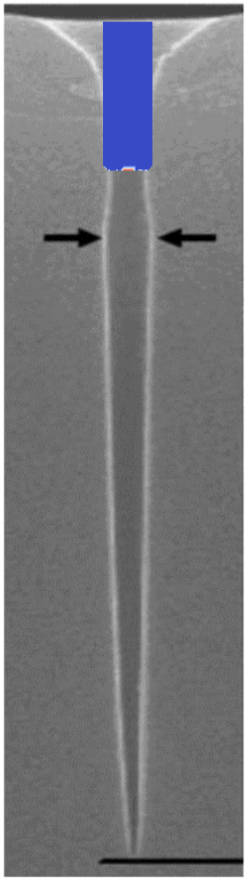

반도체 플라즈마 공정을 위한 3차원 식각 형상 시뮬레이션

- K-SPEED -

㈜ 경원테크

유동훈

회사소개

http://www.kw-tech.co.kr

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- 설 립 일 1998년 7월 10일
- 대표이사 서 광 원
- 임직원수 19 명
- 주요사업 연구용역, 상용 Software 개발 및 판매

인력구성

유동/공조/연소/Plasma/전산관련 학위를 가진 전문엔지니어

기술부문	영업부문	지원부문
14	3	2

사업목표

INNOBIZ 벤처 기업 Kibo 기술보증기금

종합엔지니어링 컨설팅 전문기업

- Total Engineering Consulting
- Leading Edge of Multi-Physics Simulation
- CFD Solution Provider

해외 업무제휴사

제품의 성능향상 및 기술교류를 위해 협력관계유지

Simerics, Inc. TECHNOLOGY BY DESIGN www.simerics.com

CEI www.ensight.com

reaction DESIGN http://www.reactiondesign.com/

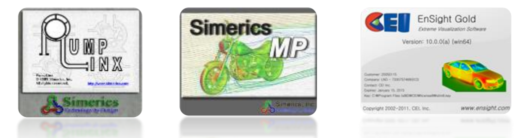
cpfd COMPUTATIONAL PARTICLE FLUID DYNAMICS http://cpfd-software.com/

WAVE FRONT www.wavefront.co.jp

국산소프트웨어 개발사업

http://www.kw-tech.co.kr

- K-SPEED : 반도체, 디스플레이의 핵심공정인 식각 및 증착공정을 위한 물성, 표면반응, 이온거동 해석용 Software 개발
(경원테크/국가핵융합연구소/한국표준과학연구원/전북대/부산대 협업)
- FANDAS : 축류형, 원심형 및 재생형송풍기 Fan 형상설계 S/W
- K-Plasma : 반도체 공정해석용 PIC기반 해석용 S/W



소프트웨어 판매사업

CFD/Plasma/PIC/유동층/Post-Processor등 공학용 S/W

- SimericsMP 범용 CFD 해석용 S/W
Flow, Heat, Cavitation, Turbulence, Species, Particle
- PumpLinx 펌프 전용 CFD 해석용 S/W
축류, 원심 펌프를 비롯, 특히 용적펌프와 Cavitation 유동해석에 강점
- Barracuda 유동층(Fludized Bed) 해석 전용 S/W
Turbulent Fludized Bed, Cyclone, CFB Combustor CFD Riser, FCC Regenerator
- Particle-Plus PIC(Particle-in-Cell)기반의 Plasma 해석 S/W
- DSMC-Neutrals 저압 유동 전용 S/W
- CHEMKIN 연소/화학반응 해석 전용 S/W
- EnSight CFD/FEA용 Post-Processor 전문가시화 S/W

Opening thoughts

Emerging issues in semiconductor plasma etch processing for next generation semiconductor devices

Bottleneck for predictable modeling of semiconductor plasma etch processing

Introduction to our 3D feature profile simulation for plasma processing

Development and applications of 3D feature profile simulator in plasma etch processing

Development of Plasma Reactor Modeling and Bulk Plasma Database, Verification of Modeling works

Hash map based 3D multiple level set algorithm

Ballistic transport module using GPU platform

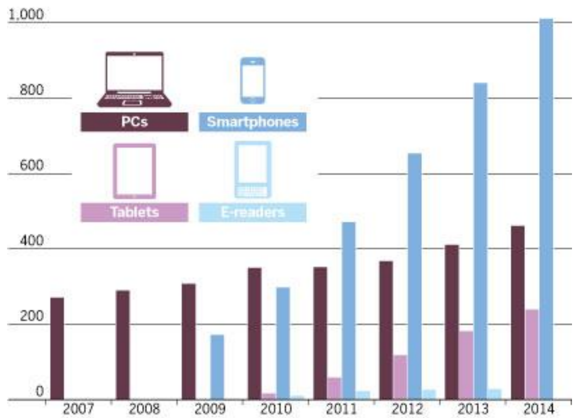
Surface chemical reaction modeling for plasma etching process

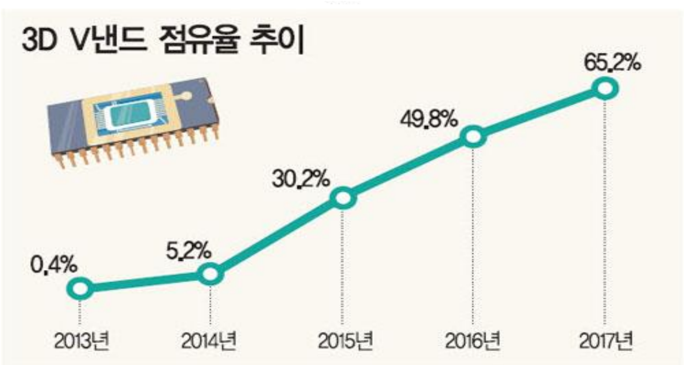
Unified algorithm :bulk plasma, plasma-surface interaction, ballistic transport, charge-up and
3D moving algorithm

Case studies using unified 3D feature profile simulation

Emerging issue in semiconductor plasma etch processing for next generation semiconductor devices

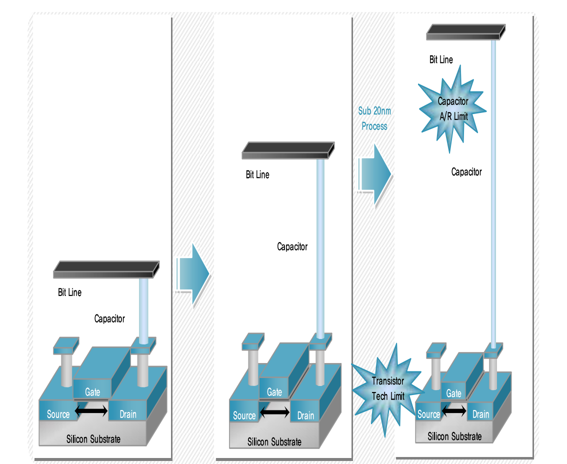
- **Worldwide unit sales (millions)**



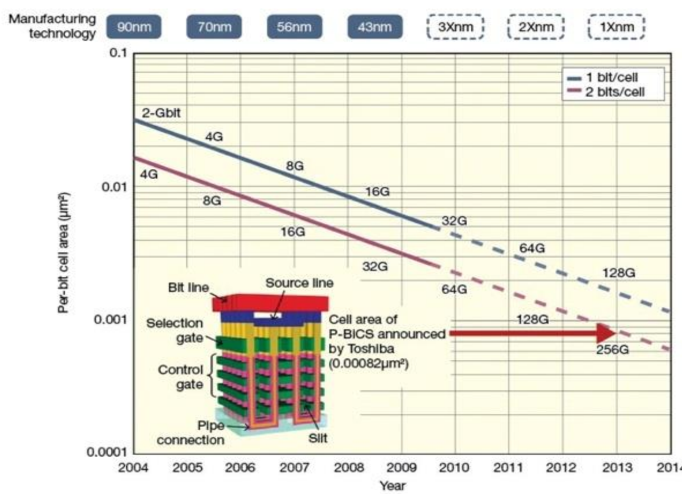


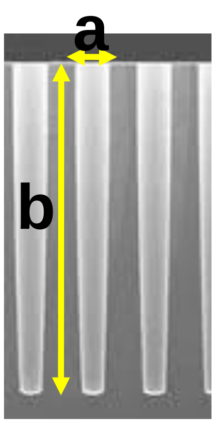
〈자료:IHS아이서플라이〉

- **Emerging Issues in High Aspect Ratio Contact Hole Etching**



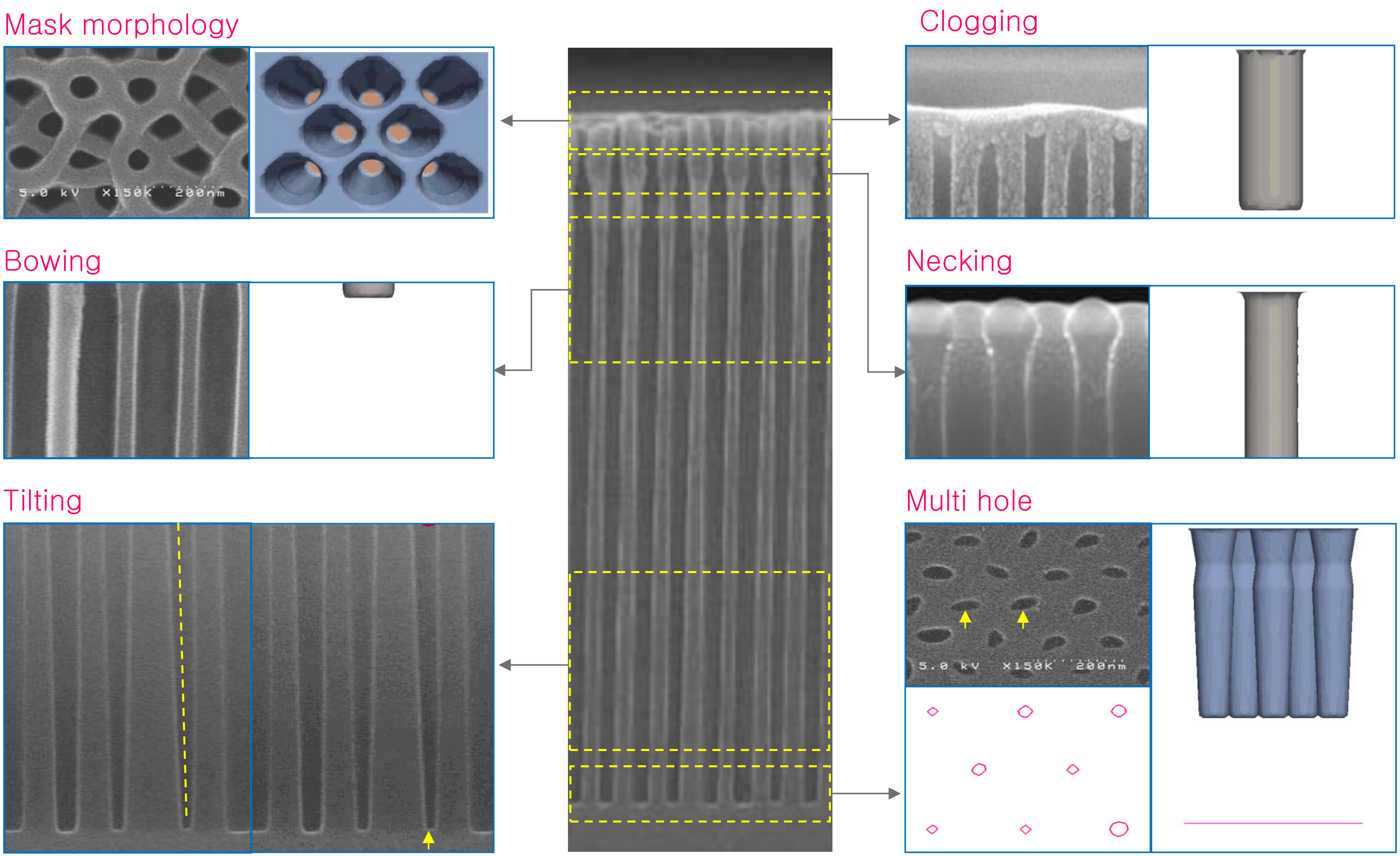
자료: 메리츠종금증권 리서치센터





Aspect Ratio=b/a

Emerging issue in semiconductor plasma etch processing for next generation semiconductor devices



Bottleneck for the predictable plasma process simulation

Current research status

- Modeling and simulation research has made impressive progress toward both improving our fundamental understanding of and providing design assist for new equipment and progress

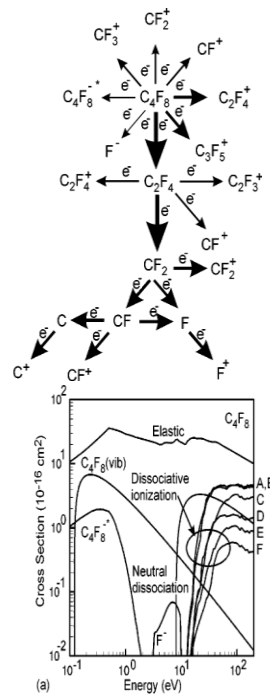
- In spite of huge contributions in academic researches, there are no realistic and predictable modeling and simulation tools of equipment and processes for plasma process due to the complexity and difficulty.

