Multi-Scale Process TCAD at the Institute for Microelectronics, TU Wien

Lado Filipovic

CDL for Multi-Scale Process Simulation for Semiconductor Devices and Sensors

Institute for Microelectronics, TU Wien

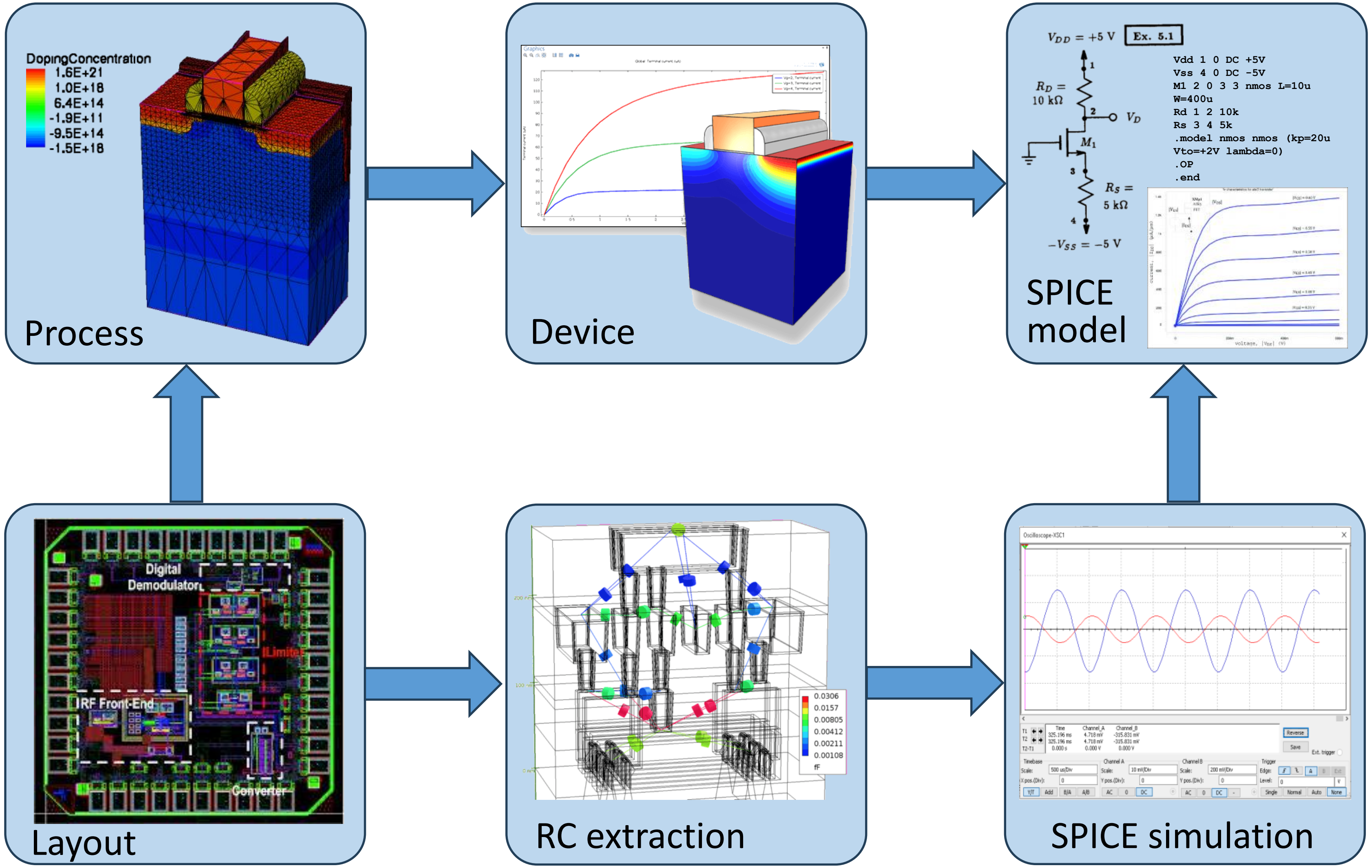
Federal Ministry
Republic of Austria
Labour and Economy

Outline

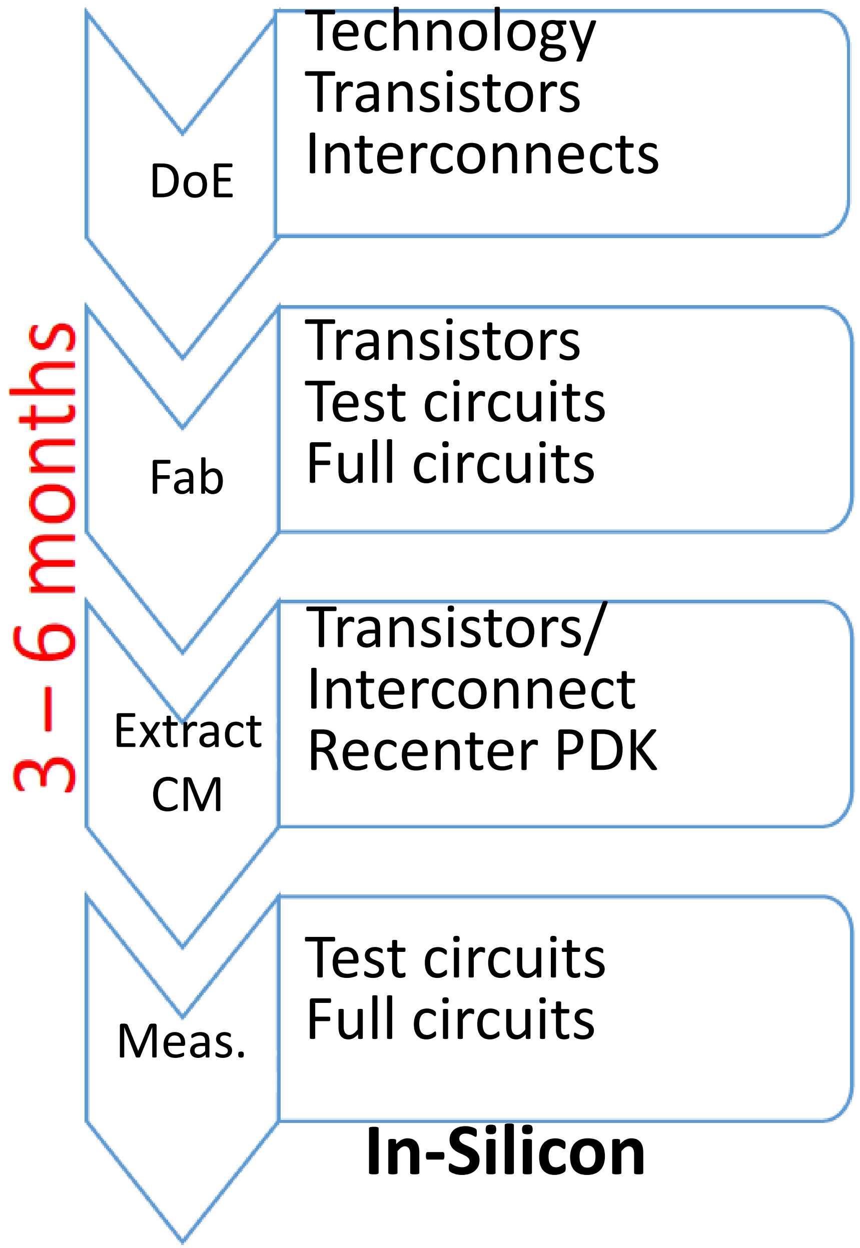
- **Technology Computer-Aided Design (TCAD)**
- ViennaPS Framework
- Process Simulation
  - Chemical Vapor Deposition
  - Plasma Etching
- Link to Equipment Settings

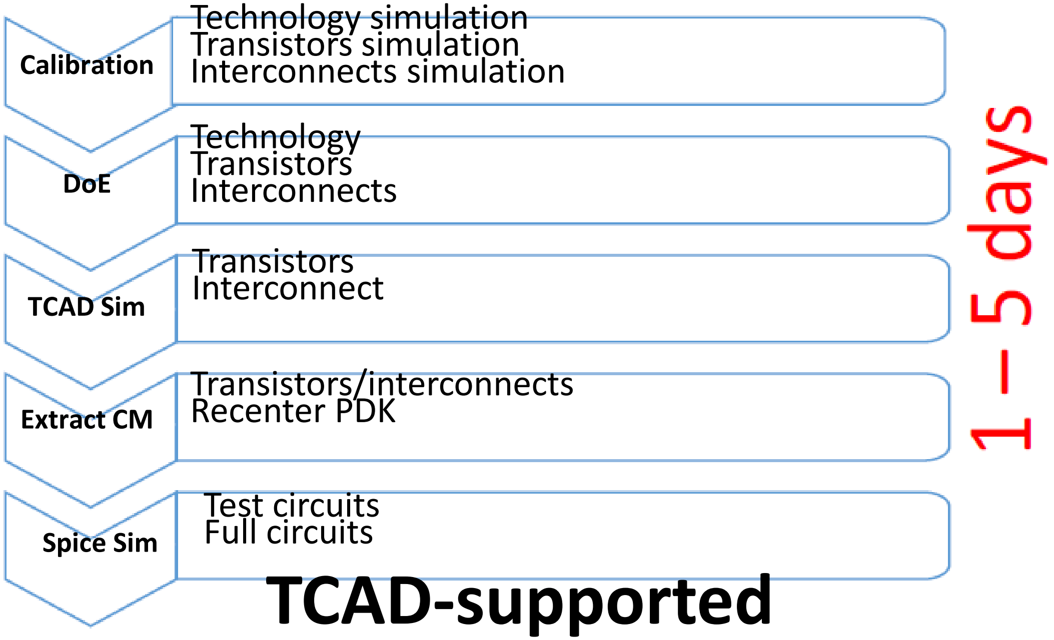
What is TCAD?

- Simulation tools used to model semiconductor fabrication and operation



Why TCAD?

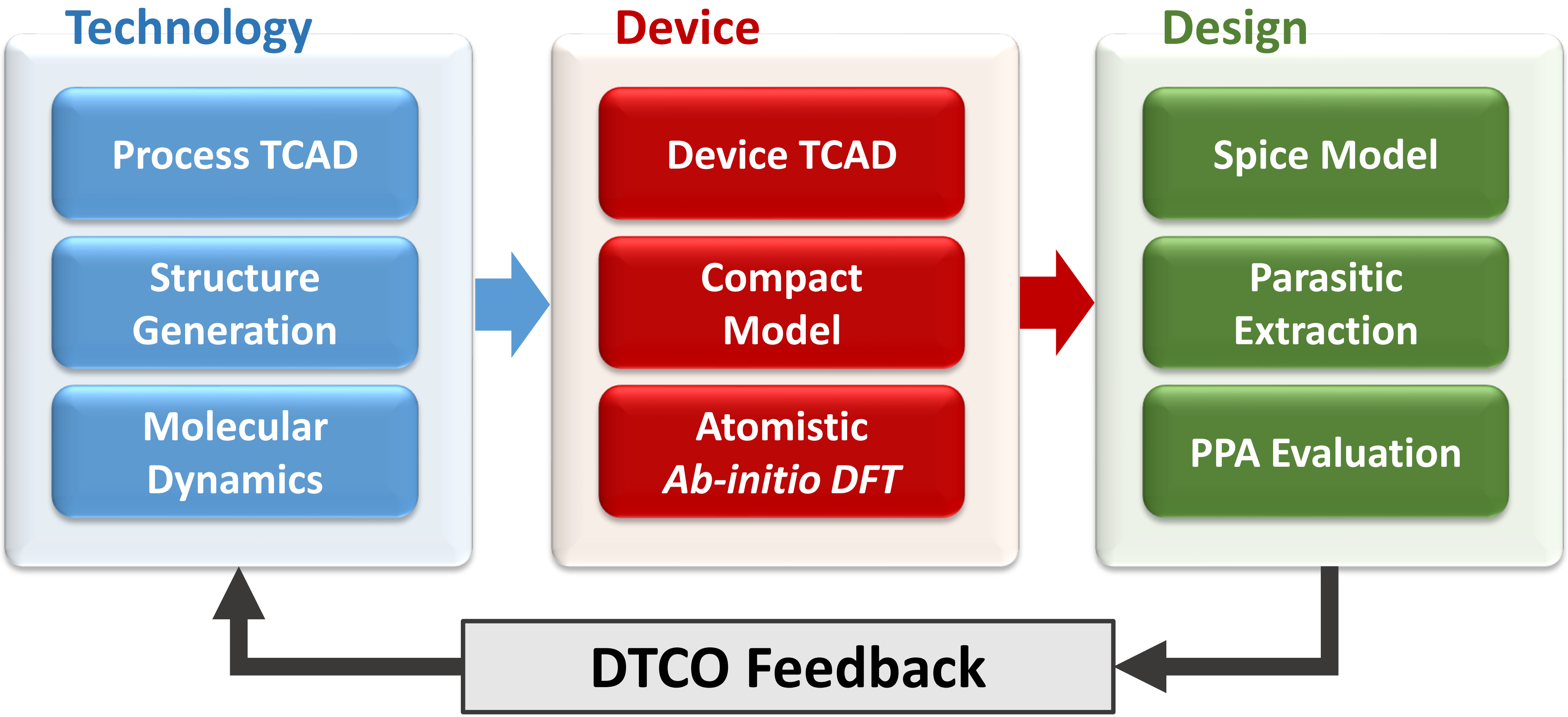




- ITRS estimated technology development cost and time reduction from the use of TCAD of about 30%
- Allows to “see” inside the device
  - Measurements: This is **what** happens
  - TCAD: This is **why** it happens
- Can visualize and evaluate information which is difficult or impossible to measure

TCAD-Supported Design-Technology Co-Optimization (DTCO)

- Physics-based TCAD can be used to optimize and propose designs



TCAD-Supported Design-Technology Co-Optimization (DTCO)

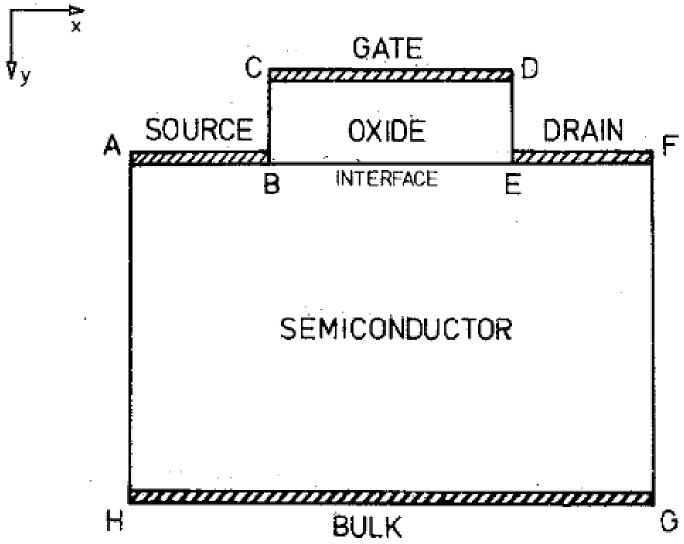
- First 2D MOSFET simulator from the Institute for Microelectronics in 1980

1540 IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. ED-27, NO. 8, AUGUST 1980

MINIMOS—A Two-Dimensional MOS Transistor Analyzer

SIEGFRIED SELBERHERR, MEMBER, IEEE, ALFRED SCHÜTZ, AND HANS WOLFGANG PÖTZL, MEMBER, IEEE

Abstract—We describe a user-oriented software tool—MINIMOS—for the two-dimensional numerical simulation of planar MOS transistors. The fundamental semiconductor equations are solved with sophisticated programming techniques to allow very low computer costs. The program is able to calculate the doping profiles from the technological parameters specified by the user. A new mobility model has been implemented which takes into account the dependence on the impurity concentration, electric field, temperature, and especially the distance to the Si-SiO_2 interface. The power of the program is shown by calculating the two-dimensional internal behavior of three MOST's with 1-μm gate length differing in respect to the ion-implantation steps. In this way, the threshold voltage shift by a shallow implantation and the suppression of punchthrough by a deep implantation are demonstrated. By calculating the output characteristics without and with mobility reduction, the essential influence of this effect is shown. From the subthreshold characteristics, the suppression of short-channel effects by ion implantation becomes apparent. The MINIMOS program is available for everyone for just the handling costs.

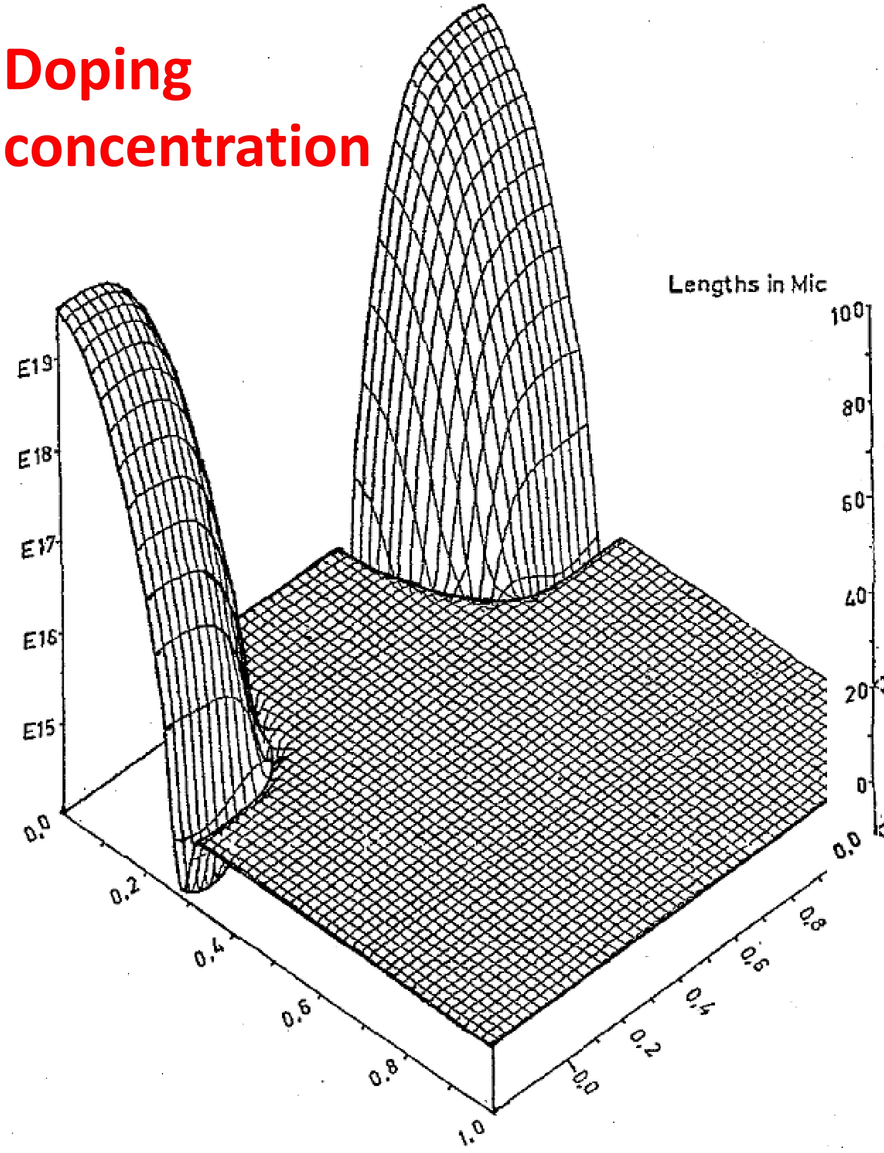



```
ONE - MICRON ANALYSIS   (DEVICE 1)
DEVICE    CHANNEL=N   GATE=AL   TOX=500.E-8   W=10.E-4   L=1.E-4
BIAS      UD=2.   UG=0.
PROFILE   NB=1.E15   ELEM=PH   DOSE=1.E15   AKEV=40   TOX=500.E-8
+         TEMP=1000   TIME=900
END
```

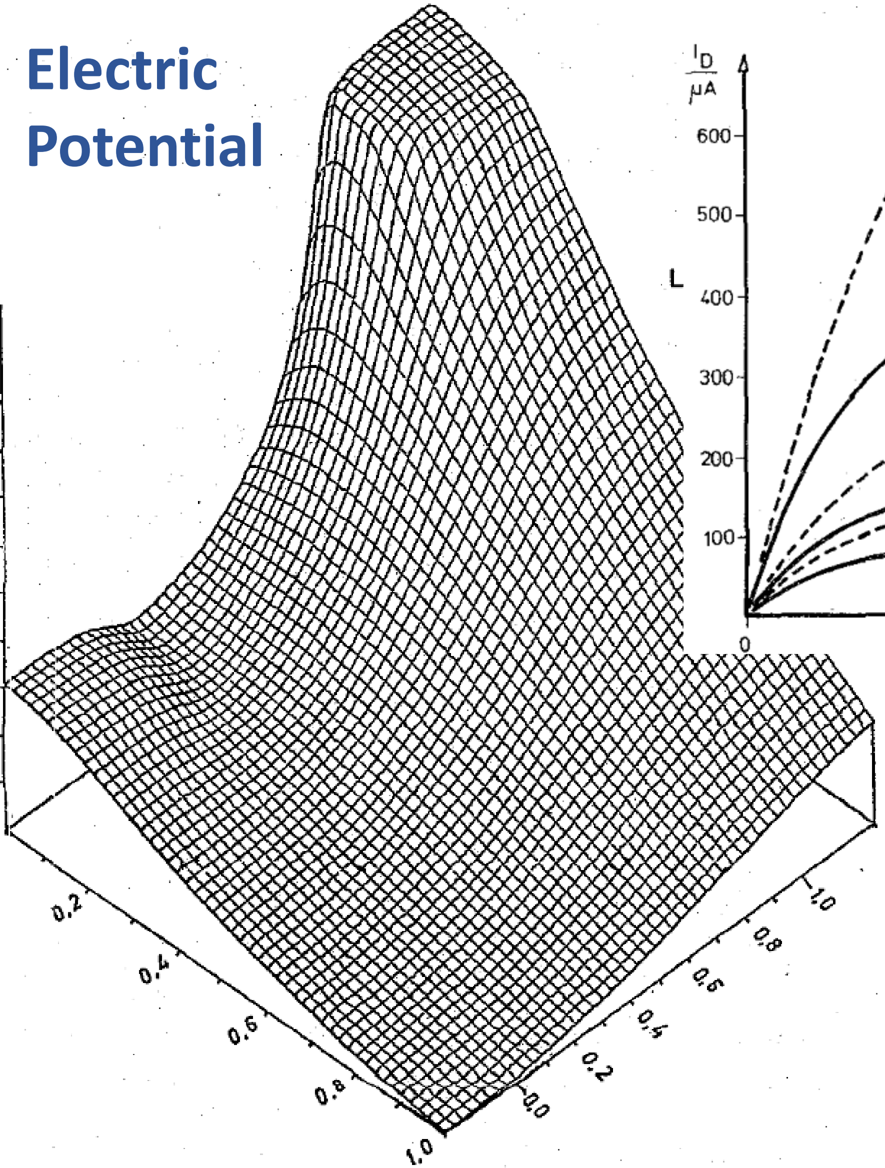
TCAD-Supported Design-Technology Co-Optimization (DTCO)

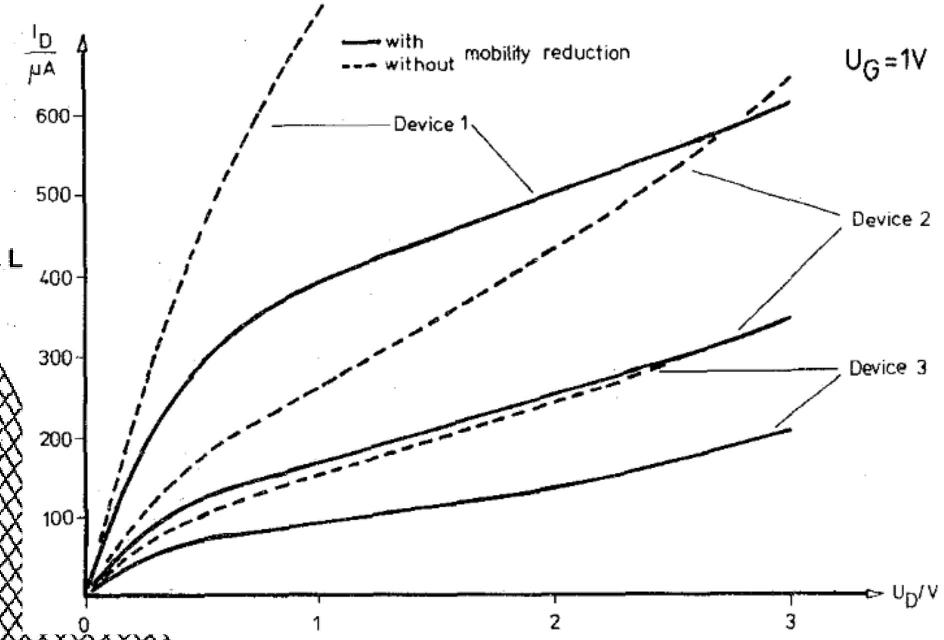
- First 2D MOSFET simulator from the Institute for Microelectronics in 1980

Doping concentration



Electric Potential



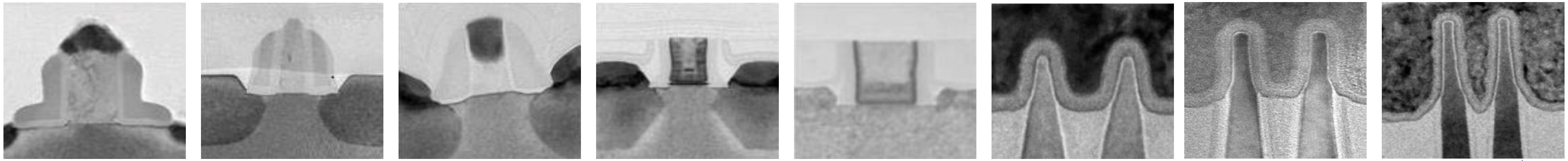


I_D-V_G curves

Field Effect Transistor Scaling

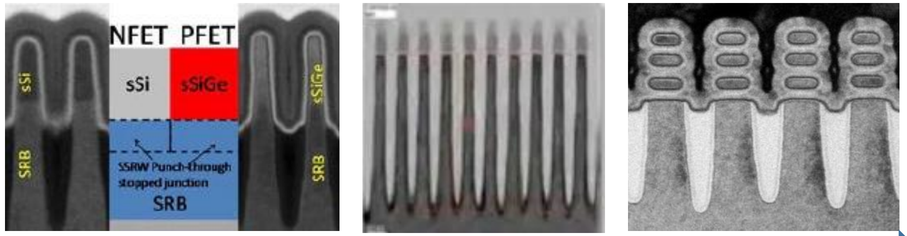
- Over the last 2 decades the planar MOSFET has undergone significant redesigns

130nm 2002	90nm 2004	65nm 2006	45nm 2008	32nm 2010	22nm 2012	14nm 2014	10nm 2016

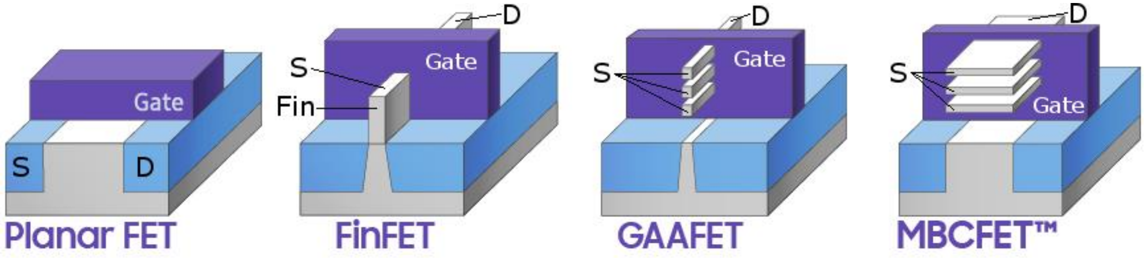


Strain engineering → High-k & Metal gate → FinFET

7nm 2018	5nm 2020	3nm 2024?



FinFET → Gate-All-Around?



