2016/5/18

Application of Rarefied Flow & Plasma Simulation Software

DSMC-Neutrals

PARTICLE-PLUS

WAVE FRONT

Yokohama City in Japan

Profile of Wave Front Co., Ltd.

Name : Wave Front Co., Ltd.
Incorporation : March 1990
Head Office : Yokohama in Japan

Business Description

(1) CFD(Computational Fluid Dynamics)&Plasma Software, Sales & Consulting Services
(2) CMMS(Computerized Maintenance Management System) Software, Sales, Consulting and Implementation services

Software Products sold in Foreign Countries

(1) Particle-PLUS(Plasma) & DSMC-Neutrals(Rarefied Gas Flow)
(2) PM-Optimizer(CMMS) & FLIPS(Scheduler)

DSMC-Neutrals

Rarefied Neutral Gas Flow Simulation using Particle Method

WAVE FRONT

Feature

1. **Rarefied Neutral Gas Flow** Simulation Software
   based on Direct Simulation Monte Carlo (DSMC) method

2. Simulation of Thin Film Growth due to Chemical Reaction like CVD
   - **Gas Phase Chemical Reaction**
   - **Surface Chemical Reaction**

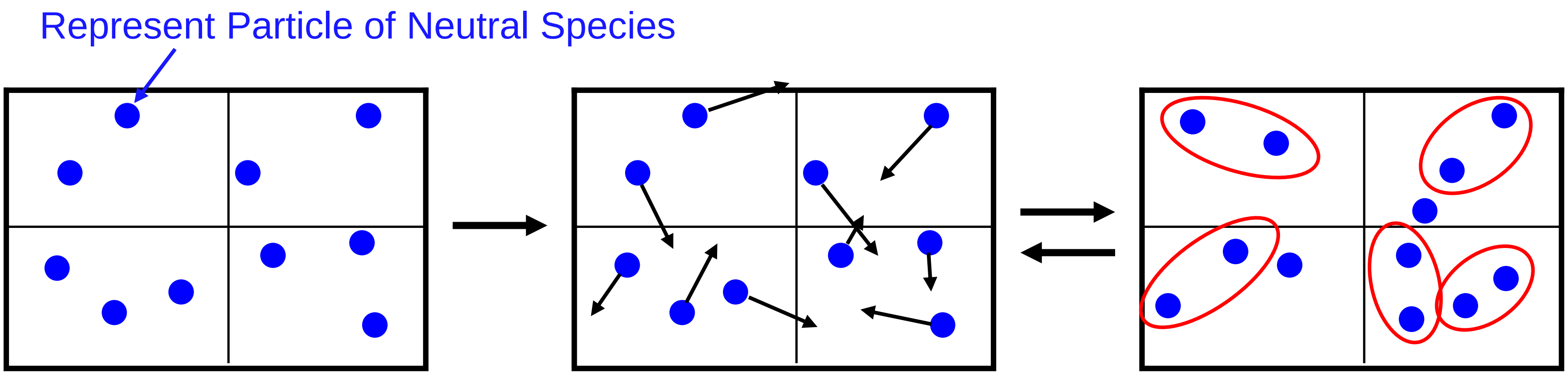
3. **Automatic and Very Fast Mesh Generation**

4. **Unstructured Mesh** for Modeling Detail Geometry

5. **High Performance of Parallel Computing** and Applicability to Big Model

6. **No Divergence** for All Model including Bad Quality Mesh
   User can obtain solution always.

DSMC method



(1) Making Grid

Initial Particle Setup

(2) Particles Moving

Reflection on Boundary

(3) Collision between Particles

One particle collides another in the same cell.

Requirement of numerical parameters

- Cell size

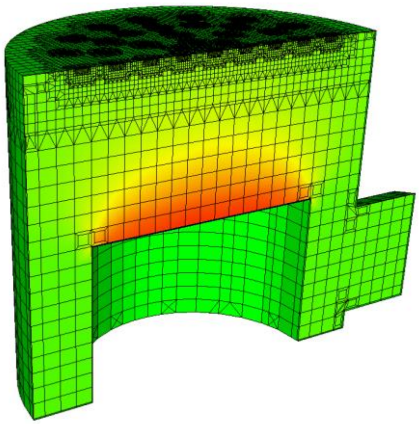
  $\Delta x < \lambda$: mean free path

- Time interval

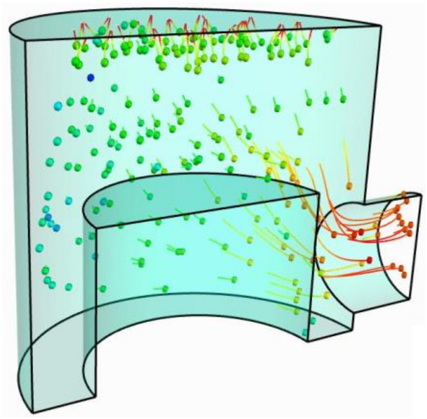
  $\Delta t < \tau$: collision time

Application examples

CVD Reactor with Showerhead

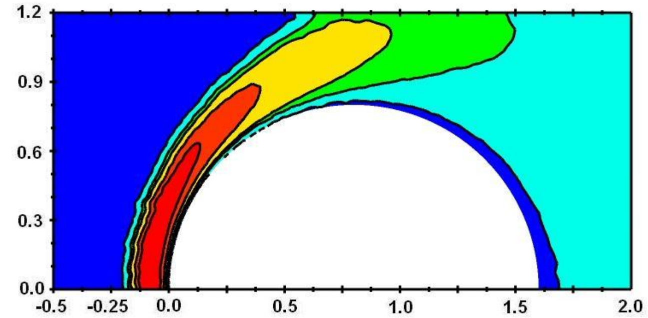


Temperature profile



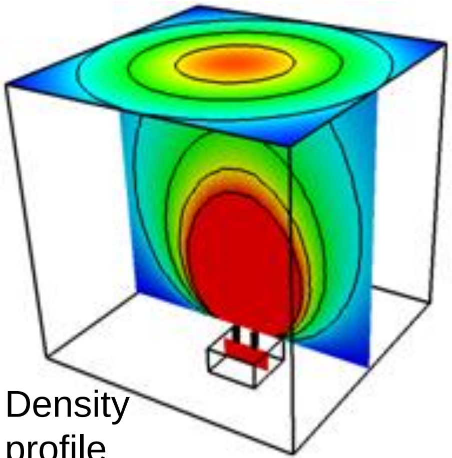
Particle Trace

Hyper Sonic Rarefied Flow



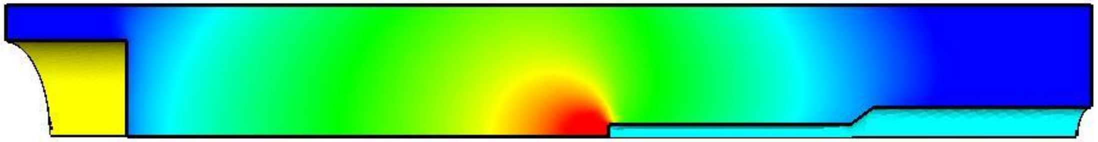
Temperature profile

LP-OVPD



Density profile

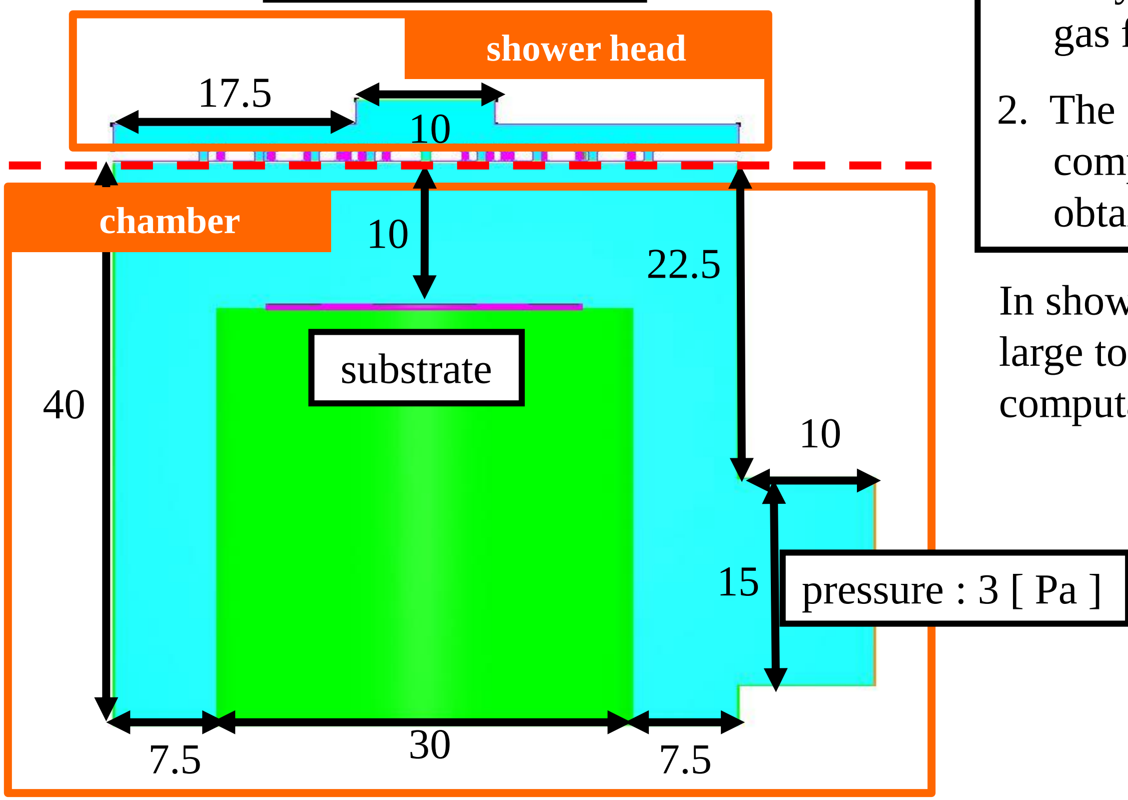
OVPD with Carrier Gas



Density profile

1. CVD model with Shower head

- N_2 : 5 [slm]
- SiH_4 : 5 [sccm]
- T : 300 [K]

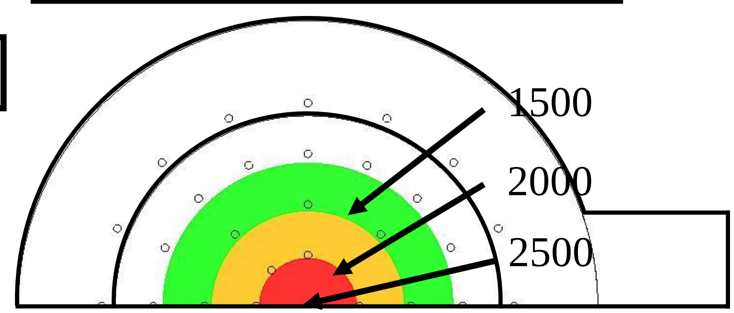


Procedure of shower head model

1. Only the shower head part is computed, where gas flow rate into the chamber is obtained.
2. The gas flow including chemical reaction is computed by using the gas flow rate which is obtained from step 1.

In shower head model, pressure difference is too large to simulation simultaneously whole computation domain.

temperature on substrate [K]



* Note that this model is just validation model in order to deposition rate depending on temperature. Therefore, computation setting is not realistic.