- Requirements to achieve the predictable simulation tools for plasma processing

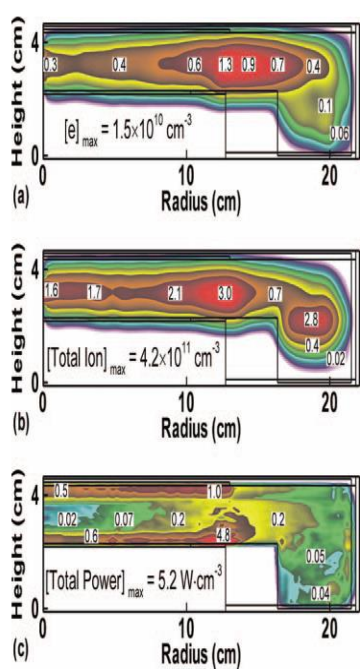
  - More completely populated bulk and surface chemical reaction database
    (CxFy/CxHxFy/Ar/O2/Additives)
  - More robust coupling of electromagnetic and plasma transport phenomena
  - Fast computational algorithms
  [MPI, GPUs]

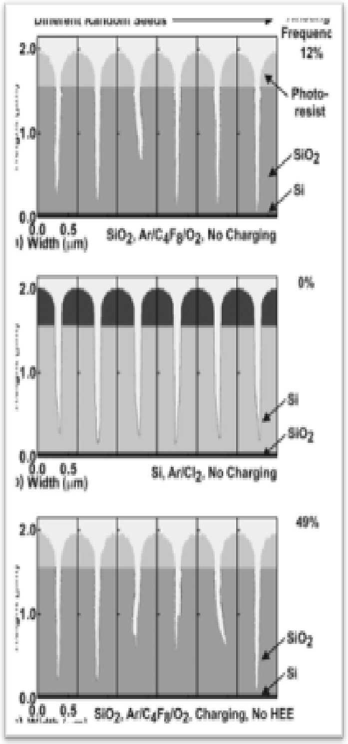
Mark J. Kushner's Group, Modeling of Ar/C_4F_8/O_2 discharges, J. Appl. Phys. 107, 023309 (2010)

Huge database



Multiscale/Multiphysics





Toward development of the realistic and predictable plasma simulator

- It is expected that the process difficulties of plasma etch increase exponentially from now.
- A plasma consortium in Korea was launched to develop the predictable and realistic plasma simulator since 2009.

NFRI 국가핵융합연구소 — Bulk plasma database and Zero-D bulk simulator

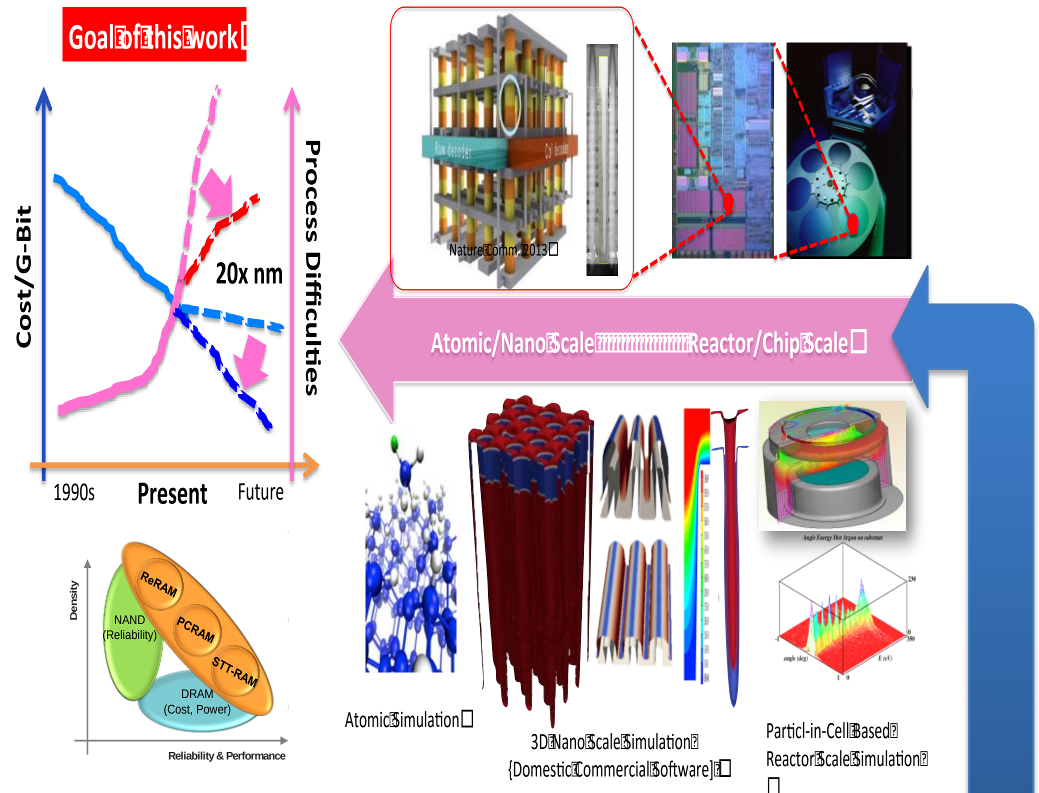
부산대학교 PUSAN NATIONAL UNIVERSITY — Particle-In-Cell based reactor simulation.

KRISS 한국표준과학연구원 — Plasma diagnostics

CHONBUK NATIONAL UNIVERSITY — Surface reaction database and feature profile simulation

KWtech 경/원/테/크 — Commercialized software [K-SPEED]

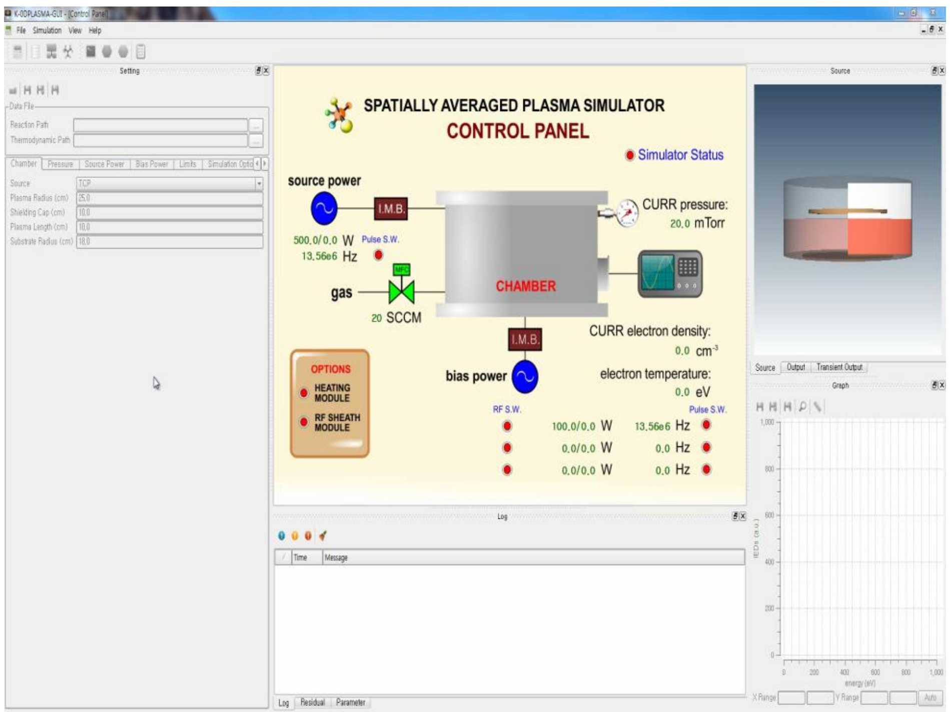
- This group has been funded by Korean government, Samsung, and SK-Hynix

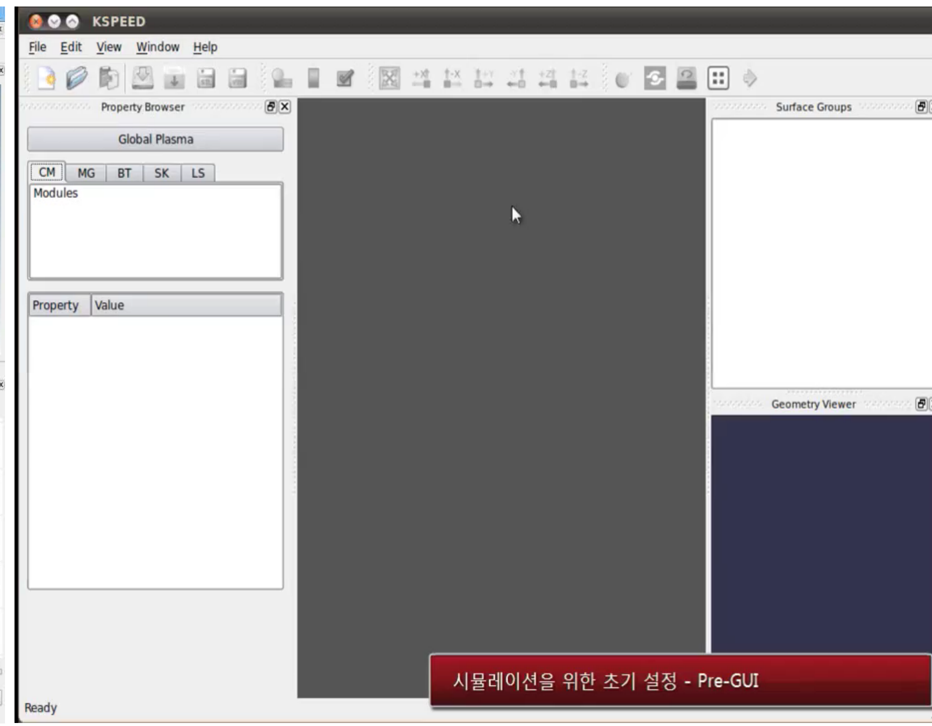


Input parameters
Geometry of dry etcher,
Process conditions [Power, Pressure, Gas flow rate & Material Inform.]