Novel materials

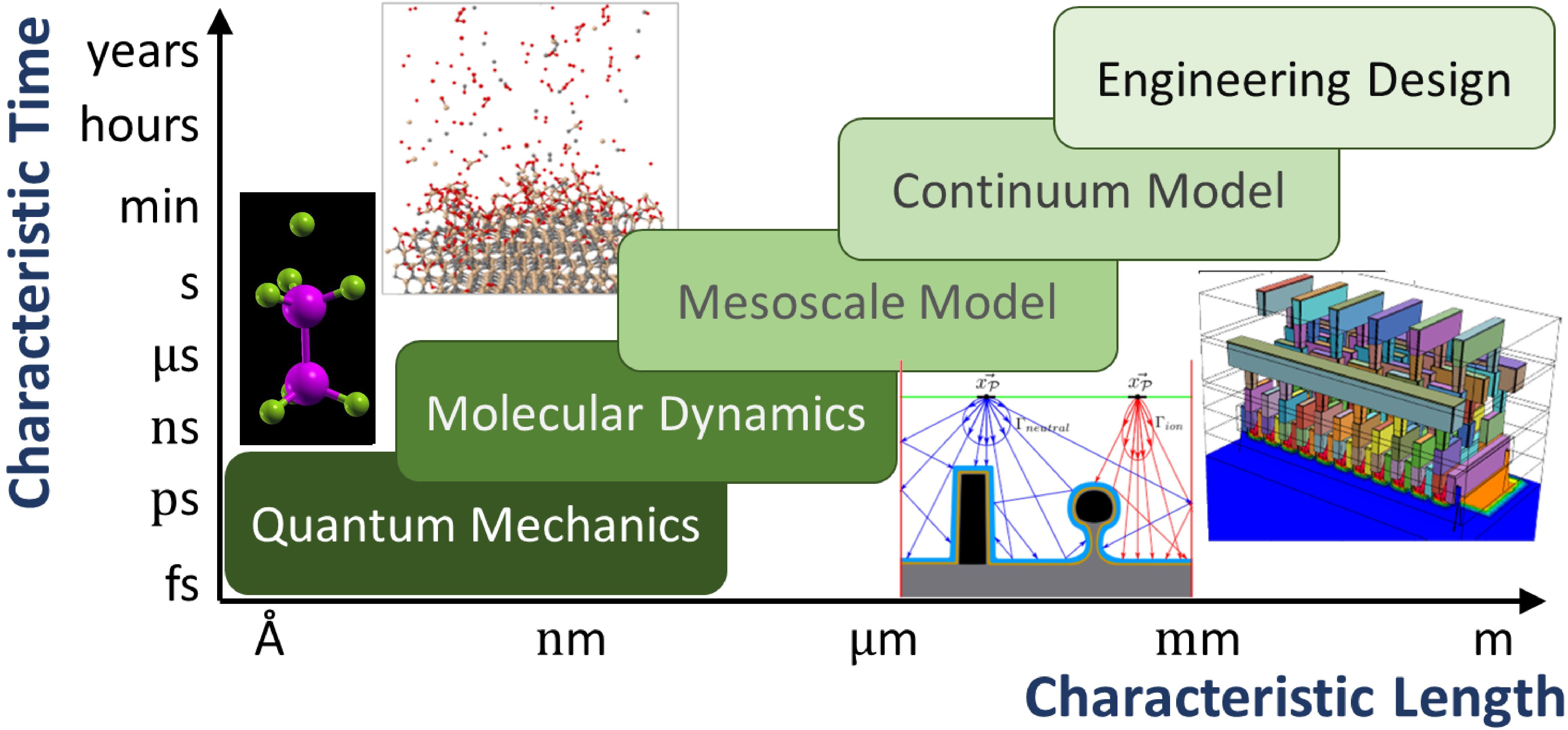
Novel geometries

More complex processes

L. Filipovic, T. Grasser (Ed.) *Miniaturized Transistors*, ISBN: 978-3-03921-010-7 (2019)

Multi-Scale Process Modeling

Approximate time and length scales covered by different approaches



Outline

- Technology Computer-Aided Design (TCAD)
- **ViennaPS Framework**
- Process Simulation
  - Chemical Vapor Deposition
  - Plasma Etching
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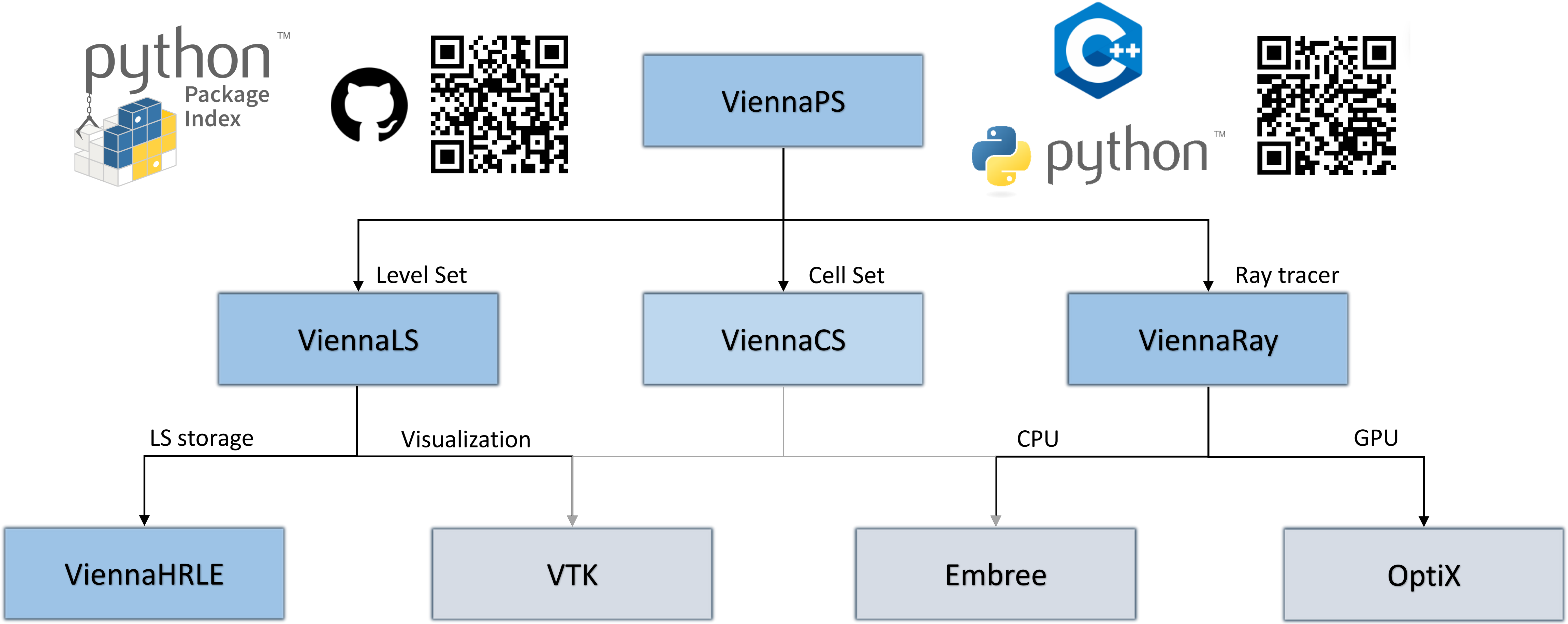
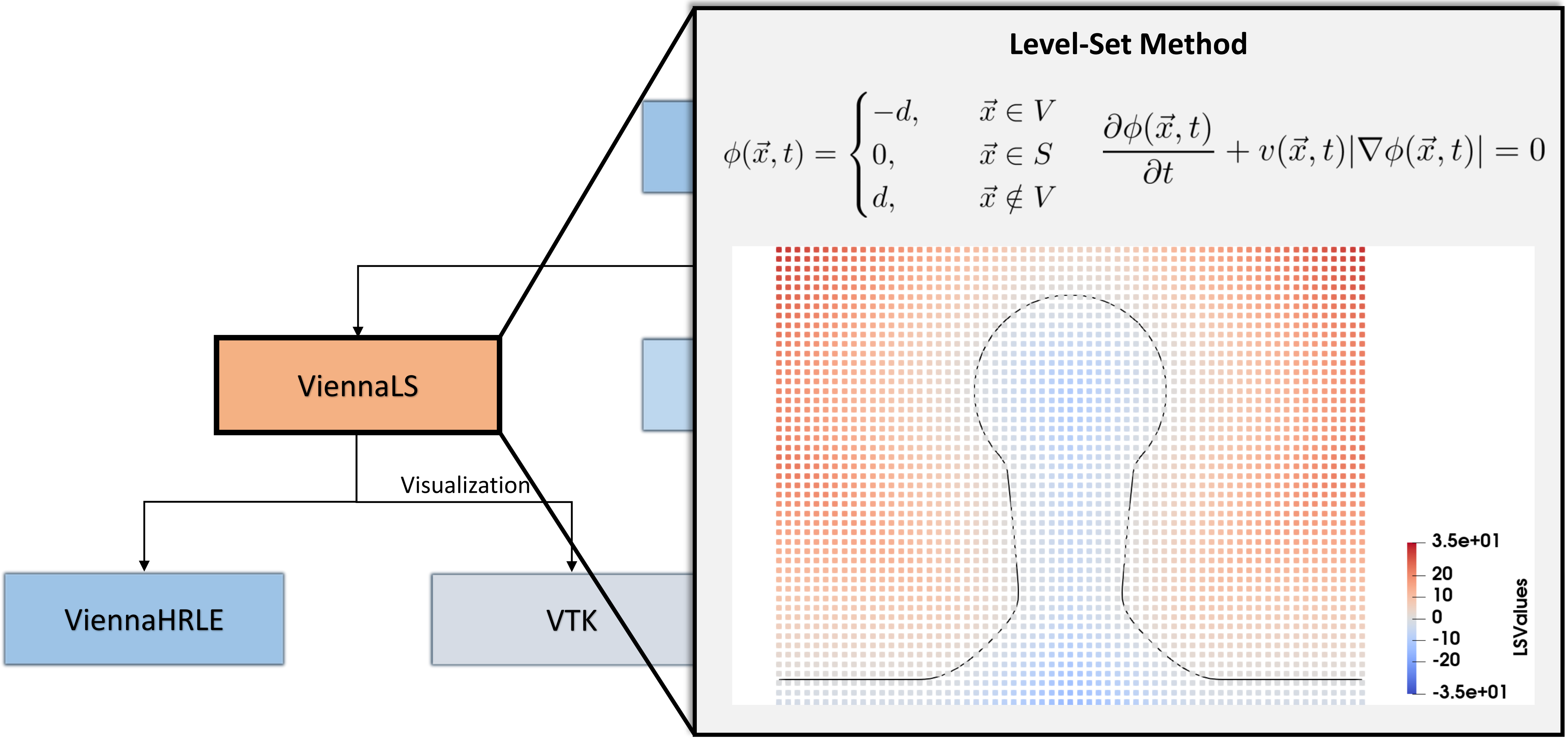
Simulation Framework



https://viennatools.github.io/ViennaPS/

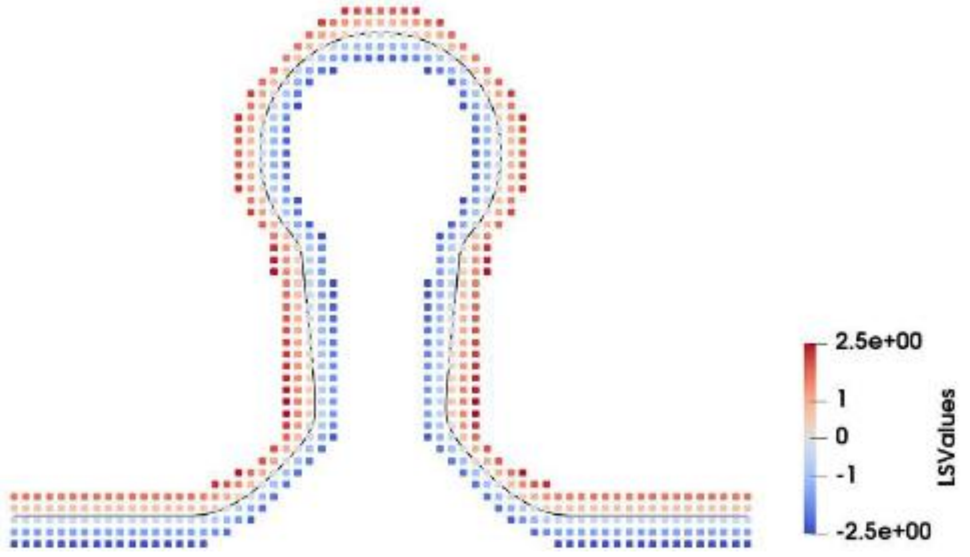
Simulation Framework



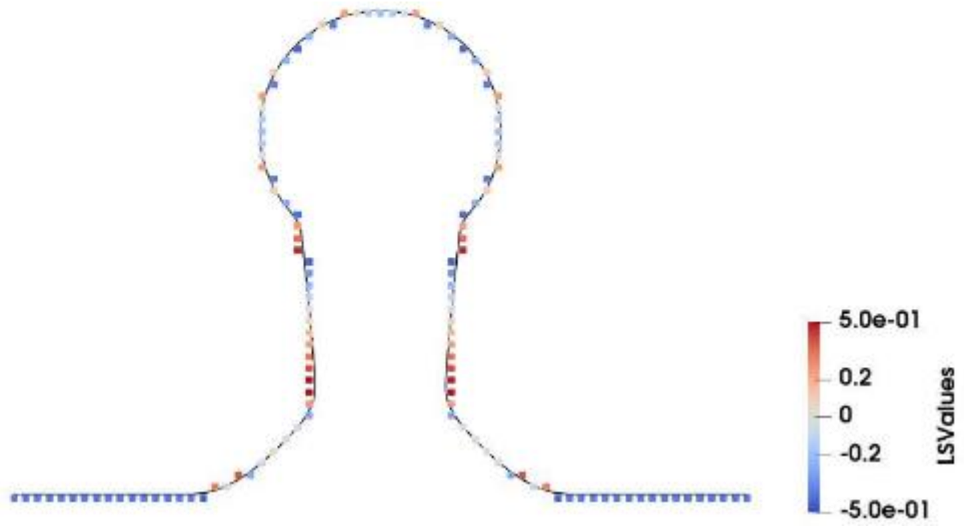
$$\phi(\vec{x},t) = \begin{cases} -d, & \vec{x} \in V \\ 0, & \vec{x} \in S \\ d, & \vec{x} \notin V \end{cases} \qquad \frac{\partial \phi(\vec{x},t)}{\partial t} + v(\vec{x},t)|\nabla \phi(\vec{x},t)| = 0$$

Simulation Framework

- Narrow- or sparse-field level set is stored (not full domain)
  X.Klemenschits, PhD, TU Wien (2022) – Section 2.3.2

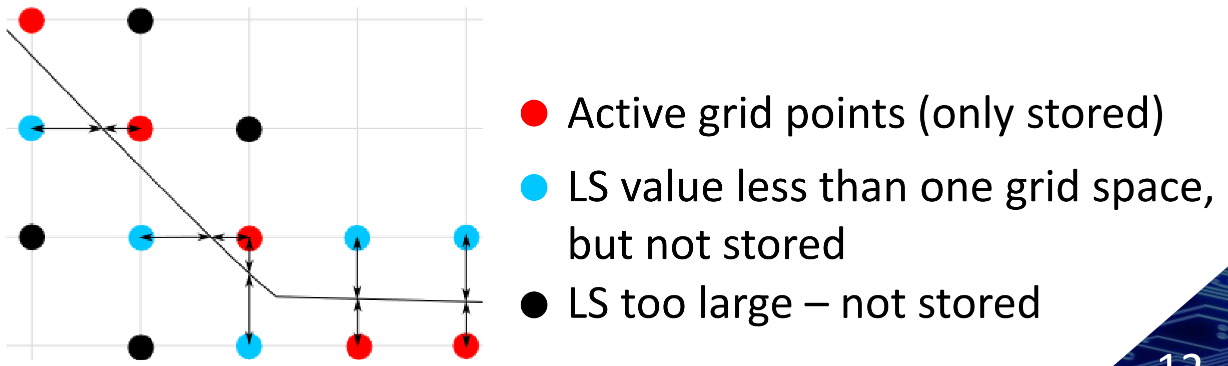


Narrow Band

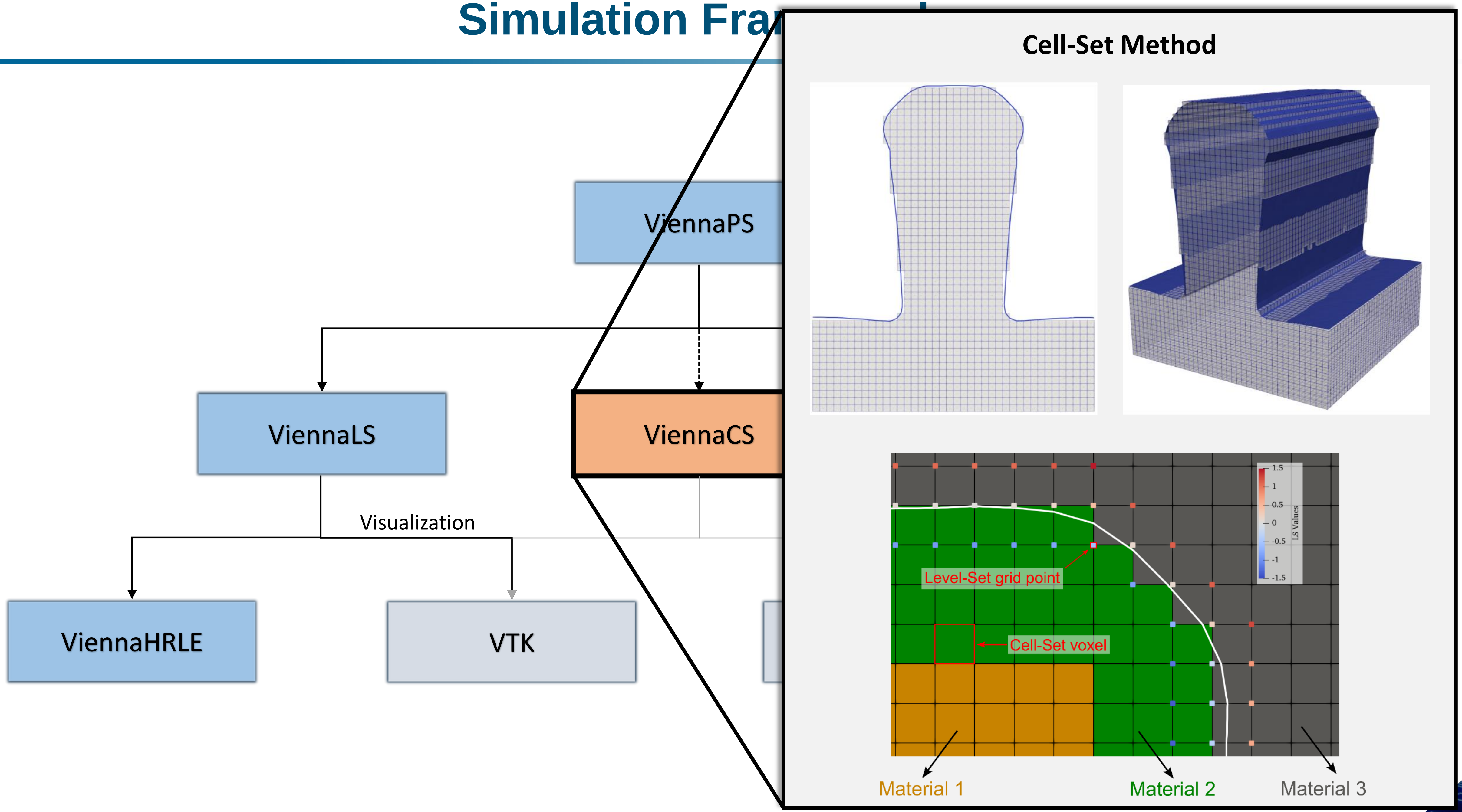


Sparse Field

- Manhattan distances are stored instead of Euclidian
- Example for the sparse field



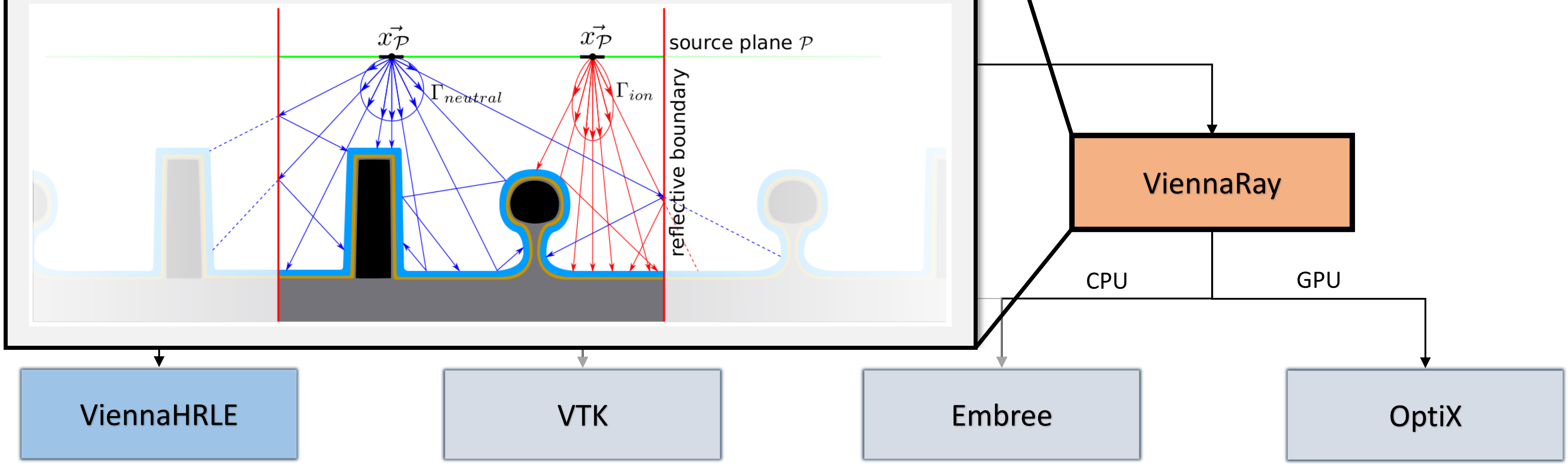
Simulation Fra



Simulation Framework

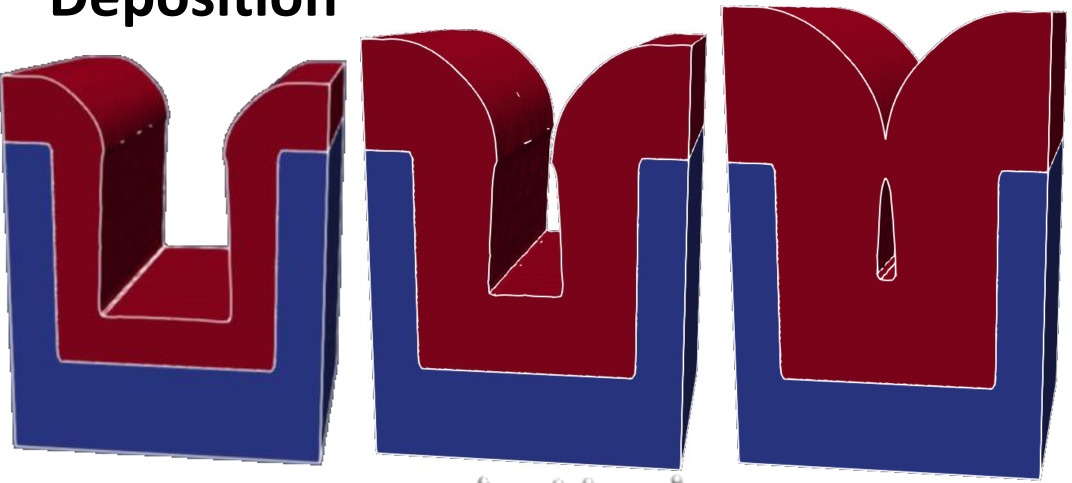
Top-Down Flux Calculation

$$\Gamma_{\text{imp}}(\vec{x}) = \beta(\vec{x}) \int_{\text{source}} \Gamma_{\text{source}}(\vec{x} - \vec{x}')\langle\vec{x}, \vec{x}'\rangle d\vec{x}' + \int_{\text{geometry}} (1 - \beta(\vec{x}'))\Gamma_{\text{refl}}(\vec{x}, \vec{x}')\langle\vec{x}, \vec{x}'\rangle d\vec{x}'$$

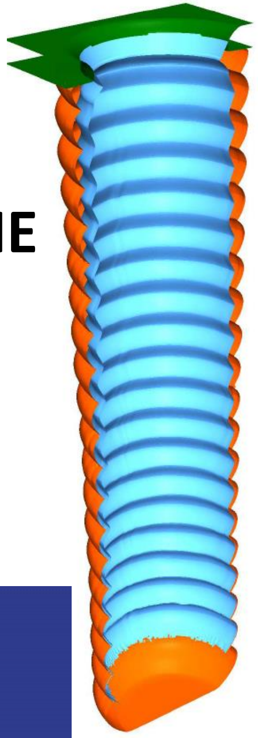


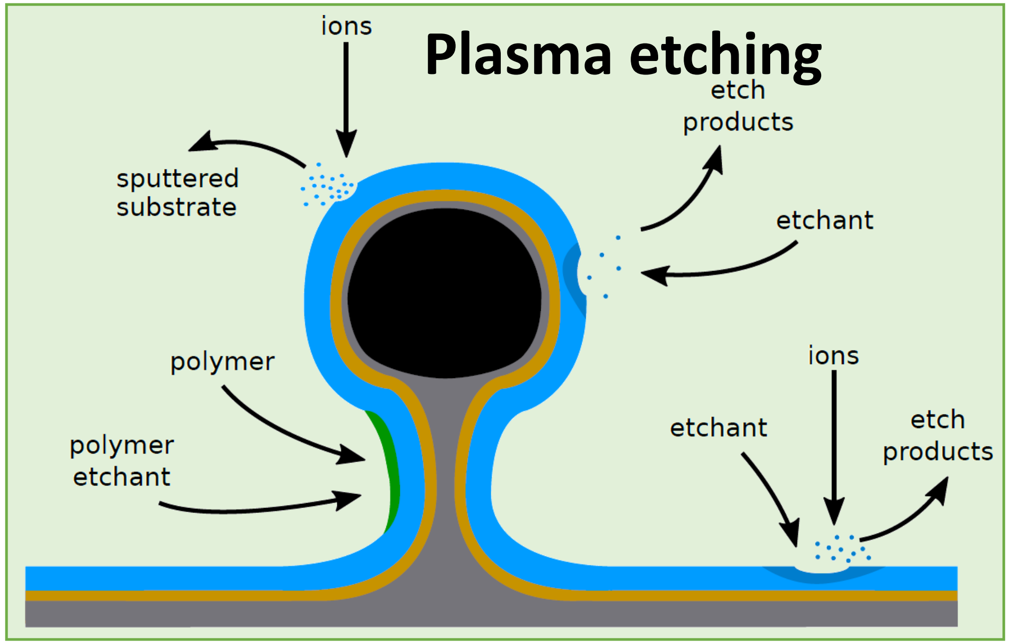
Process TCAD – Physical Modeling at Feature Scale

Deposition

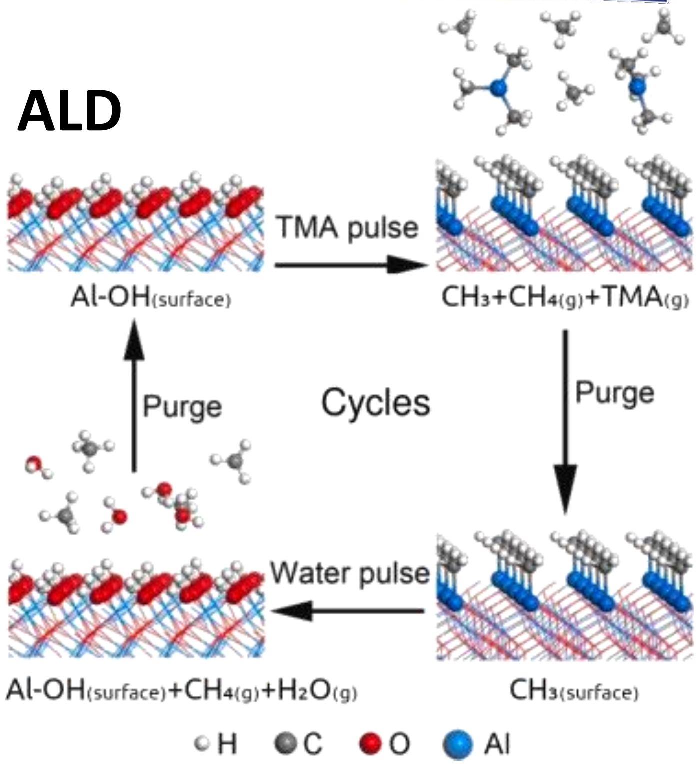


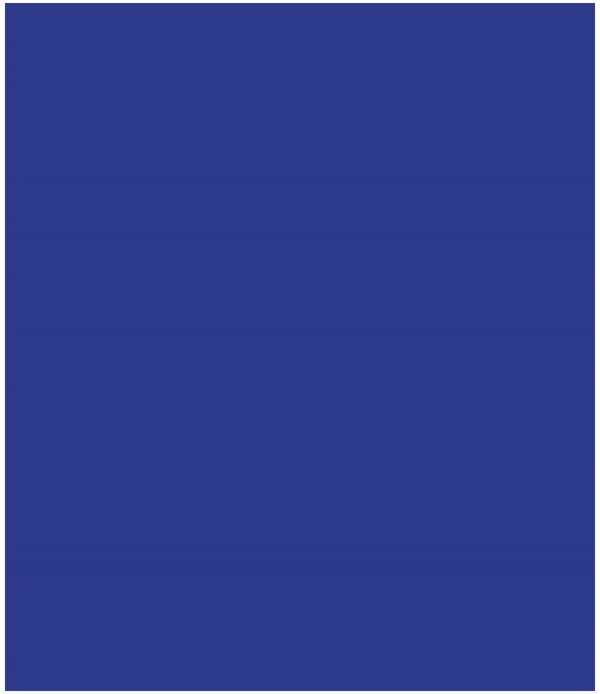
DRIE



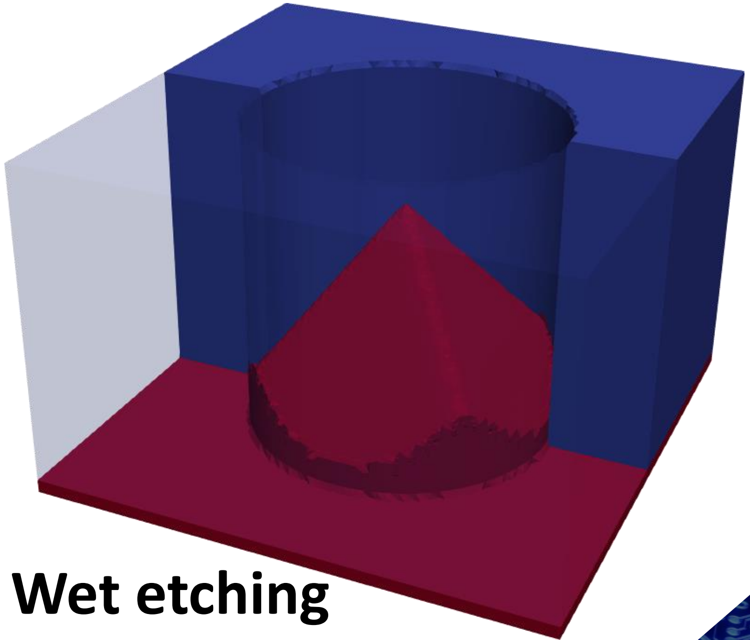


ALD





Process reliability and variability



Wet etching

Outline

- Technology Computer-Aided Design (TCAD)
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- **Process Simulation**
  - **Chemical Vapor Deposition**
  - Plasma Etching
- Link to Equipment Settings

Plasma-Enhanced Chemical Vapor Deposition (PECVD)