1. Chemical reaction of CVD model

Arrhenius equation $$k_f = \Lambda T^{\eta} \exp\left(-\frac{E_a}{T}\right)$$

Gas phase chemical reaction[*1]

Reaction equation	$\Lambda[m3/s]$	η	$E_a[K]$
SiH4 + M -> SiH2 + H2 + M	0.865	−3.54	29000

*1 J. Phys. Chem. vol.98 10138 (1994)

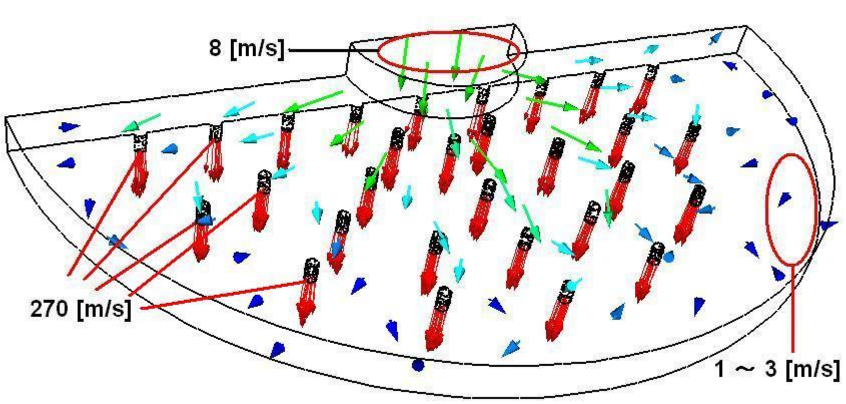
Surface reaction[*2]

Surface reaction	$\Lambda[m3/s]$	η	$E_a[K]$
SiH2 -> Si(s) + H2	1	0	0
SiH4 -> Si(s) + 2H2	0.054	0.0	9400

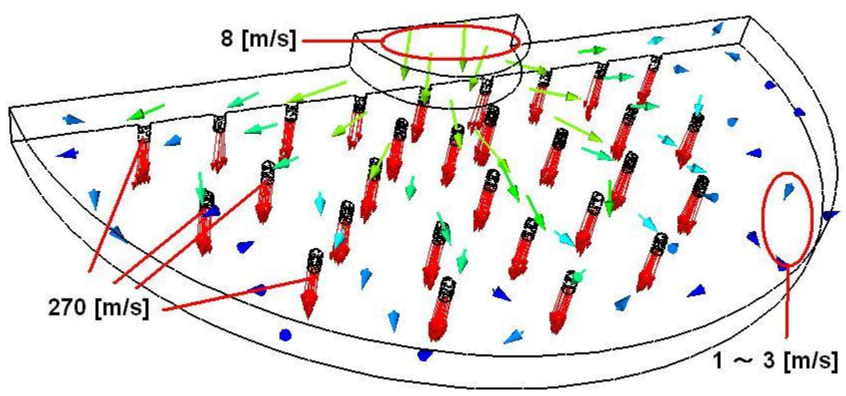
*2 J. Crystal Growth vol.126 373 (1993)

1. Shower head part

N2 flow velocity [m/s]

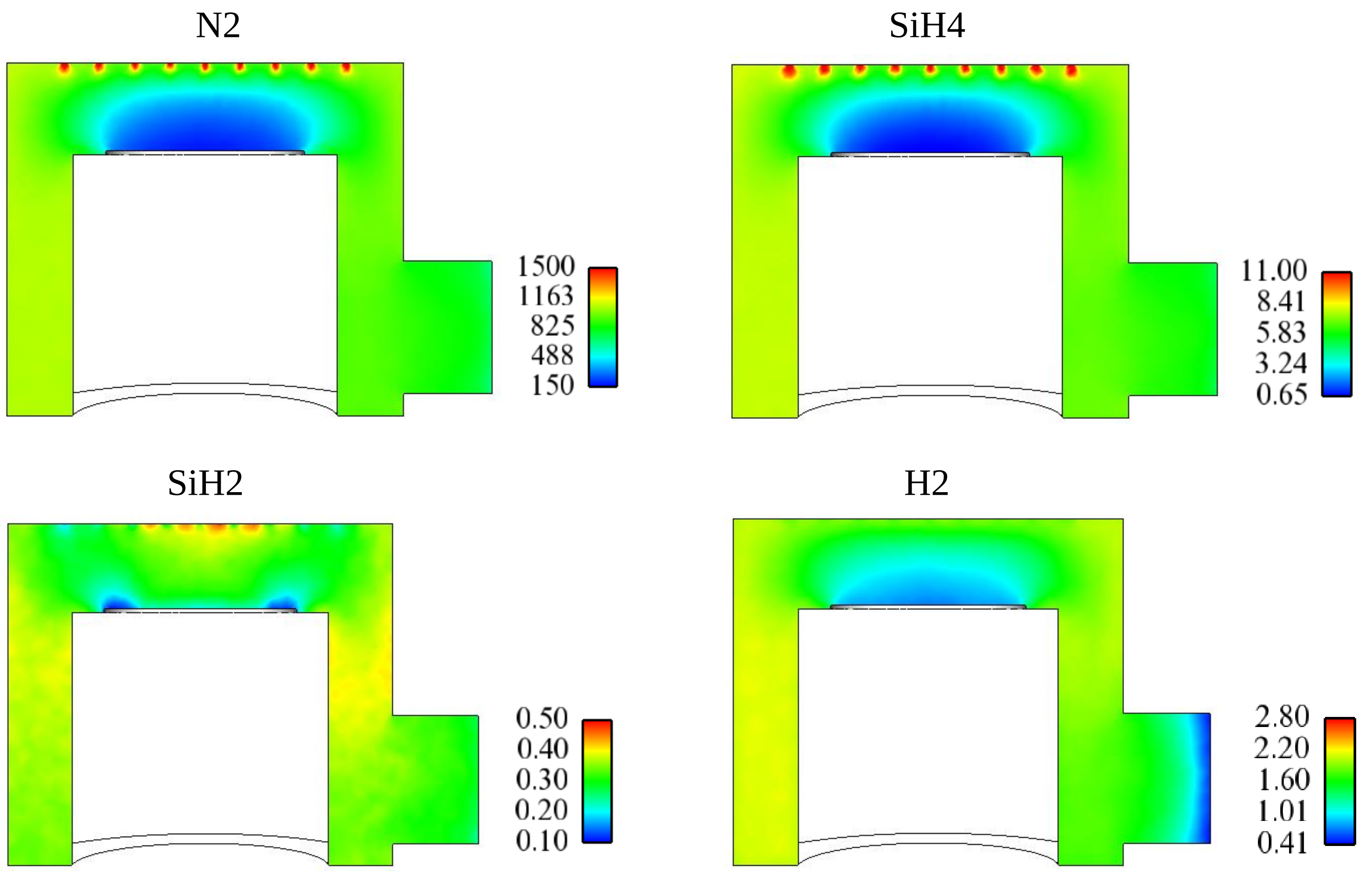


SiH4 flow velocity [m/s]

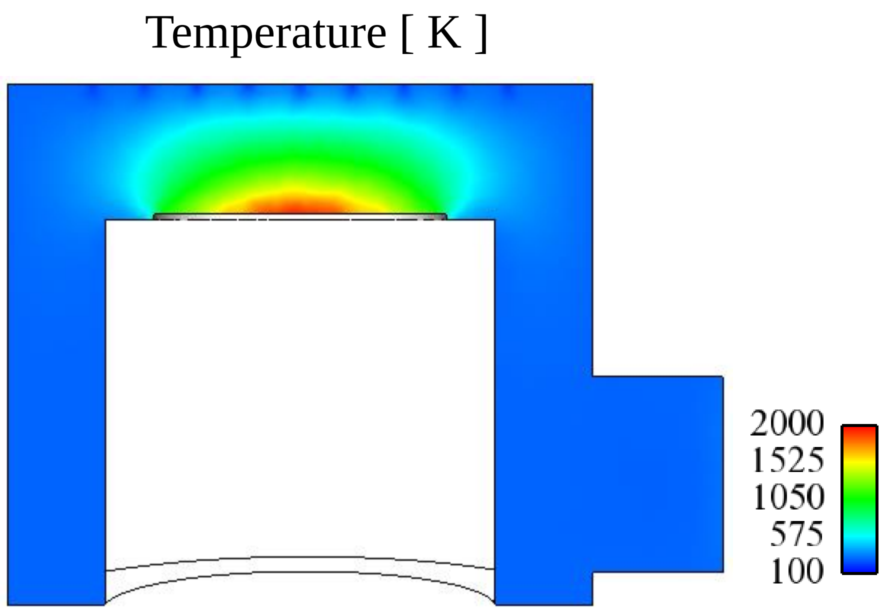


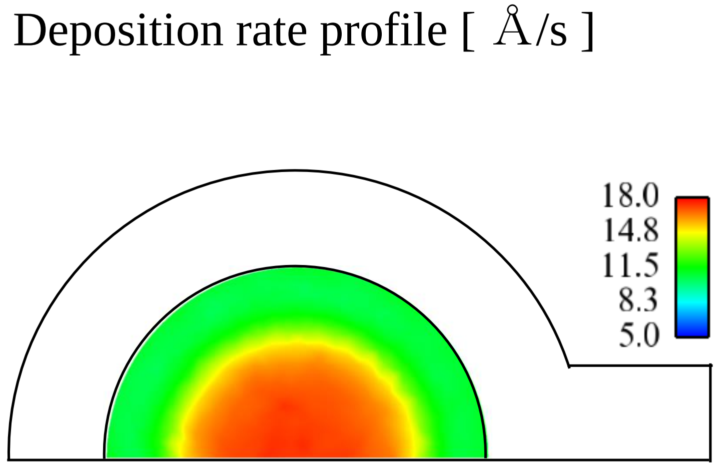
- Both flow velocity profiles is almost the same because pressure is sufficiently high.
- Gas flow rates of each shower head nozzle is obtained. The gas flow in the chamber using them.

1. Number density [10^{18} #/m^3]



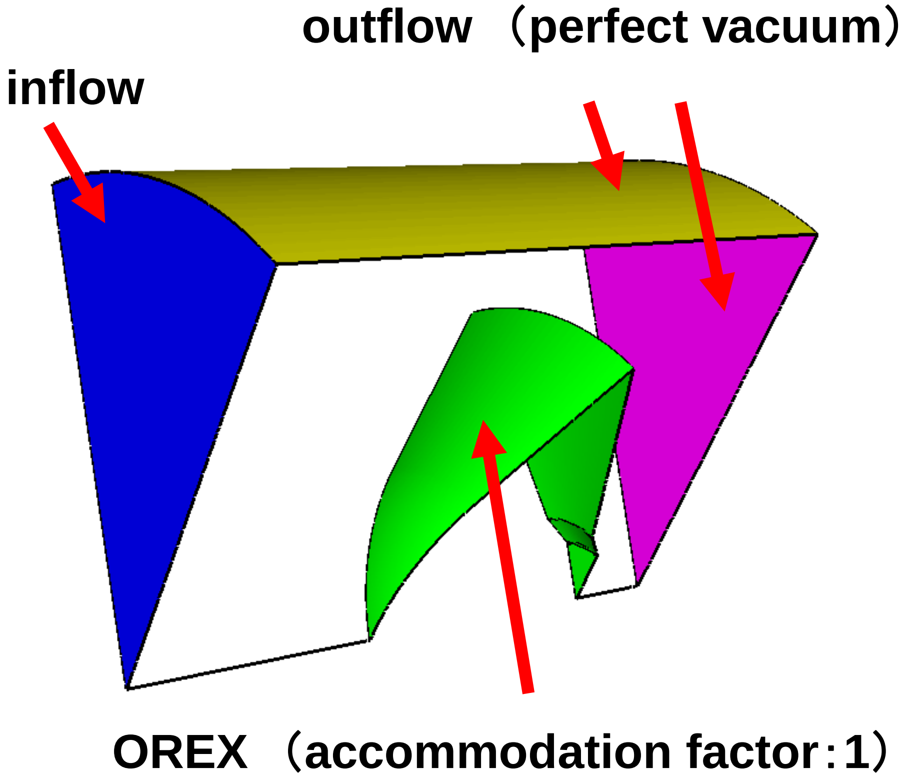
1. Temperature and depo. rate

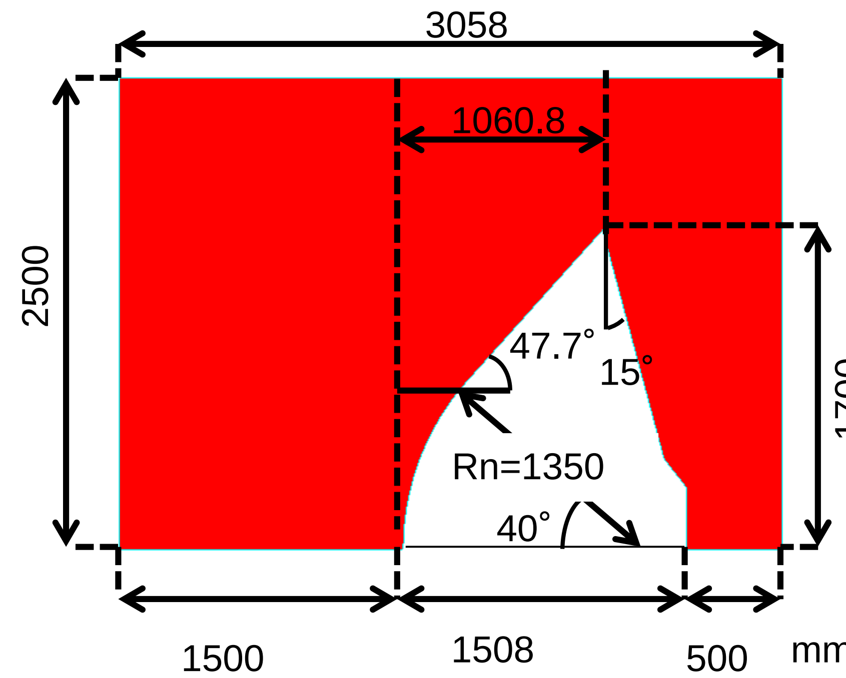




- Temperature jump is reproduce on substrate.
- The temperature dependence of deposition rate appears on the substrate.

2. Hyper Sonic Rarefied Flow





altitude [km]	flow vel. [m/s]	density [m^{-3}]	mole frac. （O2）	mole frac. （N2）	mole frac. （O）
105.0	7451.0	5.0515E+18	0.1528	0.7815	0.0657
92.8	7454.1	4.0845E+19	0.2025	0.7881	0.0094

2. Chemical reaction

Gas phase chemical reaction is computed using TCE model. The molecules used in the computation consider vibrational and rotational energy.