K-SPEED : 3D Feature Profile Simulator

Bulk plasma simulator ➕ 3D Feature profile simulator

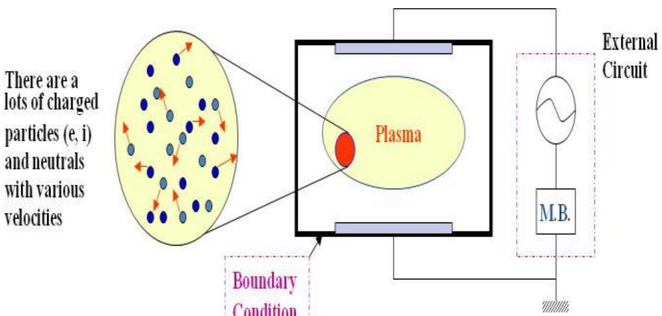




Brief introduction to bulk plasma simulation

In NFRI

Categories of bulk plasma simulation



x_i, v_i → $f(x,v,t)$ → $n(x,t), u(x,t), T_e(x,t)$

Particle Simulation

- Super-particles (one super-particle= $10^{5\sim7}$)
- Newton-Lorentz equation $\frac{d}{dt} m\mathbf{v} = \mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$,
- Poisson's equation $\nabla \cdot \varepsilon \nabla V(x,t) = -\rho(x,t)$
- Less assumptions
- Heavy computation

Kinetic Simulation

- Distribution function
- Solve Boltzmann's Equation $\frac{\partial f}{\partial t} + v \cdot \frac{\partial f}{\partial x} + \frac{qE}{m} \cdot \frac{\partial f}{\partial v} = \left.\frac{\partial f}{\partial t}\right|_c$
- Eulerian grids
- Heavy computation
- Less assumptions

Fluid Simulation

- Average f over velocity space
- Continuity eq. $\frac{\partial n_{sp}}{\partial t} + \nabla \cdot \Gamma_{sp} = S_{sp}$
- Momentum conservation eq./ Drift-diffusion approximation
- Energy conservation eq. /
- Many assumptions are used.
- Easy computation

Zero-D bulk plasma simulation – K-SPEED

Assumption : 1) Mass transport to the reactor walls is assumed to be infinitely fast,
2) The chemical reaction rate coefficients are independent of reactor conditions.
3) The flow through the reactor must be characterized by a nominal resistance time

Mass conservation and gas phase species equations

$$\frac{d(\rho V)}{dt} = \dot{m}^* - \dot{m} + \sum_{m=1}^{M} A_m \sum_{k=1}^{K_g} \dot{s}_{k,m} W_k$$

Electron energy equation for plasma systems

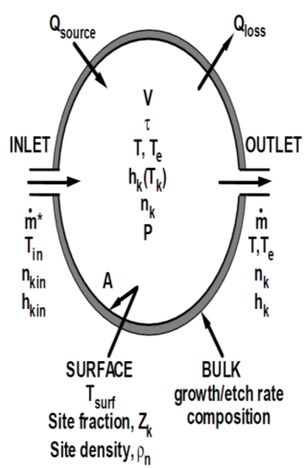
$$\rho V\left(Y_e c_{ve}\frac{dT_e}{dt} - \frac{R}{W_e}T_e\frac{dY_e}{dt}\right) = \dot{m}^* Y_e^* c_{pe}\left(T_e^* - T_e\right) + \dot{\omega}_e W_e V c_{pe}\left(T - T_e\right) - Q_{\text{loss}}^{\text{elas}} - Q_{\text{loss}}^{\text{inel}} + Q'_{\text{source}}$$

Gas energy equation for plasma systems

$$\rho V\left(\bar{c}_p(1-Y_e)\frac{dT}{dt} + Y_e c_{pe}\frac{dT_e}{dt}\right) = \dot{m}^* \sum_{k=1}^{K_g} Y_k^*\left(h_k^* - h_k\right) - V\sum_{k=1}^{K_g} h_k \dot{\omega}_k W_k - \sum_{m=1}^{M} A_m \sum_{k=1}^{K_g} h_k \dot{s}_{k,m} W_k - Q_{\text{loss}} - Q_{\text{source}}$$

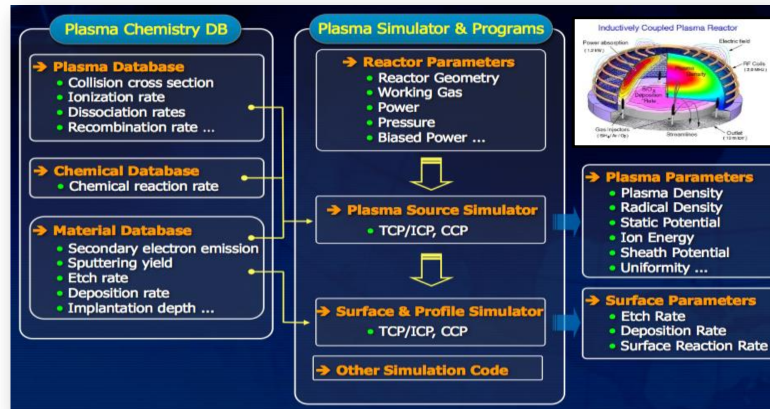
Surface species equations

$$\frac{d}{dt}\left(A_m c_k W_k\right) = A_m W_k \dot{s}_k \qquad k = K_s^f(m),\dots,K_s^l(m);\ m = 1,\dots,M$$



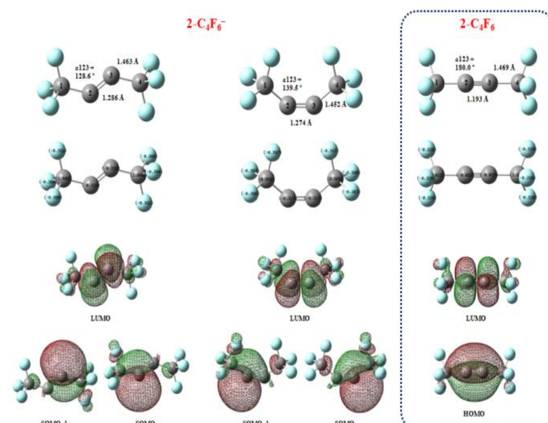
Research platform to develop bulk plasma chemistry database

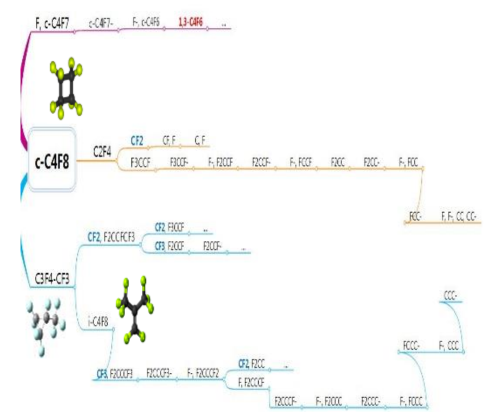
- Use the zero-D bulk simulation to develop and test bulk plasma chemistry database instead of the higher level simulation.
- Consider the power adsorption and sheath dynamics from the conventional models of ICP, CCP and pulsed plasma.
- Investigate main reaction paths of etchant gases inside bulk plasma based on the density functional theory and published data (Swarm analysis or cross section data).
- Verify the calculated or published data of bulk plasma database through comparison of plasma diagnostics as functions of plasma conditions.
  - Plasma densities
  - Radical and ion densities
- Combine with 3D feature profile simulation to support the input variables (neutral/ion flux, electron/ion energy distribution function)



C_2F_6, CHF_3, C_4F_6, $C_4F_6/O_2/Ar$, $C_4F_6/C_xF_y/O_2$, $C_4F_6/C_xF_y/CH_xF_y/O_2$

NF_3/Ar, NF_3/O_2, Ar, Cl_2, Cl_2/Ar, $BCl_3/Cl_2/Ar$, CF_4, $CF_4/O_2/Ar$, $SiH_4/O_2/Ar$, HBr/Ar, SF_6, SF_6/Ar

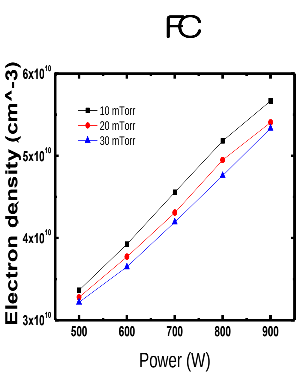


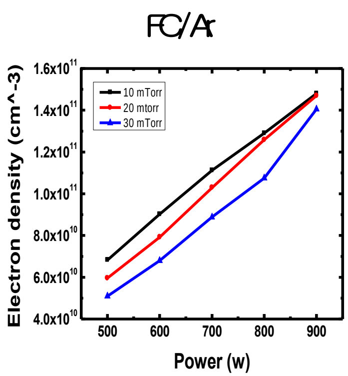


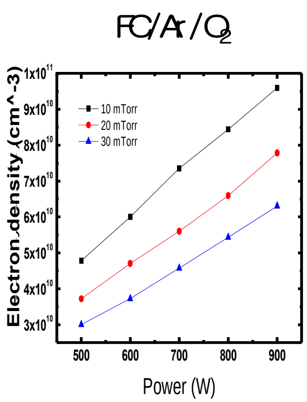
Plasma diagnostics to verify bulk plasma simulations

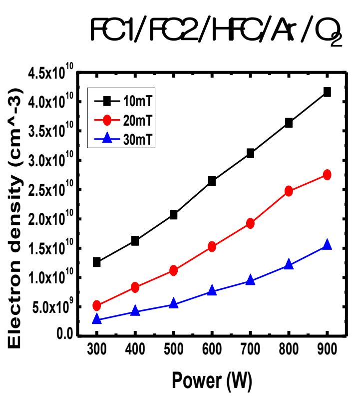
With KRISS and CNU

Plasma density and temperatures
[Langmuir probe and cutoff probe]

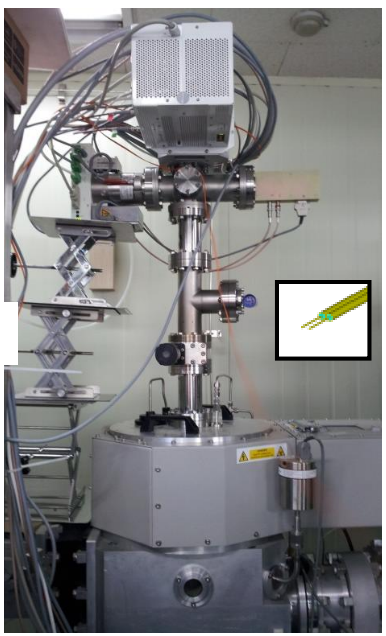








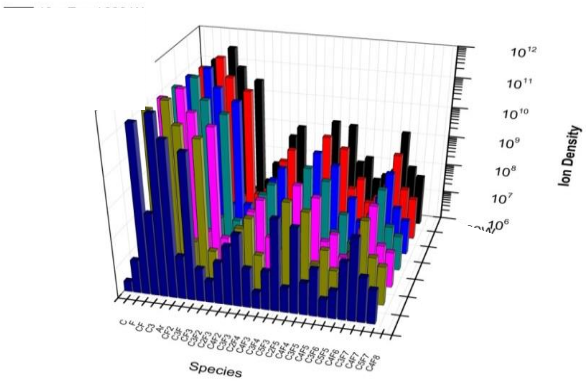
Langmuir probe and Cutoff probe



Electron density (cm^-3)

Electron density (cm^-3)

Radical and ion densities
APMS (Appearance potential mass spectroscopy)



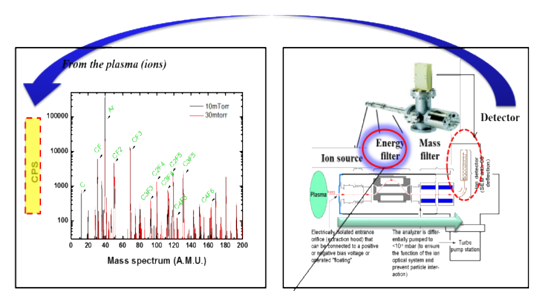


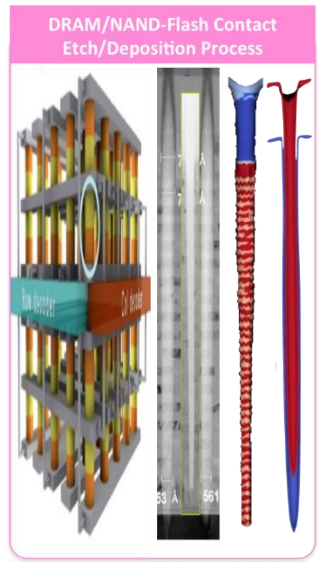
Fig. procedure schema measuring gas species or ions using a QMS

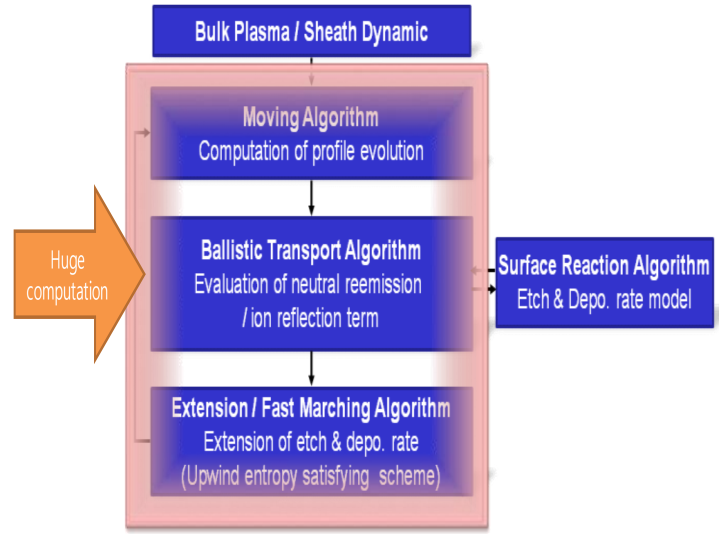
Development of 3D feature profile simulation

In CBNU

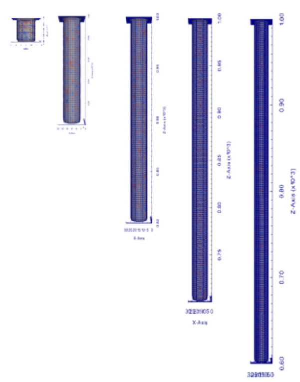
- Use the output results (incident neutral/ion fluxes, electron/ion EEDFs) of zero-D bulk simulation for 3D feature profile simulation toward the realistic plasma etch simulation.
- We developed the object-oriented numerical codes which were composed of moving algorithm, ballistic transport algorithm (neutral/ions) and surface reaction algorithm.
- Distribute the brute force computation loads of ballistic transport module to the GPU platform.