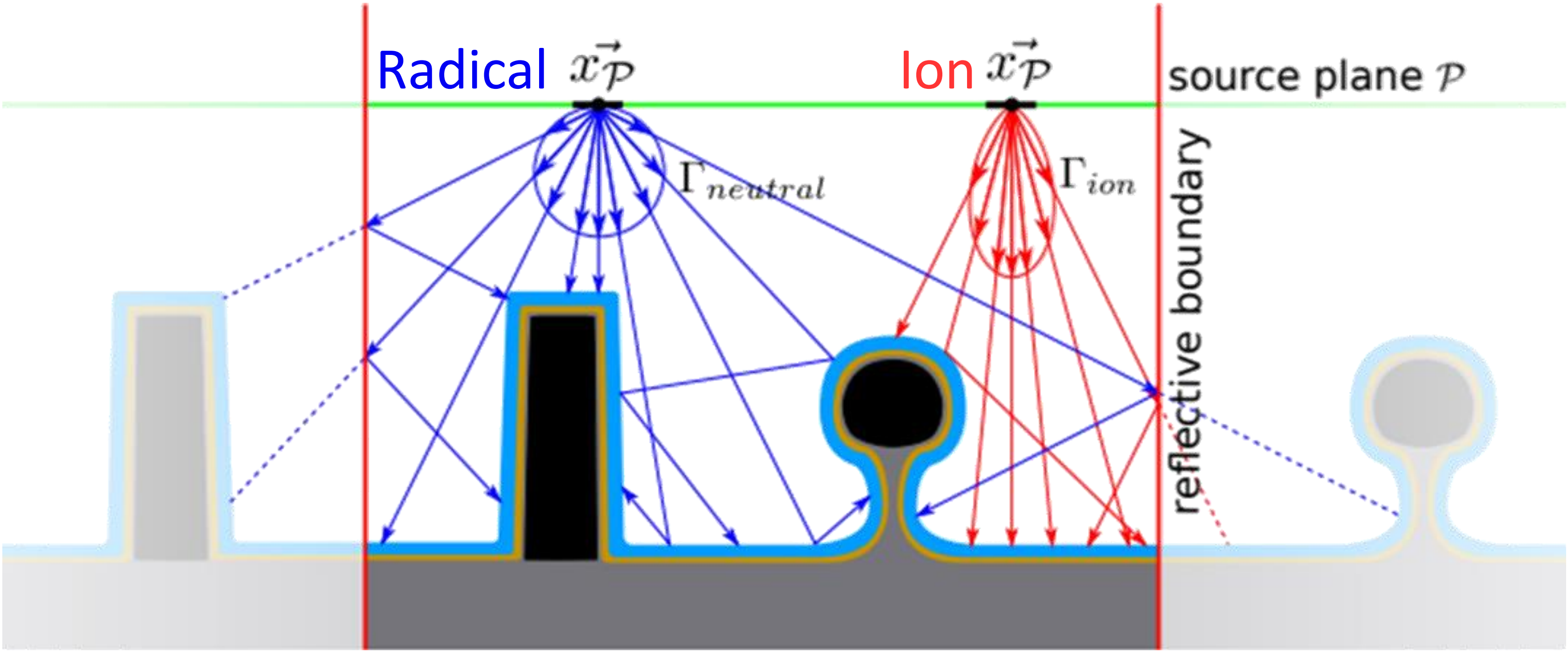
- Semi-empirical oxide PECVD from TEOS model for implemented in ViennaPS

Radical/Ion transport
in the plasma chamber

Gas Phase Flow

Flat wafer rates

Ion directionality



Plasma-Enhanced Chemical Vapor Deposition (PECVD)

- Semi-empirical oxide PECVD from TEOS model for implemented in ViennaPS

Radical/Ion transport
in the plasma chamber

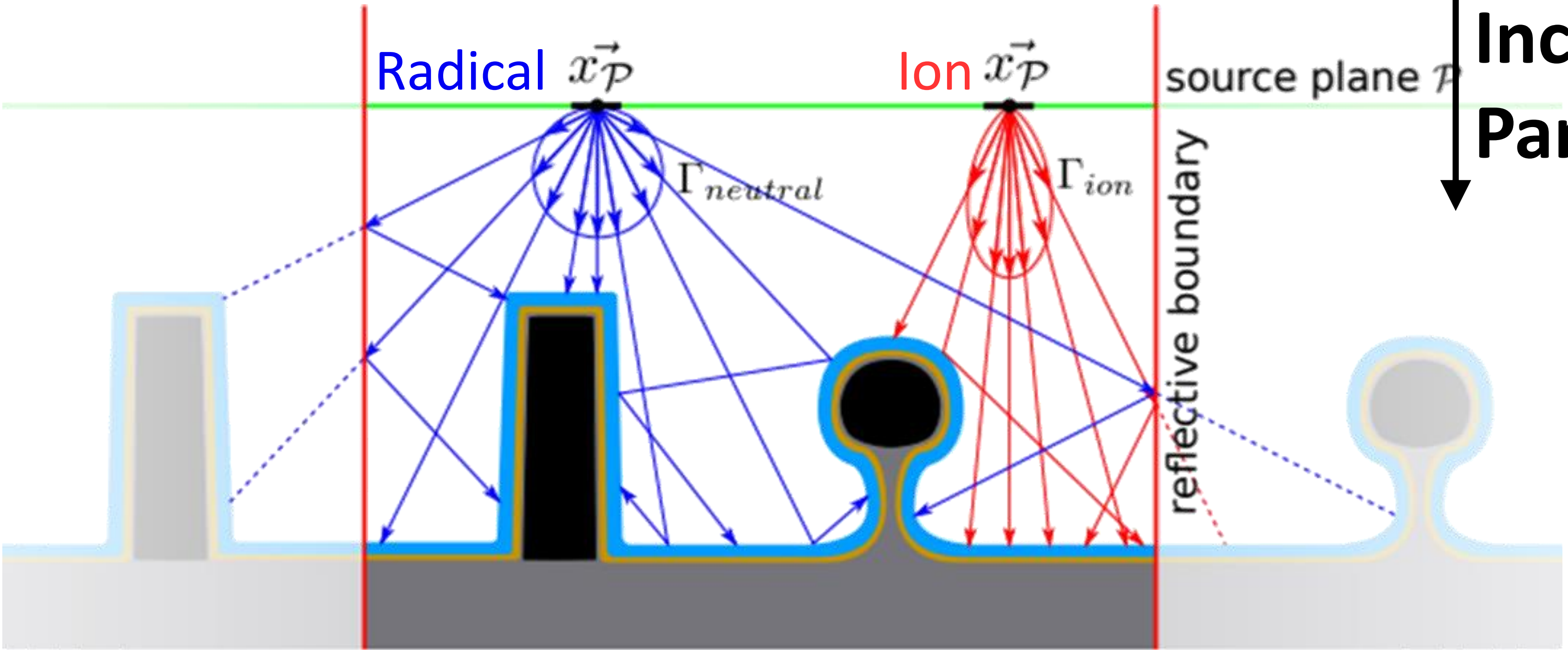
Gas Phase Flow

Rates → **Isotropy**

Radical/Ion collisions
with the surface

Ray Tracing

↓ **Incoming Particle Flux**



Plasma-Enhanced Chemical Vapor Deposition (PECVD)

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Radical/Ion transport in the plasma chamber

Gas Phase Flow

Rates

Isotropy

Radical/Ion collisions with the surface

Ray Tracing

Incoming Particle Flux

Deposition rate calculation based on fluxes

Rate Calculation

Deposition Rate v

Neutral radical contribution

Charged ion contribution

$$v = R_{rad} \cdot \Gamma_{rad}^{o_{rad}} + R_{ion} \cdot \Gamma_{ion}^{o_{ion}}$$

https://viennatools.github.io/ViennaPS/models/prebuilt/TEOSPECVD.html

S.S. Singh et al., Physics of Semiconductor Devices: 17th Int. Workshop (2013)

Plasma-Enhanced Chemical Vapor Deposition (PECVD)

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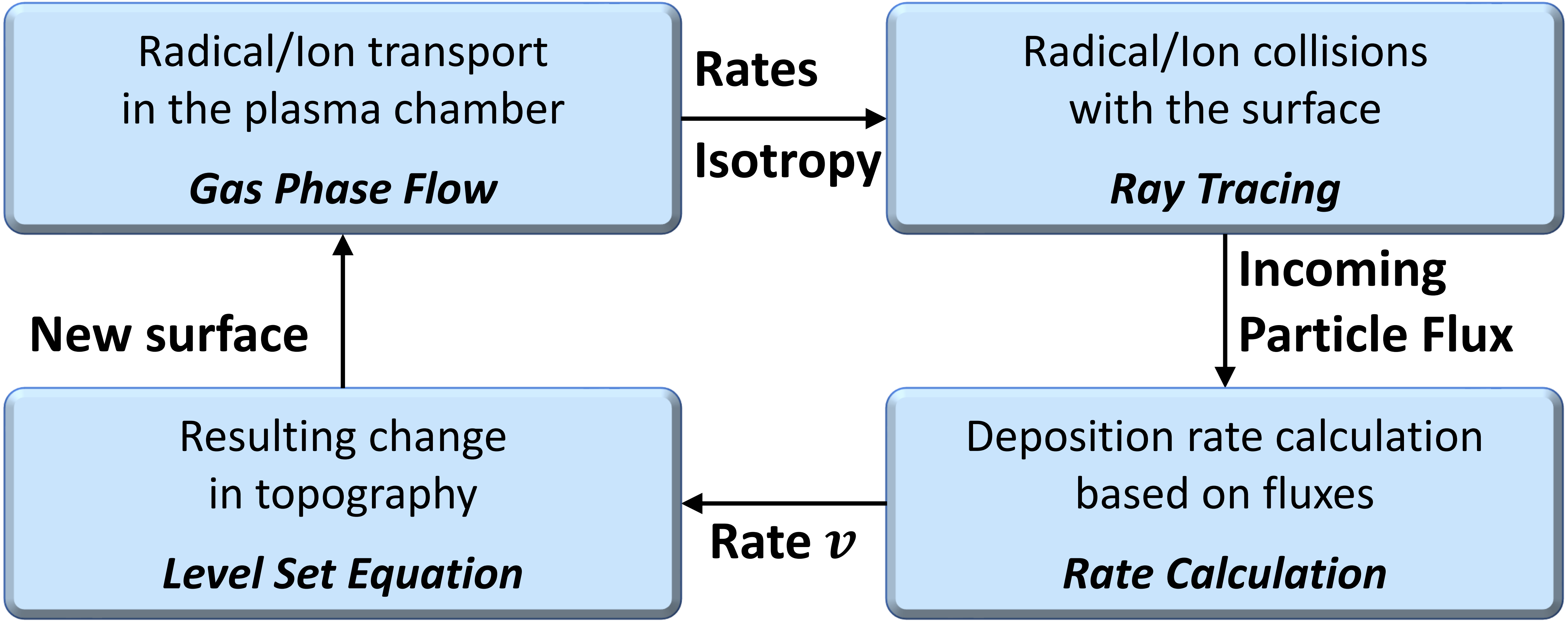


$$\frac{\delta\phi(\vec{x},t)}{\delta t} + v(\vec{x})|\nabla\phi(\vec{x},t)| = 0$$

Plasma-Enhanced Chemical Vapor Deposition (PECVD)

- Semi-empirical oxide PECVD from TEOS model for implemented in ViennaPS https://viennatools.github.io/ViennaPS/models/prebuilt/TEOSPECVD.html

Parameter	Description	Default Value
`pRadicalSticking`	Sticking probability of the TEOS precursor radicals	1.0
`pRadicalRate`	Rate of the TEOS precursor radicals	1.0
`pIonRate`	Rate of the ions	1.0
`pIonExponent`	Exponent power cosine source distribution of the ions	1.0
`pIonSticking`	Sticking probability of the ions	1.0
`pRadicalOrder`	Reaction order of the TEOS precursor radicals	1.0
`pIonOrder`	Reaction order of the ions	1.0
`pIonMinAngle`	Minimum specular reflection angle of the ions	0.0

Flat-wafer rate (analogous to source flux) X.Klemenschits, PhD, TU Wien (2022) – section 3.2.2

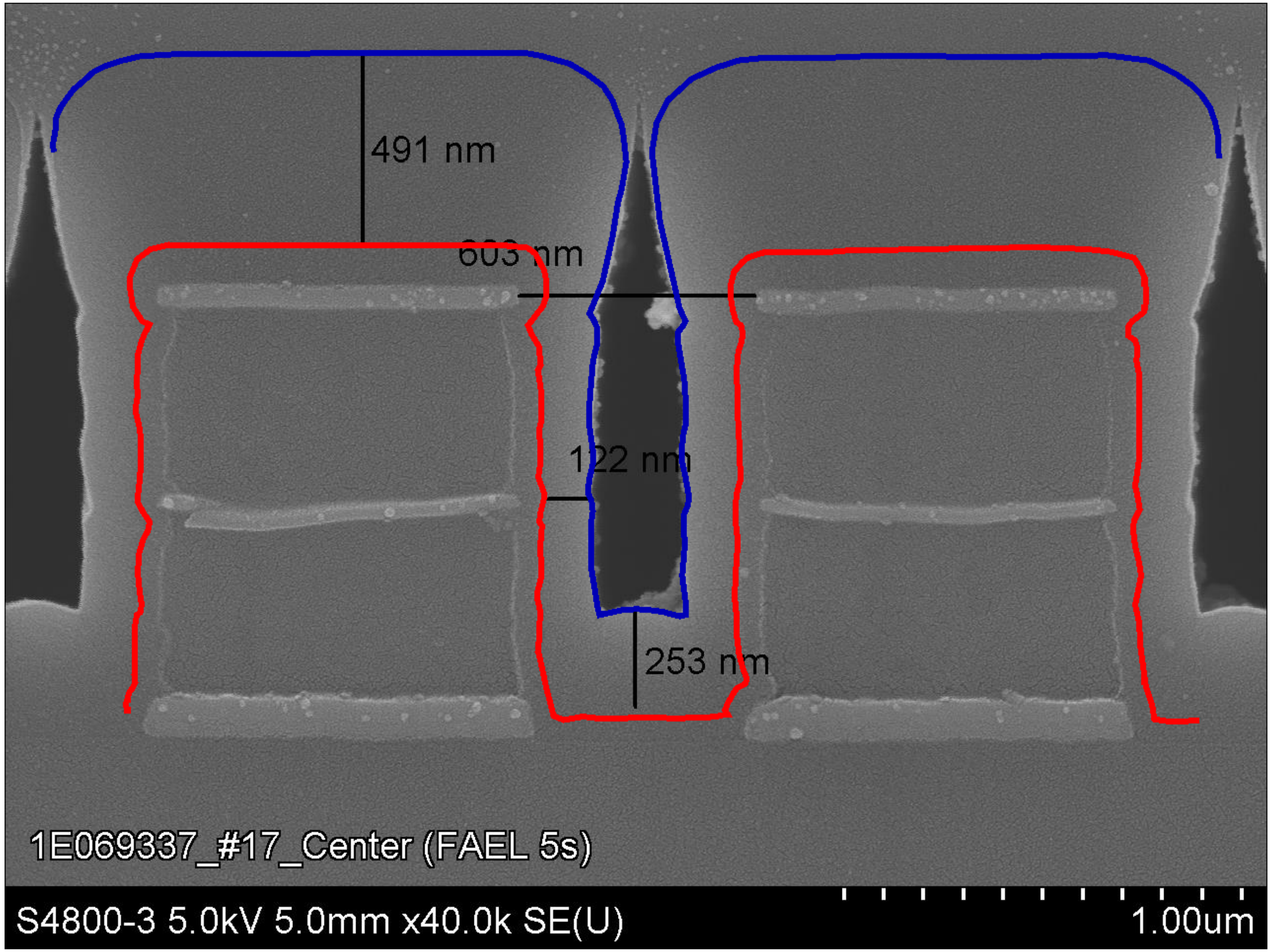
Treat potential non-linearity of the surface reactions https://www.iue.tuwien.ac.at/phd/ertl/node23.html

PECVD Parameter Search

- Use a global optimizer to find the neutral radical and ion parameters
- The parameters should ensure the deposition follows the measured profile below

Deposited oxide after TEOS PECVD

Initial topography



PECVD Parameter Search

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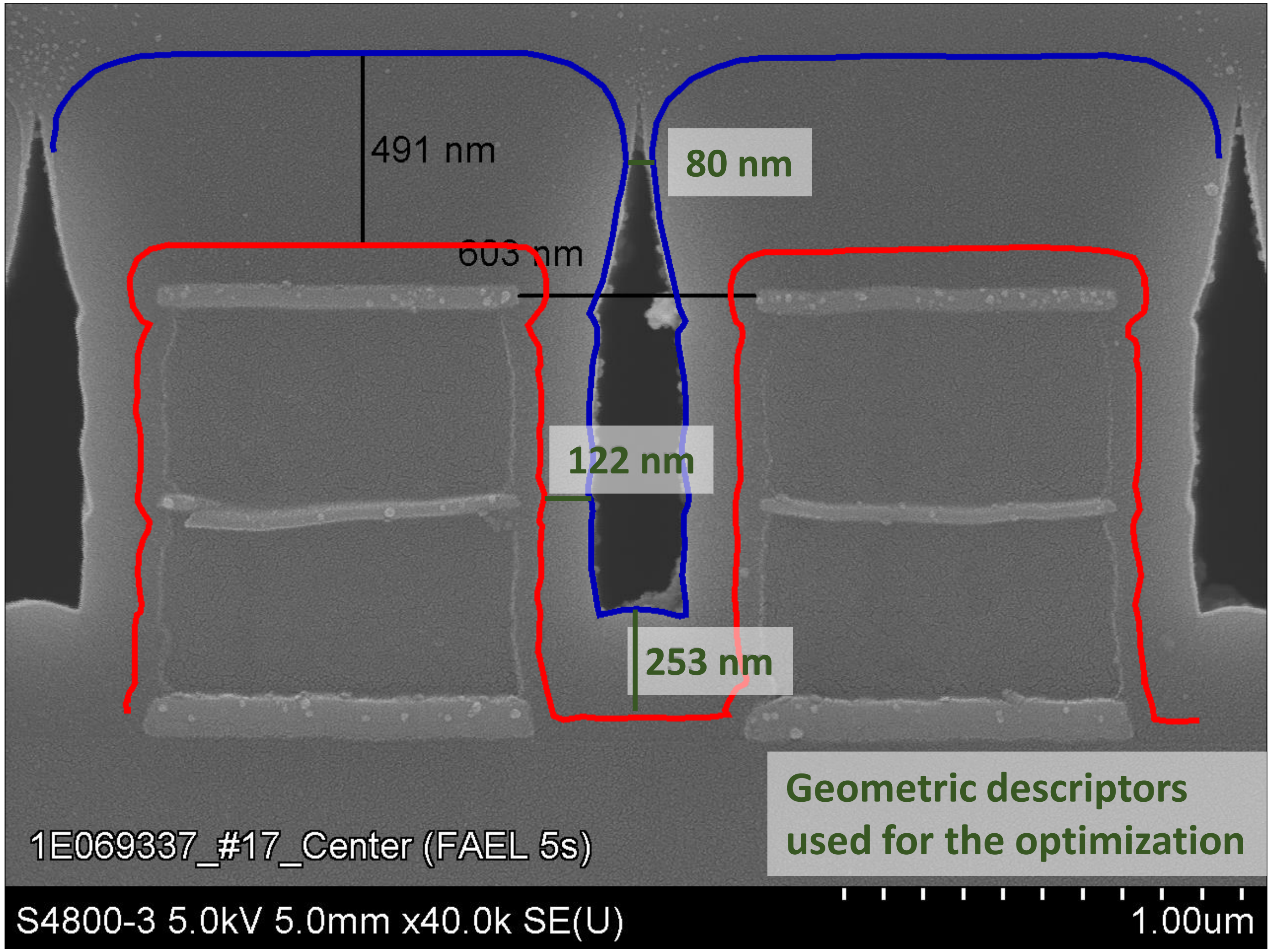
Deposited oxide after TEOS PECVD

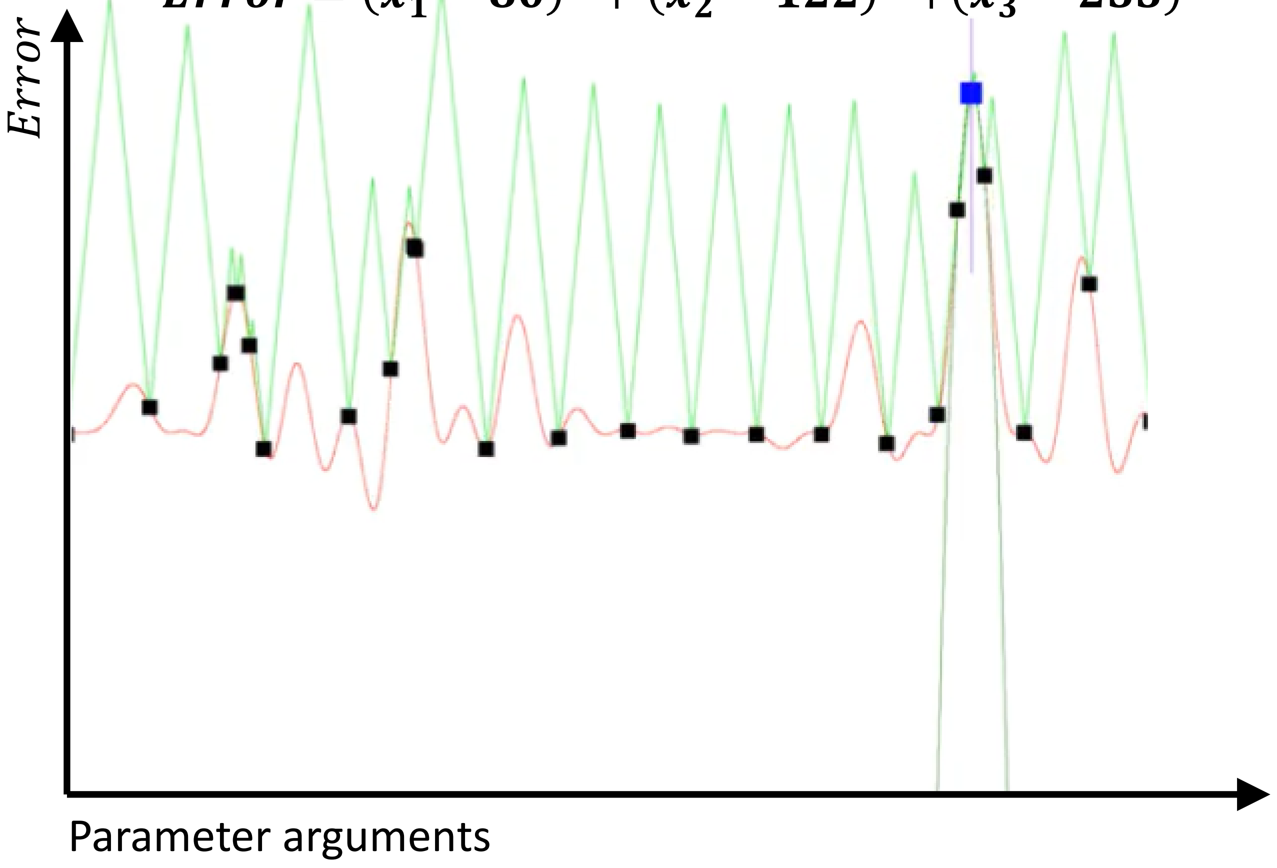
Initial topography

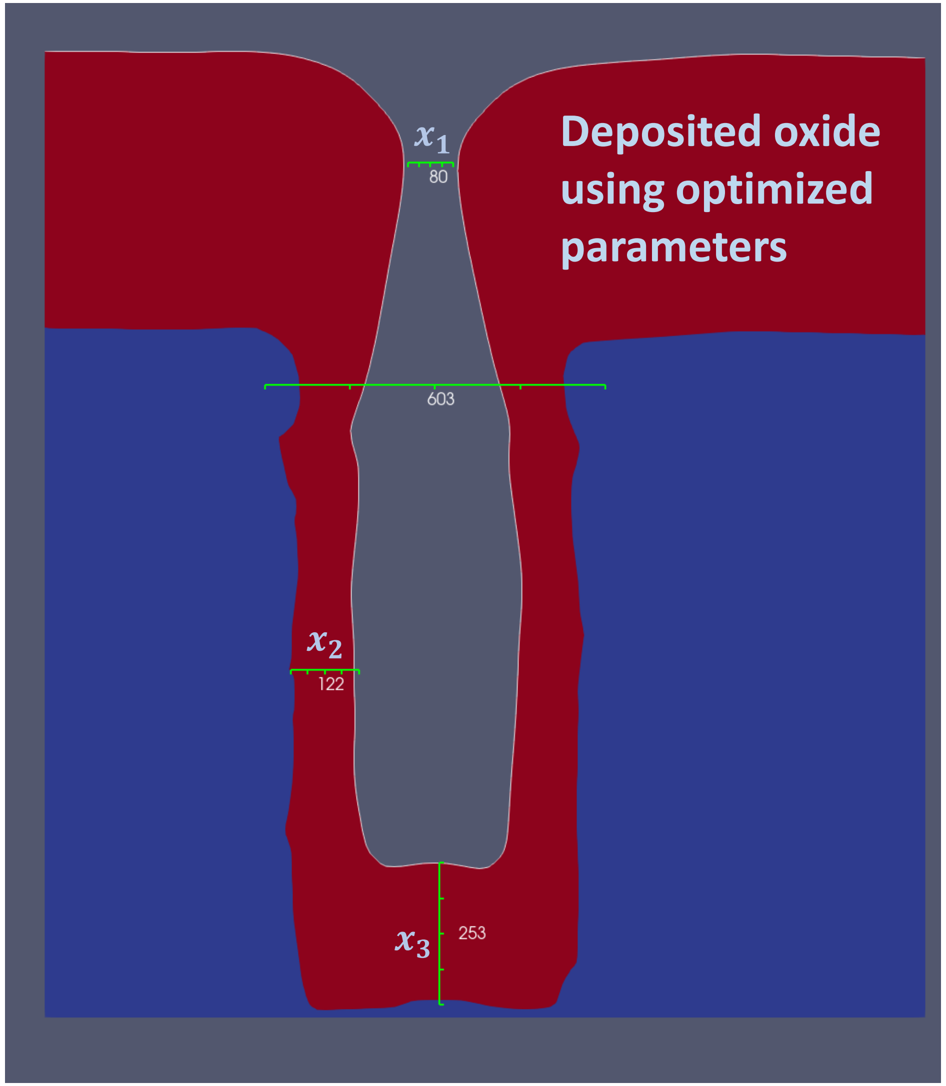


PECVD Parameter Search

- Use a global optimizer to find the neutral radical and ion parameters
  http://blog.dlib.net/2017/12/a-global-optimization-algorithm-worth.html

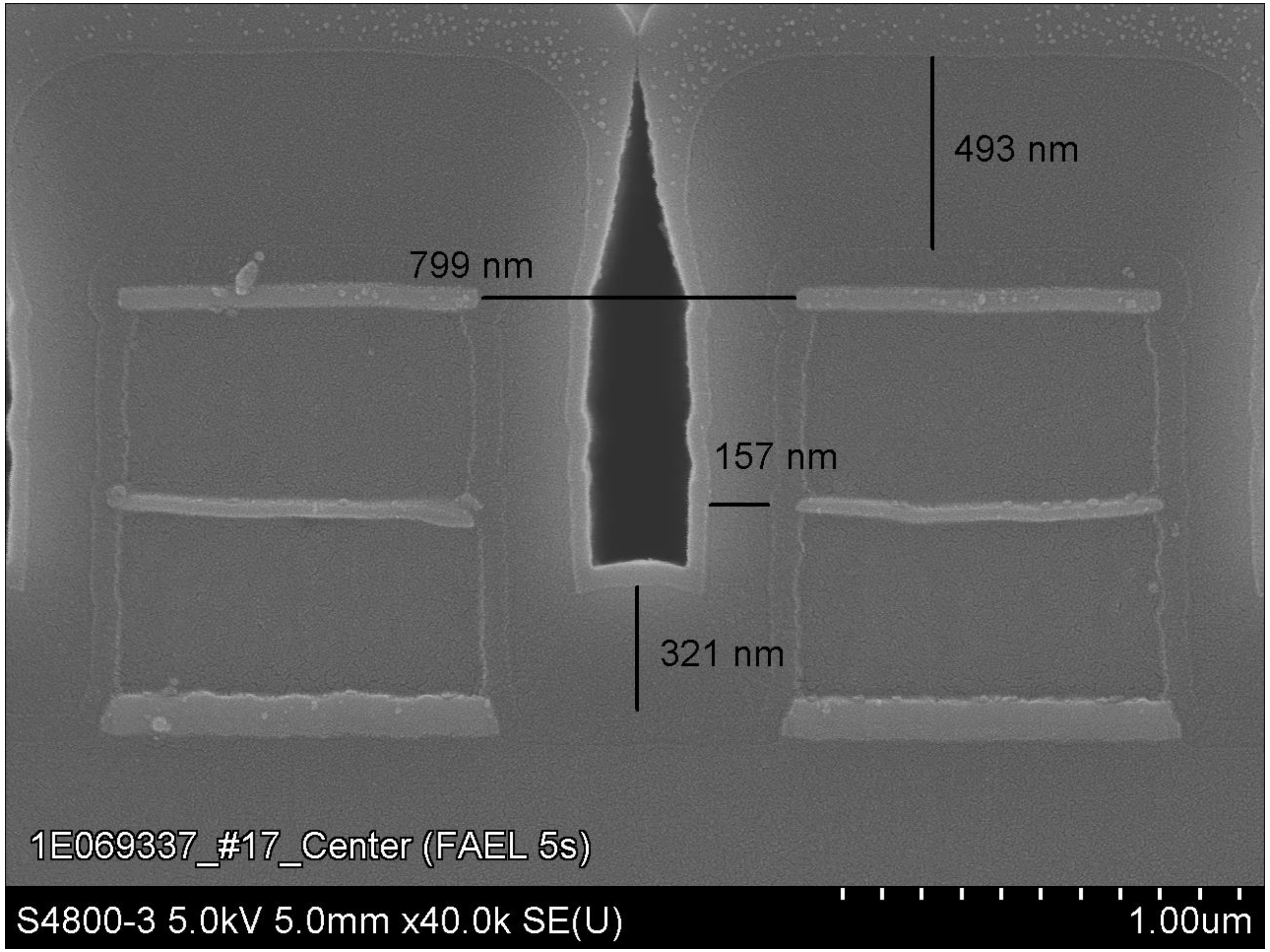
$$Error = (x_1 - 80)^2 + (x_2 - 122)^2 + (x_3 - 253)^2$$