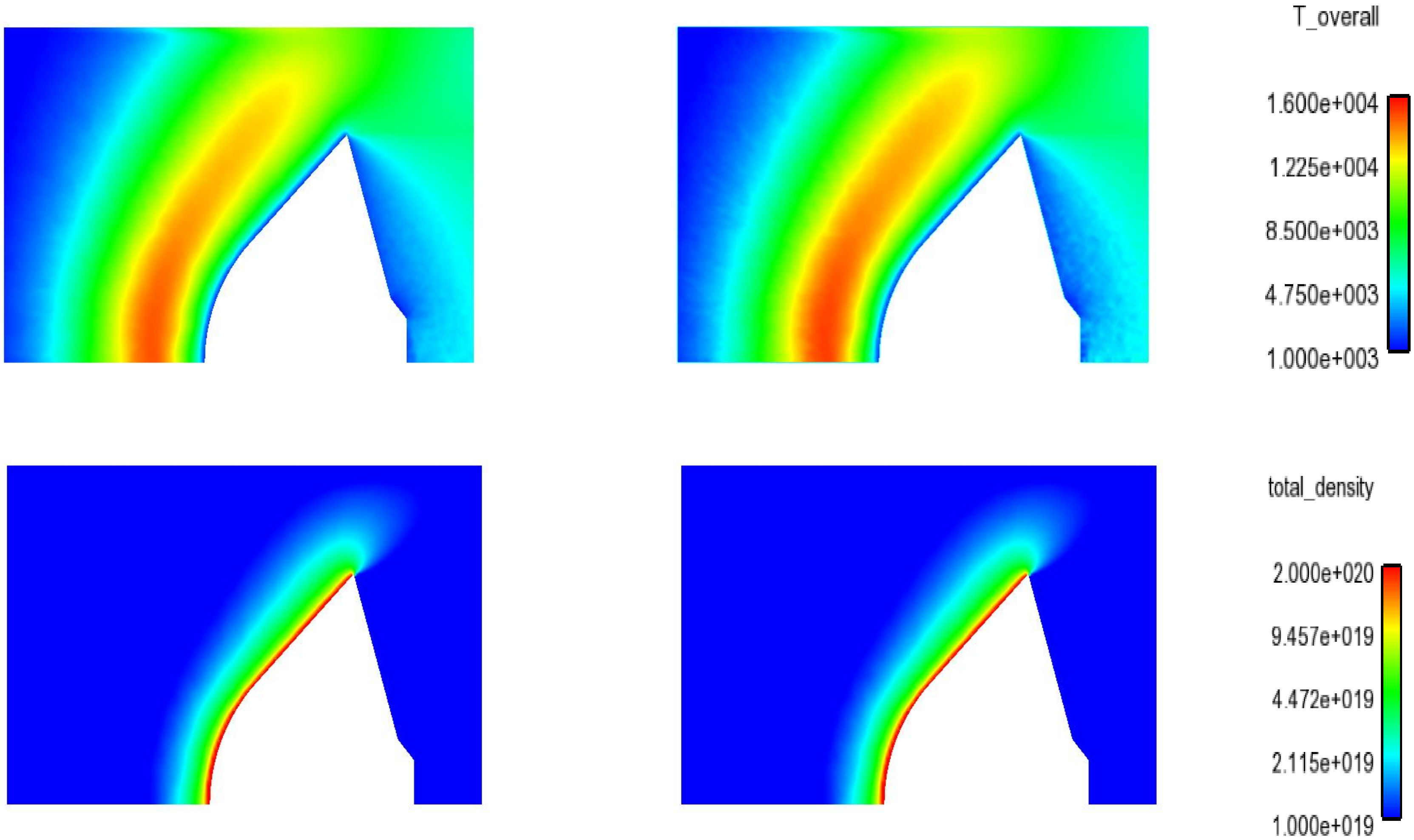
Reaction equation	A [cm^3/mol s]	B	Ea [K]
N2 + M <-> N + N + M	7.0×10^{21}	-1.6	113200
O2 + M <-> O + O + M	2.0×10^{21}	-1.5	59500
NO + M <-> N + O +M	5.0×10^{15}	0.0	75500
NO + O <-> N + O2	8.4×10^{12}	0.0	19450
N2 + O <-> N + NO	6.4×10^{17}	-1.0	38370

$$k_f = A T^B \exp\left(-\frac{E_a}{T}\right)$$

***3 Bird G. A., *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, 1st edition, Clarendon Press, Oxford, New York, 1994.**

2. Results (altitude:105 km)

with reaction without reaction



2. Heat flux [kW/m²]

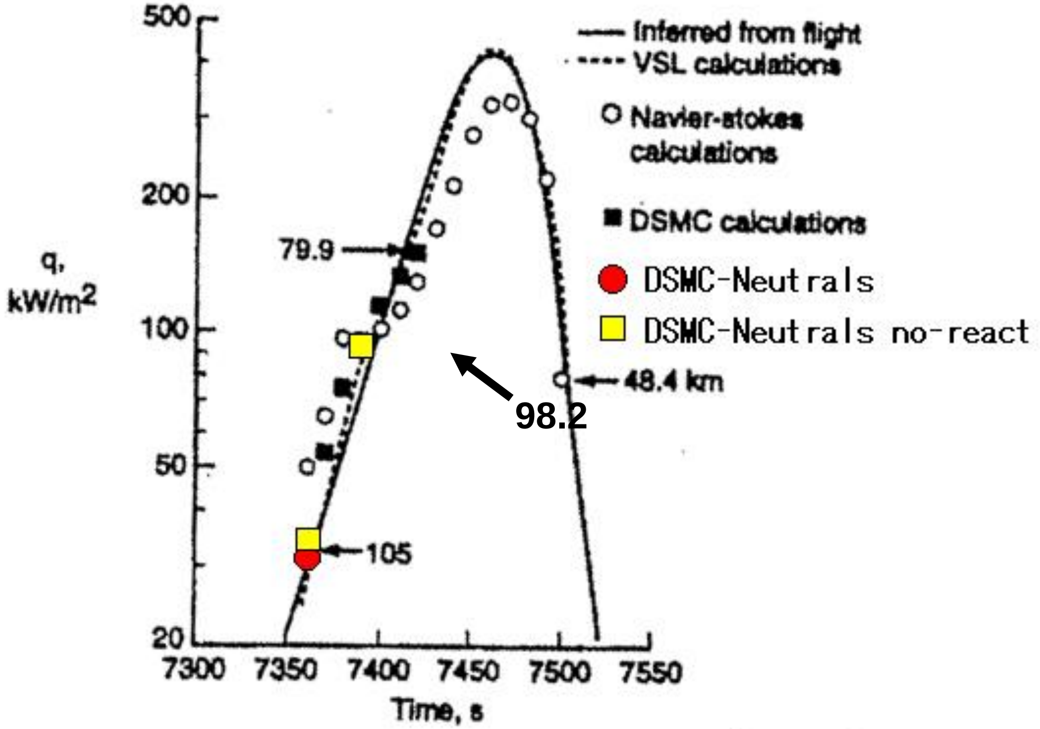


Fig 3. Comparison of flight inferred[3] stagnation-point heating rates with calculations using VSL[7], NS[6], and DSMC.

* DSMC SIMULATION OF OREX ENTRY CONDITIONS : James N. Moss, Roop N. Gupta, Joseph M. Price (Aerothermodynamics Branch, NASA Langley Research Center, Hampton, Virginia 23681-0001, USA)

2. Heating rate coefficient

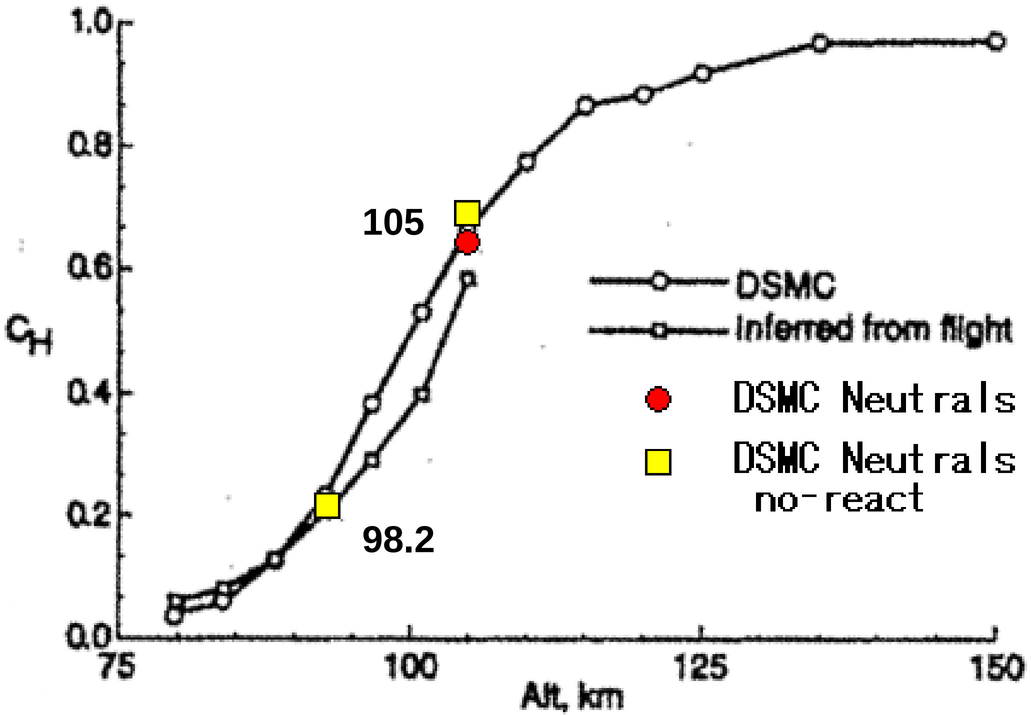


Fig. 4. Comparison of flight inferred[3] stagnation-point heating rate coefficient with DSMC results.