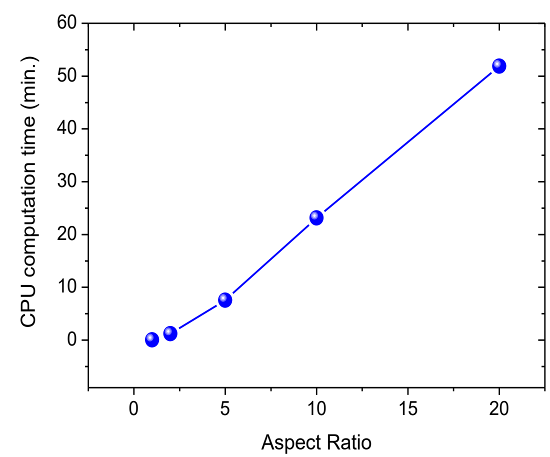
  - Based on only CPU computation, it will take few weeks for a high aspect ratio contact hole etching simulation. The computation time can't meet the industrial requirements. In addition, the charge-up simulation or multi-hole pattern simulation will take few months normally.





Computation time of neutral transport in single time step





Neutral transport inside nanoscale feature in 3D feature profile simulation

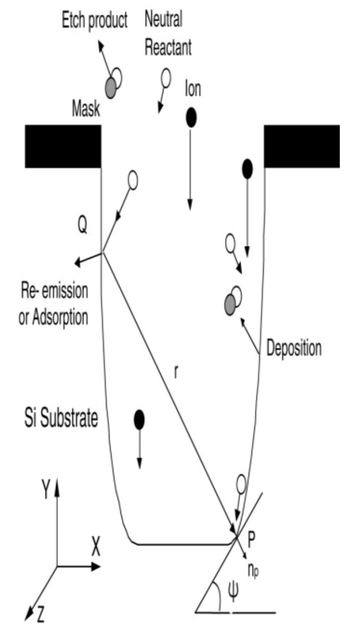
- Consider neutral transport to compute the localized incoming neutral flux (etchant or polymer precursor radicals) in an arbitrary position of nanoscale feature.
- The incoming neutral flux in an arbitrary position can be calculated by the incoming flux from the plasma source and the reemission flux from the other position.
- Deterministic Approach : The semi-analytical equation of neutral transport can be obtained by assumption of Maxwellian distribution. This equation can be solved by numerical recurrence relation. However, it is well known that the brute force computation time is required normally to compute the geometry factors such as view factor and visibility factor.

$$\Gamma_n(p) = \frac{\Gamma_{no}}{2}\int_{\theta_1}^{\theta_2}\cos(\theta - \Psi)d\theta + \int_{profile}\frac{[1 - S_c(Q)]\Gamma_n(Q)\cos\Psi_p\cos\Psi_Q}{2r}ds$$

-Numerical recurrence relation

$$\boxed{\Gamma_{R,N} = \sum_{k=1}^{n+1} W^k\Gamma_s + \Gamma_s = \left[W\sum_{k=1}^{n} W + W\right]\Gamma_s + \Gamma_s = W\Gamma_{R,N} + W\Gamma_s + \Gamma_s}$$

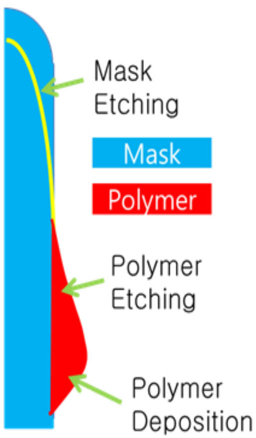
$$W_{ij} = \frac{[n_i\cdot(t_j - t_i)][n_j\cdot(t_i - t_j)n]]}{\pi\left|(t_j - t_i)\right|^3}Y_{ij}\, l_j\, [1 - S_c]$$



Y_{ij} : Visibility factor, S_c : sticking coefficient, r : distance between point i and j
t_i : Coordinates of point number I with an associated segment length l_i
$y_P(y_Q)$: angle between the line connecting P and Q and surface normal $-n_P(-n_Q)$

Neutral transport inside nanoscale feature in 3D feature profile simulation

Mask etch for deep contact hole etching

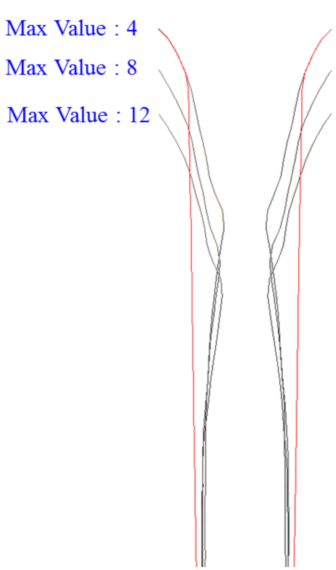


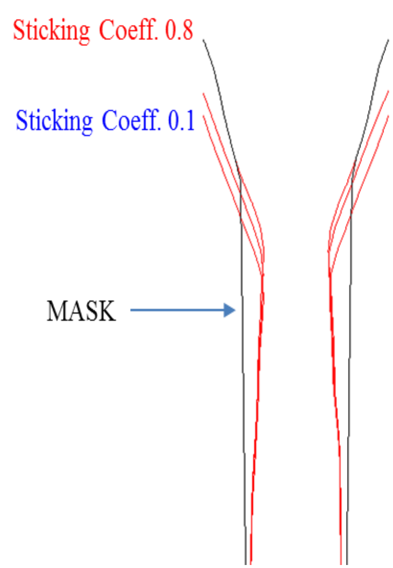
1) Mask Etching
   with Incidence Ion Angle Dependence
2) Polymer Etching
   with Incidence Ion Angle Dependence
3) Deposition of
   Polymer Radicals from Plasma
4) Re-deposition of
   Sputtered Mask Material
5) Re-deposition of
   Sputtered Polymer Material
6) Ion reflection of
   Mask and Polymer Surfaces

Multibounce algorithm for sputtered polymer flux

$$\Gamma_n(p) = \frac{\Gamma_{no}}{2}\int_{\theta_1}^{\theta_2}\cos(\theta-\Psi)d\theta + \int_{profile}\frac{[1-S_c(Q)]\Gamma_n(Q)\cos\Psi_p\cos\Psi_Q}{2r}ds$$

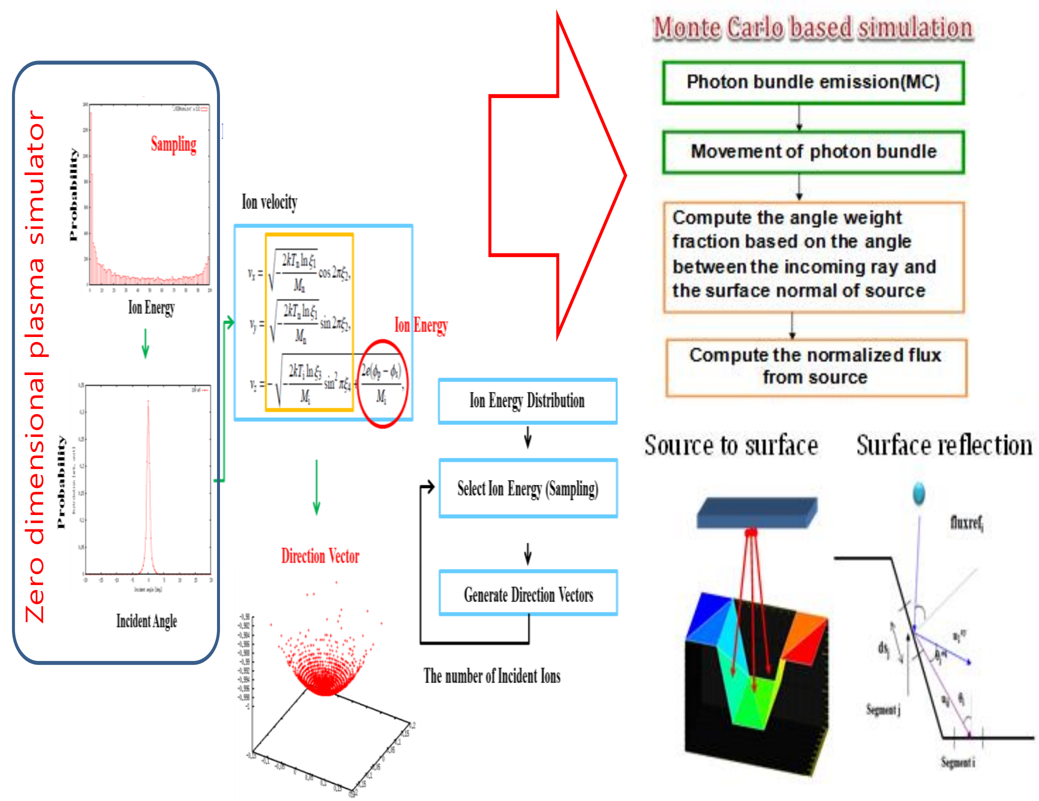
$$\Omega_{ij} = \frac{[n_i\cdot(t_j-t_i)][n_j\cdot(t_i-t_j)n]]}{\pi\left|(t_j-t_i)\right|^3}Y_{ij}\; l_j\;[1-S_c]$$





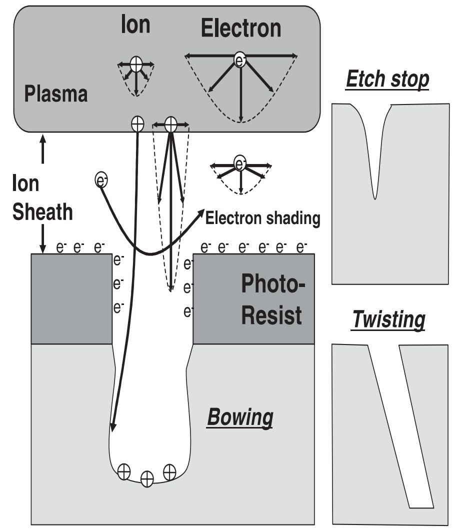
Ion transport inside nanoscale feature in 3D feature profile simulation

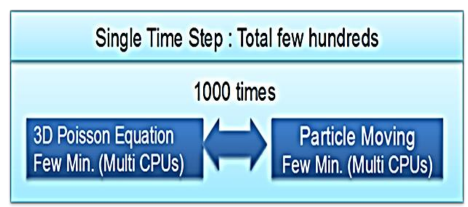
- Consider ion transport to compute the localized incoming ion flux (etchant or inert ion) in an arbitrary position of nanoscale feature.
- The incoming ion flux in an arbitrary position can be calculated by the incoming flux from the plasma sheath and the reflected flux from the other position.
- The incident ion IED or IAD via sheath region can be taken by bulk plasma simulation.
- Monte-Carlo Approach : The semi-analytical equation of ion transport is not available. In general, the charge-up simulation requires the brute force computation to compute the ion trajectory affected by the electrical field inside nanoscale feature.