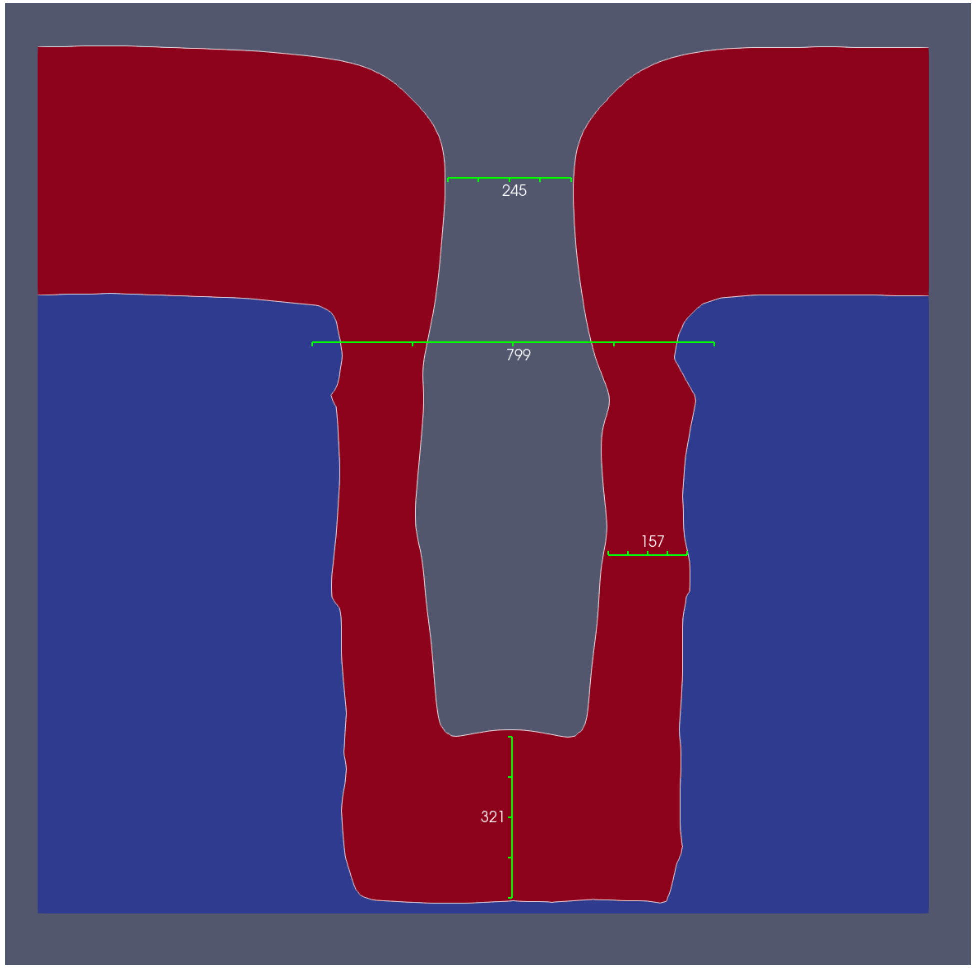




PECVD Parameter Search

- Test the optimized parameters on a different structure





- Currently enhancing the set of geometric descriptors for better optimization

Outline

- Technology Computer-Aided Design (TCAD)
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- **Process Simulation**
  - Chemical Vapor Deposition
  - **Plasma Etching**
- Link to Equipment Settings

(Physical) Plasma Etching Model

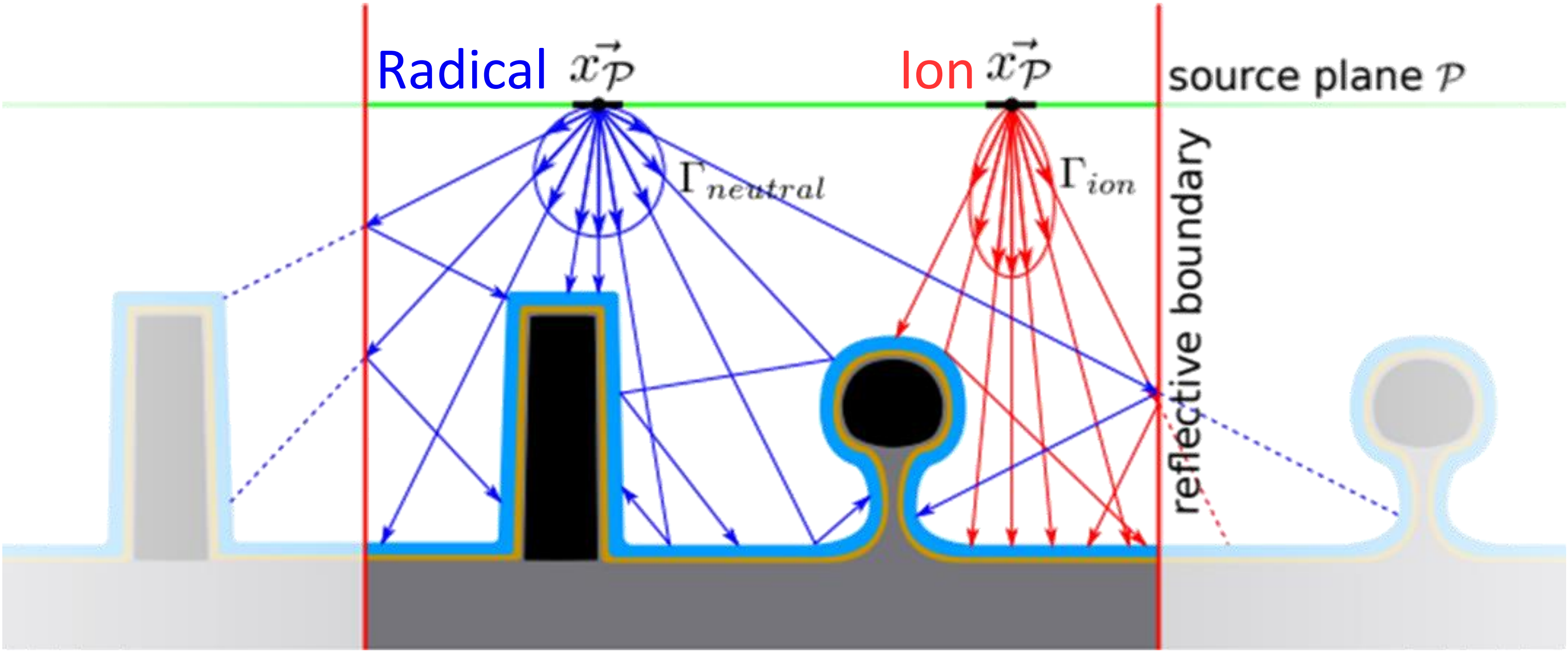
- Physical SF_6/O_2 plasma etching model implemented in ViennaPS

Molecular/Ion transport
in the plasma chamber

Gas Phase Flow

Flux at the source plane

Ion Energy distribution



(Physical) Plasma Etching Model

- Physical SF_6/O_2 plasma etching model implemented in ViennaPS

Molecular/Ion transport in the plasma chamber

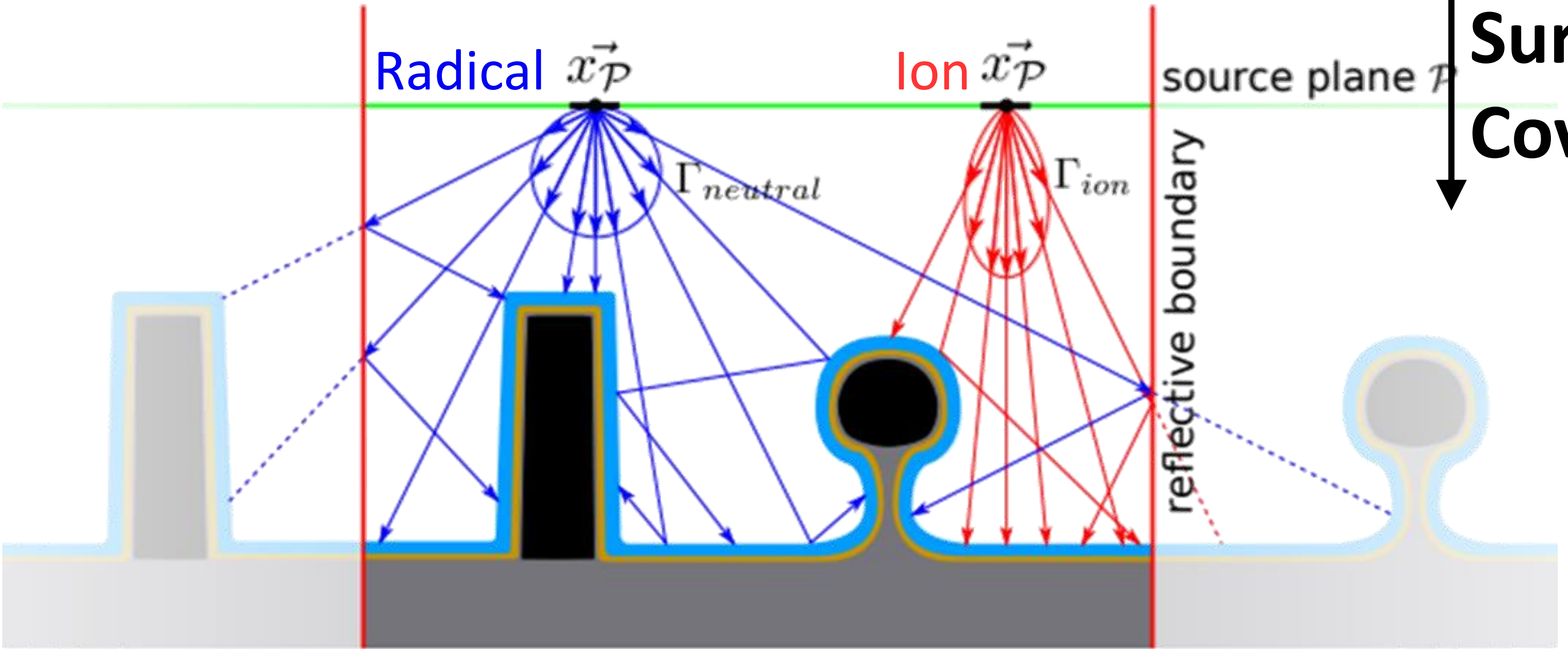
Gas Phase Flow

Flux → **Ion E**

Molecular/Ion collisions with the surface

Ray Tracing

↓ **Surface Coverages**



(Physical) Plasma Etching Model

- Physical SF_6/O_2 plasma etching model implemented in ViennaPS

Molecular/Ion transport in the plasma chamber — ***Gas Phase Flow***

→ **Flux**, **Ion E** →

Molecular/Ion collisions with the surface — ***Ray Tracing***

↓ **Surface Coverages** ↓

Chemical/physical reactions of molecules/ions on the surface — ***Monte Carlo***

← **Rates** ←

Sputtering yield (Y_F, Y_{ie}) · Ion flux (Γ_i) · Fluorine coverage (θ_F)

$$\mathrm{ER} = \frac{1}{\rho_{Si}}\left(\frac{k\sigma_{Si}\theta_F}{4} + Y_F\Gamma_i + Y_{ie}\Gamma_i\theta_F\right)$$

$$\sigma_{Si}\frac{d\theta_F}{dt} = \gamma_F\Gamma_F(1-\theta_F-\theta_O) - k\sigma_{Si}\theta_F - 2Y_{ie}\Gamma_i\theta_F$$

$$\sigma_{Si}\frac{d\theta_O}{dt} = \gamma_O\Gamma_O(1-\theta_F-\theta_O) - \beta\sigma_{Si}\theta_O - Y_O\Gamma_i\theta_O$$

R.J. Belen et al., J. Vac. Sci. Technol. A 23, 1430–1439 (2005)

(Physical) Plasma Etching Model

- Physical SF_6/O_2 plasma etching model implemented in ViennaPS

Molecular/Ion transport in the plasma chamber

Gas Phase Flow

Flux

Ion E

Molecular/Ion collisions with the surface

Ray Tracing

Surface Coverages

Chemical/physical reactions of molecules/ions on the surface

Monte Carlo

Rates

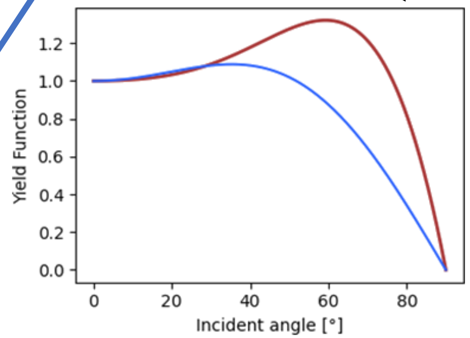
Angle- and **energy**-dependent ion flux

$$\Gamma(\vec{x}) = N\left(\sqrt{E} - \sqrt{E_{th}}\right) f(\theta)$$

Ion energy randomly distributed with a Gaussian distribution

Threshold energy for etching

Yield function depending on incident angle

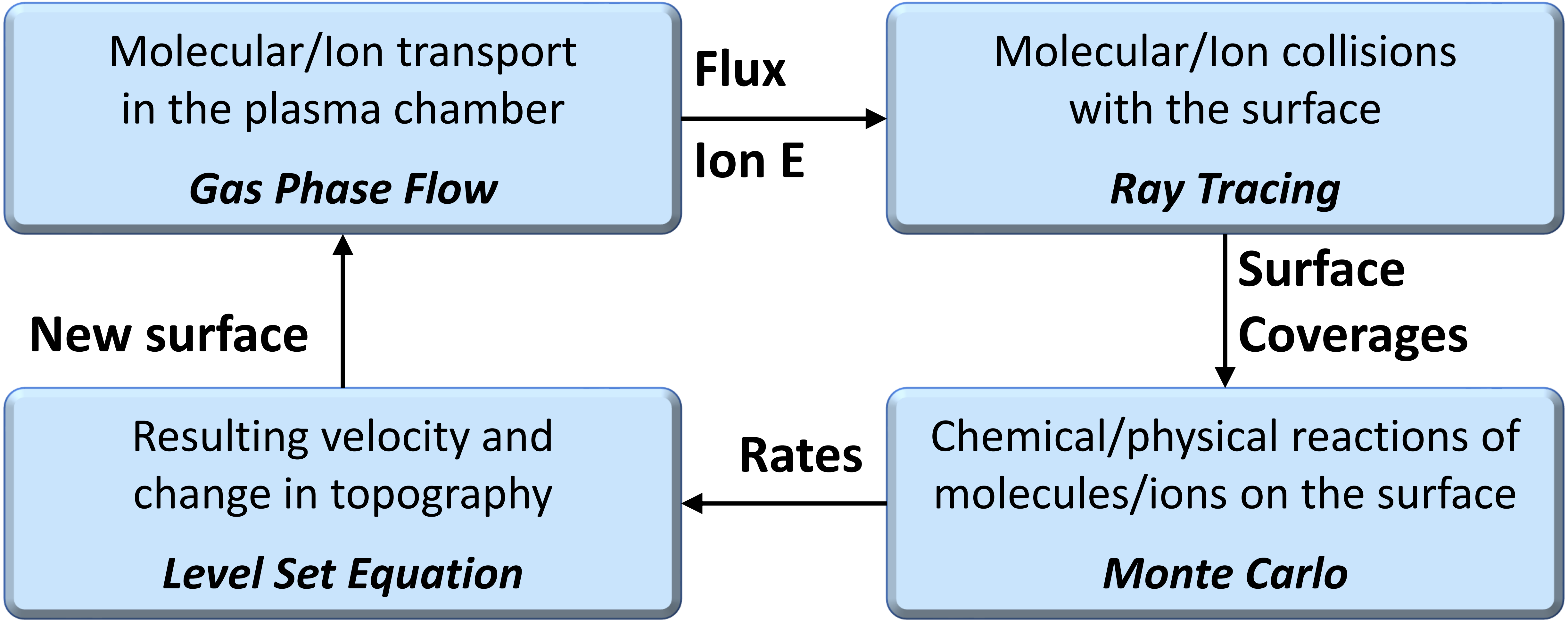


X.Klemenschits, PhD, TU Wien (2022) – Section 3.2.4

https://viennatools.github.io/ViennaPS/models/prebuilt/SF6O2Etching.html

(Physical) Plasma Etching Model

- Physical SF_6/O_2 plasma etching model implemented in ViennaPS



$$\frac{\delta \phi(\vec{x},t)}{\delta t} + v(\vec{x})|\nabla \phi(\vec{x},t)| = 0$$

(Physical) Plasma Etching Model

- SF_6/O_2 etching model implementation in ViennaPS
  https://viennatools.github.io/ViennaPS/models/prebuilt/SF6O2Etching.html

Parameter	Description	Type
`ionFlux`	Ion flux for the SF_6O_2 etching process.	`double`
`etchantFlux`	Etchant flux for the SF_6O_2 etching process.	`double`
`oxygenFlux`	Oxygen flux for the SF_6O_2 etching process.	`double`
`meanEnergy`	Mean energy of ions (eV).	`NumericType`
`sigmaEnergy`	Energy distribution standard deviation (eV).	`NumericType`
`ionExponent`	(Optional) Exponent in the power cosine source distribution of ions for initial directions. Default is set to 100.	`NumericType`
`oxySputterYield`	(Optional) Oxygen sputtering yield. Default is set to 2.	`NumericType`
`etchStopDepth`	(Optional) Depth at which etching should stop. Default is negative infinity.	`NumericType`

Cosine distribution from the source plane (even distribution)
X.Klemenschits, PhD, TU Wien (2022) – section 3.2.2

Assuming Gaussian energy distribution

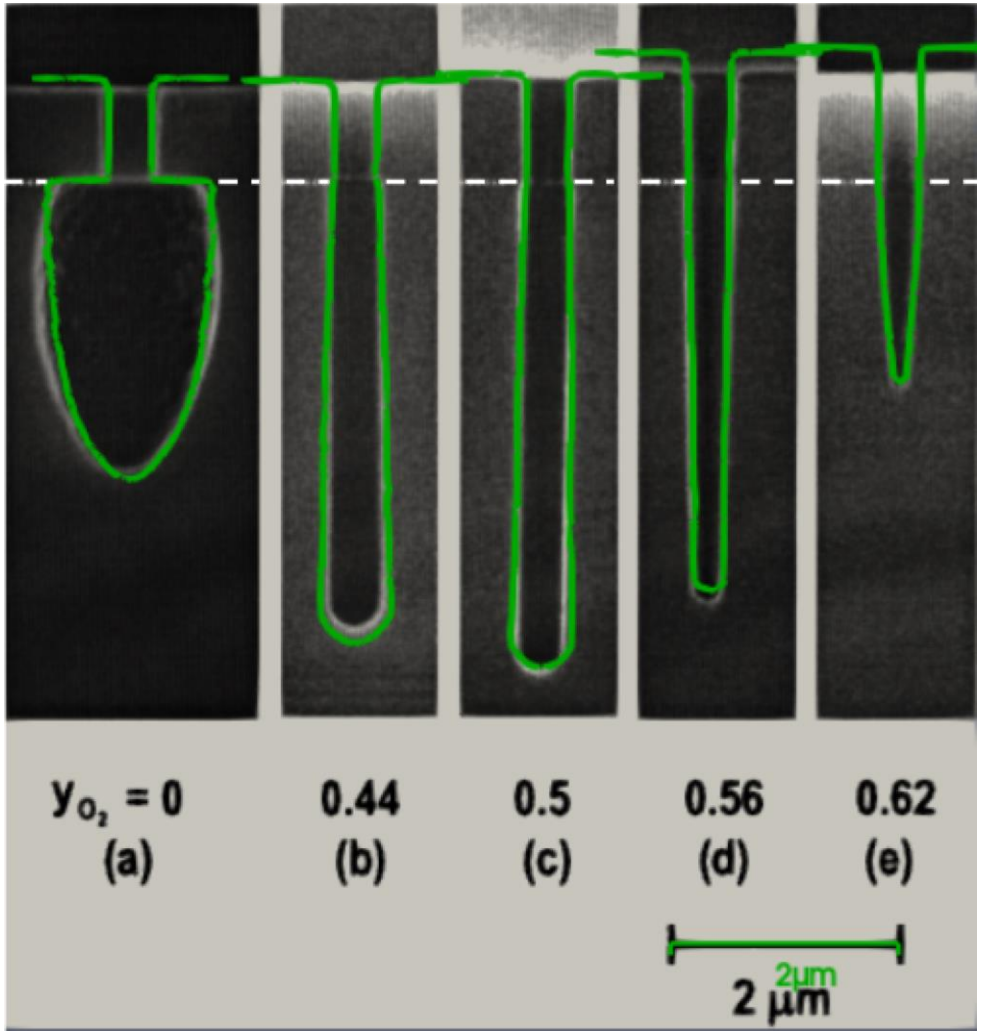
Power cosine distribution from the source plane (more vertical due to E-field)
X.Klemenschits, PhD, TU Wien (2022) – section 3.2.2

Belen et al., *J.Vac.Sci.Technol.A* 23 (2005) / R.A. Gottscho et al. *J.Vac.Sci.Technol.B* 10 (1992)

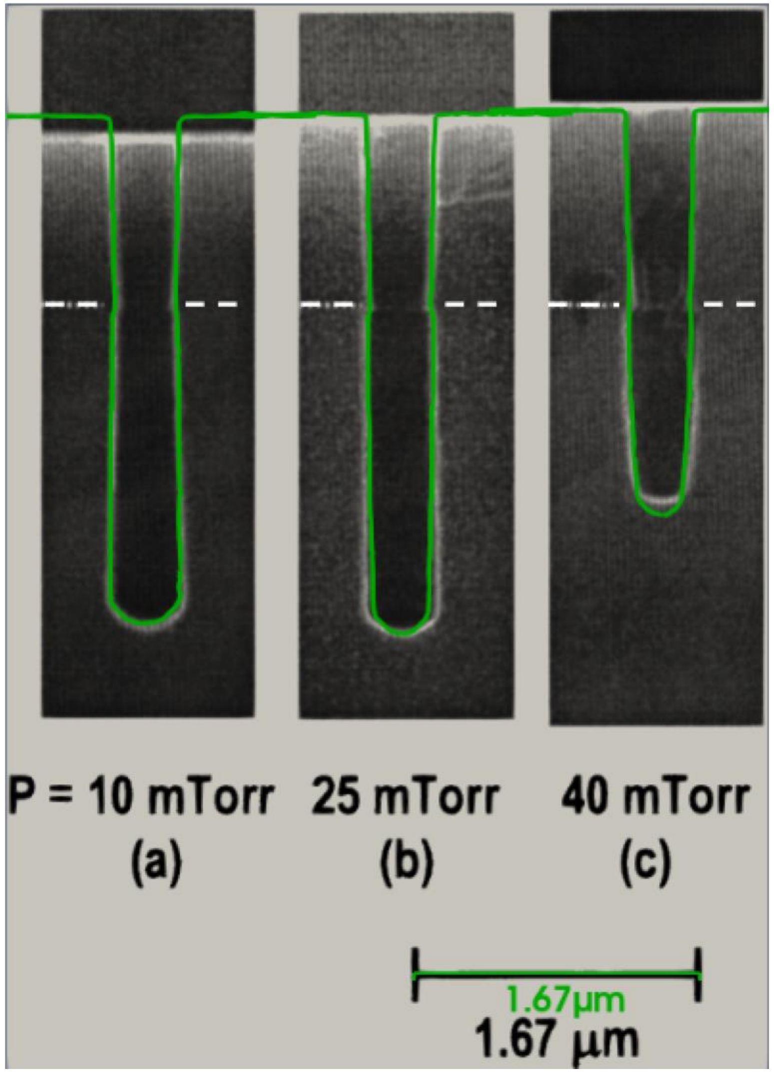
(Physical) Plasma Etching Model

- SF_6/O_2 etching model implementation in ViennaPS

Calibrated model



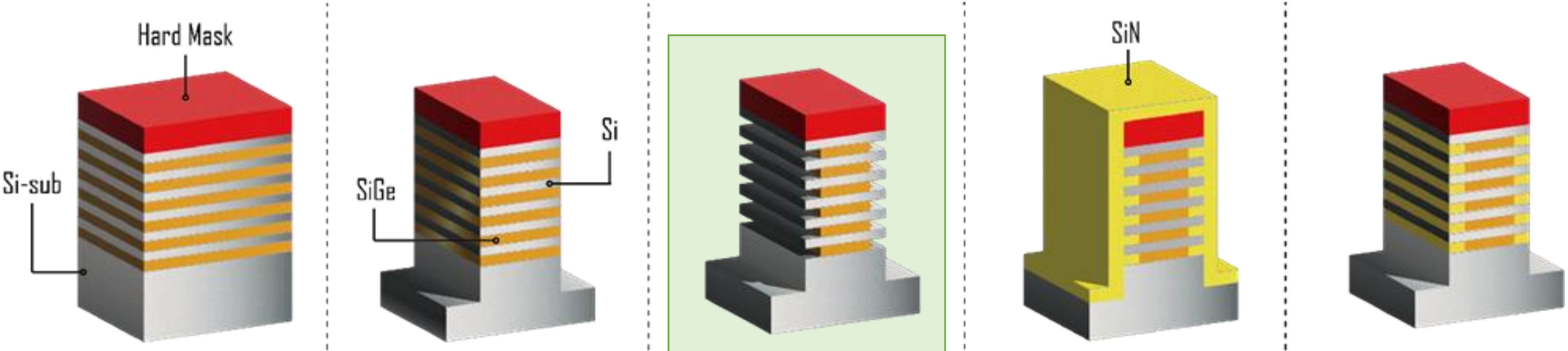
O_2 to SF_6 ratio



Pressure

(Physical) Plasma Etching Model

Example: Formation of a Si channel for GAA transistors



(a) epitaxy of Si/SiGe stacks and hard mask growth

(b) anisotropic etching of Si/SiGe stack and Si substrate

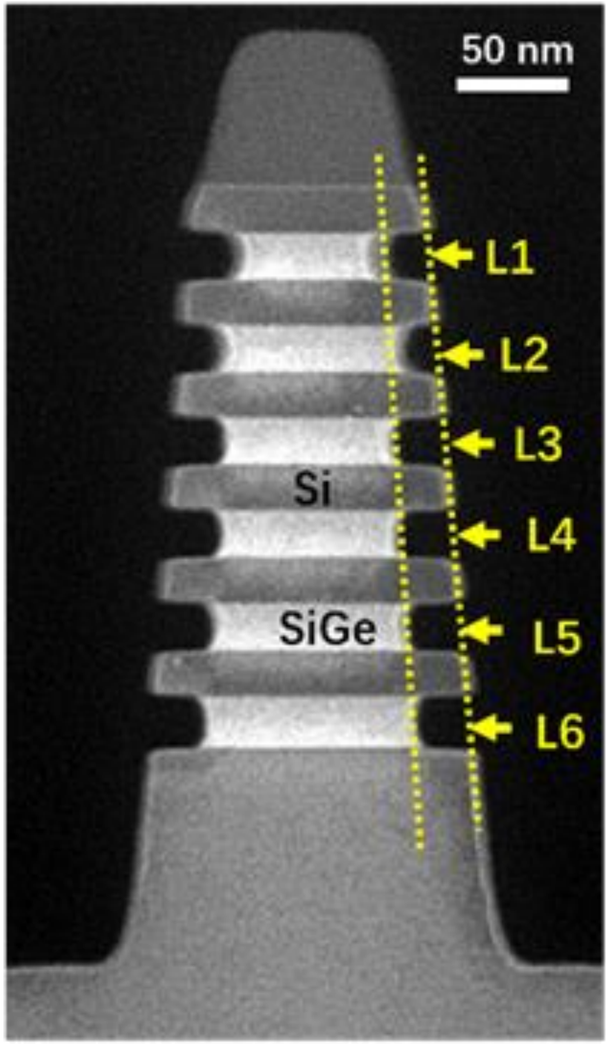
(c) lateral etching of SiGe layers

(d) inner spacer material SiN filling

(e) etch back of SiN film

(Physical) Plasma Etching Model

Selective SiGe etching in a CF_4/O_2 plasma



- Recipe:

Pressure:	10 - 40 mTorr
RF plasma power:	600 W
CF_4 flow:	100 sccm
O_2 flow:	20 sccm
He flow:	8 sccm
Temperature:	60 °C

H. Shao et al., *ACS Appl. Electron. Mater.* (in submission)

(Physical) Plasma Etching Model

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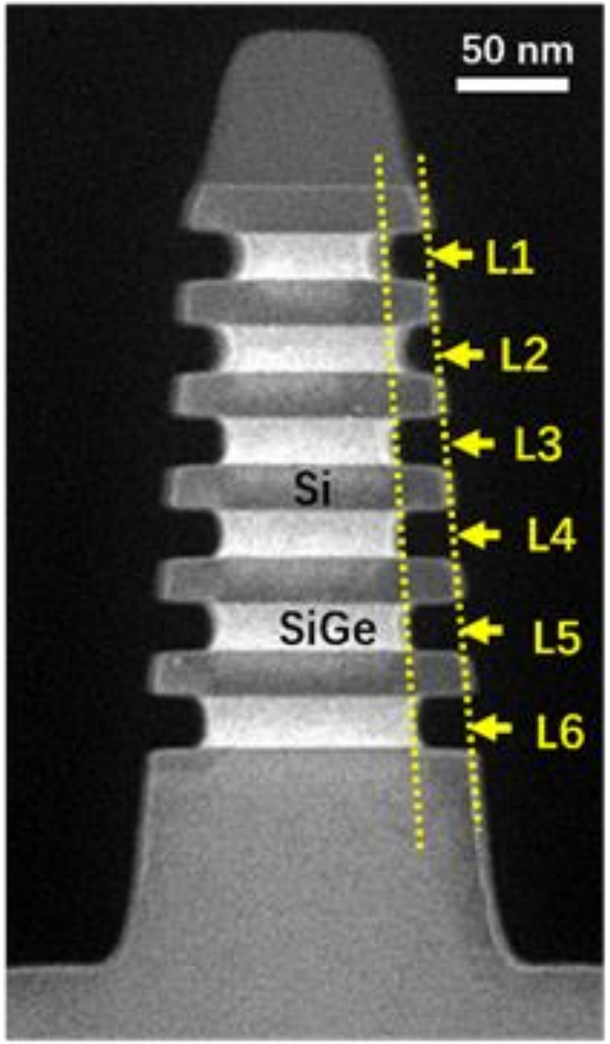