C_H

$$C_H = \frac{2q}{\rho V^3}$$

mass density in atmospheric pressure

$$\rho = \frac{\sum_s M_s n_s}{N_A}$$

q : heat flux

M_s : atomic mass

n_s : No. density

N_A : Avogadro constant

V : OREX's velocity

Low Pressure Plasma Simulation using Particle Method

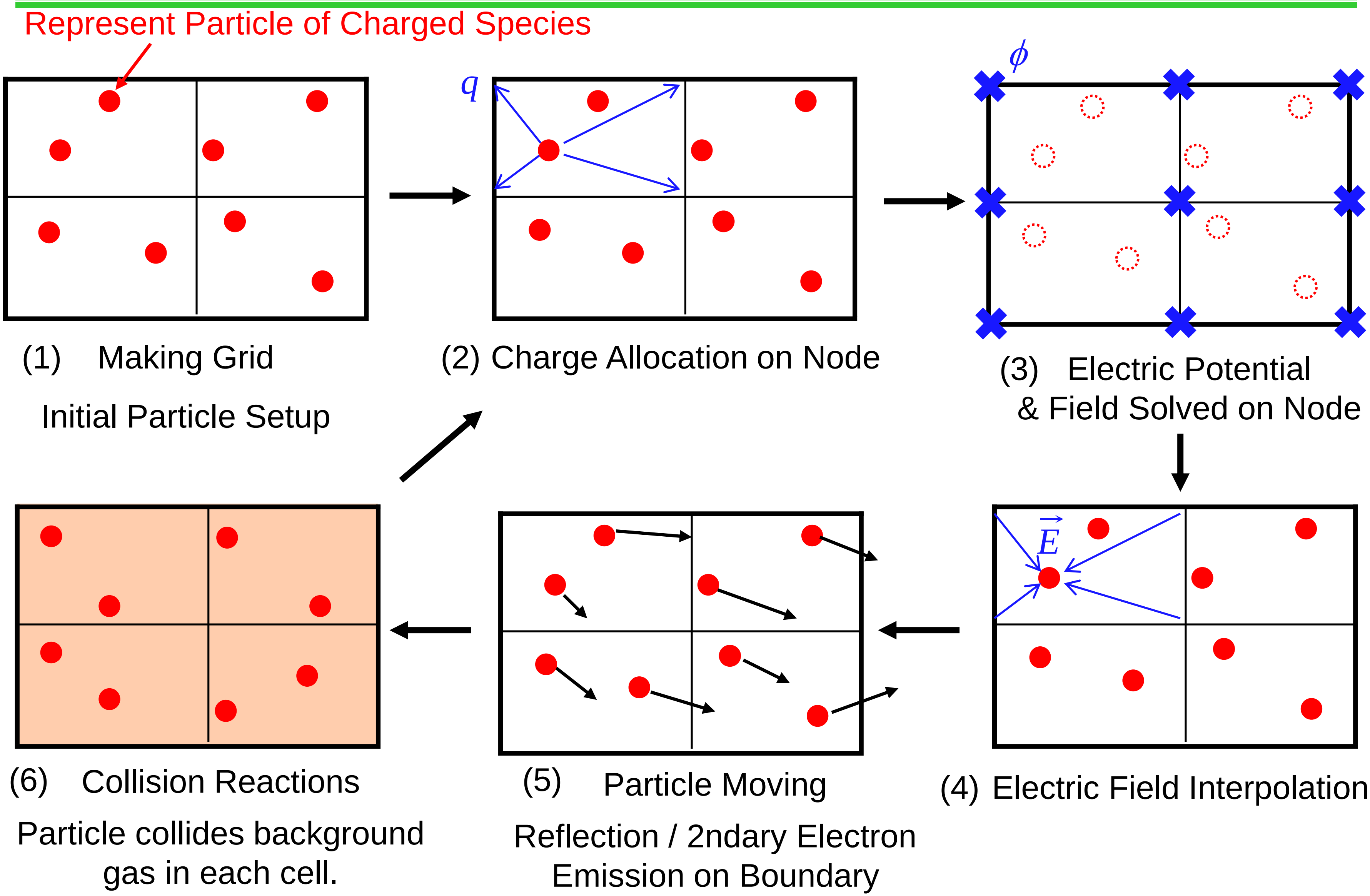
Feature of Particle-PLUS

1. **Plasma Simulation Software Package for Law Pressure**

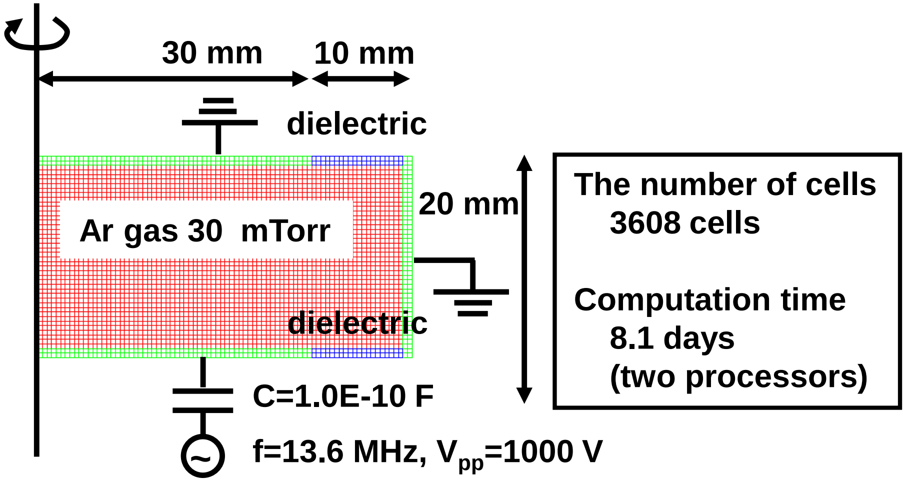
2. Composition of Main Two Modules,
   Plasma Module : based on Particle-in-Cell (PIC) method
   Neutral Module : based on DSMC method

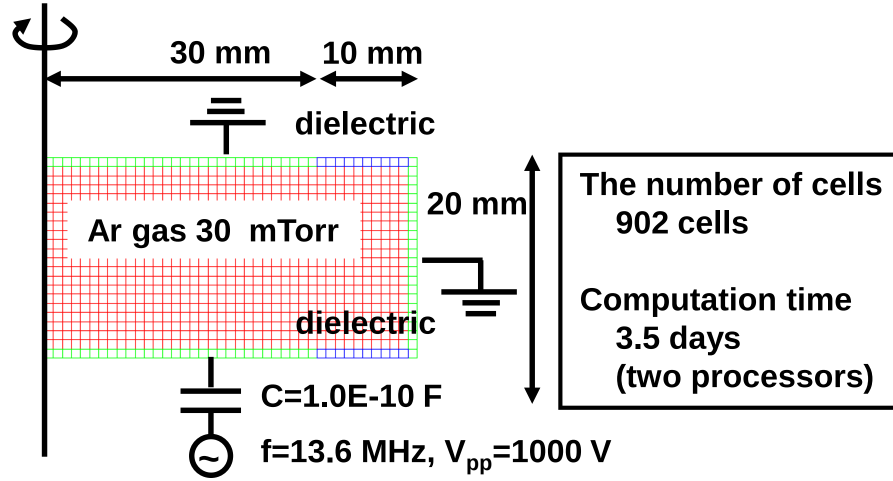
3. Simulation of Thin Film Growth due to Magnetron Sputtering
   - **Background Gas Flow** : Neutral Module
   - **Magnetic Field by External Magnet** : Plasma Module
   - **Collision Reactions by Electron/Ion Impact** : Plasma Module
   - **Secondary Electron Emission** : Plasma Module
   - **Sputtering of Target Atom** : Neutral Module
   - **Motion of Sputtered Atom** : Neutral Module

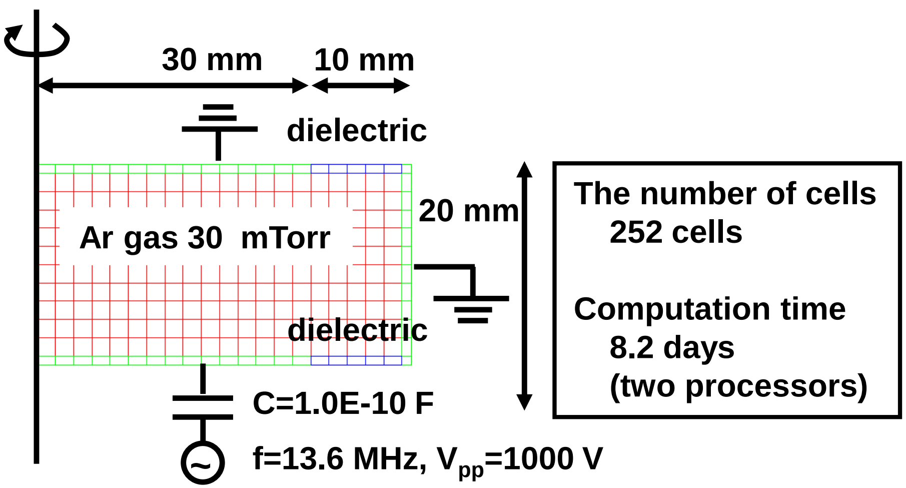
Particle in cell method



Mesh size dependence



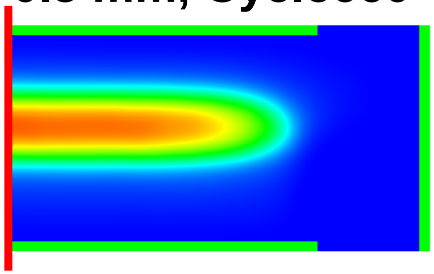




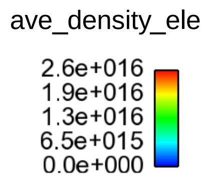
Mesh size dependence

electron density [#/m³]

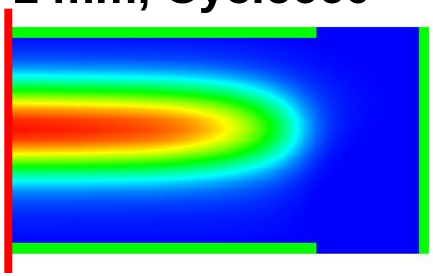
0.5 mm, Cycle660



Max=2.4x10¹⁶

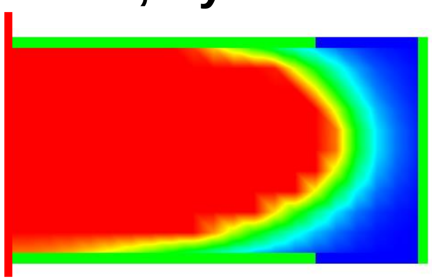


1 mm, Cycle660



Max=2.6x10¹⁶

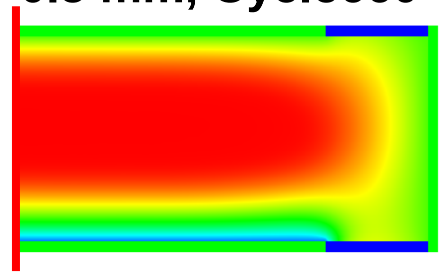
2 mm, Cycle 650



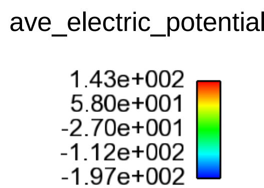
Max=2.4x10¹⁷

electric potential [V]

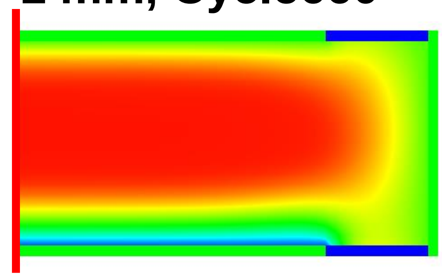
0.5 mm, Cycle660



Max= 143
Min =-156

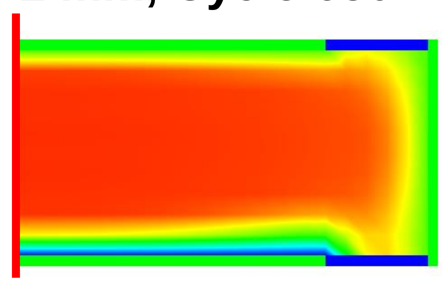


1 mm, Cycle660



Max= 137
Min =-170

2 mm, Cycle 650



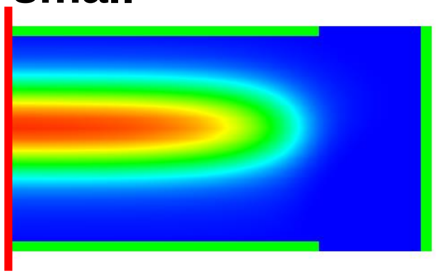
Max= 128
Min =-197

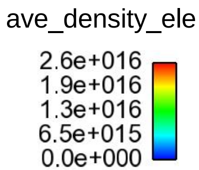
Weight of particles dependence

electron density [#/m³]

small

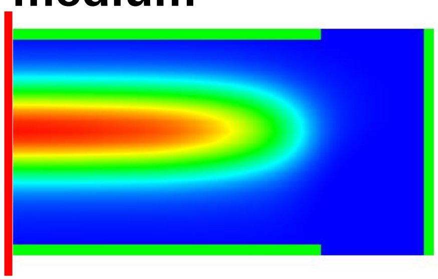
Max=2.5x10^{16}





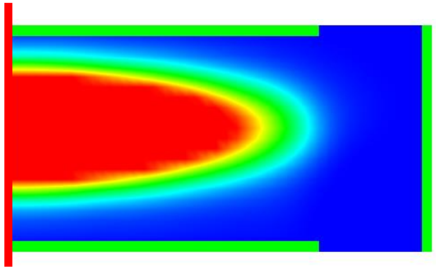
medium

Max=2.6x10^{16}



large

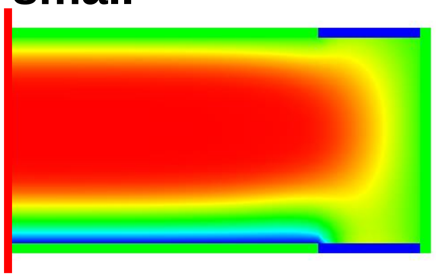
Max=7.0x10^{16}

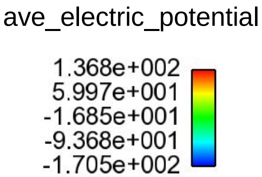


electric potential [V]