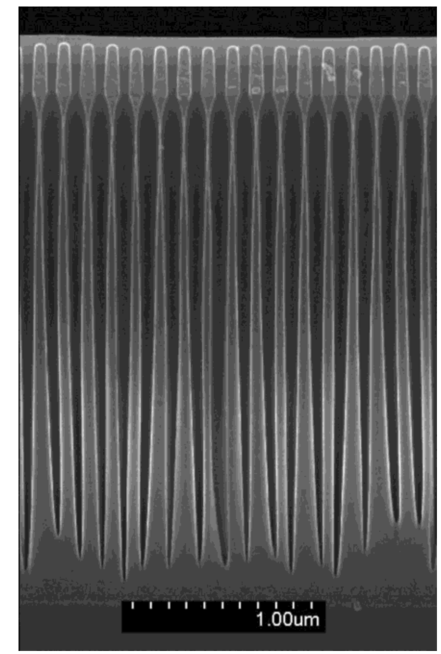
Charge-up simulation of electron and ion transport inside nanoscale feature

- The generation of the abnormal profiles, such as bowing, etch stops and twisting, has been reported in high-aspect-ration hole etching. In particular, twisting is one of the severest problems in nanoscale device fabrication. Recently, some researches pointed out that the abnormal profiles such as twisting profiles are caused by the distortion of the ion trajectory.
- Ions are accelerated into holes by the ion sheath, while electrons cannot go into holes due to their isotropic velocity distribution. Due to this “electron shading effect”, the bottom of contact holes is positively charged, which affects the ion trajectory significantly.
- The phenomena is still one of the controversial topics due to its inherent complexity such as the unknown charge-up behaviors of polymer passivation layer or oxide. To avoid this effect, we need to precisely control charge accumulation on the wafer surface.
- This simulation also requires the brute force computation to compute the ion trajectory and electrical field.





CPU based computation can't meet goal of engineering software



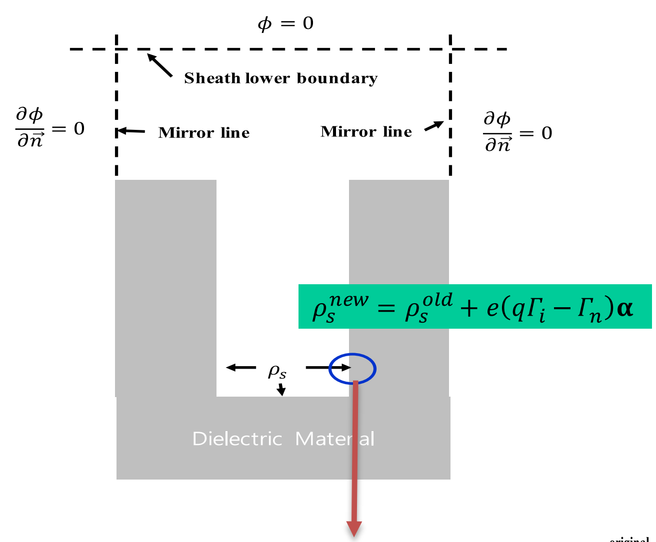
Japanese Journal of Applied Physics **49** (2010) 04DB14 **REGULAR PAPER**

Prediction of Abnormal Etching Profile in High-Aspect-Ratio Via/Hole Etching Using On-Wafer Monitoring System

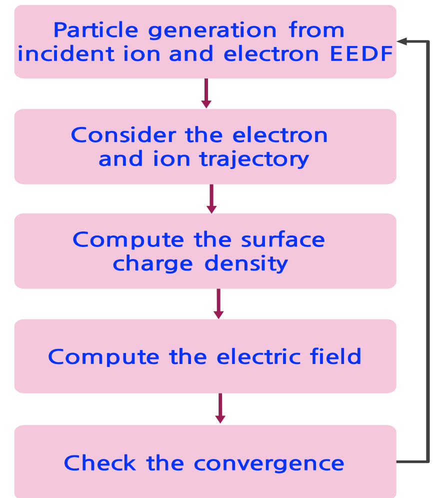
Hiroto Ohtake, Seiichi Fukuda, Butsurin Jinnai, Tomohiko Tatsumi[1], and Seiji Samukawa*

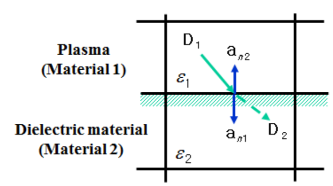
Charge-up simulation of electron and ion transport inside nanoscale feature

- Take the electron and ion EEDF from bulk plasma simulator, and generate particle by MC approach.
- Launch and trace the individual electron and ion particles. The surface charge density is computed by the arrival fluxes of electron and ions.
- Consider the charge redistribution to avoid the highly localized charge buildup.
- Apply the boundary element method(BEM) for the numerical solution of the electric field integral equation.
- Develop fully GPU code for computation of BEM, electron and ion trajectory.



$$\rho_s^{new} = \rho_s^{old} + e(q\Gamma_i - \Gamma_n)\boldsymbol{\alpha}$$





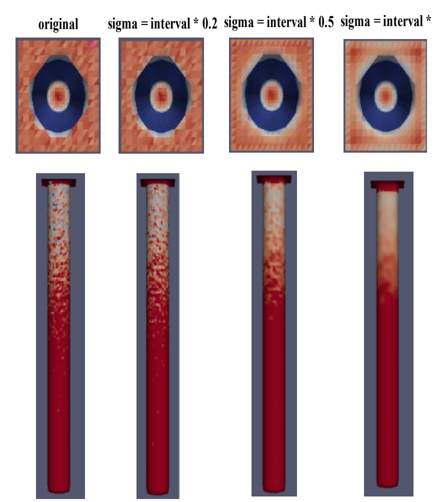
$$a_{n1} \cdot (\mathbf{D}_2 - \mathbf{D}_1) = \rho_s$$

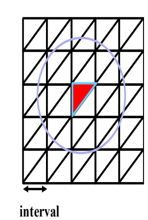
$$D_{2n} - D_{1n} = \rho_s$$

$$E_{1n} = -\frac{\rho_s}{\varepsilon_1} + \frac{\varepsilon_2}{\varepsilon_1} E_{2n} \quad (\because D_{1n} = \varepsilon_1 E_{1n})$$

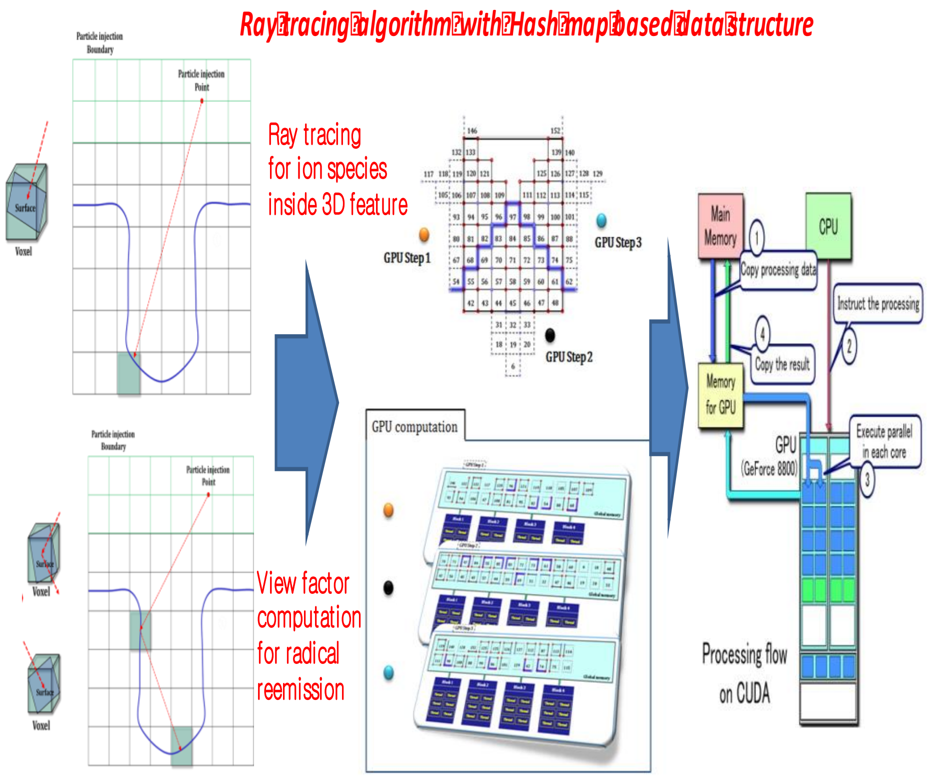
$$E_{1n} = -\frac{\rho_s}{\varepsilon_1} \quad (\boldsymbol{if} E_{2n} = \mathbf{0})$$

$$E_{1n} = -\nabla\phi_{1n} = -\frac{\partial \phi_1}{\partial n} = -\frac{\rho_s}{\varepsilon_1}$$



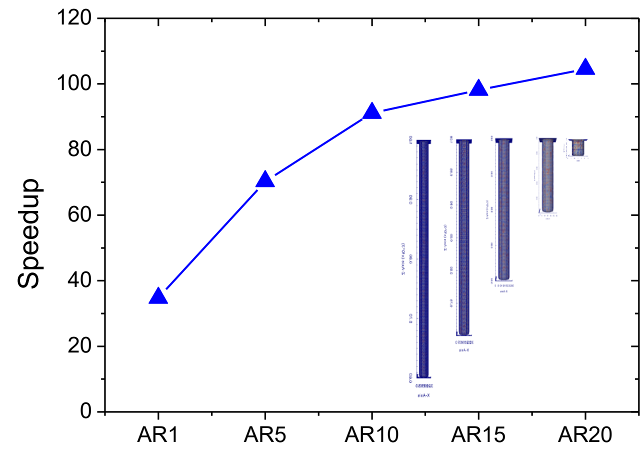


GPU computation for ballistic and charge-up simulation

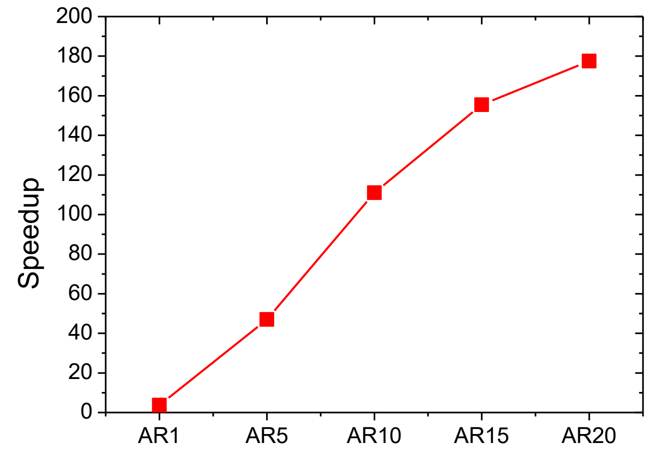


NVIDIA GeForce GTX TITAN X

Picture		Core clock	1002 MHz
		Boost Clock	1089 MHz
		Memory Clock	1753 MHz
		Memory Bus	384-bit
GPU	28nm GM200-400	Memory	12GB GDDR5
CUDA Cores	3072	Bandwidth	336 GB/s
TMUs	192		

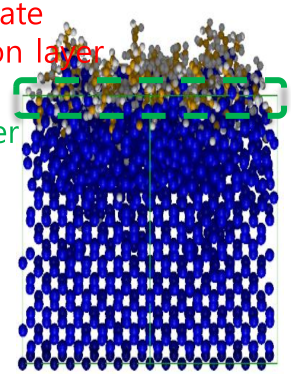


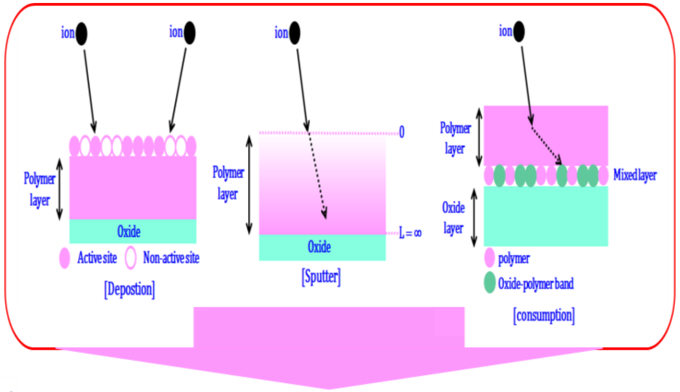
Ion transport

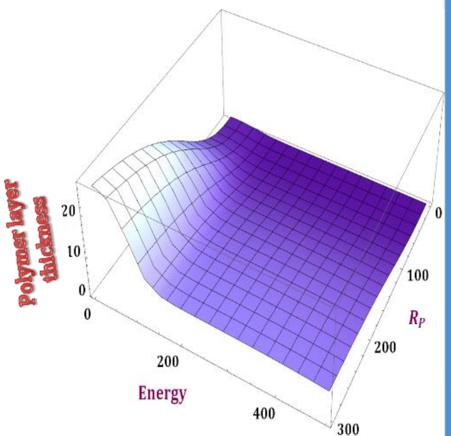


Surface reaction for 3D feature profile simulation

- We develop global two-layer model for flurocarbon/hydroflurocarbon plasma, in order to consider the plasma etch under the existence of the steady-state polymer passivation layer.
- The thickness of the steady-state passivation layer can be computed by our two-layer models.
- The ion energy loses during penetration of the steady-state passivation layer. The penetrated ions can take part in oxide etch at the mixed layer.
- In our model, the detailed kinetic models were used for computation of etch rate with assumption of the modified Langmuir-Hinshelwood mechanism.
- The key parameters such as reaction rate coefficients, incidence ion angular dependence, and sticking coefficients can be obtained by Molecular Dynamic and fitting experimental data.