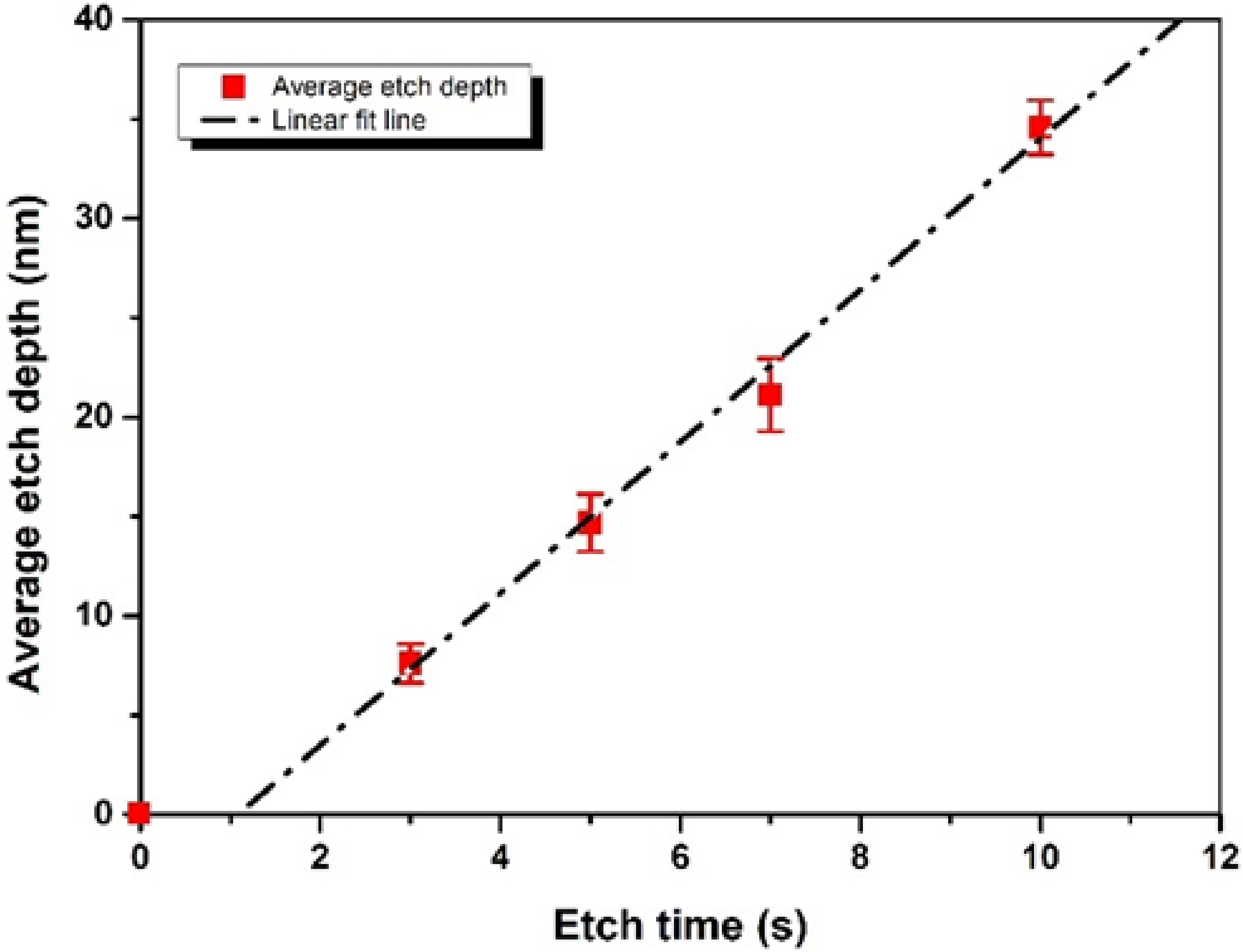

H. Shao et al., *ACS Appl. Electron. Mater.* (in submission)

(Physical) Plasma Etching Model

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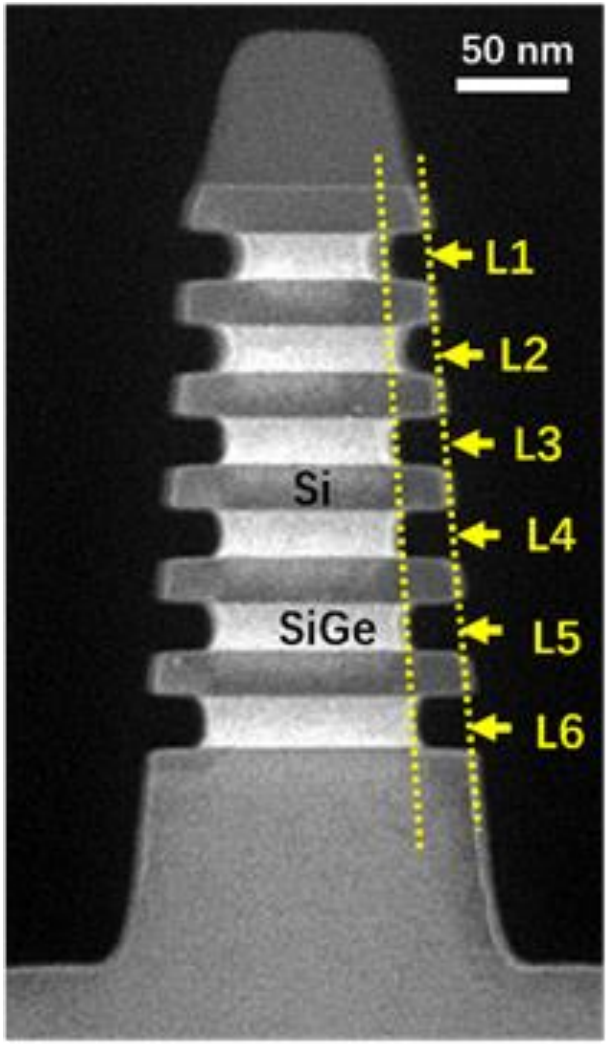

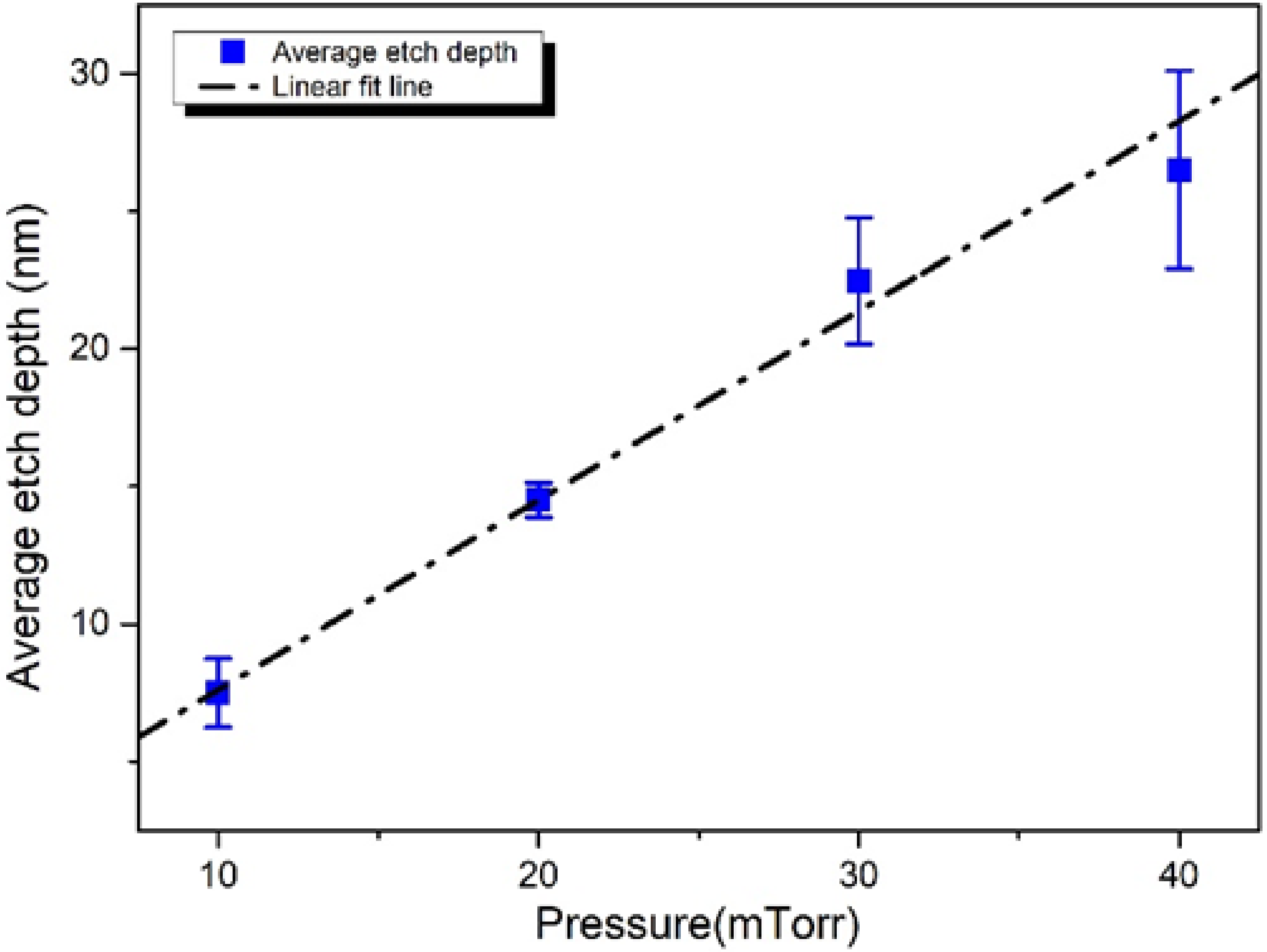

H. Shao et al., *ACS Appl. Electron. Mater.* (in submission)

(Physical) Plasma Etching Model

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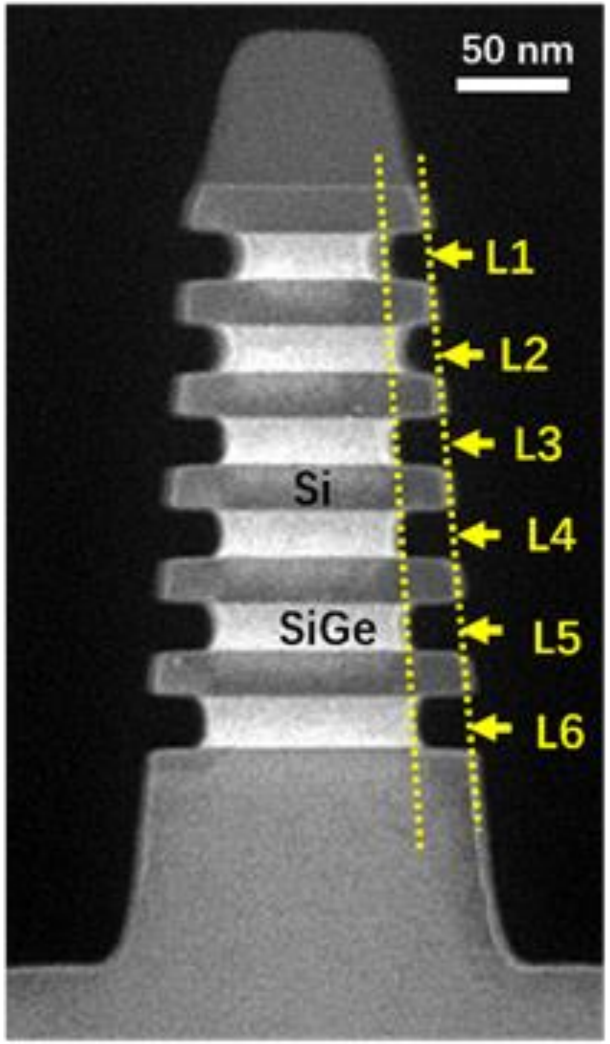


- Etching is isotropic and selective against Si
- Where does the selectivity come from?
- **Bond strengths?**

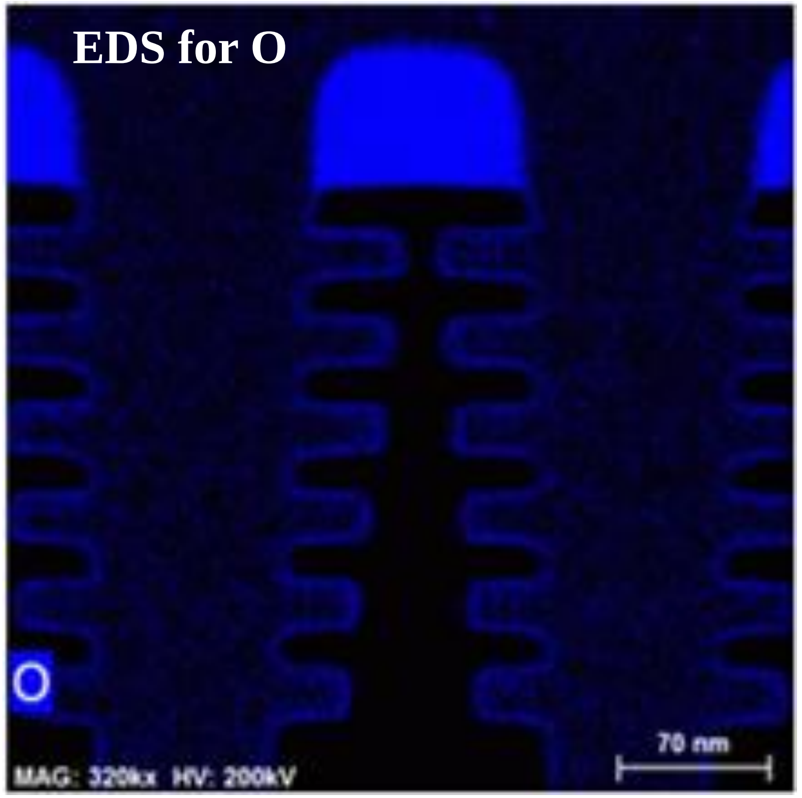
Bond	Dissociation energy
Si-Si	310 kJ/mol = 3.21 eV
Ge-Ge	274 kJ/mol = 2.84 eV
Si-Ge	297 kJ/mol = 3.08 eV
Si-O	800 kJ/mol = 8.29 eV
Ge-O	657 kJ/mol = 6.81 eV

Bond Dissociation Energies, in CRC Handbook of Chemistry and Physics, CRC Press, 2012

H. Shao et al., *ACS Appl. Electron. Mater.* (in submission)

(Physical) Plasma Etching Model

Selective SiGe etching in a CF_4/O_2 plasma



Etching one pillar

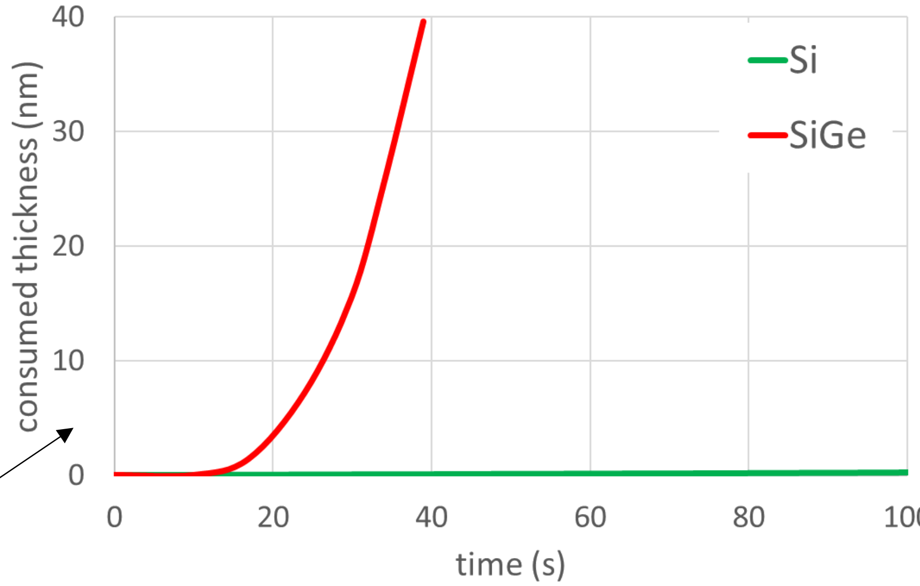
- Etching is isotropic and selective against Si
- **Surface oxidation?**

$$\sigma \frac{d\theta_F}{dt} = \gamma_F \Gamma_F (1 - \theta_F - \theta_O) - k\sigma\theta_F$$

F coverage

$$\sigma \frac{d\theta_O}{dt} = \gamma_O \Gamma_O (1 - \theta_F - \theta_O) - \beta\sigma\theta_O$$

O coverage



With native oxide

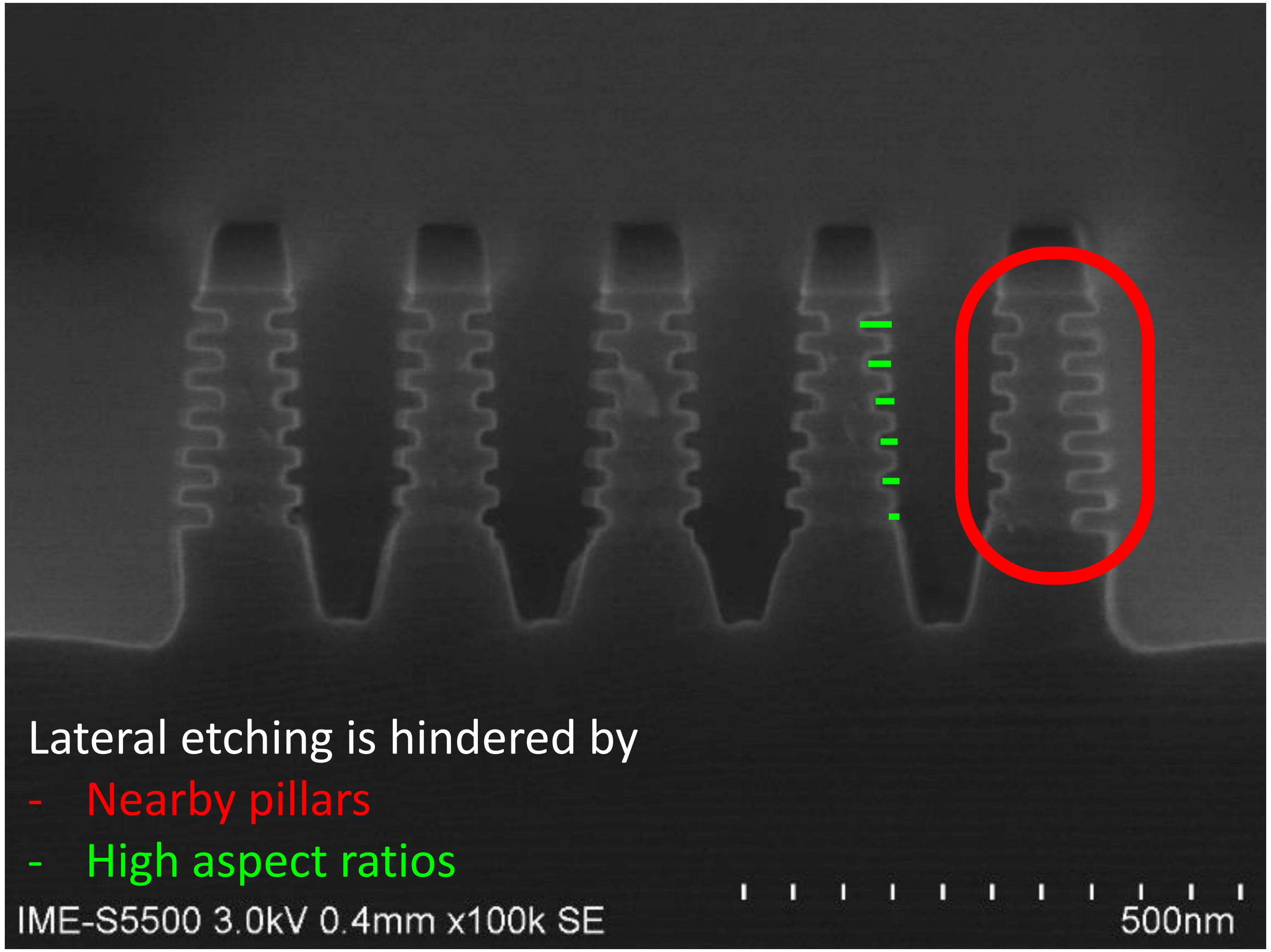
- Surface oxidation will hinder Si etching more than SiGe etching

H. Shao et al., *ACS Appl. Electron. Mater.* (in submission)

E. Pargon et al., *J. Vac. Sci. Technol. A* 37 (2019)

(Physical) Plasma Etching Model

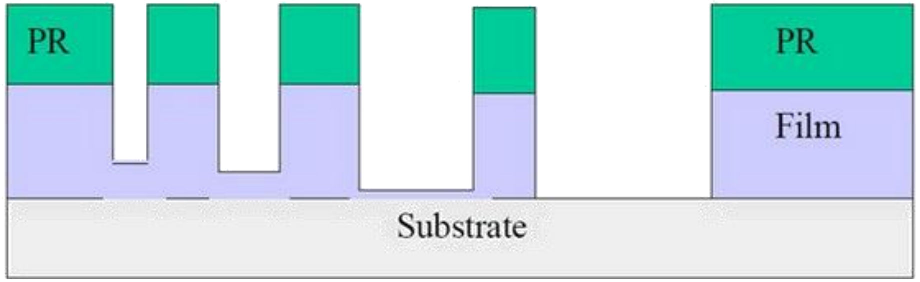
Selective SiGe etching in a CF_4/O_2 plasma



Etching multiple pillars side-by-side

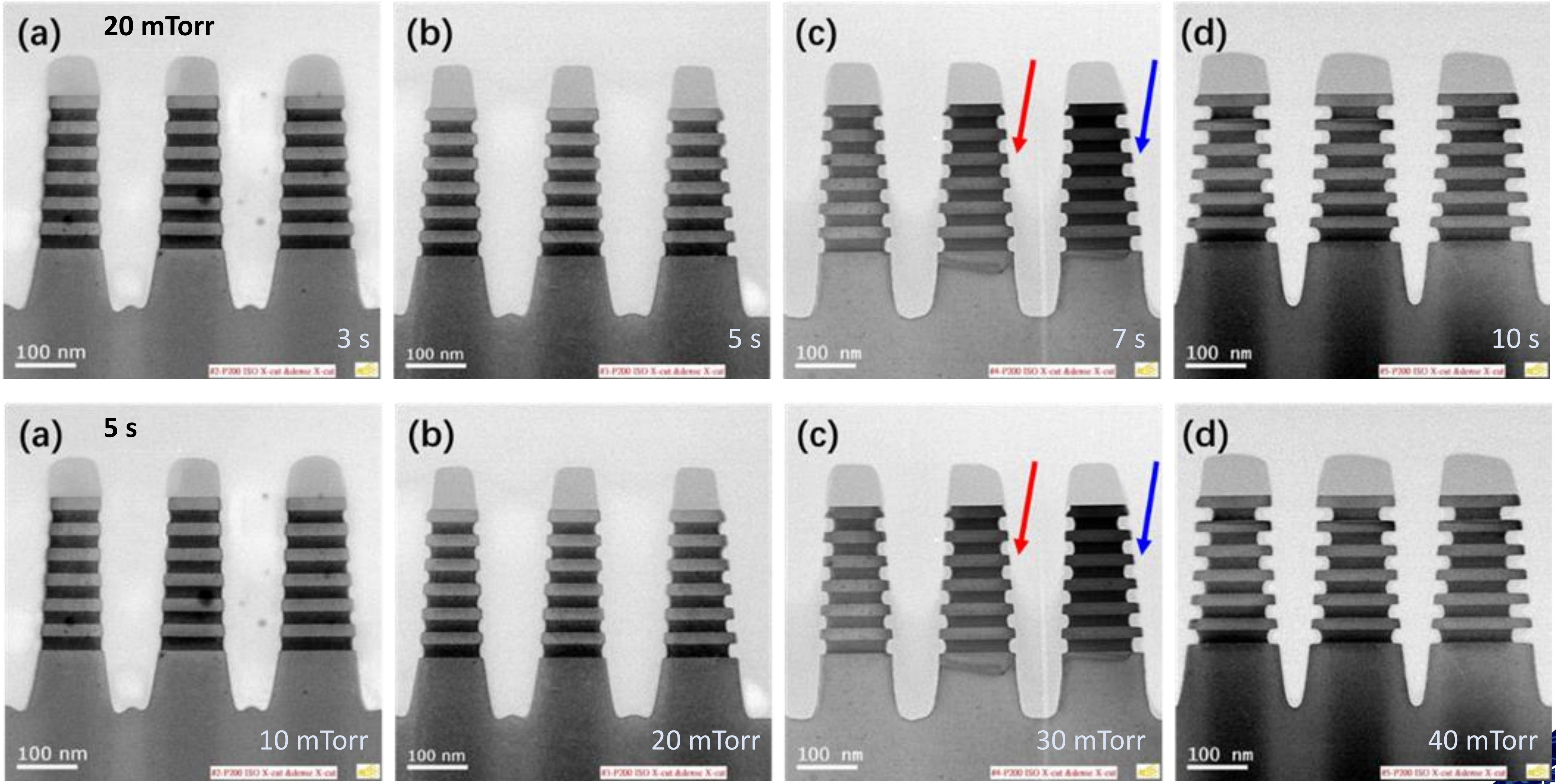
H. Shao et al., *ACS Appl. Electron. Mater.* (in submission)

- Typically, we want to place many devices near each other
- This can cause microloading



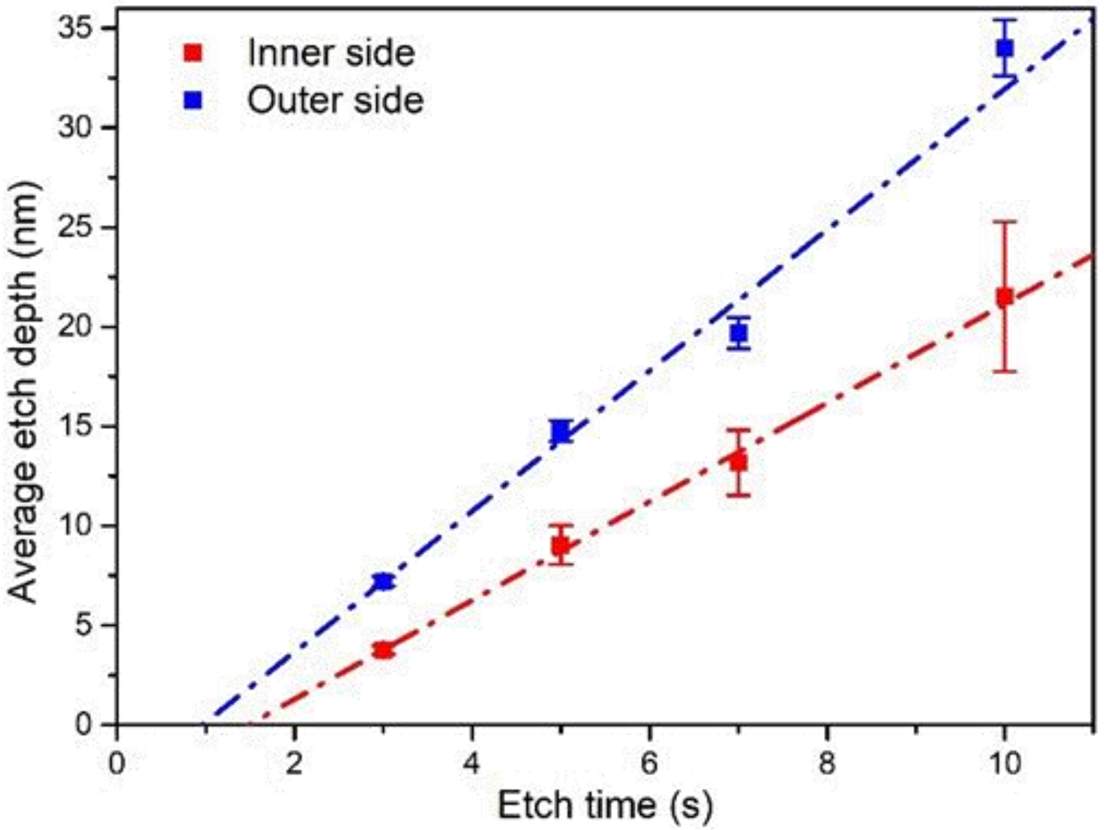
- This effect can be captured using Monte Carlo ray tracing

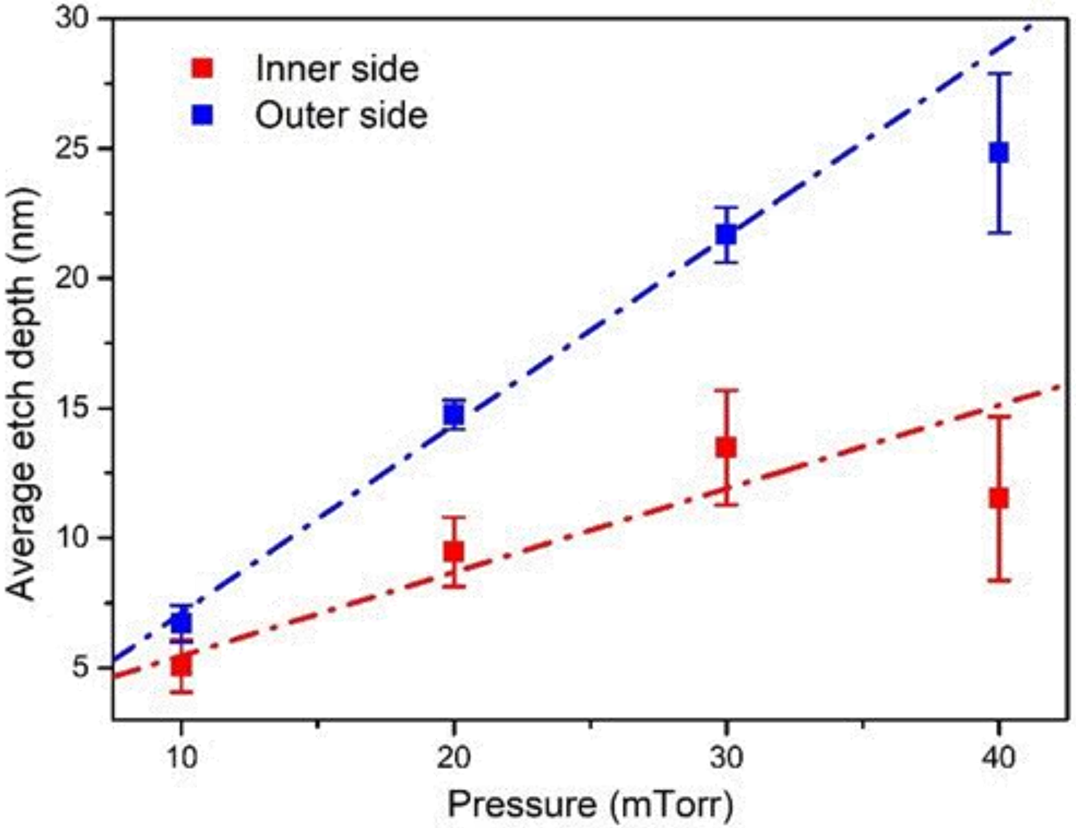
(Physical) Plasma Etching Model



(Physical) Plasma Etching Model

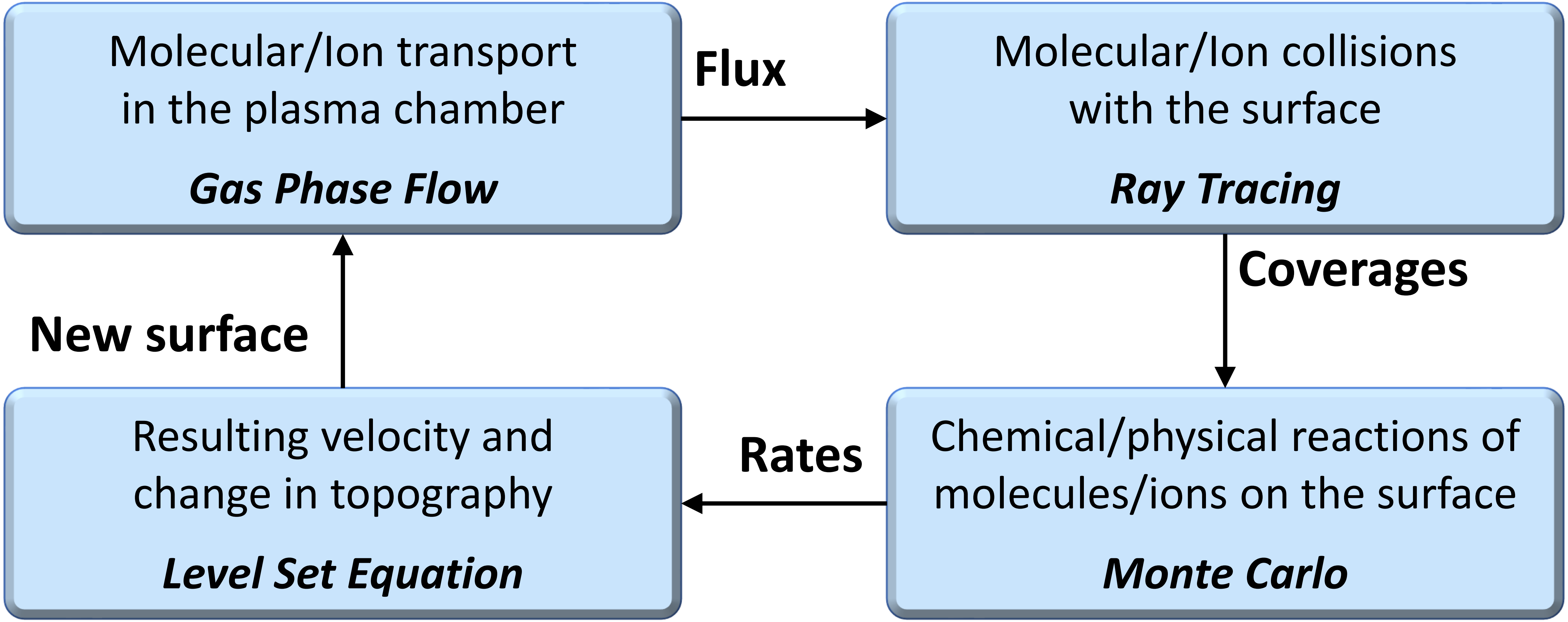
- Loading is clearly visible for inner side pillars
- Etch depth reduces deeper inside the trench





