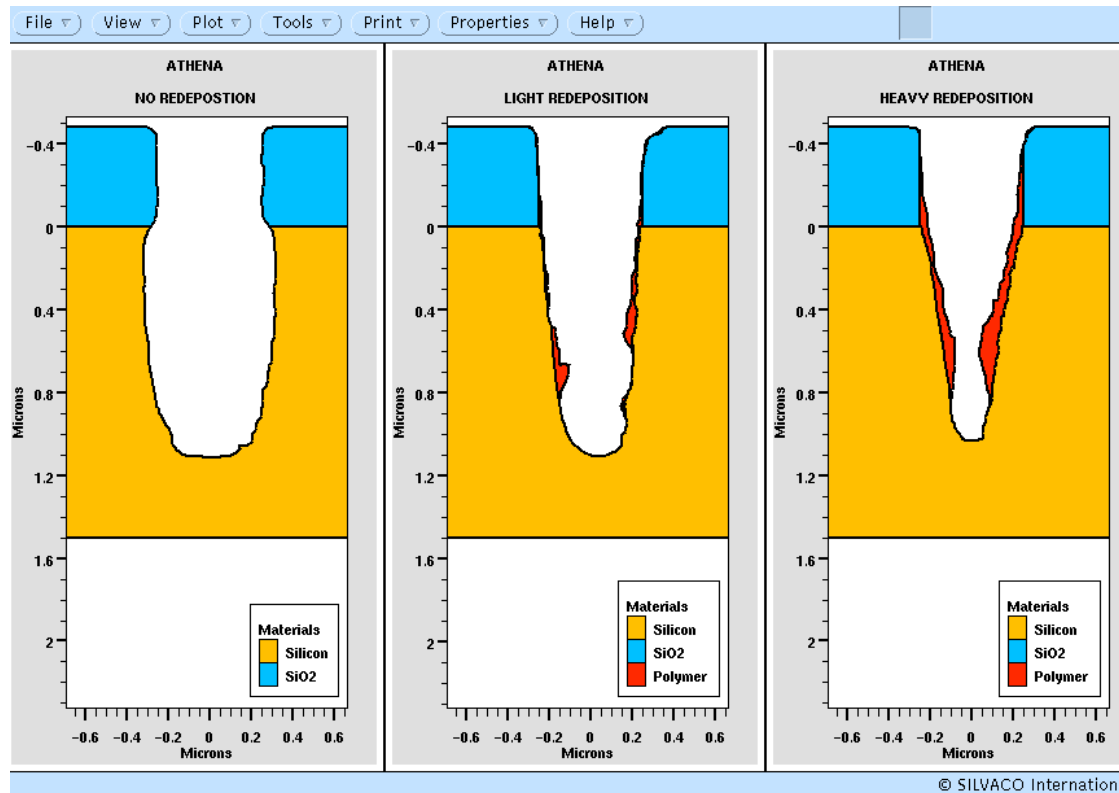
Effect of Polymer Re-Deposition



- Comparison of silicon trench etch with and without polymer redeposition



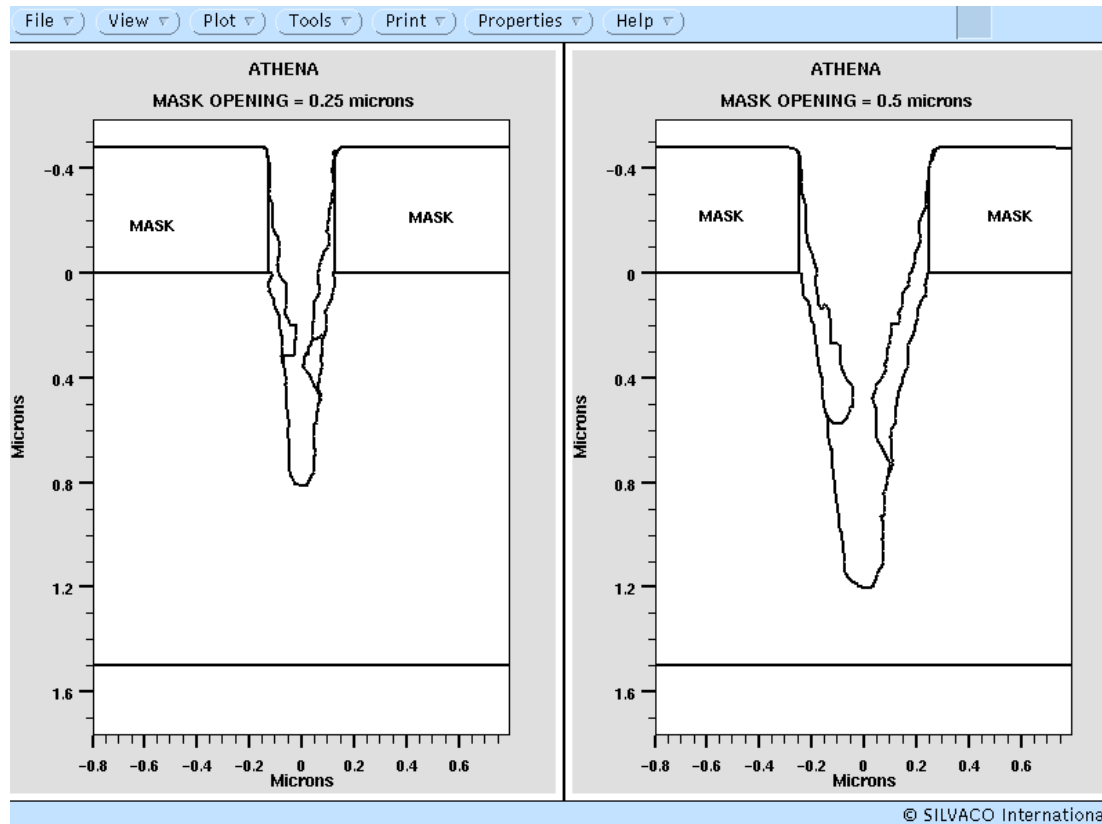
Deep Trench Etch Profiles



- Demonstration of the effect of redeposition on trench sidewall Angle



Mask Opening



- Etch depth varies with the size of the mask opening as the redeposited material restricts etching the bottom of the trench

Chemical Mechanical Polishing in ATHENA



ATHENA
Process Simulation Framework

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Overview

- Effective planarization is an increasingly important process in any submicron VLSI device technology
- For five or more layer technology at least one layer should be perfectly planar
- Lack of planarity may cause serious problems for lithography and dry etching in sub 0.5 micron processes
- Increasingly popular planarization technique is CMP in which the wafer is held on a rotating carrier while its face is pressed against a polishing pad covered with a slurry of an abrasive material
- Allows very high degree of planarization because it is nonlocal process determined by the topography of the surrounding features
- Simulation of the process is very important due to its strong dependency on the device layout, pattern density, and topography from previous oxidations, etches, and depositions



Applications

- Emerged as a preferable planarization technique for several advanced technologies
- Main application is planarization of intermetal layer dielectric in multilayer interconnects
- has also been used to obtain high degree of planarity in submicron trench isolation process in MOS technology
- Similar techniques have been used for bipolar device isolation
- Such isolation techniques are extremely important when thermal constraints do not allow a more conventional LOCOS processing of silicon



Hard and Soft CMP Models

- Two different models (hard polishing and soft polishing) are implemented into ATHENA/ELITE
- Both models are phenomenological and based only on wafer topography
- They do not account for stresses of the polishing pad, fluid flow, removal of material by erosion, etc.
- The hard polishing model takes into account only nonplanarity of the wafer surface and adjusts the polish rate accordingly