Global Two-Layer Model for $C_xF_y/CH_{x1}F_{y1}/Ar/O_2$ plasma-surface reaction

- Activated site balance

$$\frac{d\theta_A}{dt} = \Gamma_{io} Y_A (1-\theta_A) - \Gamma_P S_A \theta_A = 0$$

- Steady-state Polymer Layer

$$\frac{d}{dt}[L(E)] = \Gamma_P S_P (1-\theta_A) + \Gamma_P S_A \theta_A - \int_{\Gamma_{ip} Y_{P(z=L(E))}}^{\Gamma_{ip} Y_{P(z=0)}} d\left(\Gamma_{ip} Y_P\right) - \Gamma_{ip} Y_M \theta_{\text{Mixed Layer}} = 0$$

$$\text{where } \theta_A = \left(1 + \frac{\Gamma_n(0) S_A}{\Gamma_i(0) Y_A}\right)^{-1}, \Gamma_i(l) = \Gamma_i(0)\exp\left(-\frac{l}{\lambda}\right), \text{and } E(l) = E(0)\exp\left(-\frac{2l}{\lambda}\right)$$

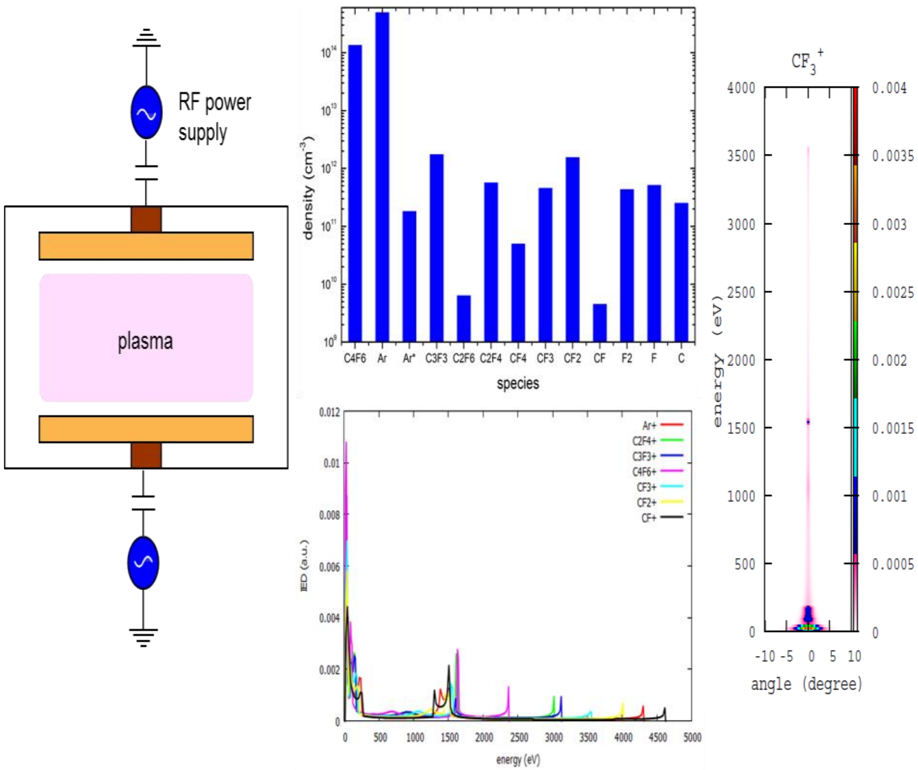
- PLED (Polymer Layer based Etching & Deposition) regime

$$EY = Y_S(1-\theta_{PLED})$$
$$= 2.0 \times A_S e^{-L(E)/\lambda}\left(\sqrt{Ee^{-2L(E)/\lambda}} - \sqrt{E_{th.S}}\right)\left(1 - \theta_{\text{Mixed Layer}}\right)$$

Case study I : Fluorocarbon/Ar/O2 CCP Plasma

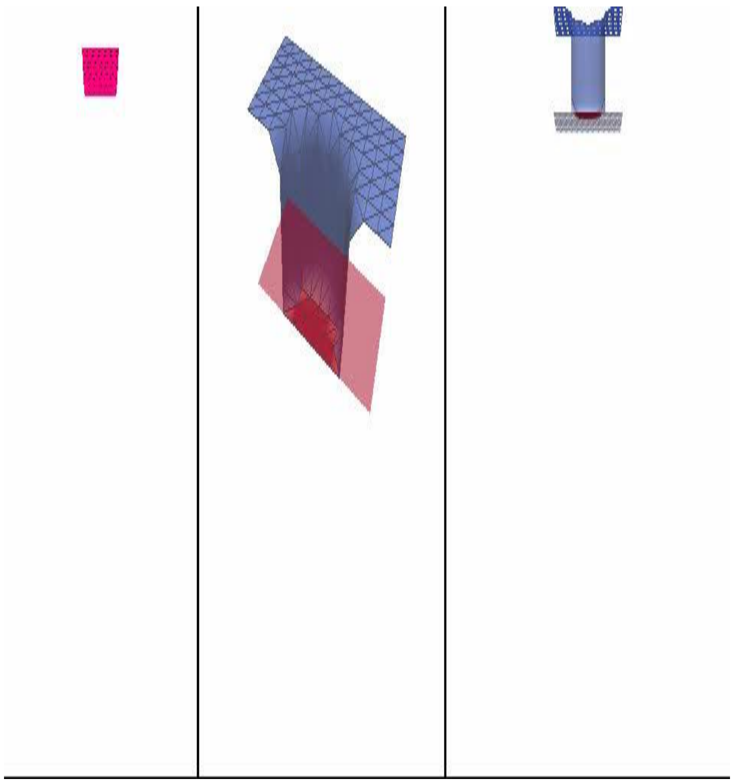
Bulk plasma simulation using Zero-D simulator

Neutral/Ion Flux, Ion IED & IAD →



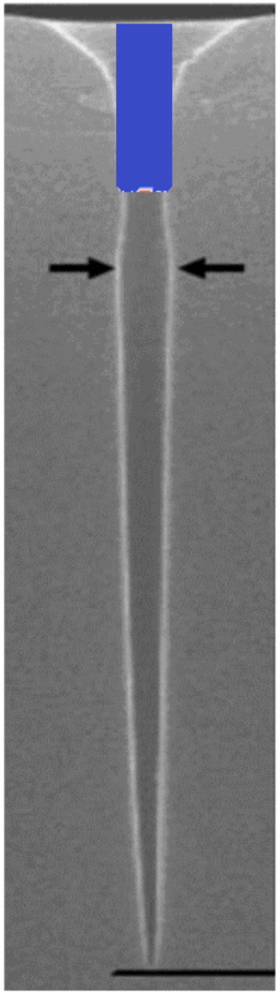
3D feature profile simulation

Bowing and necking formation

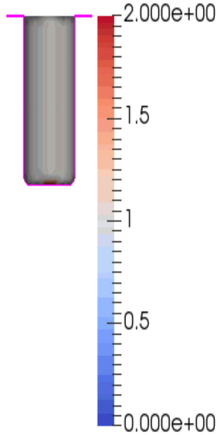


Case study I : Fluorocarbon/Ar/O2 CCP Plasma

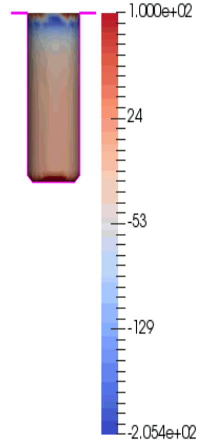
Reference



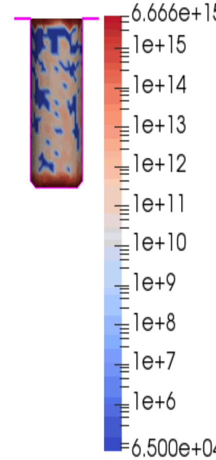
Material



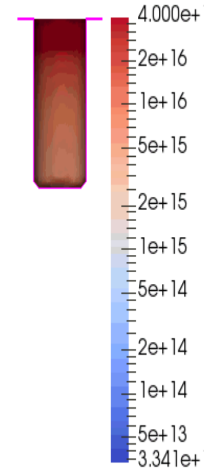
Etch Rate



Ion Flux



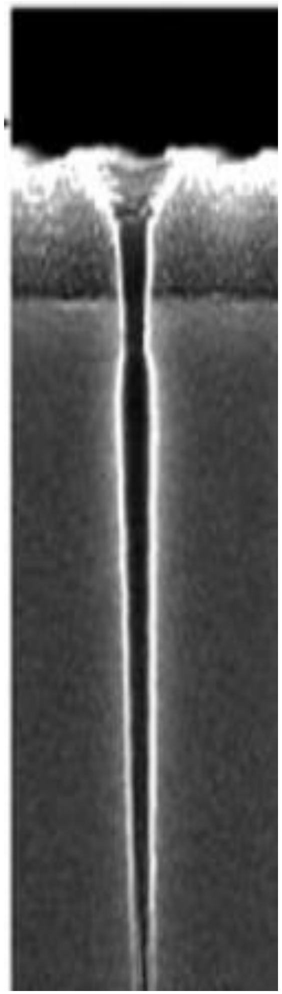
Neutral Flux



T. F. Yen et al., Microelectronics Eng., 82 (2005) 129

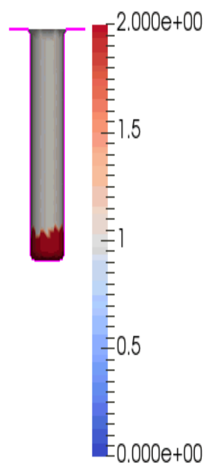
Case study I : Fluorocarbon/Ar/O2 CCP Plasma

Reference

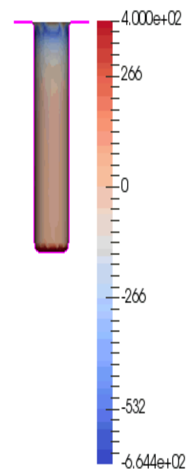


G.Y. Yeom etc, J. Vac. Sci.