(Physical) Plasma Etching Model

- Plasma etching model as implemented in ViennaPS – single reactive species

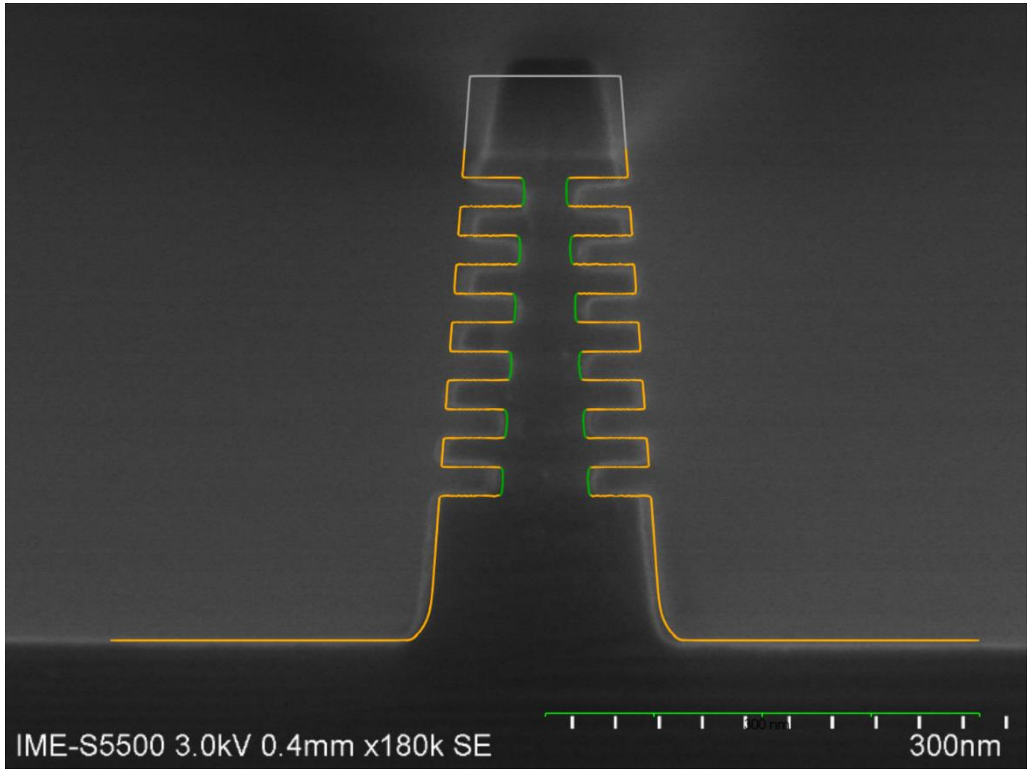


$$\frac{\delta\phi(\vec{x},t)}{\delta t} + v(\vec{x})|\nabla\phi(\vec{x},t)| = 0$$

J. Bobinac et al., *Miromachines* 14 (2023)

(Physical) Plasma Etching Model

Selective SiGe etching in a CF_4/O_2 plasma



Etching one pillar

- Etching is isotropic and selective against Si
- At the feature scale, we track coverages of adsorbed Fluorine θ_F and Oxygen θ_O

$$\sigma \frac{d\theta_F}{dt} = \gamma_F \Gamma_F (1 - \theta_F - \theta_O) - k\sigma\theta_F$$

$$\sigma \frac{d\theta_O}{dt} = \gamma_O \Gamma_O (1 - \theta_F - \theta_O) - \beta\sigma\theta_O$$

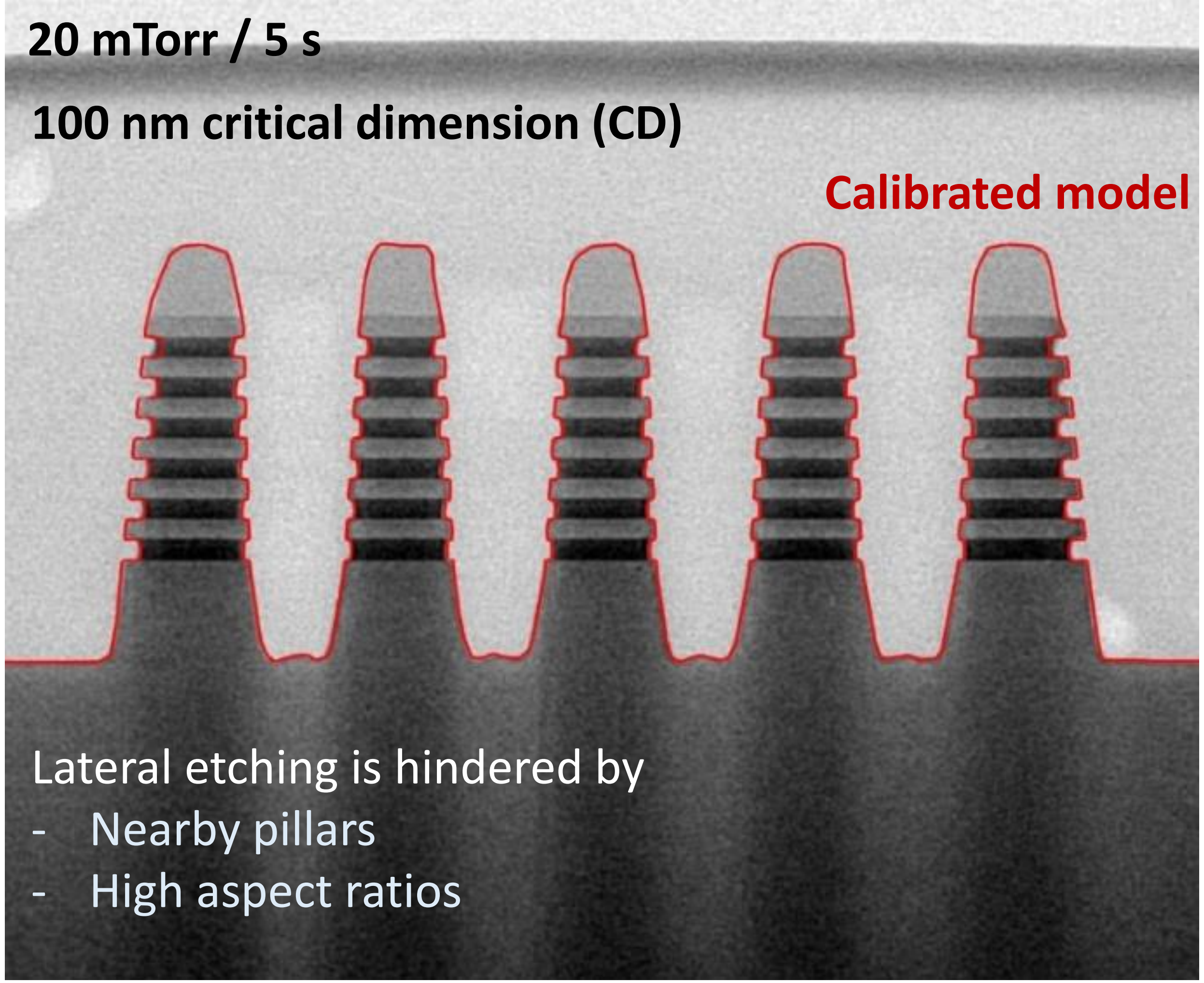
- The etch rate is then

$$v(\vec{x}) = \frac{1}{\rho}\left(\frac{k\sigma\theta_F}{4}\right)$$

$$\frac{d\phi(\vec{x},t)}{dt} = v(\vec{x})|\nabla\phi(\vec{x},t)|$$

(Physical) Plasma Etching Model

Selective SiGe etching in a CF_4/O_2 plasma



Etching multiple pillars side-by-side

H. Shao et al., *ACS Appl. Electron. Mater.* (in submission)

Calibrate the model using the results of the multi-pillar fabricated sample by adjusting the flux and sticking coefficient

$$\sigma \frac{d\theta_F}{dt} = \gamma_F \Gamma_F (1 - \theta_F - \theta_O) - k\sigma\theta_F$$

$$\sigma \frac{d\theta_O}{dt} = \gamma_O \Gamma_O (1 - \theta_F - \theta_O) - \beta\sigma\theta_O$$

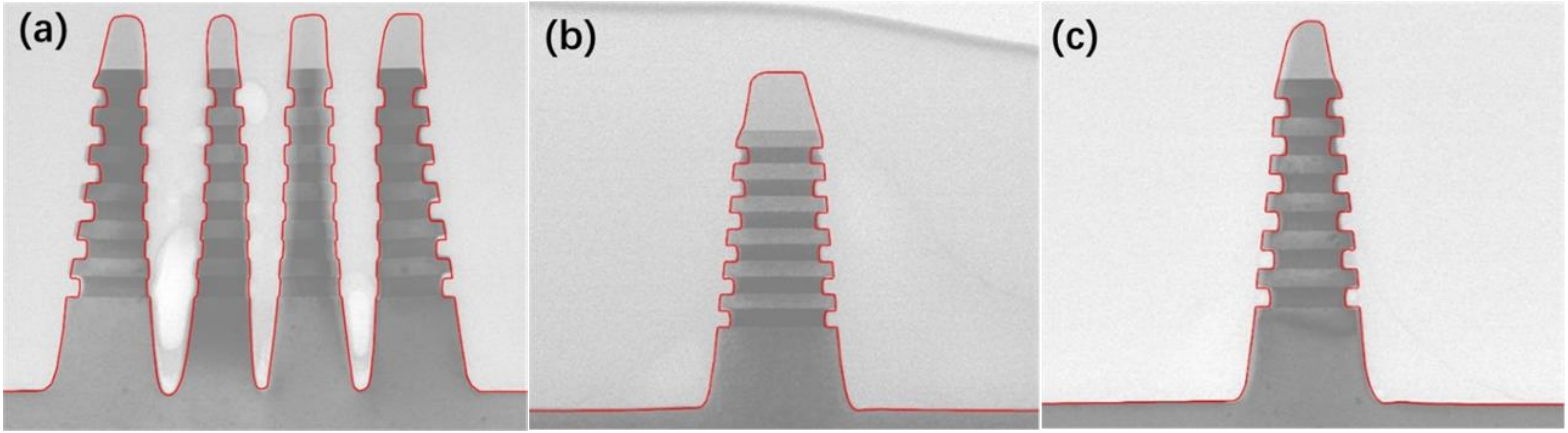
$$v(\vec{x}) = \frac{1}{\rho}\left(\frac{k\sigma\theta_F}{4}\right)$$

(Physical) Plasma Etching Model

Apply the calibrated model on different geometries

5 s etch at 20 mTorr pressure

Calibrated model



Multi-pillar 50 nm CD | **Single pillar 100 nm** | **Single pillar 50 nm**

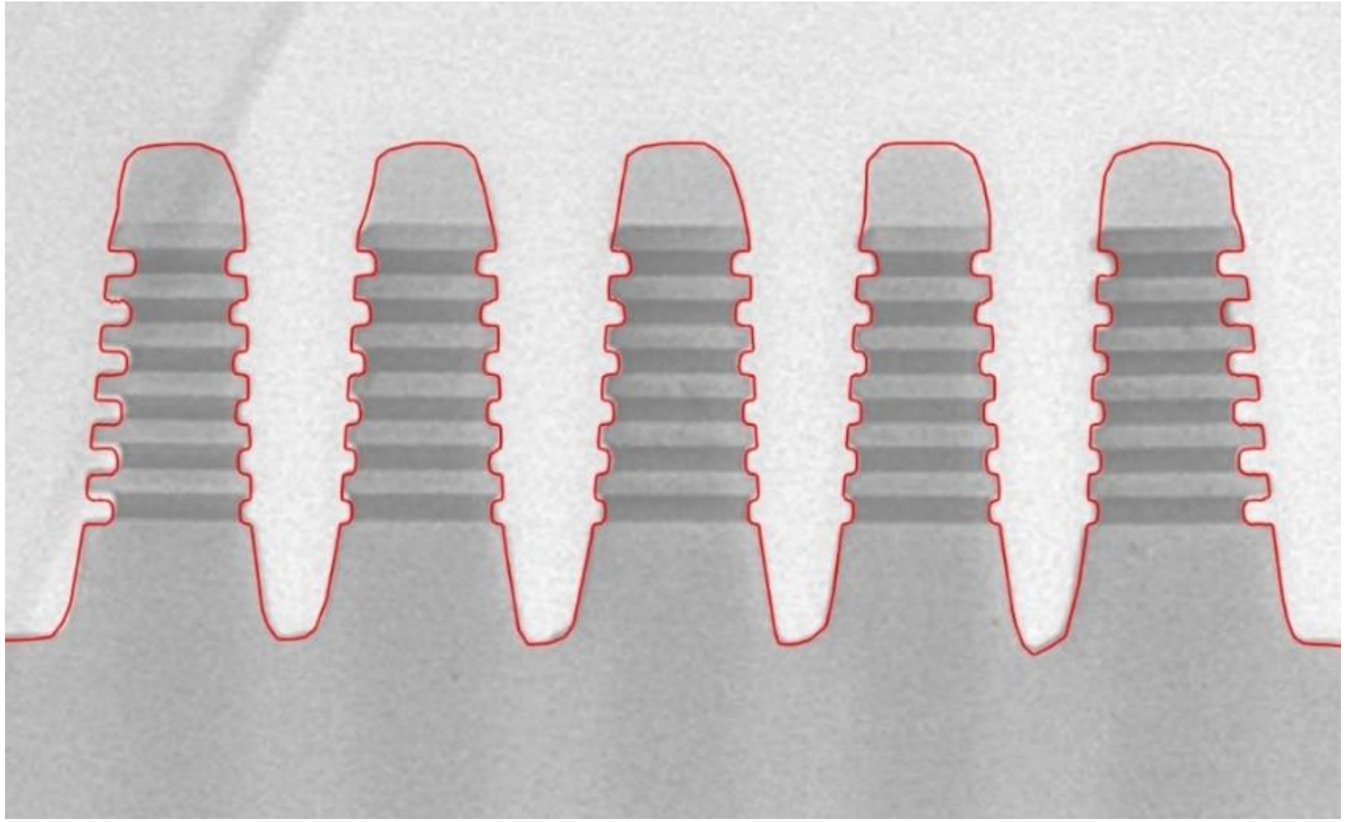
H. Shao et al., *ACS Appl. Electron. Mater.* (in submission)

(Physical) Plasma Etching Model

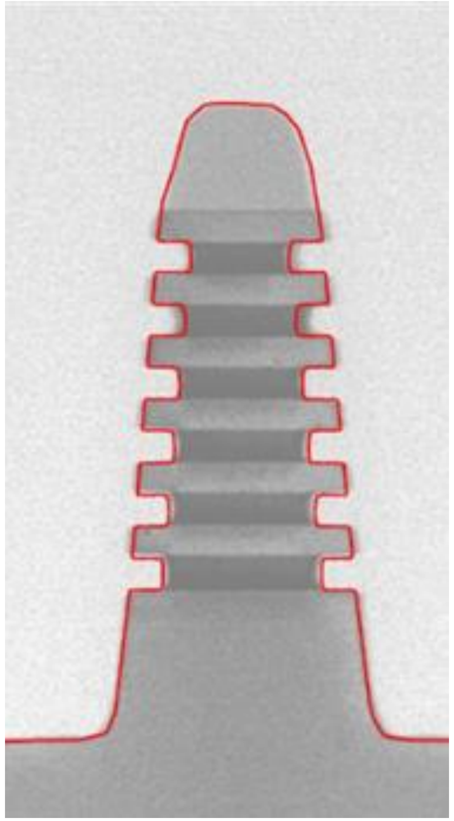
Apply the calibrated model on different geometries

5 s etch at 40 mTorr pressure

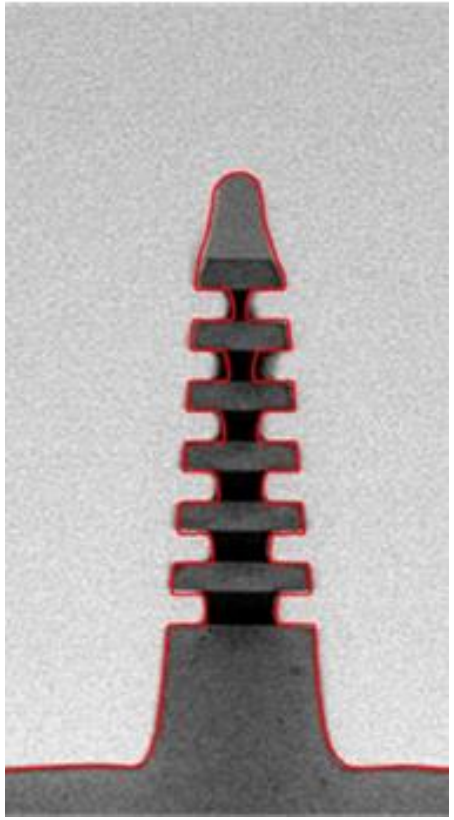
Calibrated model



Multi-pillar 100 nm CD



Single pillar 100 nm

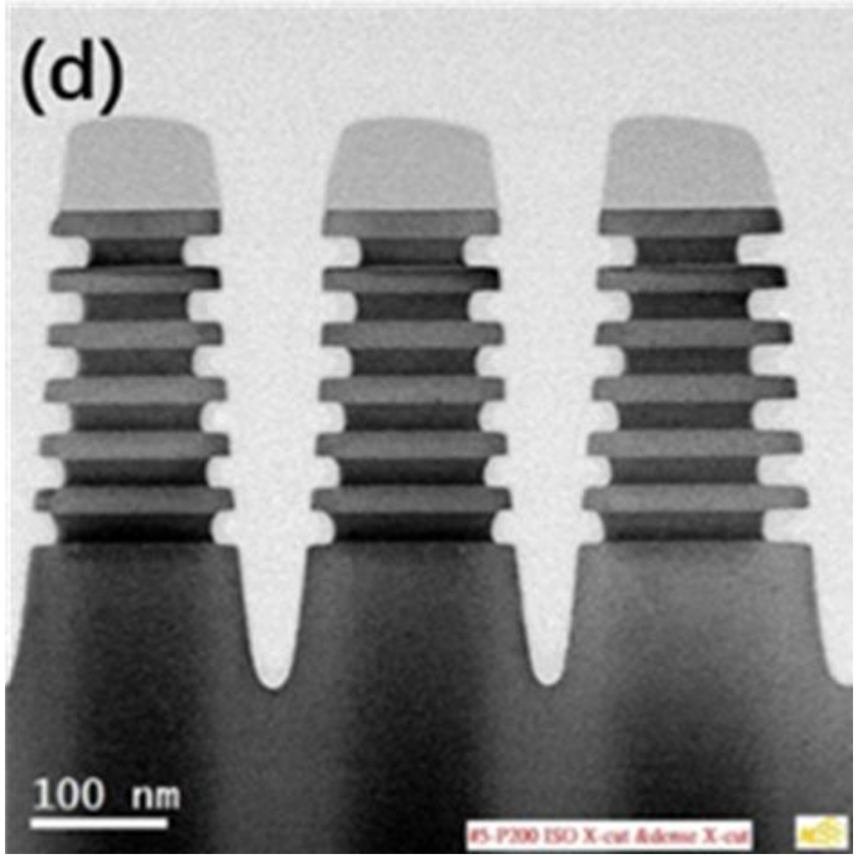


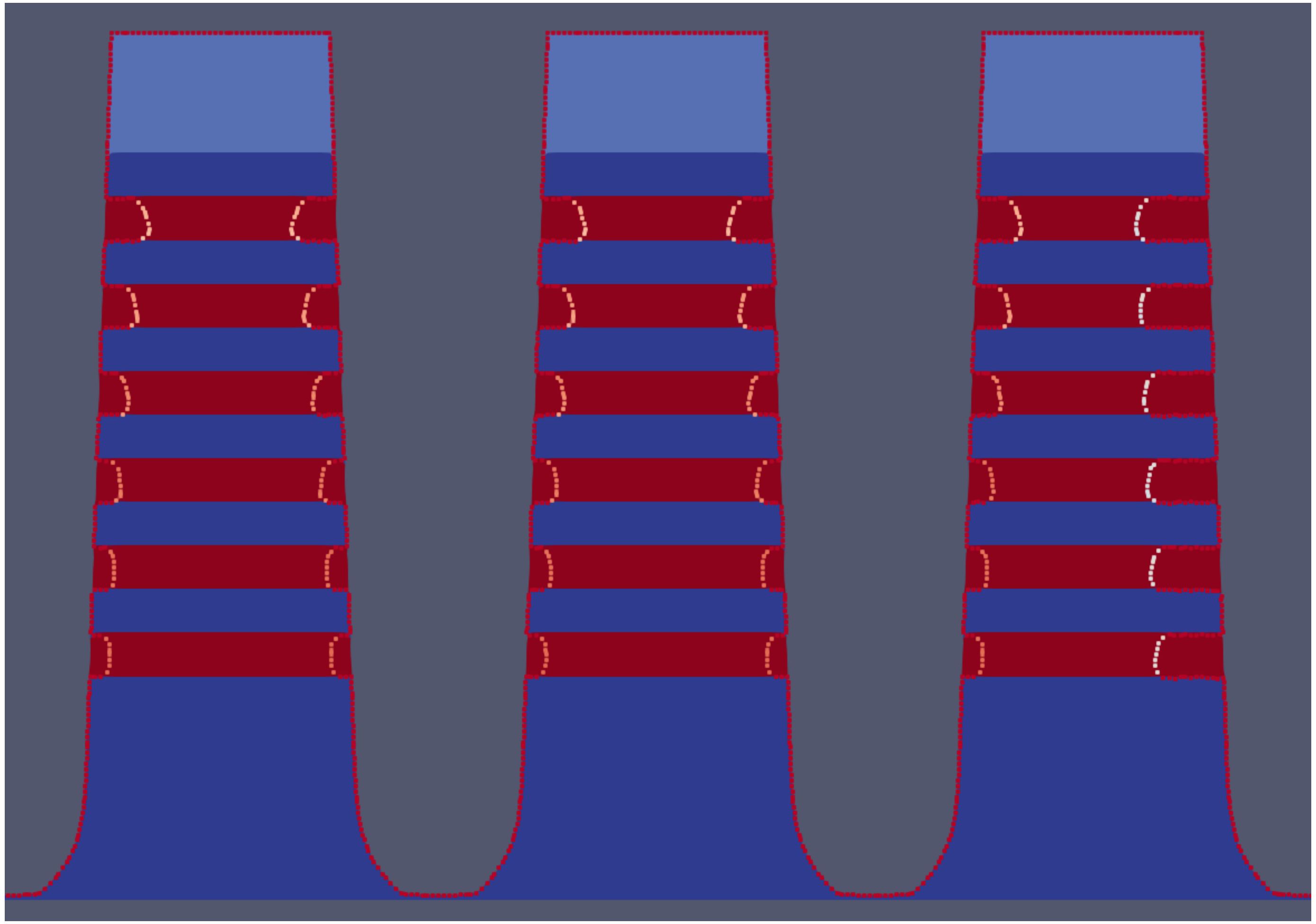
Single pillar 50 nm

H. Shao et al., *ACS Appl. Electron. Mater.* (in submission)

Plasma Etching Parameter Search

- Use a global optimizer to find the parameters for the etching model
- Need to extract all latera etch depths automatically





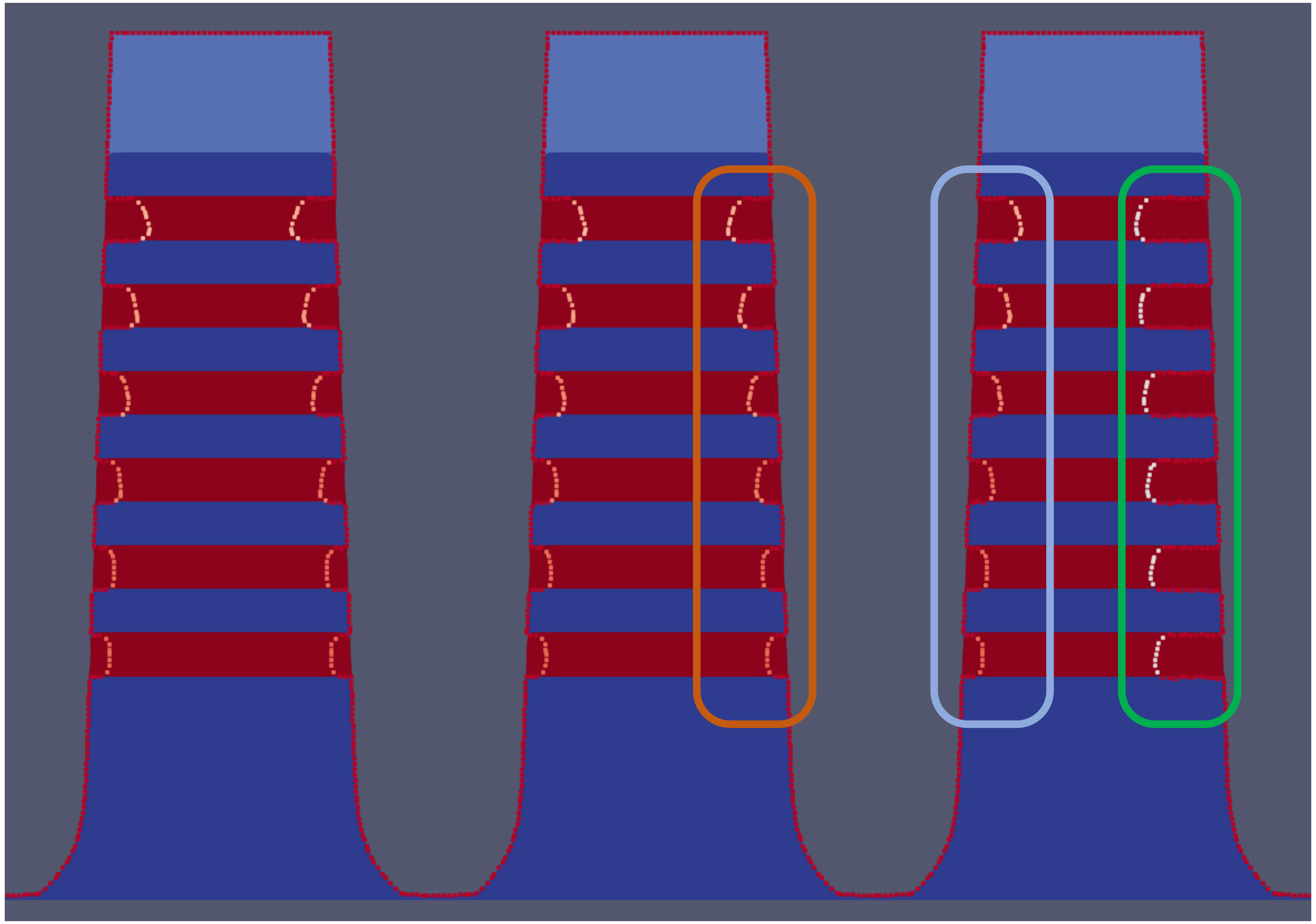
H. Shao et al., *ACS Appl. Electron. Mater.* (in submission)

Plasma Etching Parameter Search

- Use a global optimizer to find the parameters for the etching model
- Need to extract all latera etch depths automatically

- We extract the depths matrix:

```
[[... 20.8 21.  20.8 21.  20.8 33.9]
 [... 16.7 16.7 16.7 16.9 16.8 33.5]
 [... 14.1 14.1 13.9 14.  13.9 33. ]
 [... 11.5 11.6 11.6 11.7 11.7 32.9]
 [... 10.2 10.2 10.1 10.3 10.3 32.8]
 [...  9.2  9.2  9.2  9.2  9.2 31.9]]
```