- The soft polishing model accounts for flexibility and hardness of the polishing pad and reasonably defines the dependence of polish rate on the wafer shape



ATHENA/Elite Syntax

- The CMP module uses syntax similar to that of the etch simulation in Athena/Elite
- The **RATE.POLISH** statement is used to define the type of polishing to be used as well as the model parameters
- The hard and soft models could be used separately or simultaneously
- A small isotropic removal portion could be added using the **ISOTROPICAL** parameter which is usually much smaller than the lowest polishing rate
- The **POLISH** statement defines the time of polishing process as well as time and spatial discretization used in simulation



Hard Polishing Model

- This is a simplified version of a model by Burke (P.A. Burke, Proc. VMIC Conf. 1991, pp.379-384)
- The model uses a constant polish rate for areas above $Y_{max} - dx$ and zero for areas below $Y_{max} - dy$. The rate is calculated from the pattern factor

$$\text{hardRate} = \text{max.hard} * (1 - \text{pf}) + \text{min.hard} * \text{pf}$$

- where : max.hard and min.hard are maximum and minimum polish rates specified in micron/sec, etc.
- pf is the pattern factor which is estimated as follows:

$$\text{pf} = \frac{\text{length of the surface (at } Y_{max} - dy)}{\text{total length of the surface}}$$

where: ymax is vertical position of current highest point; and dy is an average vertical shift during one time step



Soft Polishing Model

- Uses mathematical models of J. Warnock (J Electrochem. Soc. V. 138, pp. 2398 - 2402, 1991)
- Models the pad flexibility (hard or soft) via the **LENGTH.FAC** parameter
- Models texture of the pad surface with the parameter **HEIGHT.FAC**
- Models erosion due to chemical slurry via the **KINETIC.FAC** parameter and **ISOTROPICAL** component
- The **SOFT** rate and **ISOTROPICAL** rates can be set for each material



Conclusion

- ATHENA is based on a unified string/grid algorithm capable to simulate technology processes in structures consisting from many material regions of arbitrary geometry
- Combination of SSuprem4 and Elite within ATHENA framework allows to simulate complex process sequences which include both in-wafer and topography steps