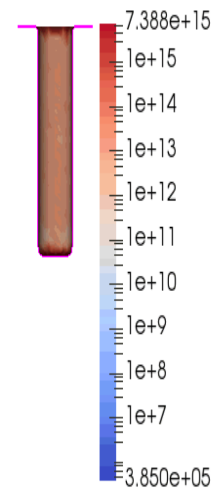
Material



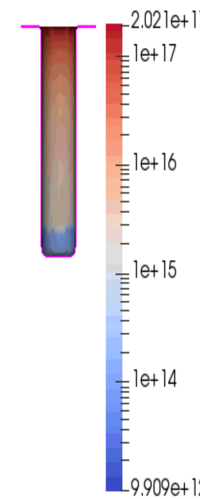
Etch Rate



Ion Flux

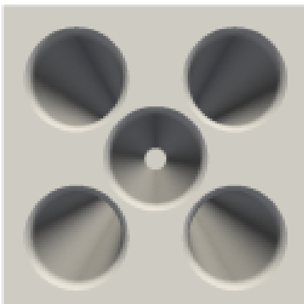


Neutral Flux

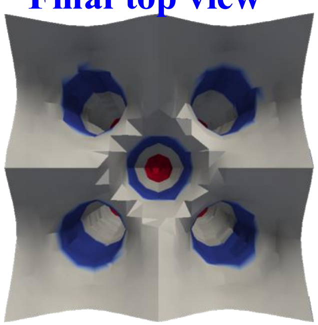


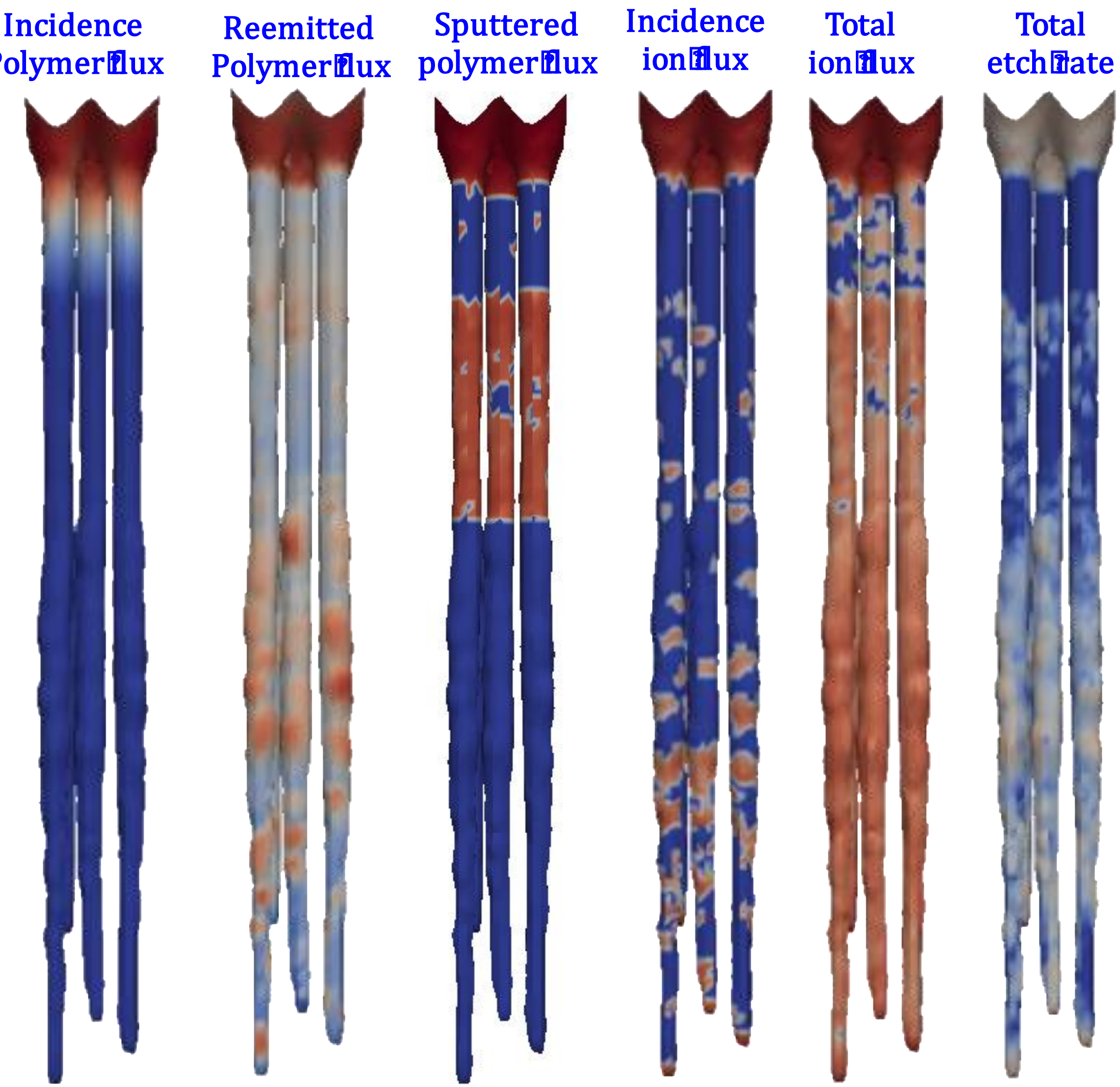
Case study I : Mask pattering issue under FC/Ar/O2 CCP Plasma