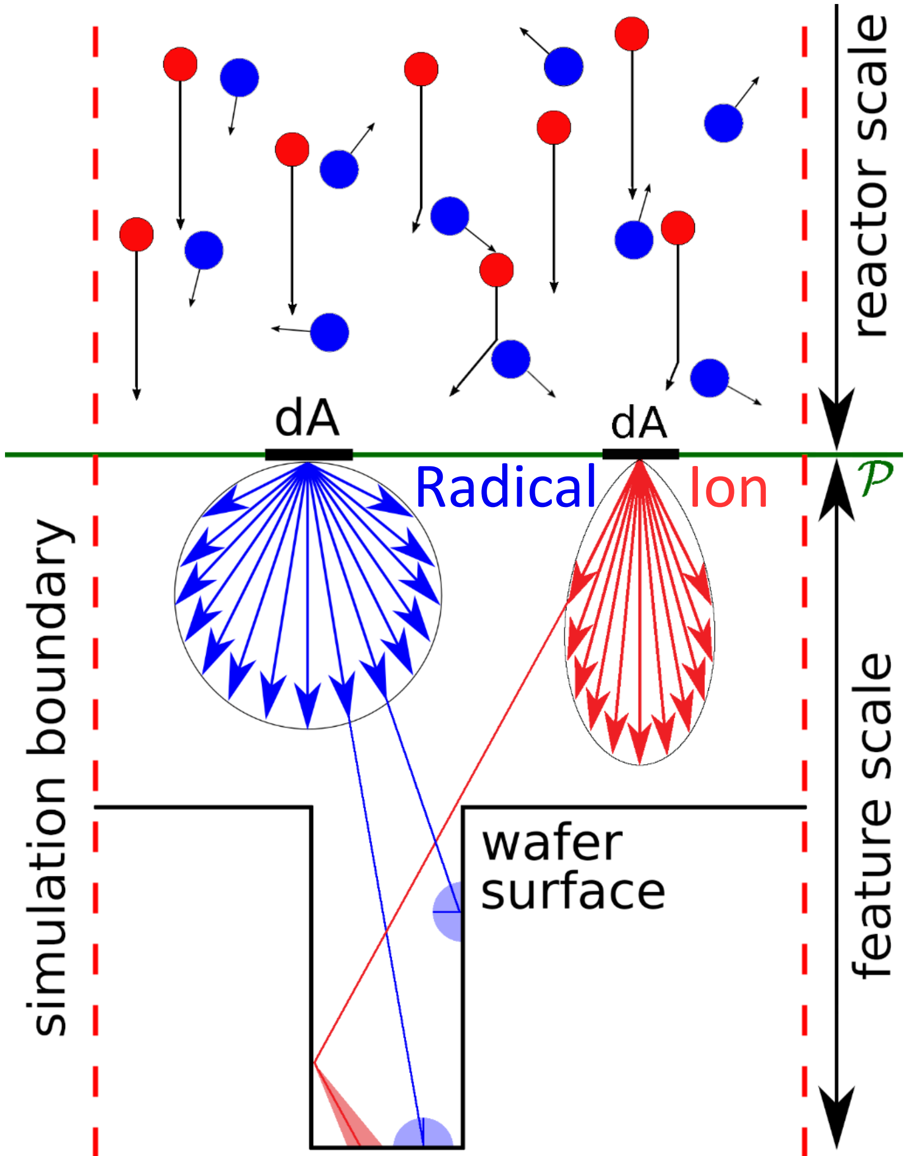
- Use the matrix elements to define the optimization target

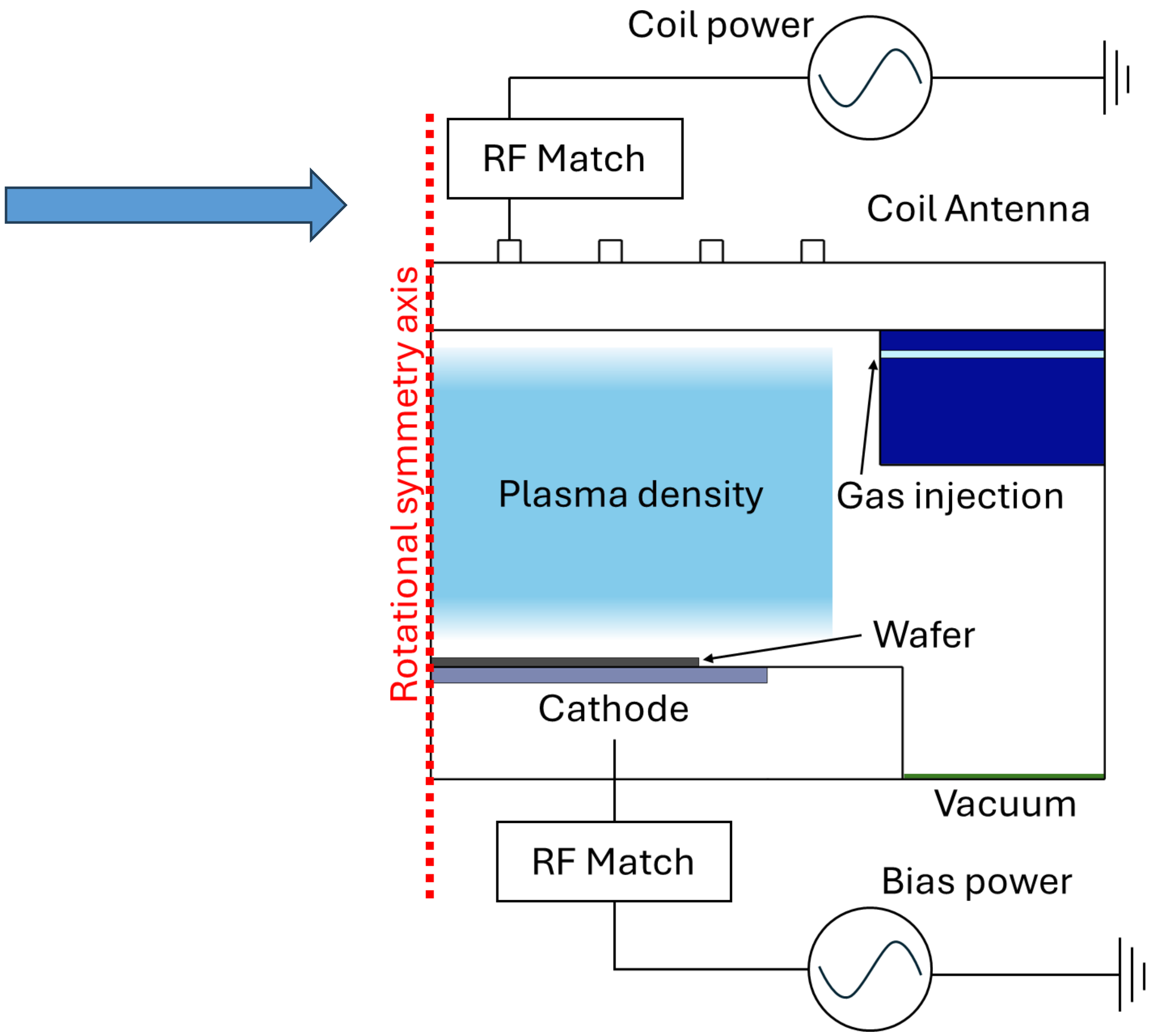
Outline

- Technology Computer-Aided Design (TCAD)
- ViennaPS Framework
- Process Simulation
  - Chemical Vapor Deposition
  - Plasma Etching
- **Link to Equipment Settings**

Multi-Scale Plasma Etching Model

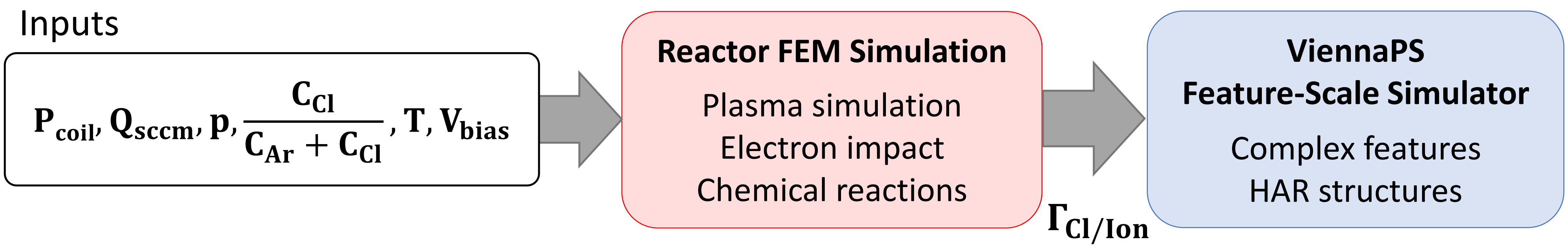
- Merging the reactor and feature scales





Multi-Scale Plasma Etching Model

- We combine reactor simulation (FEM) with ViennaPS topography simulations (LS)
- Implementation for Cl_2/Ar plasma:



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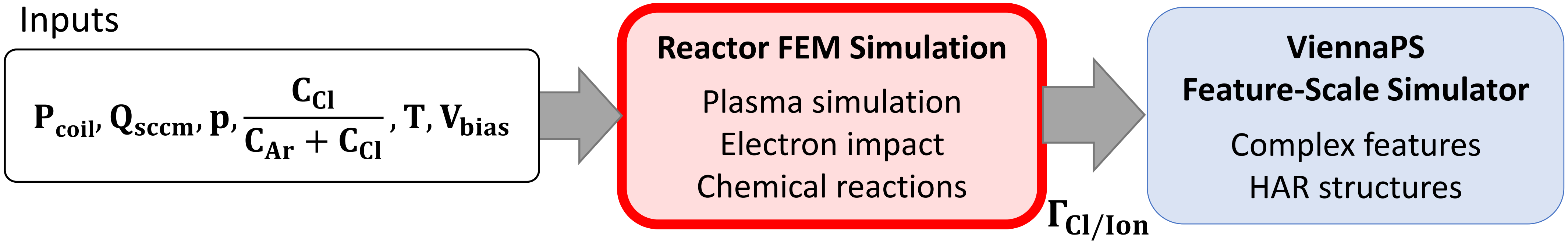
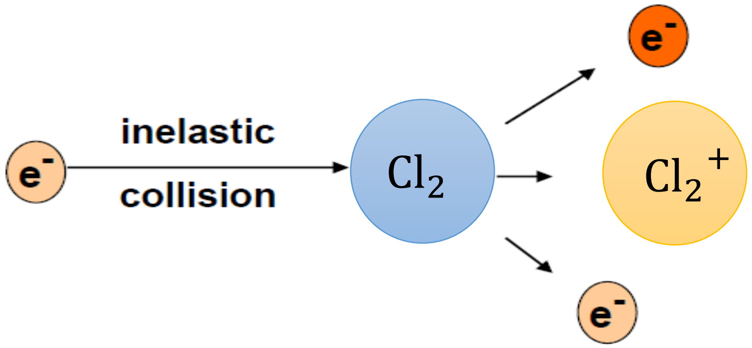
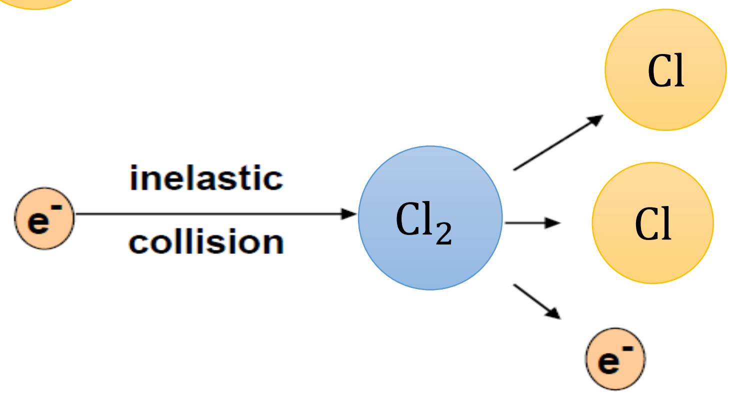


- Reactor simulation:
  - Ionization:
    $e^- + Cl_2 \rightarrow 2e^- + Cl_2{}^+$
  - Dissociation:
    $e^- + Cl_2 \rightarrow e^- + Cl + Cl$
  - Excitation:
    $e^- + Ar \rightarrow Ars + e^- \rightarrow Ar + e^- + \hbar\omega$





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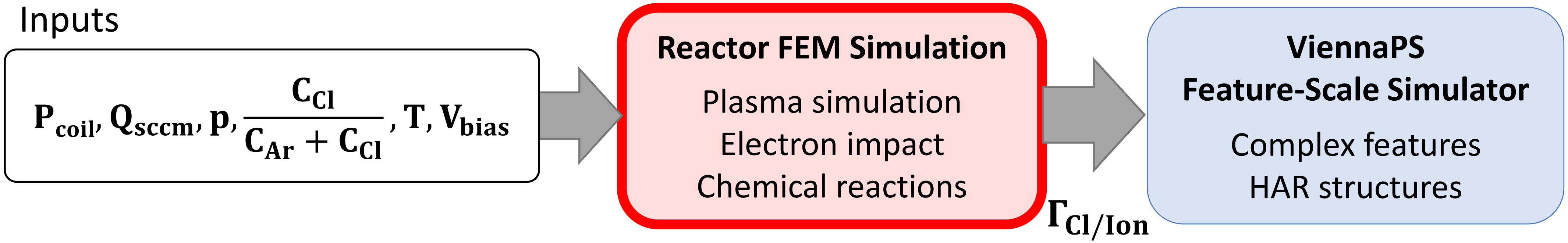
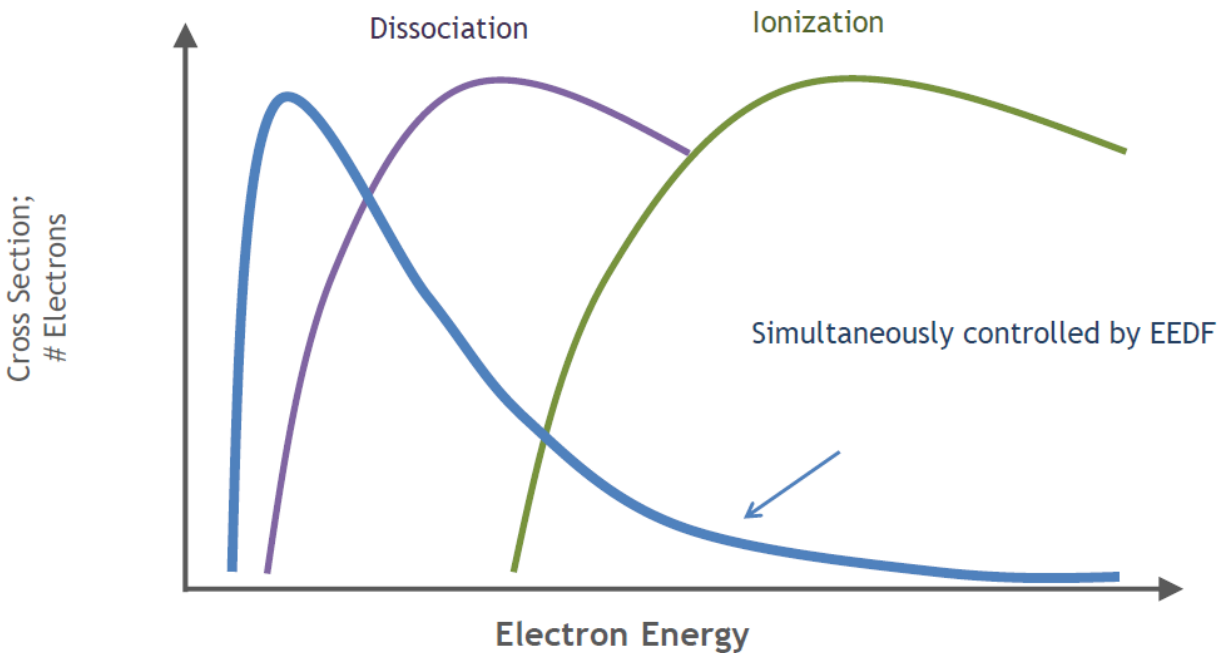


- Reactor simulation:
  - Ionization:
    $$e^- + Cl_2 \rightarrow 2e^- + {Cl_2}^+$$
  - Dissociation:
    $$e^- + Cl_2 \rightarrow e^- + Cl + Cl$$
  - Excitation:
    $$e^- + Ar \rightarrow Ars + e^- \rightarrow Ar + e^- + \hbar\omega$$



Multi-Scale Plasma Etching Model

- We combine reactor simulation (FEM) with ViennaPS topography simulations (LS)
- Implementation for Cl_2/Ar plasma:

Inputs

$$P_{coil}, Q_{sccm}, p, \frac{C_{Cl}}{C_{Ar} + C_{Cl}}, T, V_{bias}$$

→

Reactor FEM Simulation

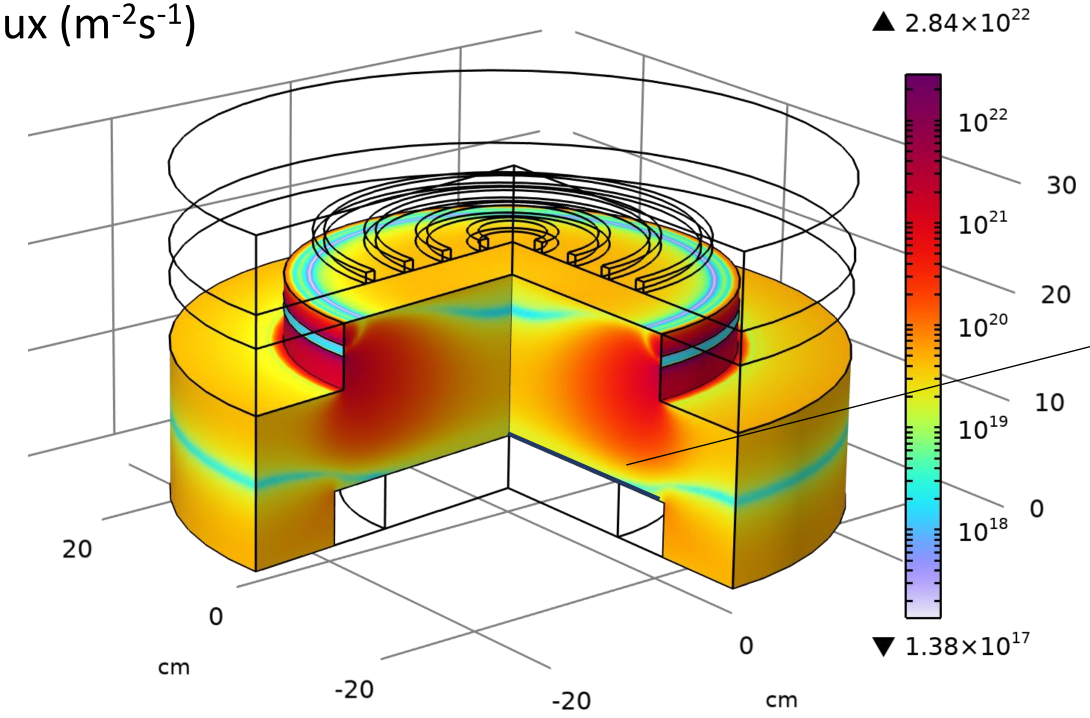
Plasma simulation
Electron impact
Chemical reactions

→

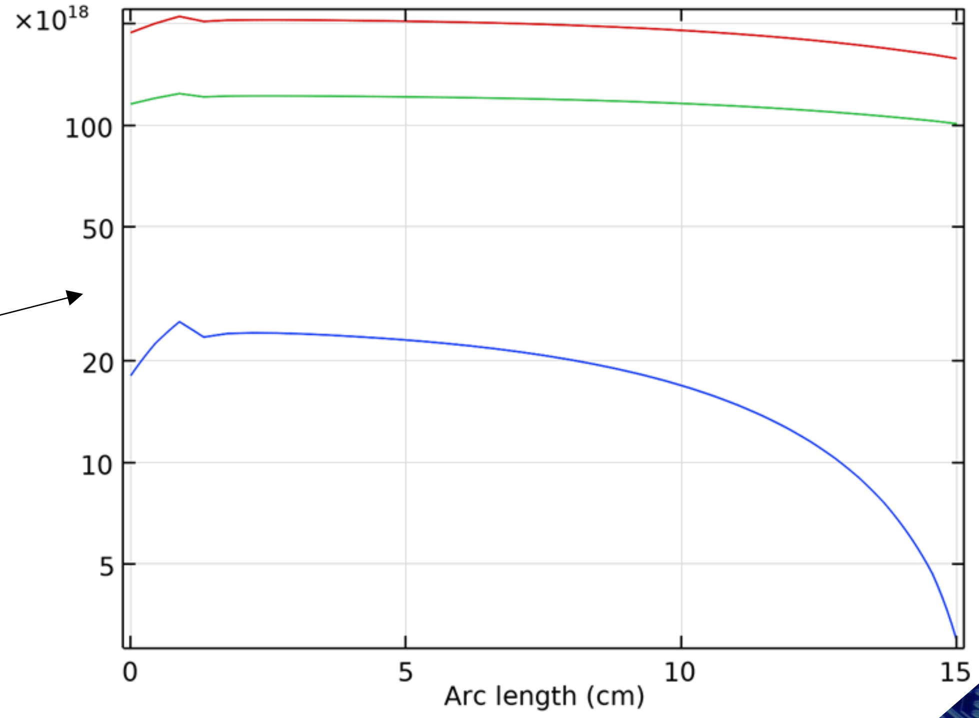
ViennaPS
Feature-Scale Simulator

Complex features
HAR structures

Cl flux ($m^{-2}s^{-1}$)



$\Gamma_{Cl/Ion}$



Multi-Scale Plasma Etching Model

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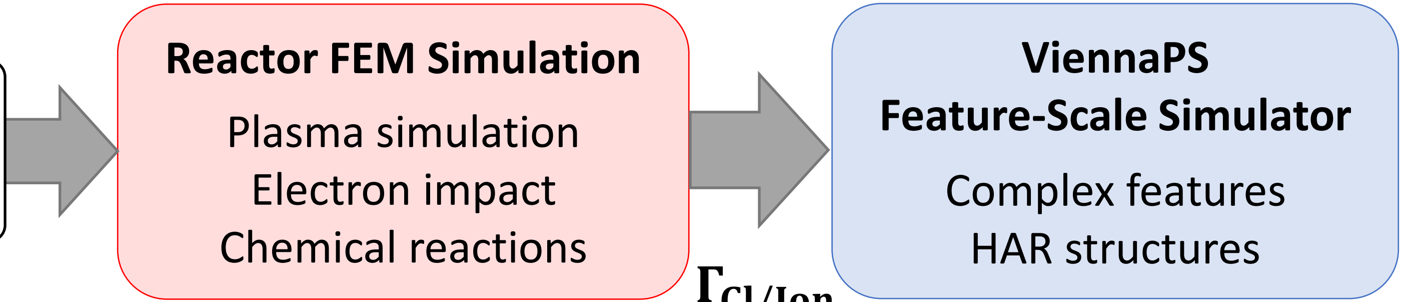

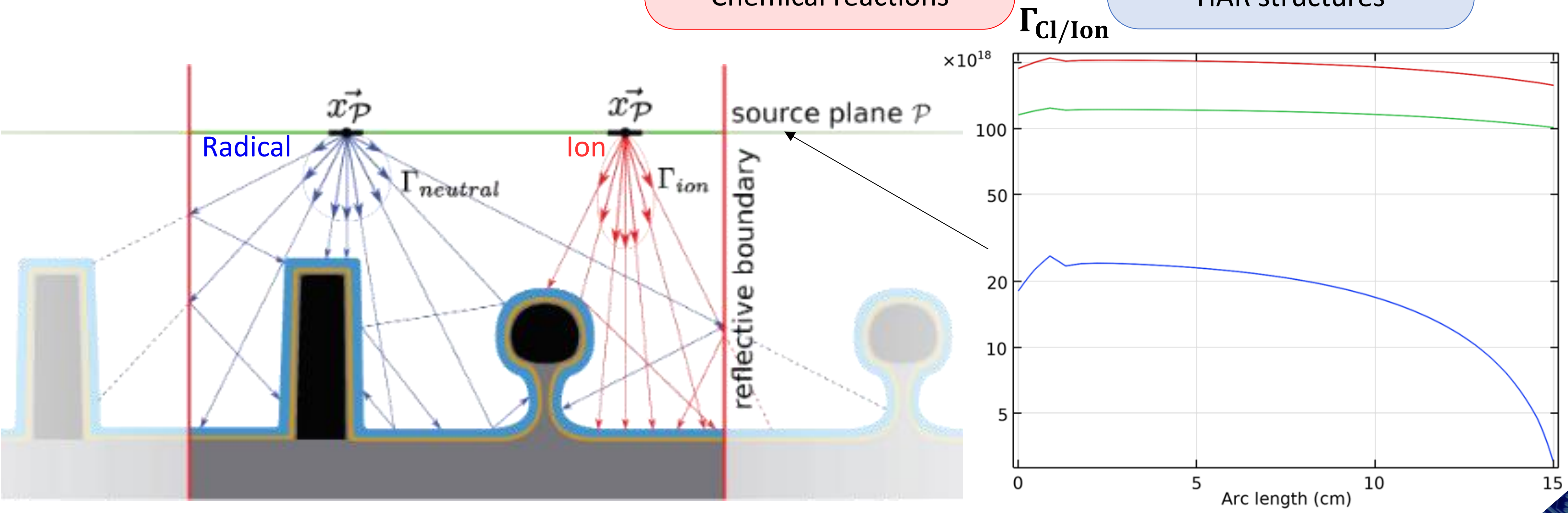

Multi-Scale Plasma Etching Model

- We combine reactor simulation (FEM) with ViennaPS topography simulations (LS)
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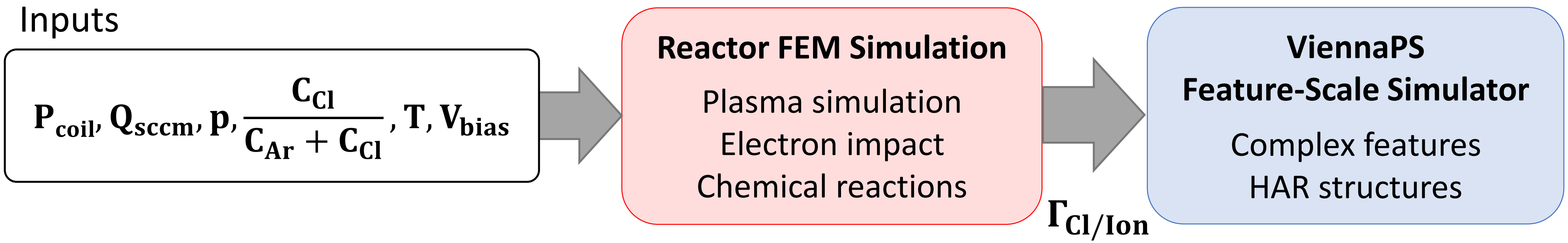


- We test Cl2/Ar plasma chamber simulations for 18 750 combinations

Coil power P_{coil} **(W):**	200,	300,	400,	500,	600	
Gas flow Q_f **(sccm):**	50,	75,	100,	125,	150	
Pressure p **(Torr):**	0.007,	0.01,	0.013,	0.016,	0.019	
Cl_2 concentration ratio $C_{Cl_2}/(C_{Cl_2}+C_{Ar})$:	0.55,	0.65,	0.75,	0.85,	0.95	
Temperature T **(°C):**	25,	35,	45,	55,	65	
Bias voltage V_{bias} **(V):**	0,	-30,	-60,	-90,	-120,	-150

Multi-Scale Plasma Etching Model

- **Generation** of a multi-variable spline interpolation model

Inputs

$$P_{coil}, Q_{sccm}, p, \frac{C_{Cl}}{C_{Ar} + C_{Cl}}, T, V_{bias}$$

Reactor FEM Simulation

Plasma simulation
Electron impact
Chemical reactions

ViennaPS Feature-Scale Simulator

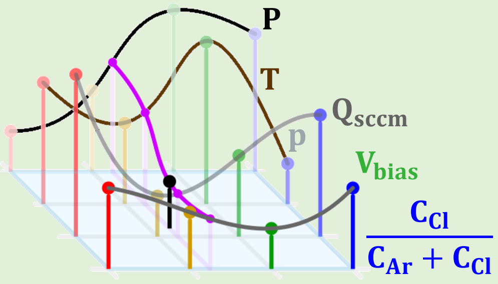
Complex features
HAR structures

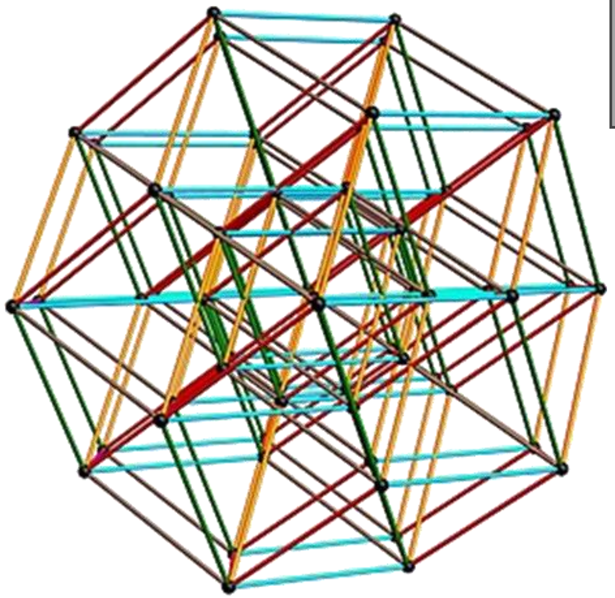
$\Gamma_{Cl/Ion}$

$\Gamma_{Cl/Ion}$

Multi-Variable Spline Interpolation Model

$$\Gamma_{Cl/Ion}\left(P_{coil}, Q_{sccm}, p, \frac{C_{Cl}}{C_{Ar} + C_{Cl}}, T, V_{bias}\right)$$