small

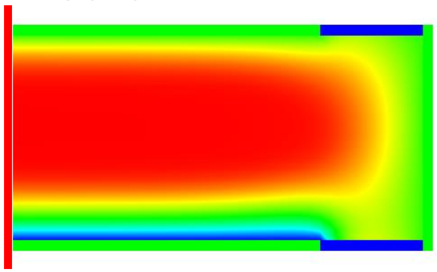
Max= 136.6
Min =-170.5





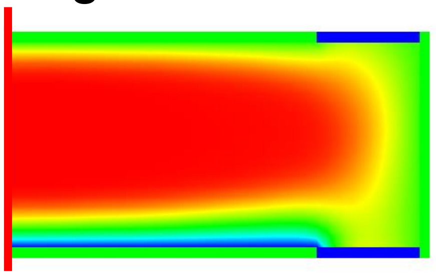
medium

Max= 136.8
Min =-170.2



large

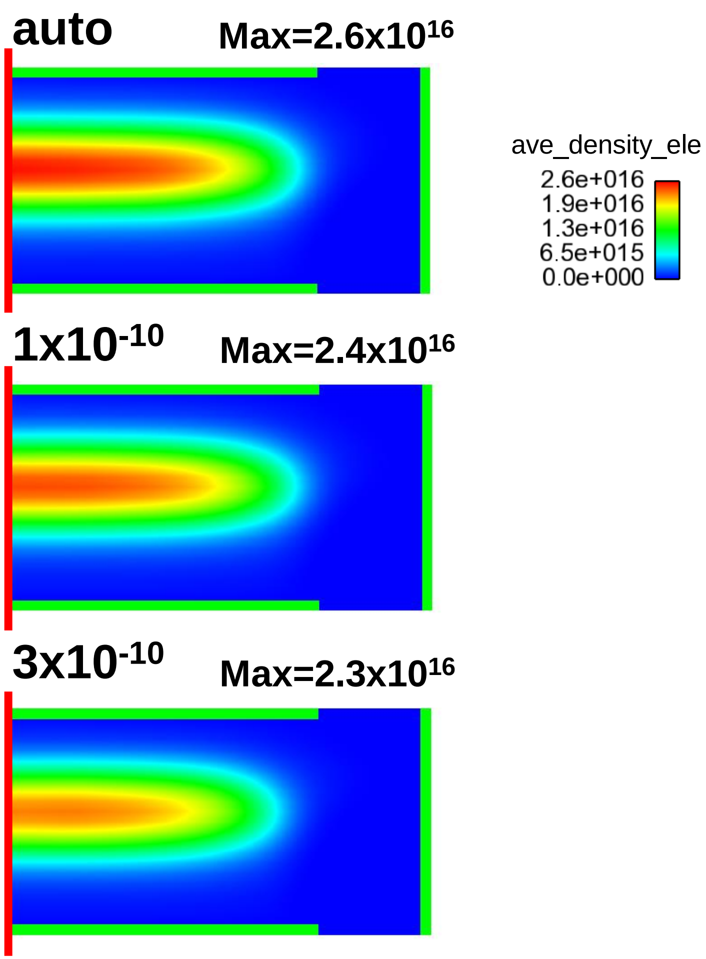
Max= 138.5
Min =-171.5



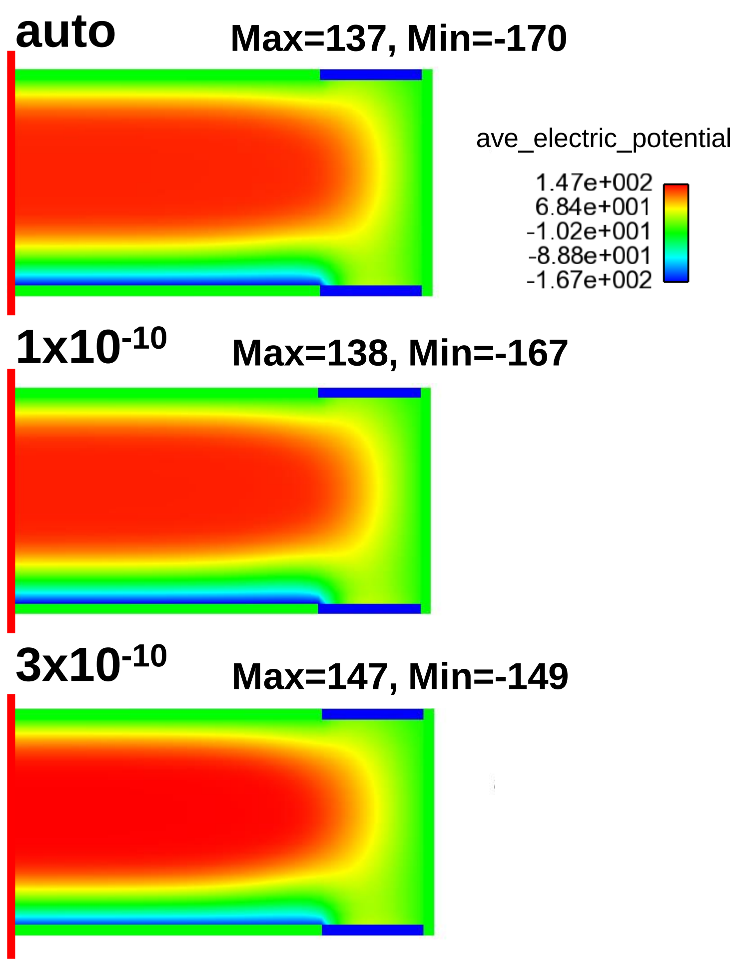
* The weight is the number of molecules represented by a super particle.

Time step dependence

electron density [#/m³]



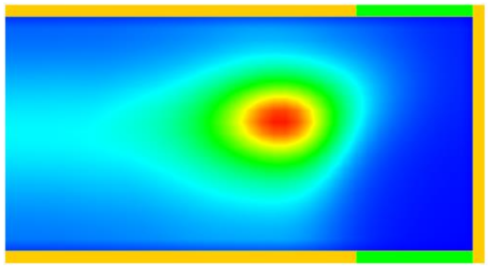
electric potential [V]



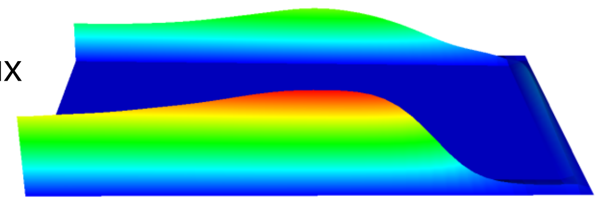
Application example

Capacitively Coupled Plasma (CCP)

Ion Density

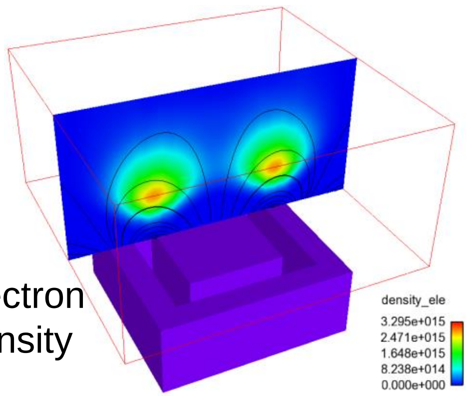


Ion Flux

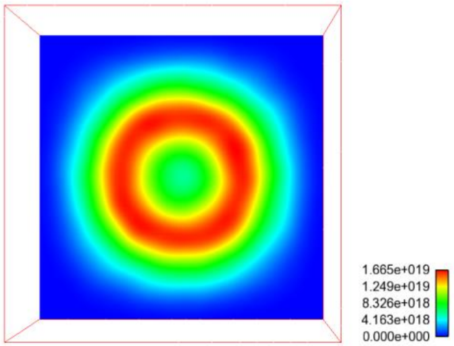


Magnetron Sputtering

Electron Density



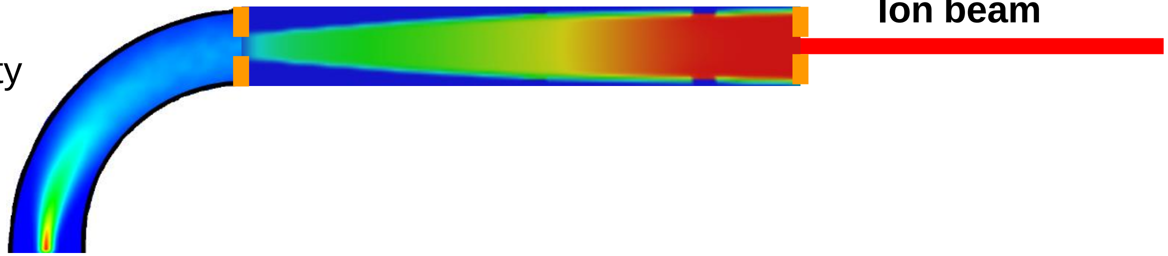
Ion Flux



Ion Beam Spectrometry & Acceleration

Velocity profile

Density profile

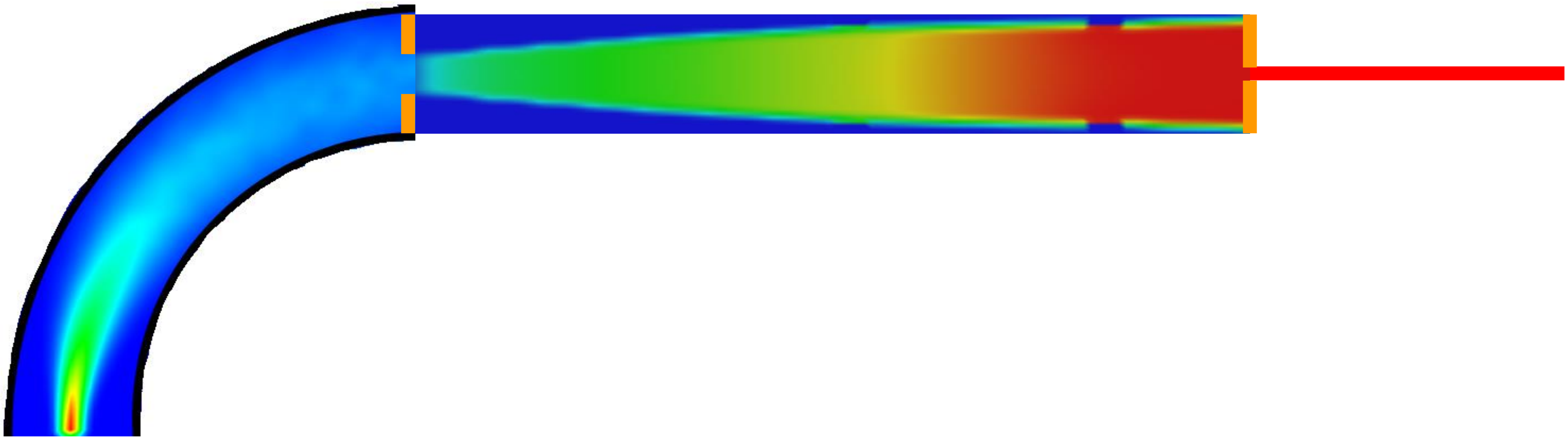


Ion beam

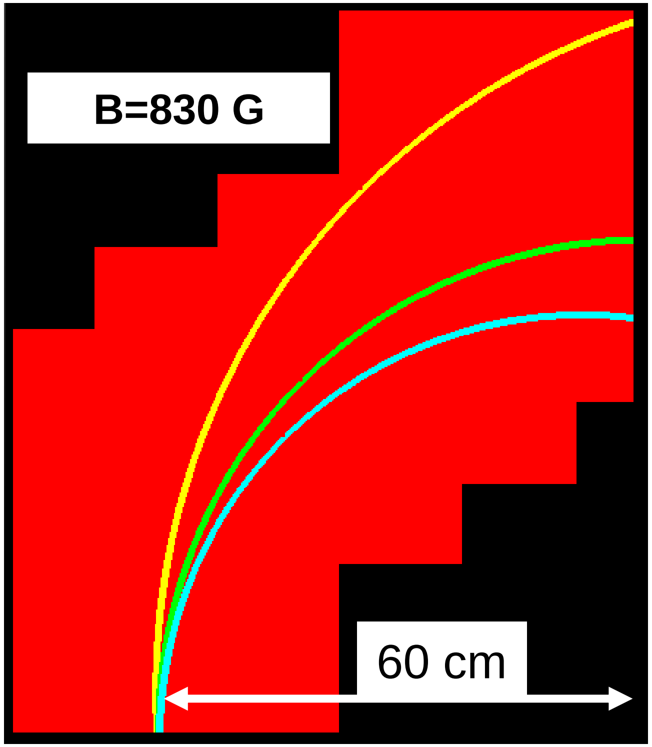
1. Ion implant process

Ion beam analysis **Ion beam accelerate** **Ion beam**

Density profile Velocity profile



1. Ion implant process



Mg^+, C^+, Be^+ (E=100 eV)

Mg^+ (M=24, R=87 cm)

C^+ (M=12, R=60 cm)

Be^+ (M=9, R=52 cm)

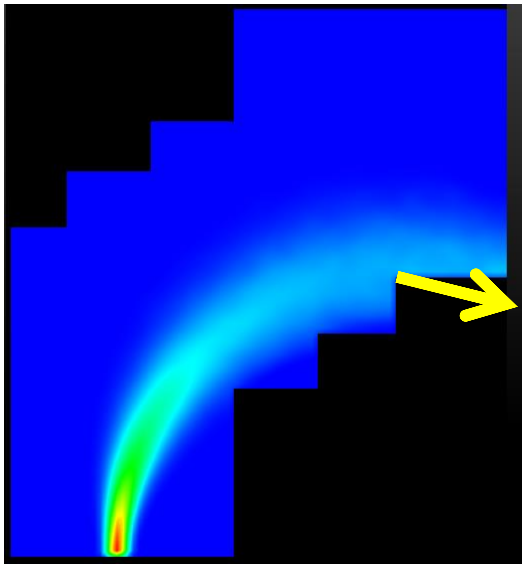
M : molecular weight, R : radius of ion flight pass

Radius of ion flight pass

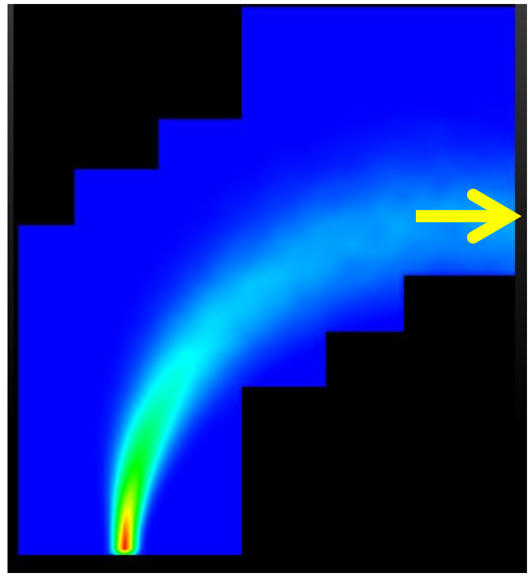
$$R = \frac{mv}{qB} = \frac{\sqrt{2mE}}{qB}$$

The radius of ion flight pass is proportional to root of ion energy. The results of Particle-PLUS agree with analysis results.