Initial top view

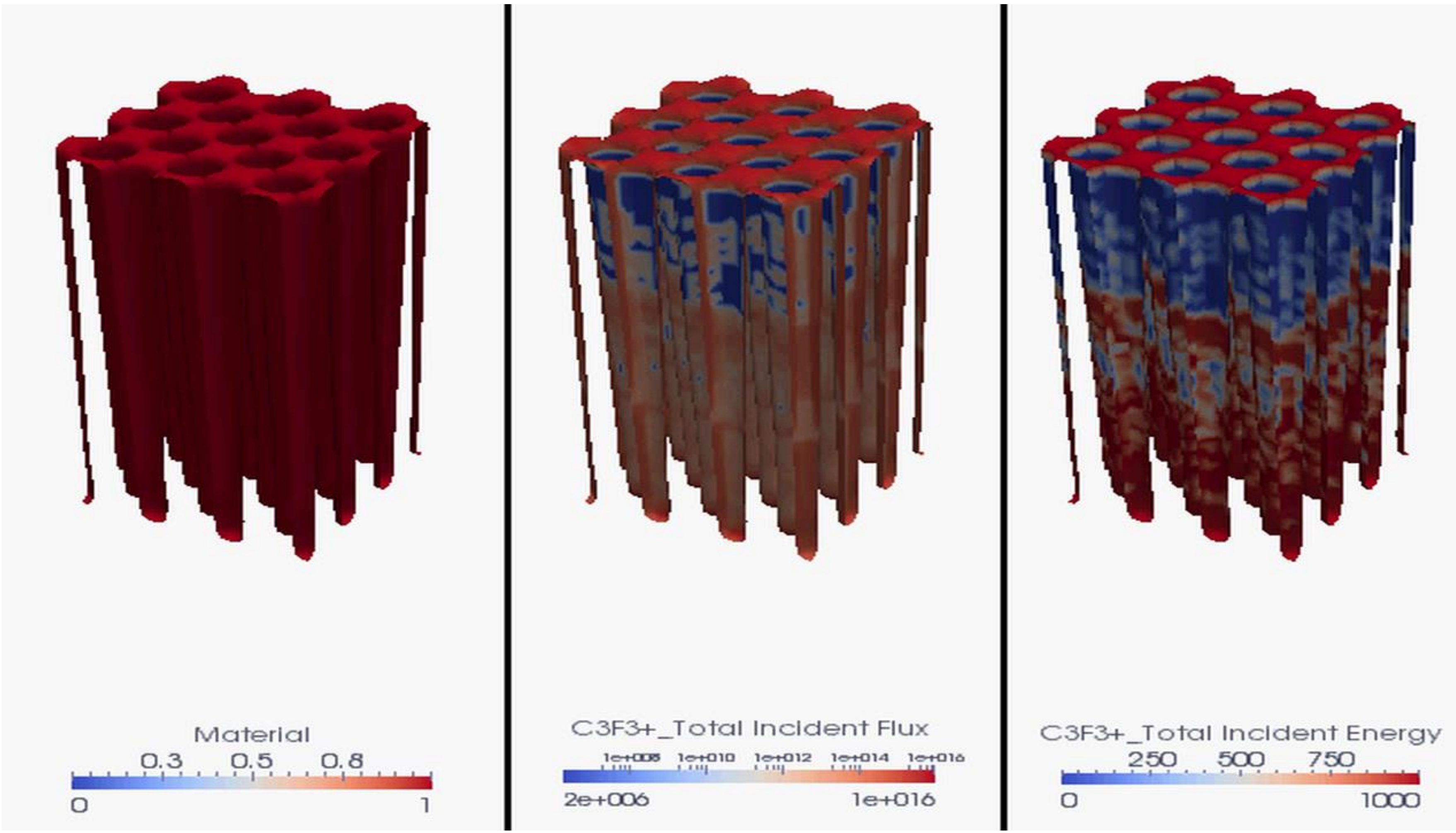


Final top view

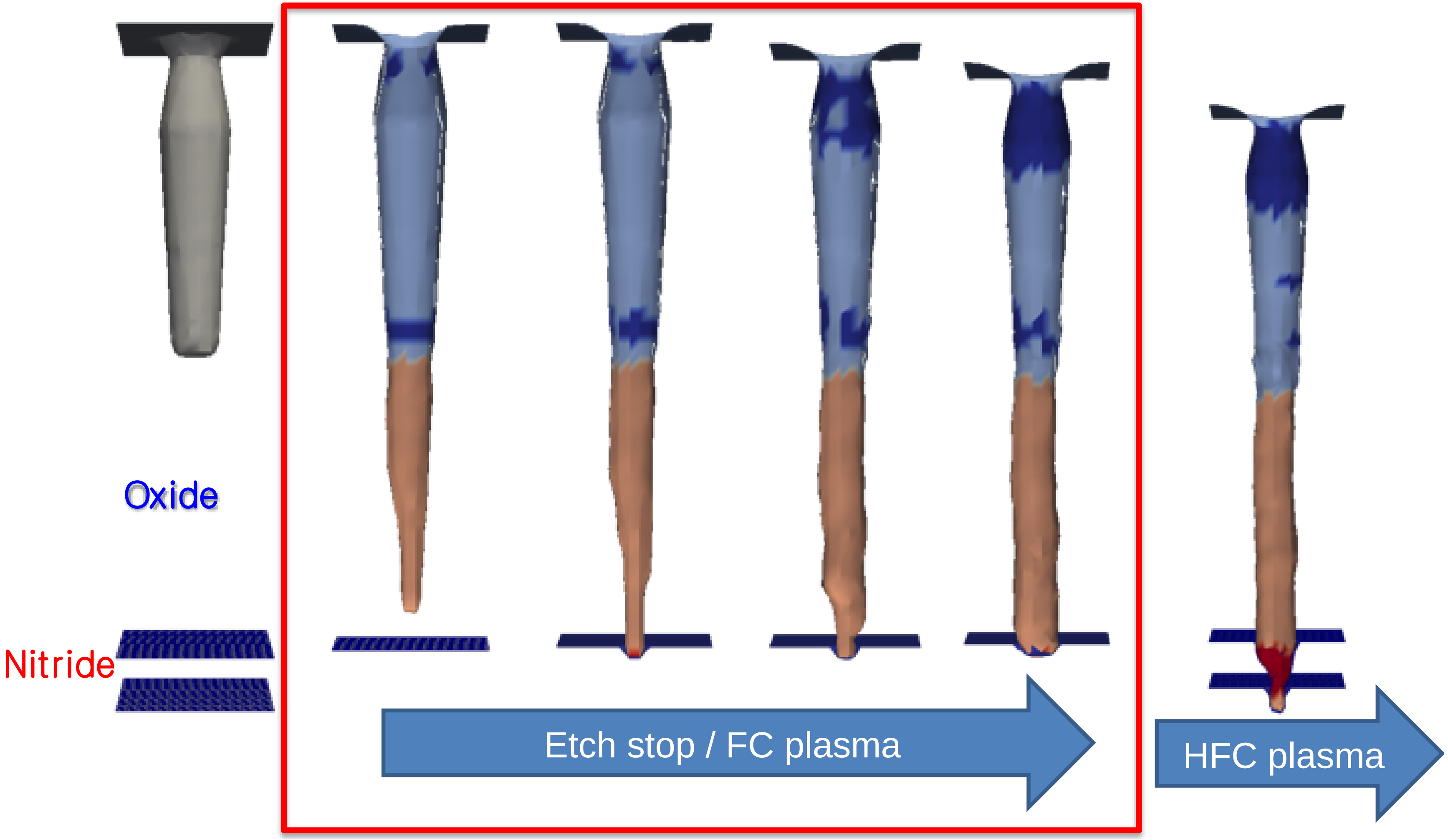




Case study II : Large area simulation



Case study III : Oxide etch stop & Continuous nitride etch



Case study IV : Charge-up simulation

Single time step : few hundreds hours

1000 times

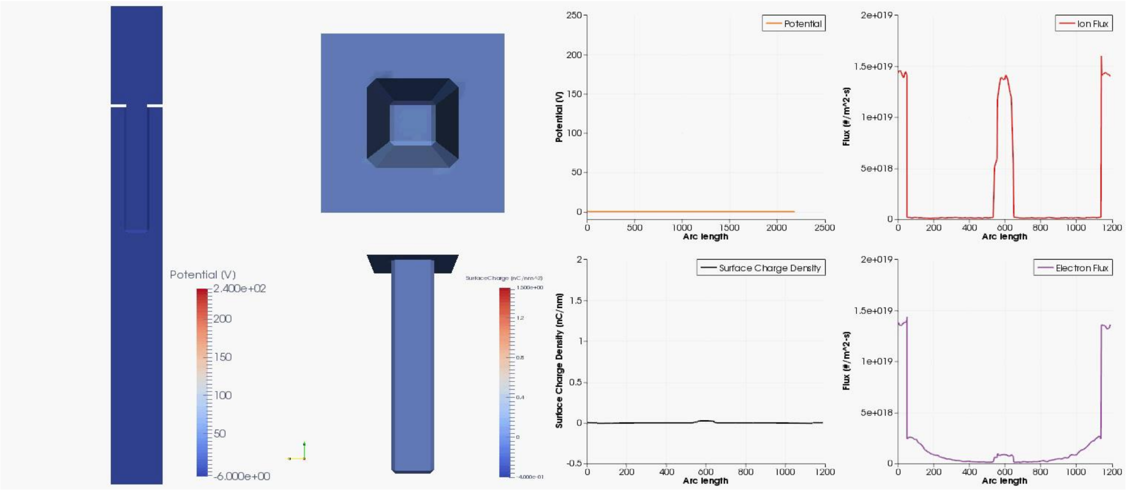
3D Poisson Equation Few Min. (Multi CPUs) ⟷ Particle Moving Few Min. (Multi CPUs)

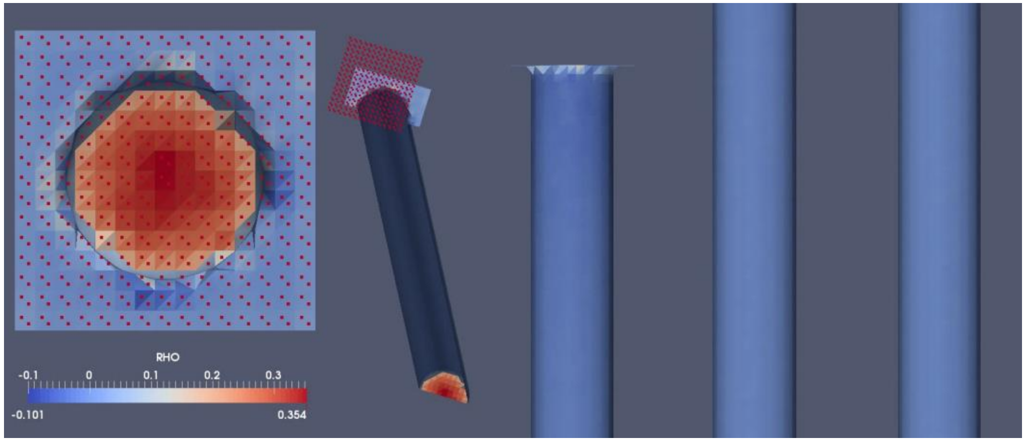
CPU based computation can't meet goal of engineering software

Single time step : few hundreds min.

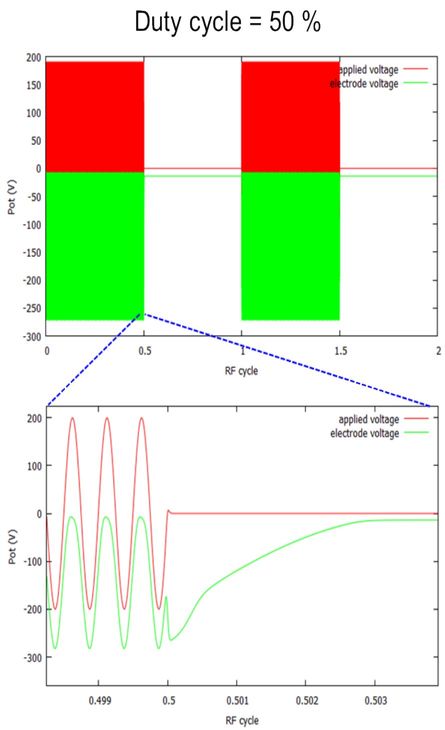
1000 times

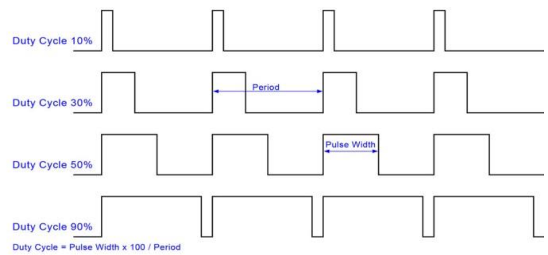
3D Poisson Equation [GPU] Few seconds ⟷ Particle Moving [GPU] Few seconds

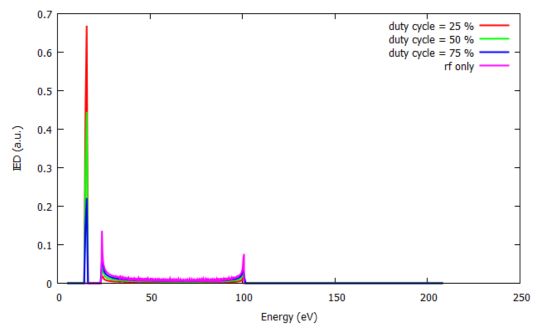


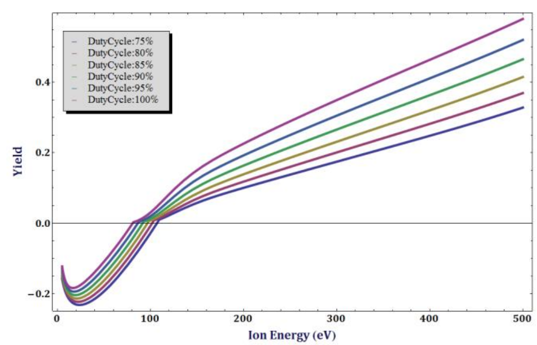


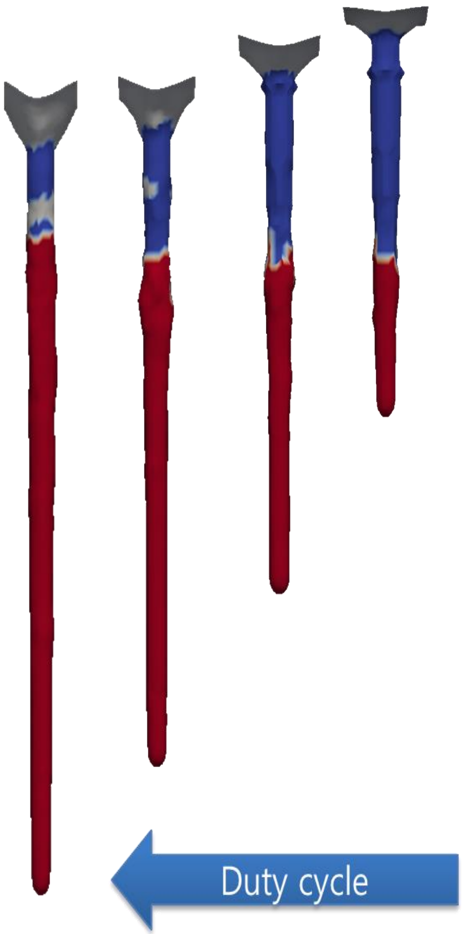
Case study V : Pulsed fluorocarbon plasma



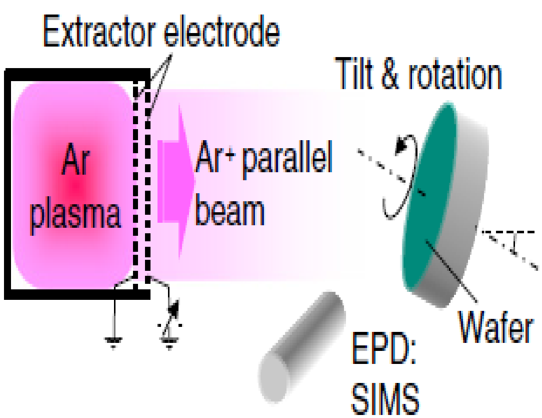


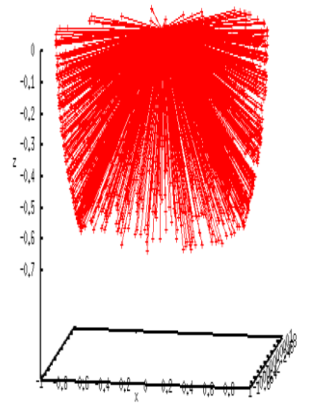


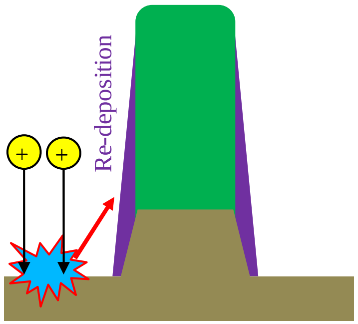




Case study VI : Plasma etch simulation for MTJ material







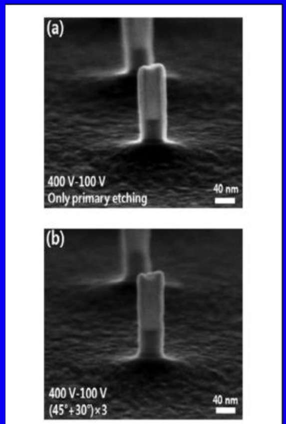
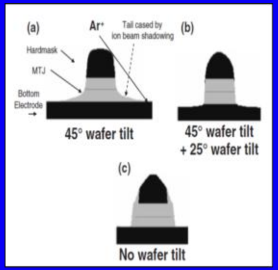


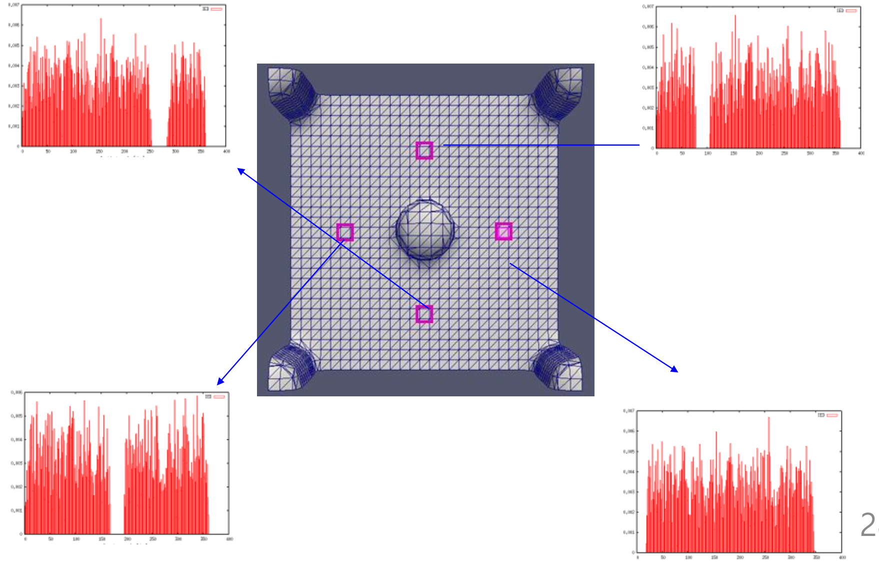
FIG. 2. Scanning electron micrograph of the MTJ structures (a) after IBE process at 45° for 18 min, and (b) after (3 min at 45° then 3 min at 30°) × 3 multi-step IBE for 18 min.

*S Chun, JAP, **111**, 07C722, 2012*



*K Sugiura, JJAP, **48**, 08HD02, 2009*

▪ **Reduce sidewall redeposition using multi-step ion beam etching**



감사합니다.