Multi-Scale Plasma Etching Model

- **Application** of a multi-variable spline interpolation model

Inputs

$$P_{coil}, Q_{sccm}, p, \frac{C_{Cl}}{C_{Ar} + C_{Cl}}, T, V_{bias}$$

Reactor FEM Simulation

Plasma simulation
Electron impact
Chemical reactions

ViennaPS
Feature-Scale Simulator

Complex features
HAR structures

$\Gamma_{Cl/Ion}$

Multi-Variable Spline Interpolation Model

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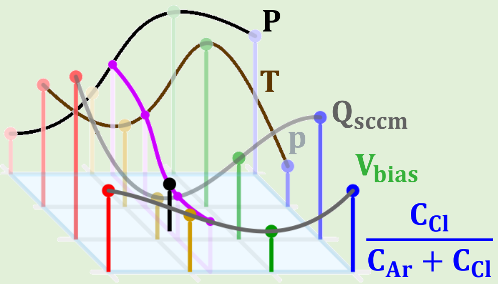
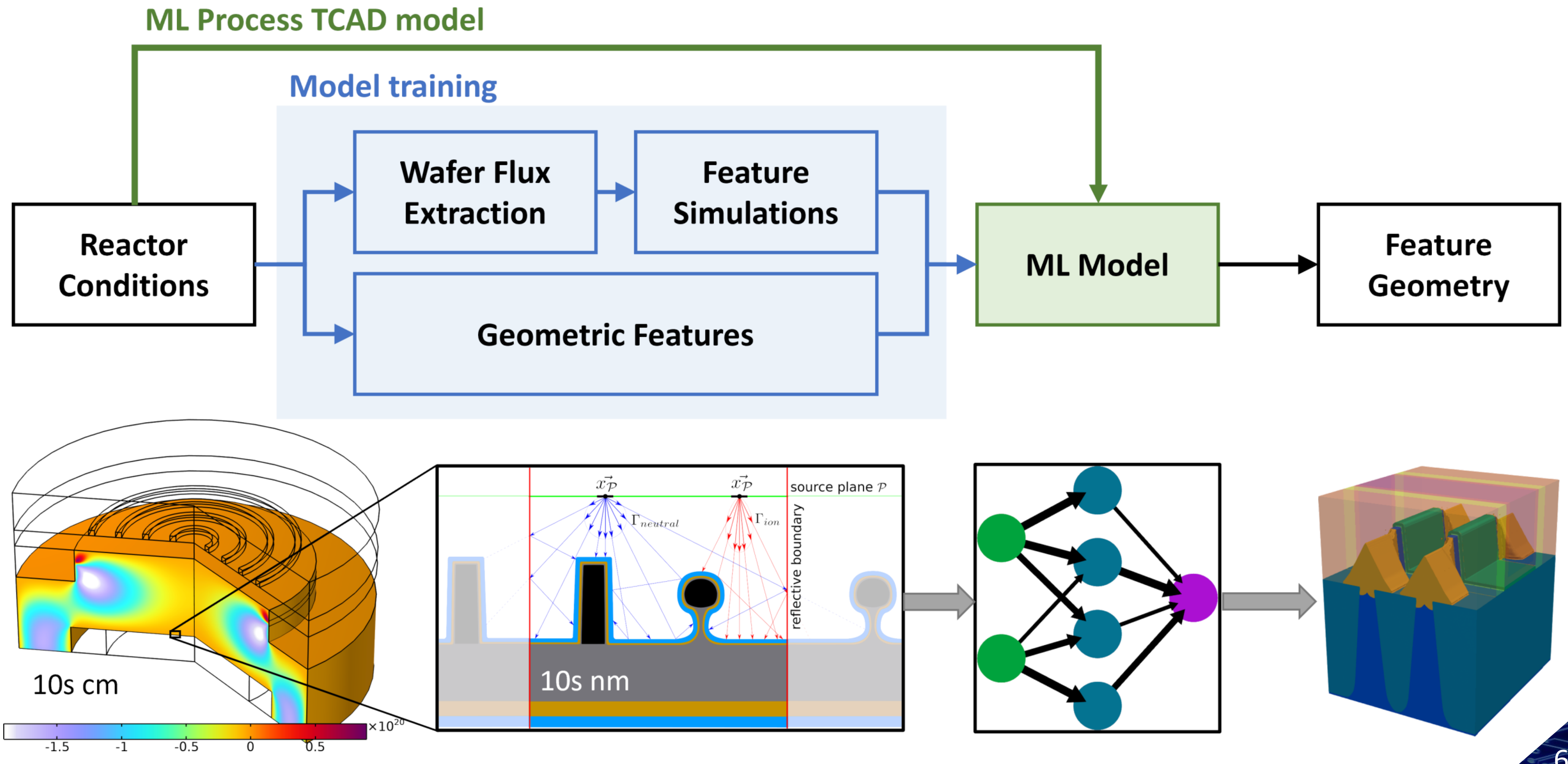


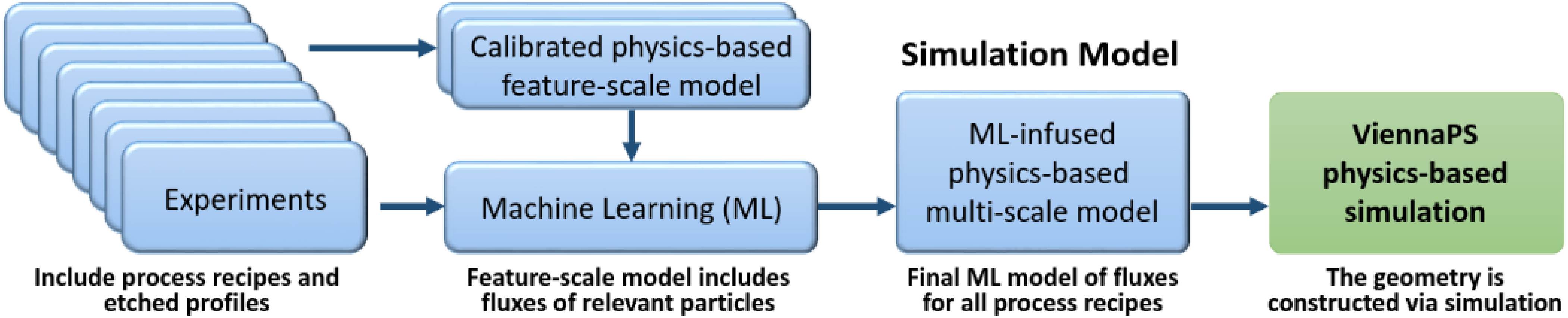
Alternative Approaches with Machine Learning



Alternative Approaches with Machine Learning

- Design an SF_6/O_2 model based on experimental data*

p	y_{O_2}	V_b	Γ_F	Γ_O	Γ_i	A_O
25	0.4375	120	5500	1500	10	3
25	0.5000	120	5000	2500	10	3
25	0.5625	120	4500	6000	10	2
25	0.6250	120	4000	10000	10	1
10	0.5000	20	2000	1000	20	3
25	0.5000	20	5000	2500	10	3
40	0.5000	20	7500	6000	5	3
5						
25						
75						

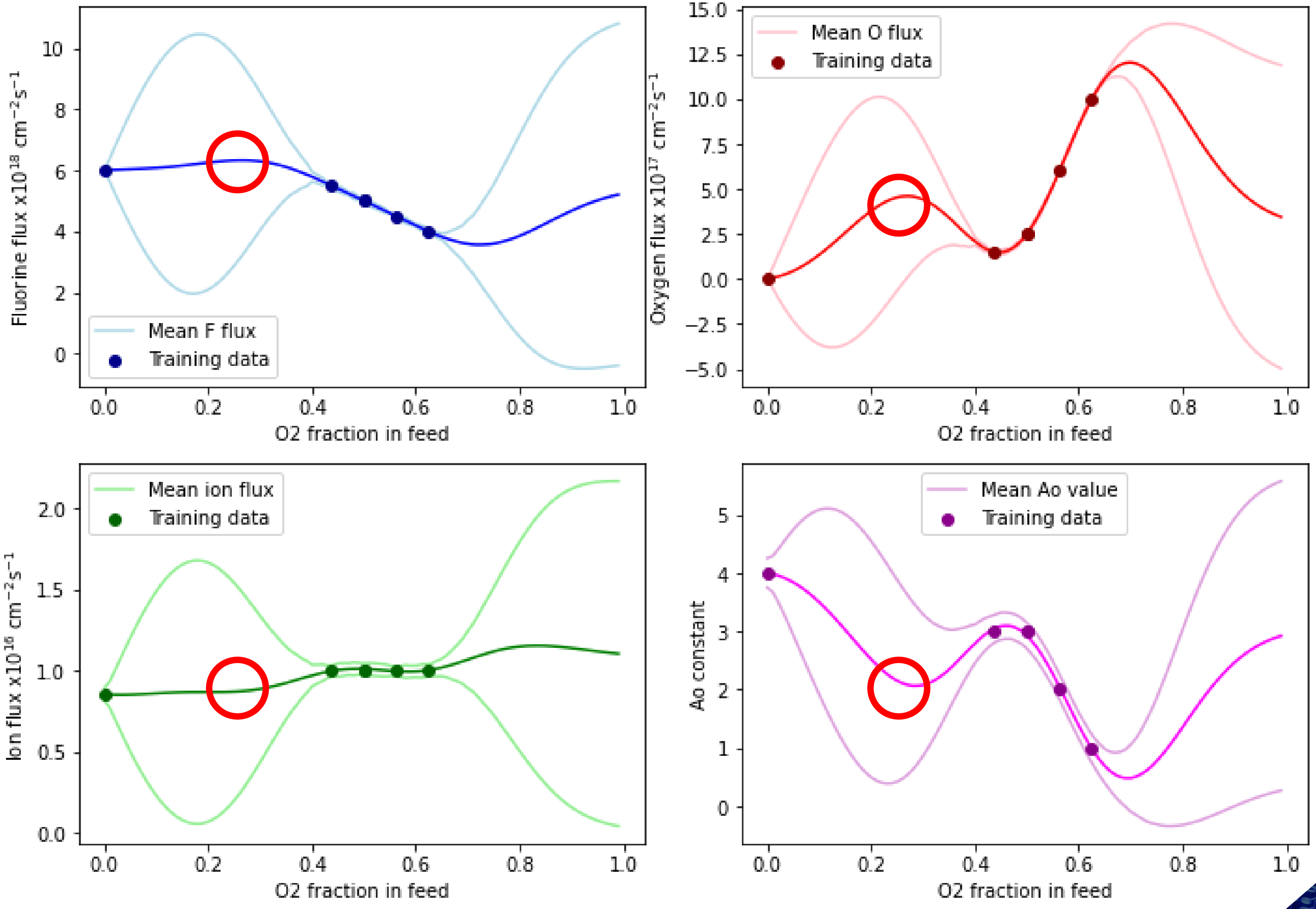


*Data from several publications by Belen et al. and Gomez et al., *Journal of Vacuum Science & Technology A*, 2004-2005

Alternative Approaches with Machine Learning

Gaussian Process Regression – Squared exponential kernel

- Good fit within known data range
- Large waviness causes poor estimation in regions where data is not available
- Standard deviation provides (un)certainty estimate
- Certainty estimate suggests where more training data is needed



Alternative Approaches with Machine Learning

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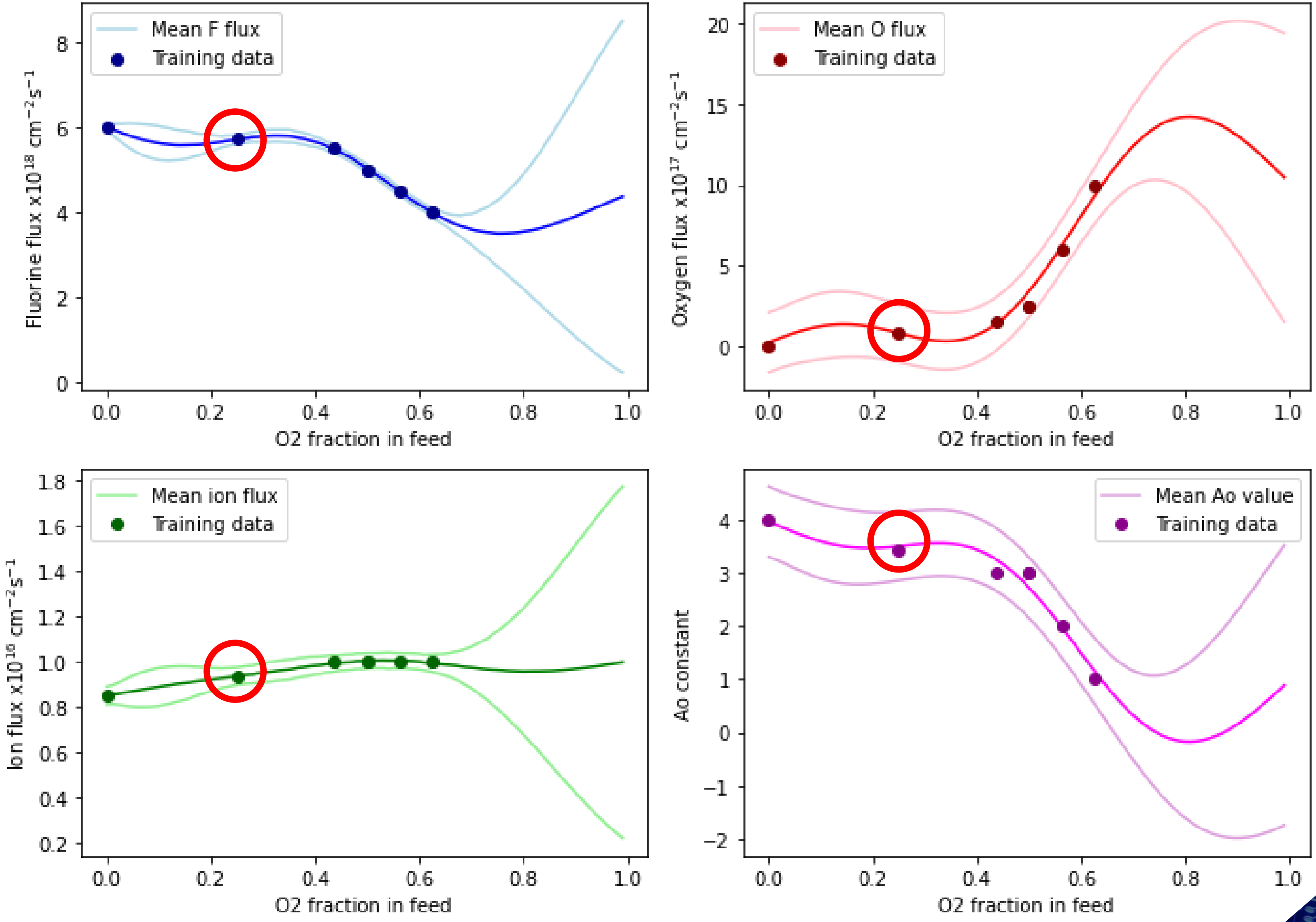
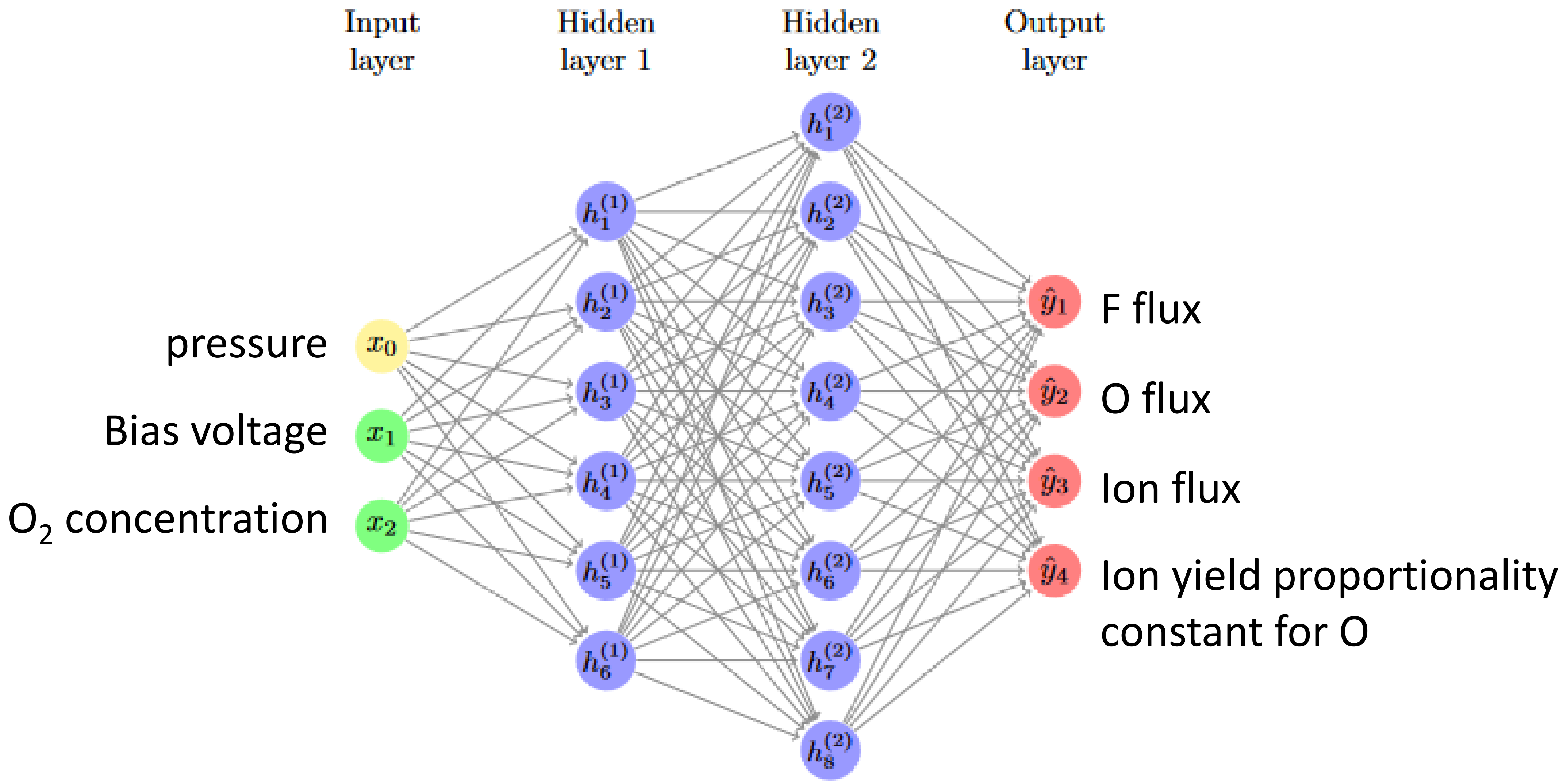


Alternative Approaches with Machine Learning

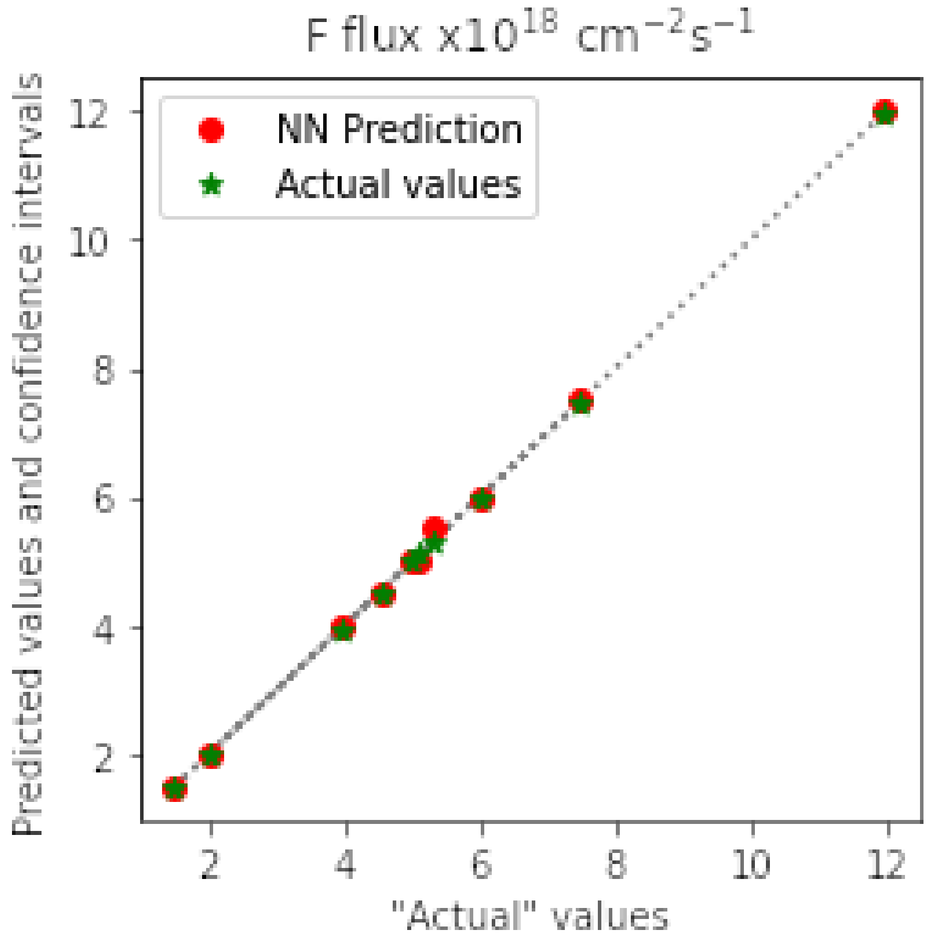
Neural Network – Hidden Layer with 12 Nodes

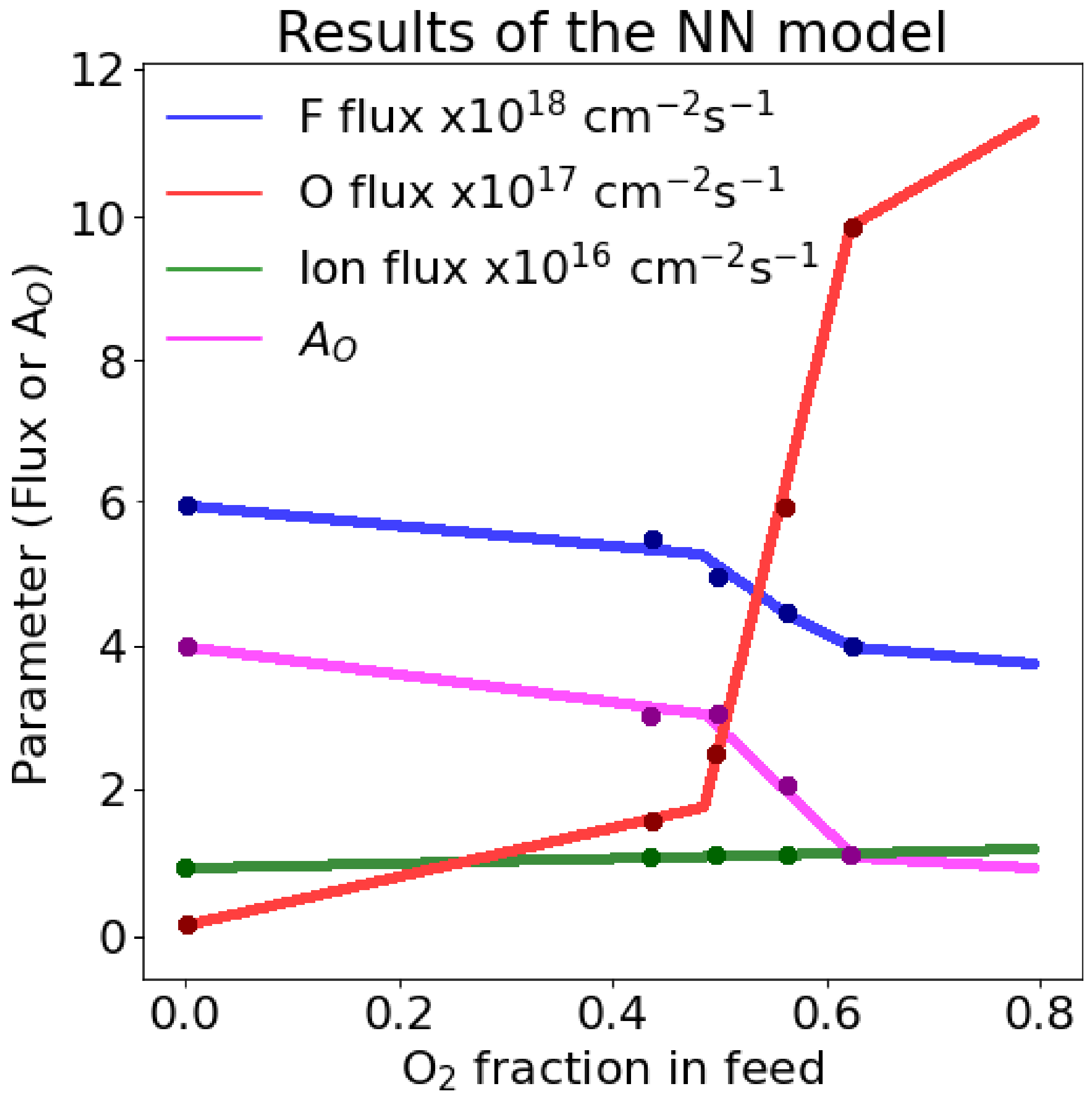


Alternative Approaches with Machine Learning

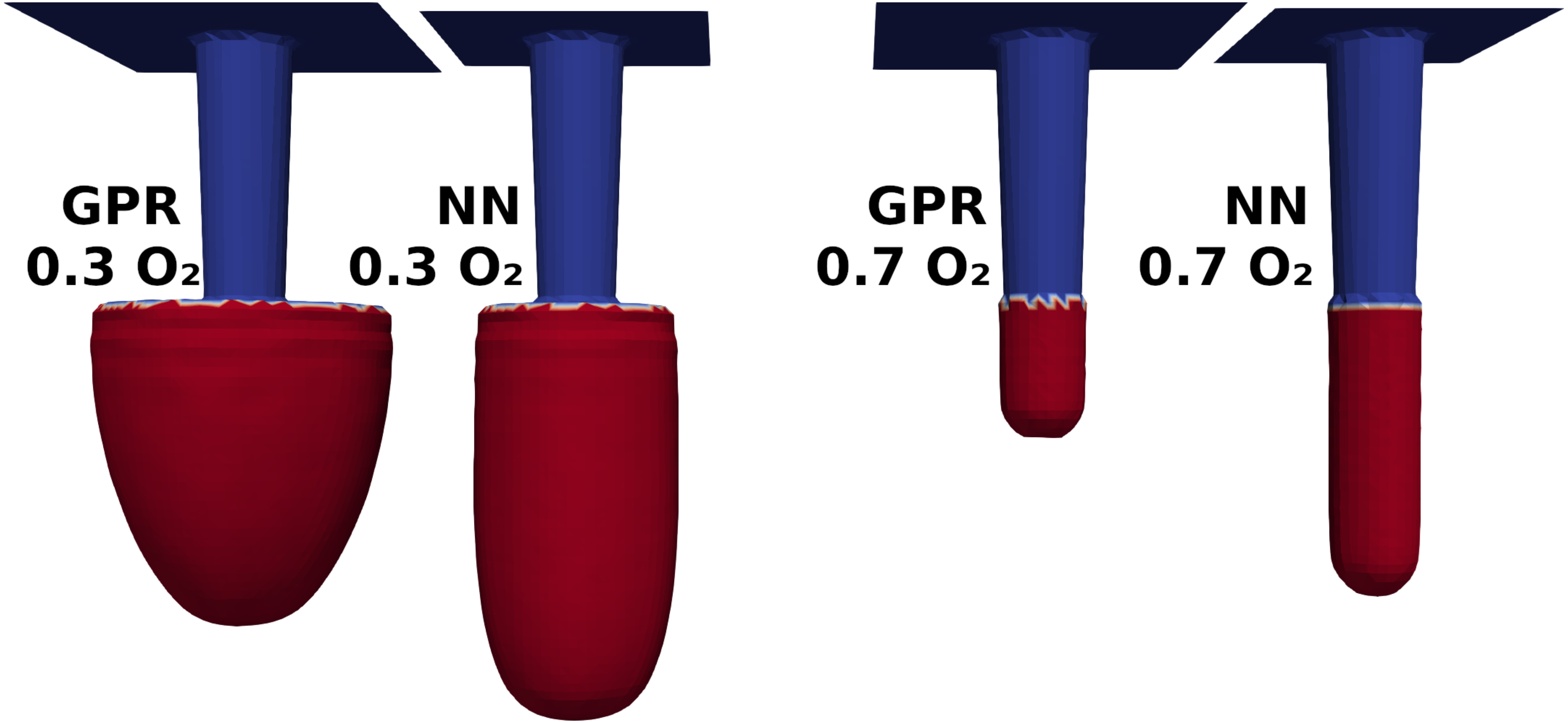
Neural Network – Hidden Layer with 12 Nodes

- Rectified linear unit activation
- Qualitatively reasonable results



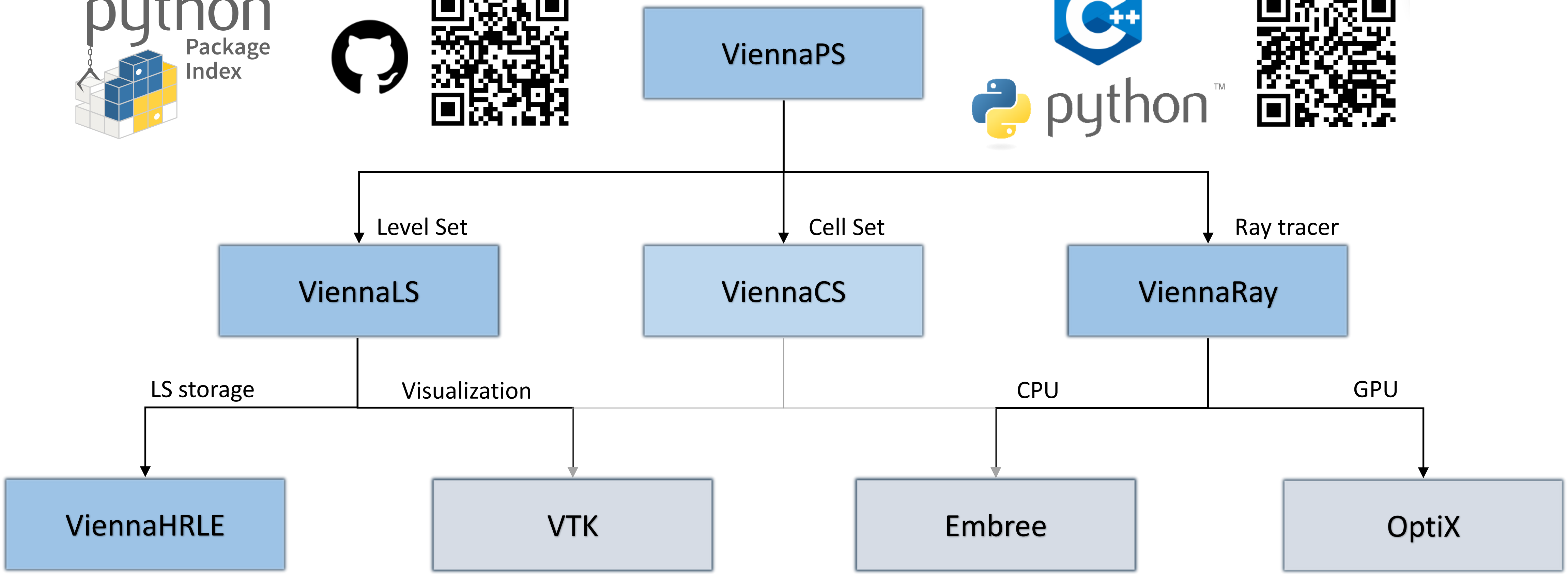


Comparison between GPR and NN



Simulation Framework

- ViennaPS: Process simulator and emulator (installable through pip)



- Link to equipment information through:
  - Physical simulations
  - Optimization
  - Machine learning

https://viennatools.github.io/ViennaPS/

pip install ViennaPS