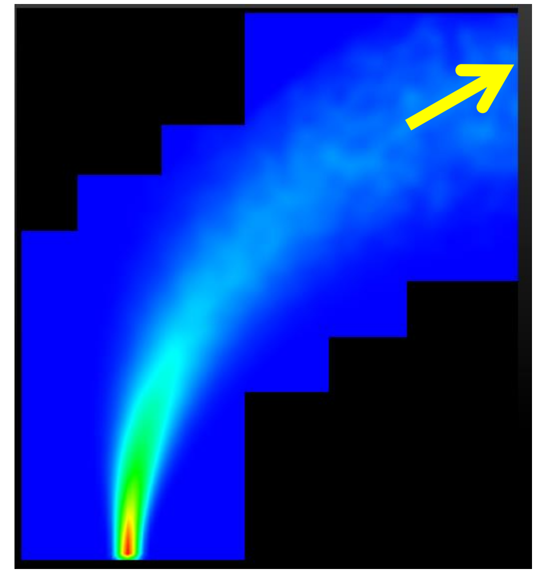
1. Ion implant process



Be^+

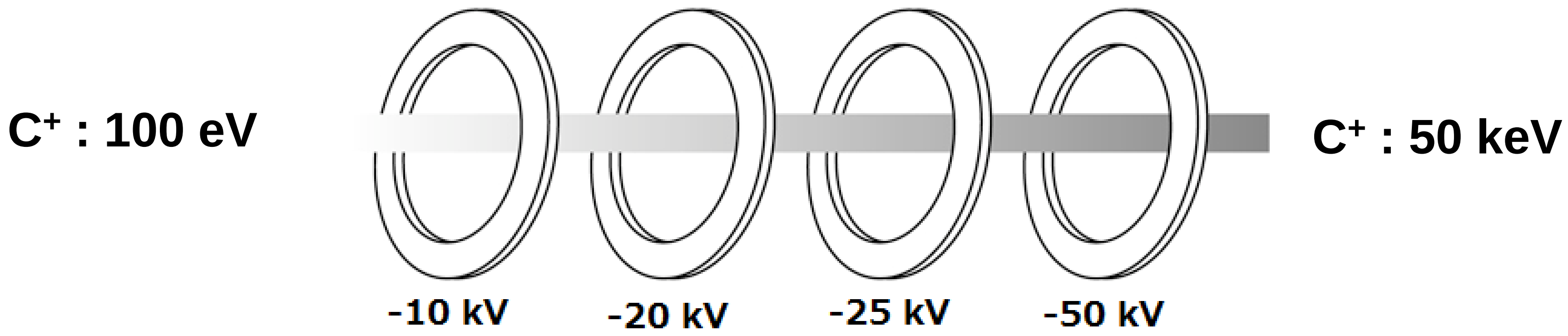


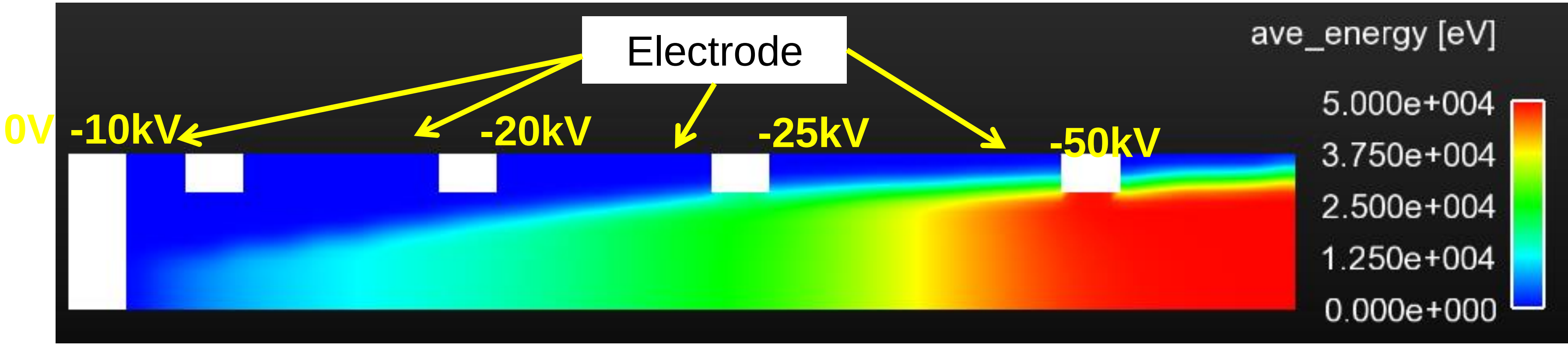
C^+



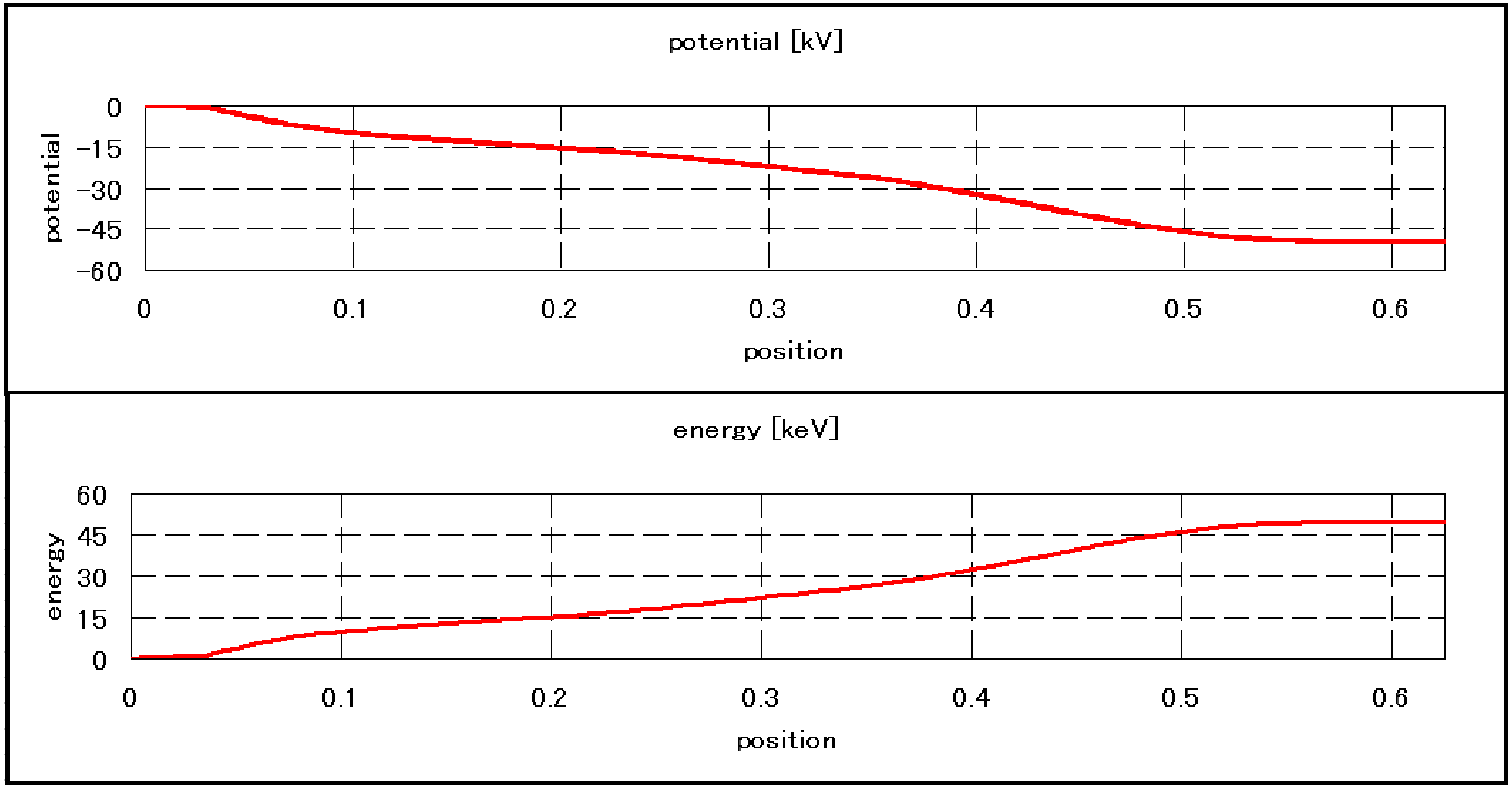
Mg^+

1. Ion implant process



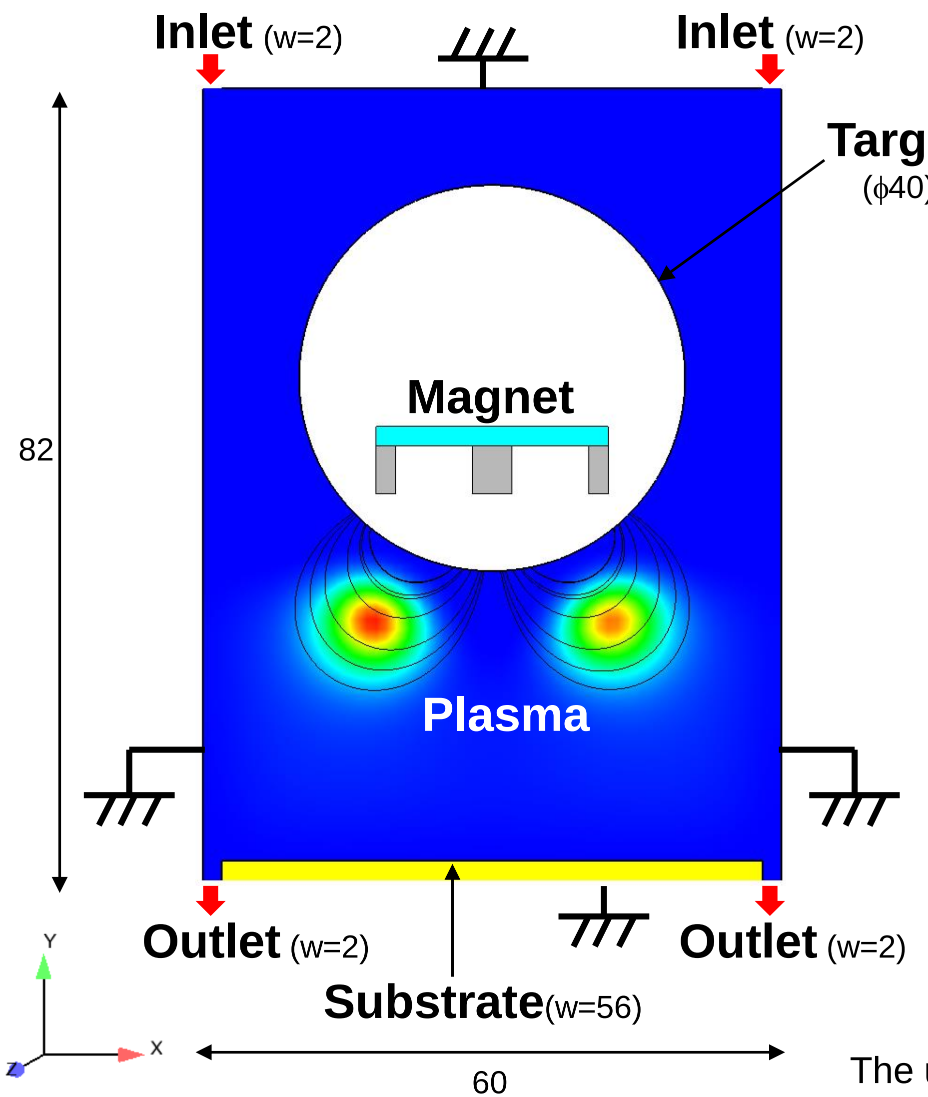


1. Ion implant process



In this simulation, elastic collision is neglected so that sum of potential and kinetic energies is conserved completely.

2. Magnetron Sputter Circular target

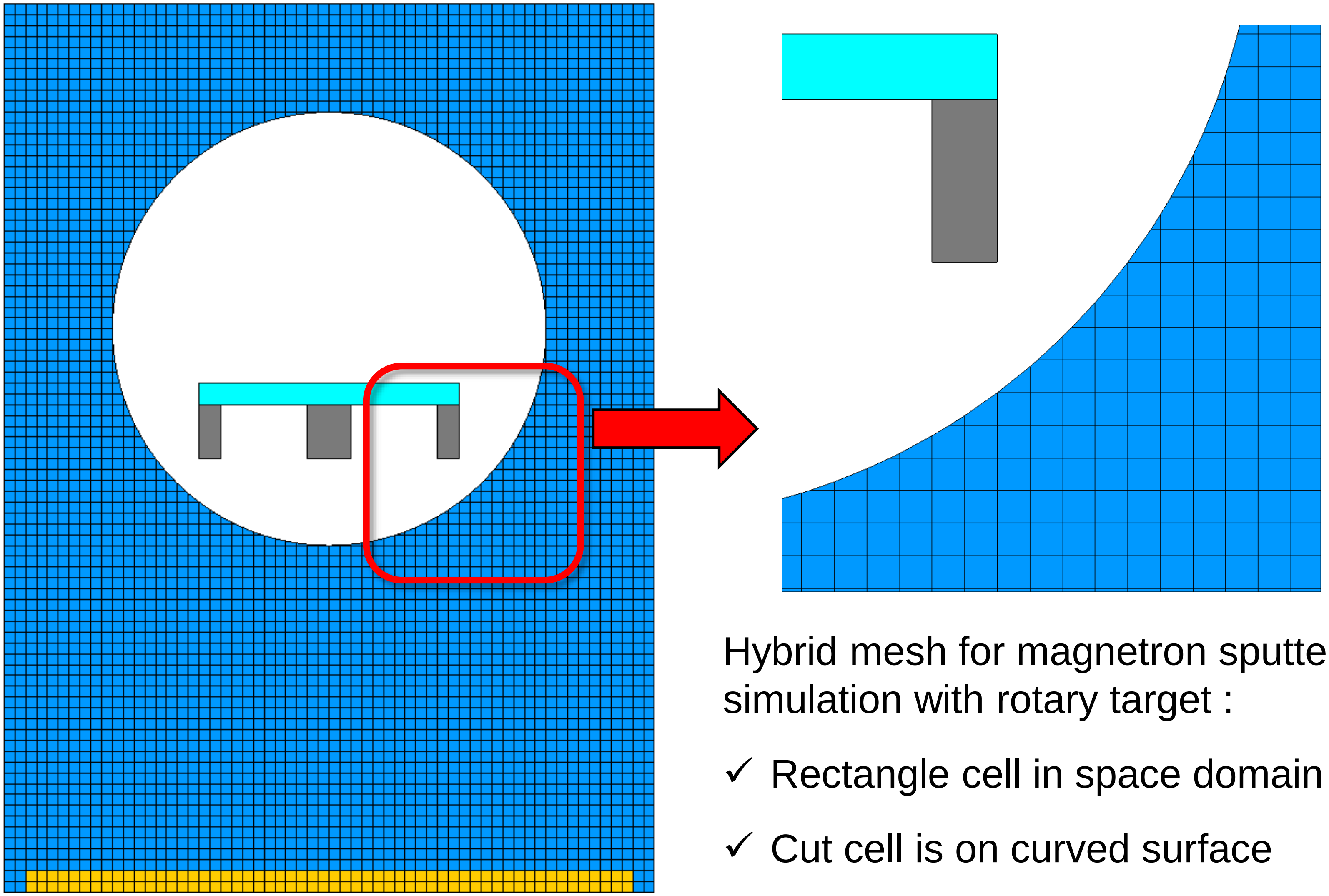


The unit is [mm].

Physical Parameters:

Inlet condition	Ar 10 sccm for each part
Outlet condition	1.0 Pa
Permanent magnet	Ferrite
Magnetic Yoke	Fe
Target material	Ta
Target-Substrate distance	30 mm
Applied voltage on target	DC -500 V

2. Cut cell mesh

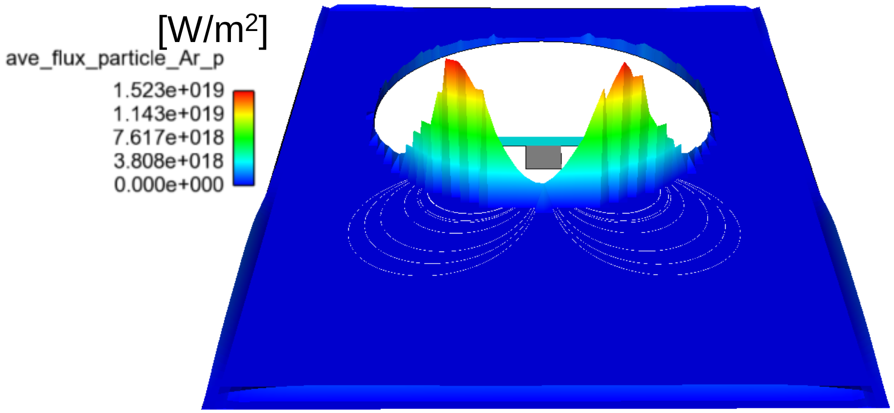


Hybrid mesh for magnetron sputtering simulation with rotary target :

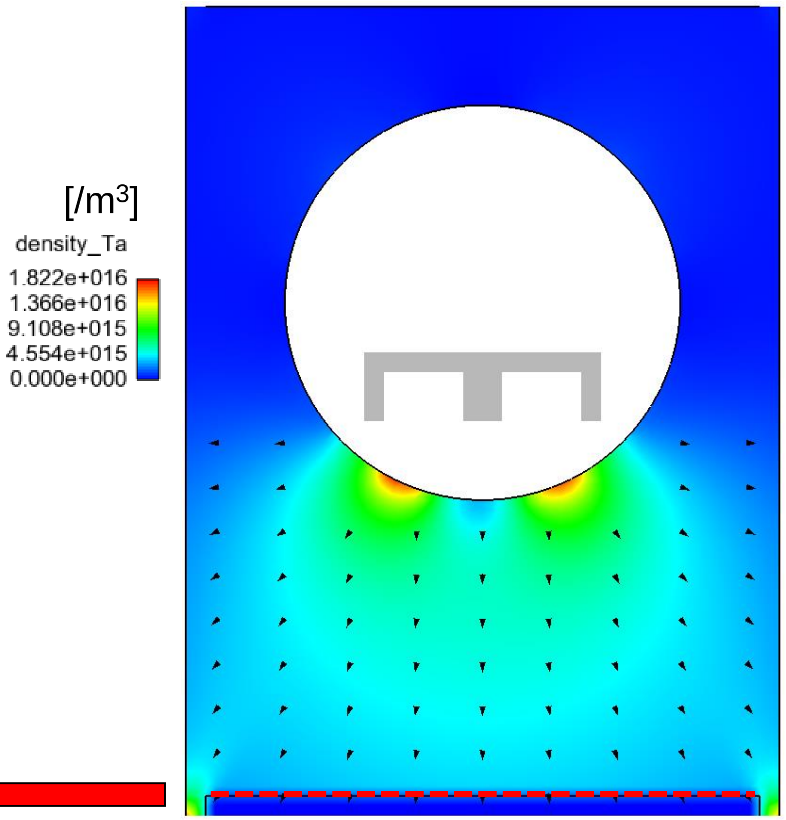
- ✓ Rectangle cell in space domain
- ✓ Cut cell is on curved surface

2. Results

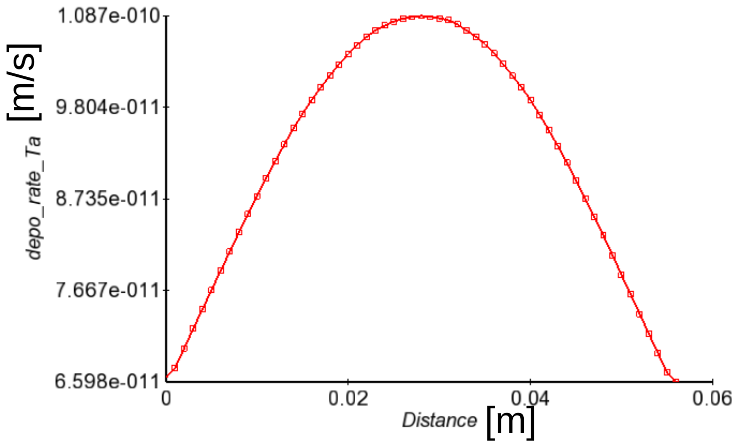
- Ar^+ Ion Energy Flux (Plasma module)



- Ta Number Density with Flow Vector (Neutral module)



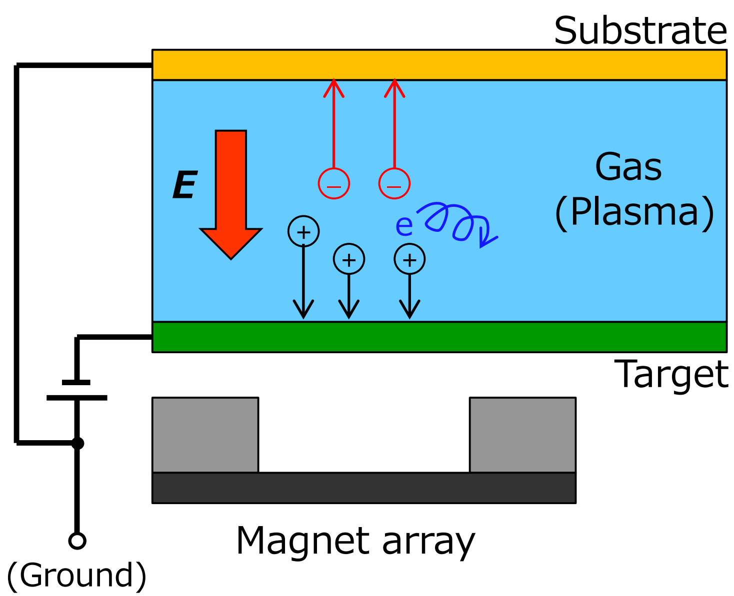
- Ta Deposition Rate on Substrate



3. Magnetron Sputter negative ion

It is easy for halogen gas, for example oxygen and fluorine, to form negative ion because of the large electron affinity. The negative ion damages substrate in DC magnetron sputtering process.

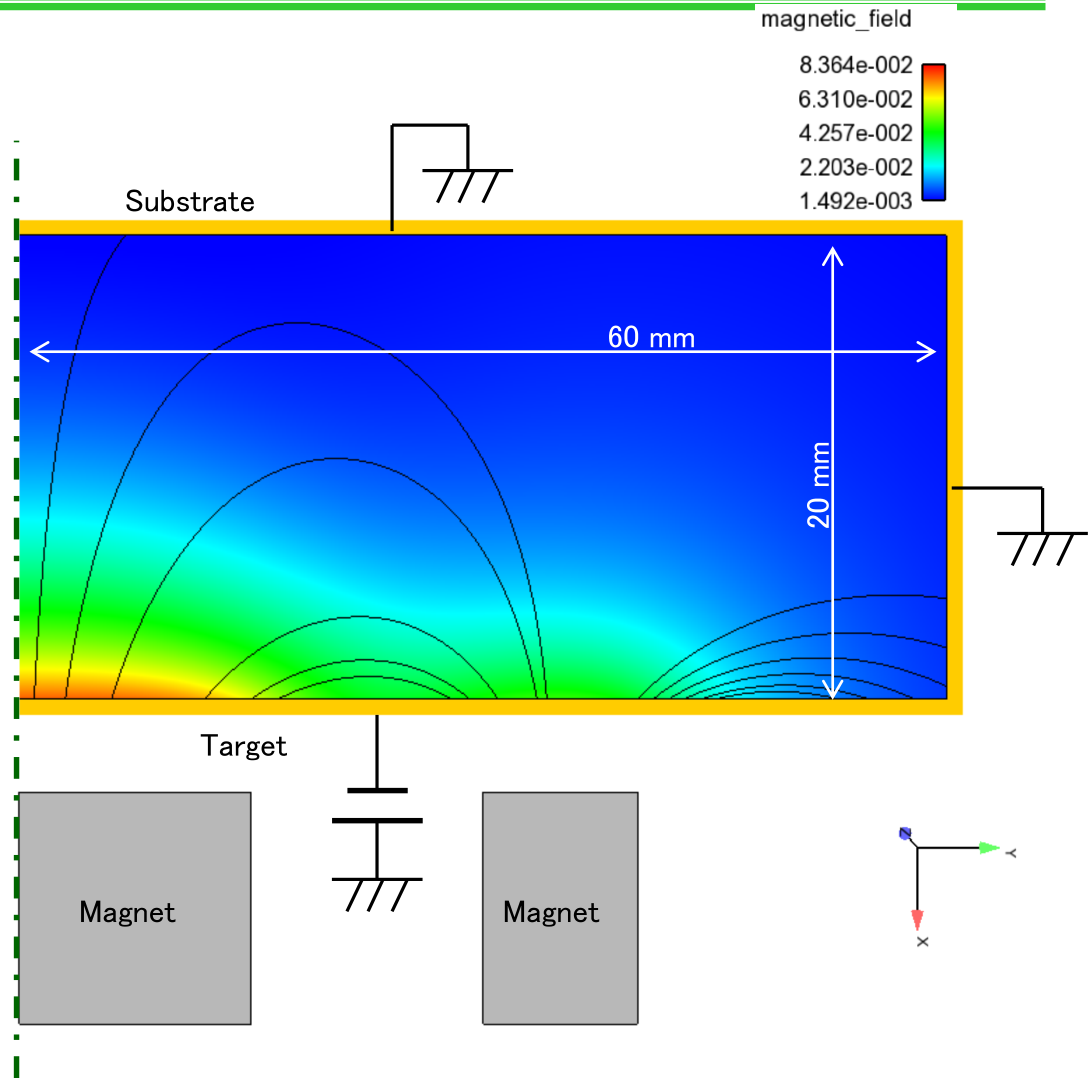
We simulate plasma including negative ions using Particle-PLUS.



- ✓ Positive ions move according to electric field, and bump into target (sputtering)
- ✓ **Negative ions move according to electric field, and bump into substrate (damage)**
- ✓ Electrons move with cyclotron motion by magnetic field.

3. Magnetron Sputter negative ion

- ✓ 2D–axisymmetric model
- ✓ Mixture of Ar and O_2, total pressure 1 Pa (0.5 Pa + 0.5 Pa)
- ✓ DC −250 [V] on target
- ✓ 2ndary electron emission coefficient 0.02



3. Gas Reaction

Collision reaction data set for O_2–Ar mixture consists of (a) pure O_2 data, (b) pure Ar data, and (c) interactions of O_2 (or products from O_2) and Ar. The data set is shown in the following table.

- Table a-1. Collision-reactions of pure O_2 system

No.	Collision reaction			Type	Reference
(1)	$e + O_2$	→	$e + O_2$	Elastic	(Phelps, 1978)
(2)	$e + O_2$	→	$e + O_2^*$	Excitation	(Phelps, 1978)
(3)	$e + O_2$	→	$e + O + O$	Dissociation	(Phelps, 1978)
(4)	$e + O_2$	→	$e + O + O^*$	Disso. Excitation	(Phelps, 1978)
(5)	$e + O_2$	→	$e + O^* + O^*$	Disso. Excitation	(Phelps, 1978)
(6)	$e + O_2$	→	$e + e + O_2^+$	Ionization	(Phelps, 1978)
(7)	$e + O_2$	→	$O^- + O$	Disso. Attachment	(Phelps, 1978)
(8)	$e + O_2$	→	O_2^-	Attachment	(Phelps, 1978)
(9)	$e + O_2$	→	$e + O^+ + O^-$	Ion-pair Formation	(Rapp et al., 1965)
(10)	$e + O_2$	→	$e + e + O^+ + O$	Disso. Ionization	(Eliasson & Kogelschatz, 1986)

3. Gas Reaction

- Table a-2. Collision-reactions of pure O_2 system

No.	Collision reaction			Type	Reference
(11)	$O_2^+ + O_2$	→	$O_2^+ + O_2$	Elastic	(Djilali & Mohammed, 2014)
(12)	$O_2^+ + O_2$	→	$O_2 + O_2^+$	Charge Transfer	(Langevin theory)
(13)	$O^- + O_2$	→	$O^- + O_2$	Elastic	(Langevin theory)
(14)	$O^+ + O_2$	→	$O + O_2^+$	Charge Transfer	(Langevin theory)

- Table b. Collision-reactions of pure Ar system

No.	Collision reaction			Type	Reference
(1)	e + Ar	→	e + Ar	Elastic	(Yamabe et al., 1983)
(2)	e + Ar	→	$e + Ar^*$	Excitation	(Yamabe et al., 1983)
(3)	e + Ar	→	$e + e + Ar^+$	Ionization	(Hayashi, 1987)
(4)	$Ar^+ + Ar$	→	$Ar^+ + Ar$	Elastic	(Phelps, 1991)
(5)	$Ar^+ + Ar$	→	$Ar + Ar^+$	Charge Transfer	(Phelps, 1991)

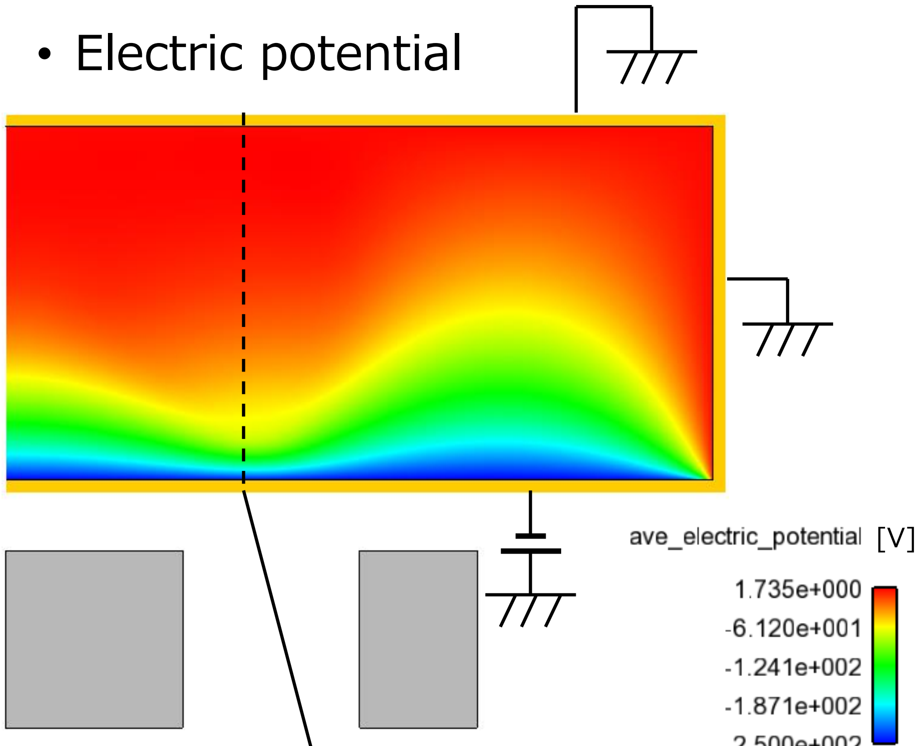
3. Gas Reaction

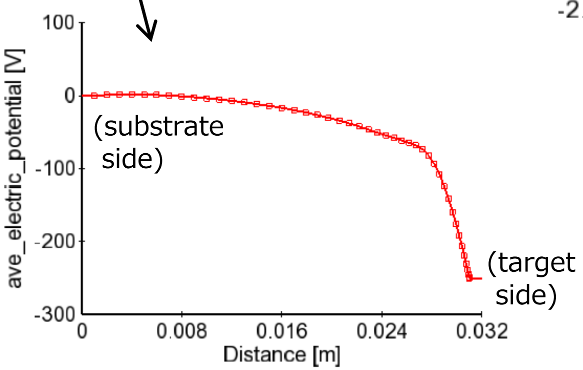
- Table c. additional collision-reactions for O_2-Ar mixture system

No.	Collision reaction			Type	Reference
(1)	$O_2^+ + Ar$	→	$O_2^+ + Ar$	Elastic	(Langevin theory)
(2)	$O^+ + Ar$	→	$O^+ + Ar$	Elastic	(Langevin theory)
(3)	$O^- + Ar$	→	$O^- + Ar$	Elastic	(Penent et al., 1987)
(4)	$Ar^+ + O_2$	→	$Ar + O_2^+$	Charge Transfer	(Langevin theory)

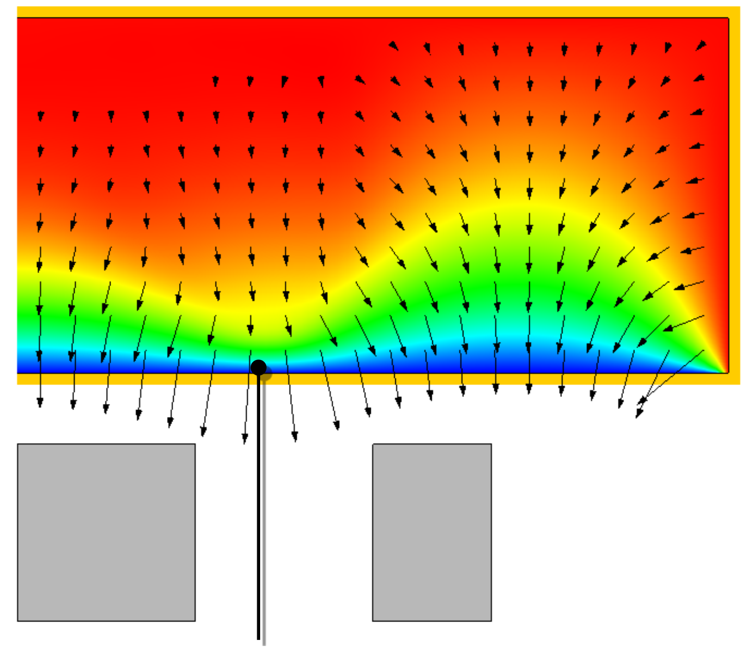
3. Results

- Electric potential





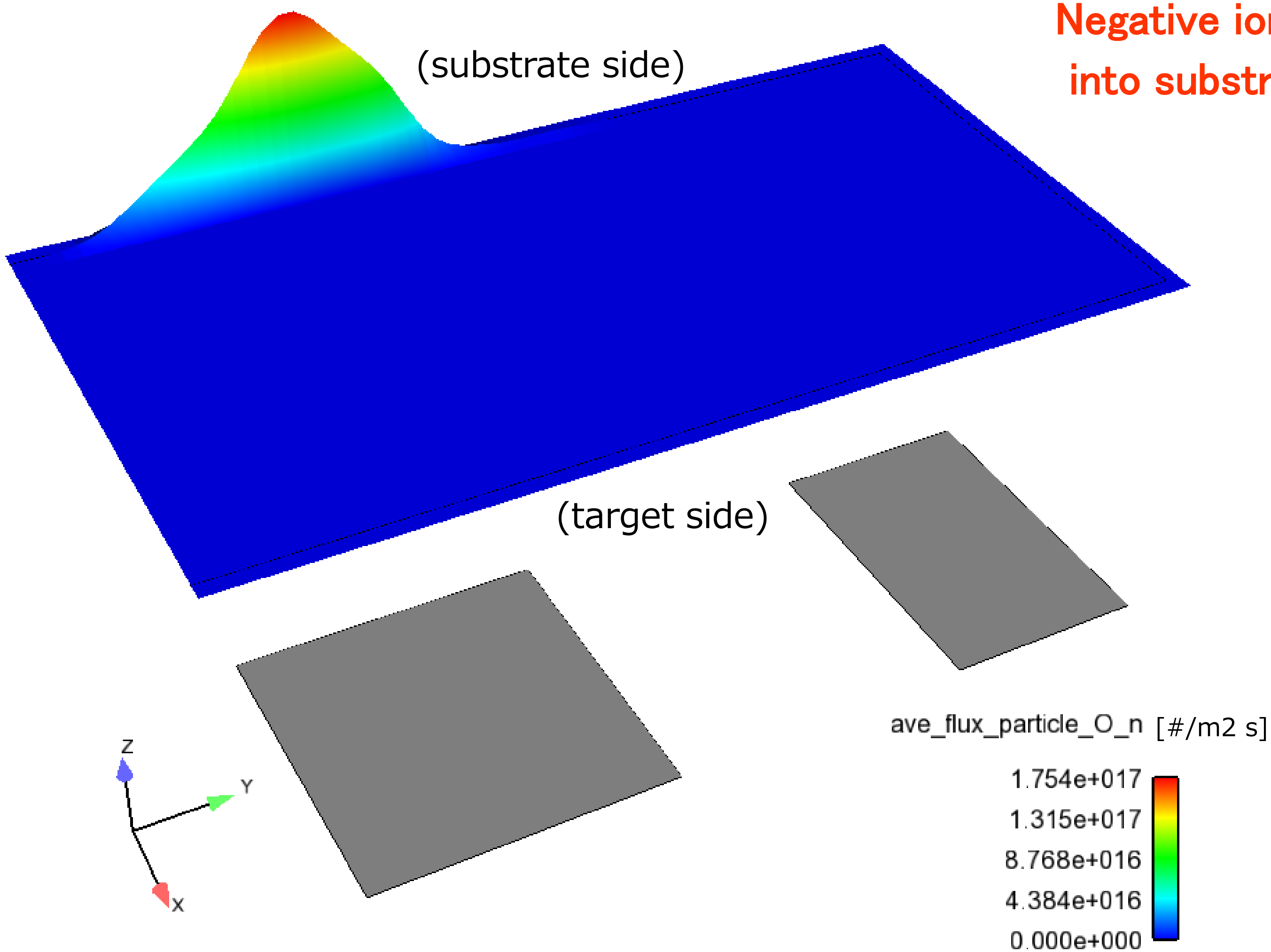
- Electric potential with electric field vector



The electric field in plasma is toward the target side.

3. Negative ion flux

- Number flux of O^{-} ion



Negative ions bump into substrate.

Summary

1. DSMC-Neutrals / Particle-PLUS are useful for simulation of magnetron sputtering.
   User can obtain profiles of background gas, magnetic field, electron/ion density, flux, erosion, deposition and so on.

2. Particle-PLUS can simulates RF magnetron plasma considering self-bias effect.

3. Particle-PLUS can simulates sputtering on circular target.

4. Particle-PLUS can simulates 3D magnetron plasma considering cross-corner effect.