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Particle-in-Cell Simulations of Plasma Discharge in DC Magnetron Sputtering

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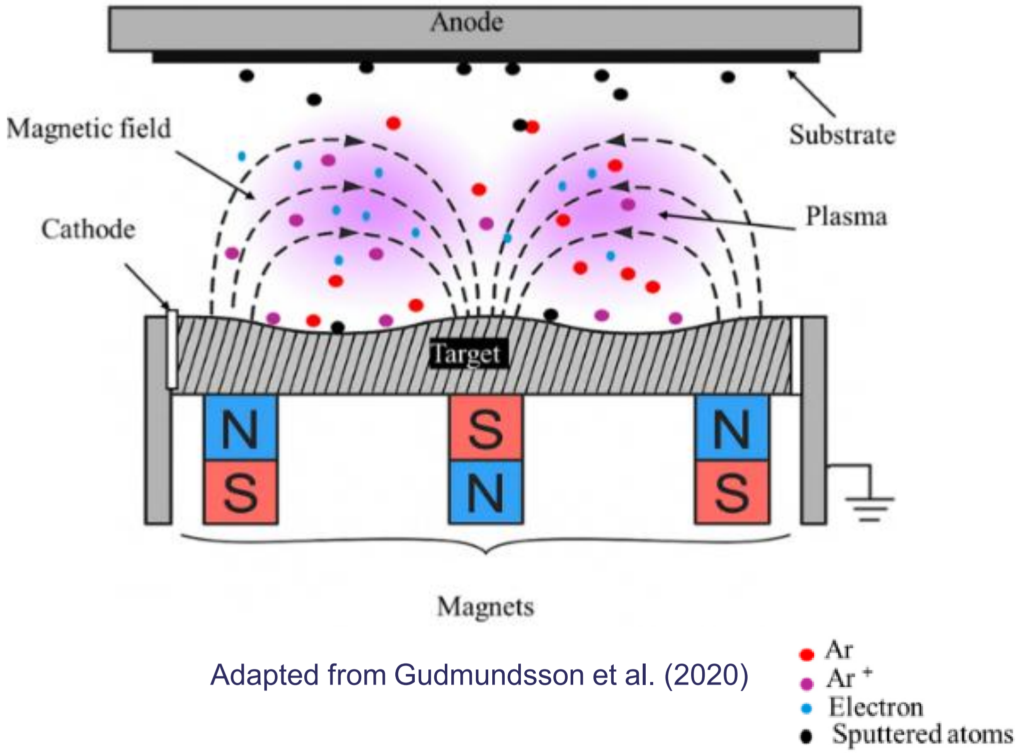
Outline

- Motivation
- Particle-in-Cell Method
- Problem Formulation
- Plasma discharge simulation results
  - Plasma Instabilities (Spokes)
- Summary & Future Outlook

Motivation

- Understanding the plasma discharge behaviour in a Magnetron important as this influences the ion energy/ flux impacting the target.
- Important to capture the electron kinetics, E×B drift, plasma instabilities & secondary electron emissions as this influences the transport of sputtered particles, ultimately affecting deposition rate and film properties.
- Plasma-kinetic models required to accurately model the non-equilibrium electron dynamics, magnetic confinement and particle–surface interactions that are not fully captured by conventional fluid models.
- Experimental diagnostics & modelling need to work hand-in-hand.



Adapted from Gudmundsson et al. (2020)

Experimental Results - Spokes

Drifting Ionization Zone in Sputtering Magnetron Discharges at Very Low Currents

André Anders, Pavel Ni, and Joakim Andersson

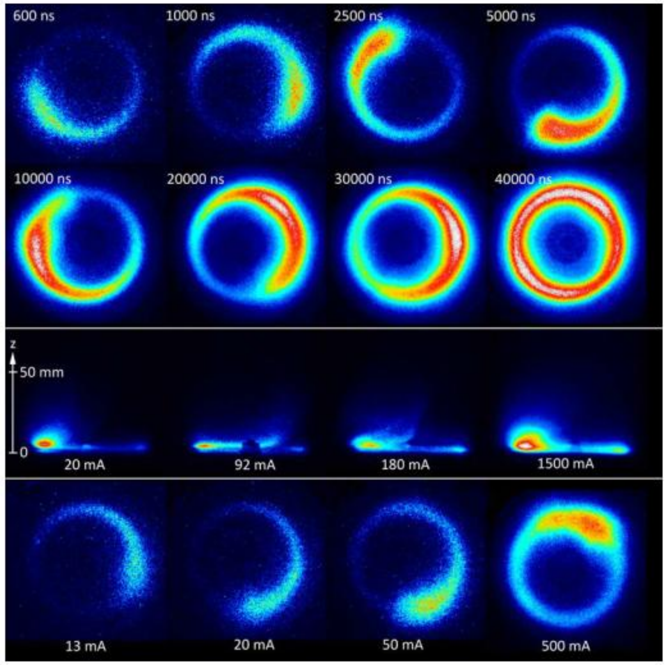
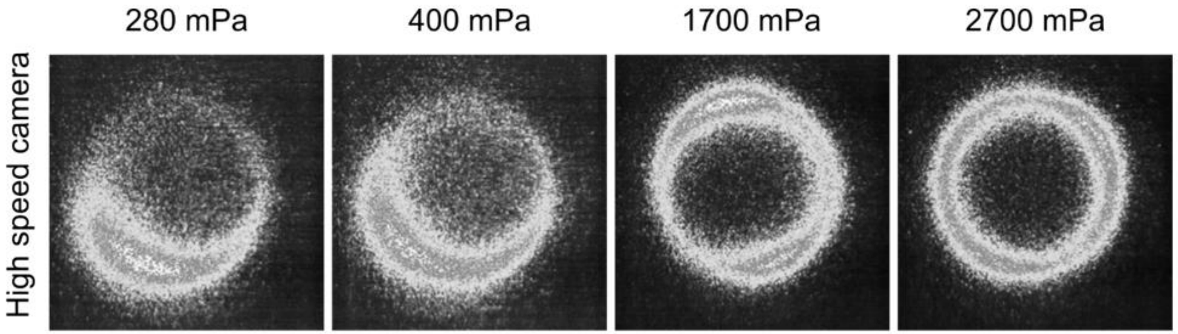


Fig. 1. False-color fast camera images of aluminum sputtered in 0.5 Pa of argon. The top 8 images show the blurring of a drifting ionization zone when the image exposure time exceeds 5 μs (the discharge current was 30 mA). The center 4 side-view images were taken with an exposure time of 500 ns for different discharge currents; z is the distance from the target surface. The lower 4 images, also taken with 500 ns exposure time, illustrate the existence of one zone at different currents. Note that the camera was always in the linear regime; the image intensifier's gain had to be increased to make plasma visible at short exposures, and decreased to avoid saturation at long exposures, and hence the apparent brightness should be judged with caution.

- Spoke instability typical in $\boldsymbol{E} \times \boldsymbol{B}$ discharges like Magnetron discharges.
- They appear as localized zones of high excitation and ionization rate moving along the racetrack.
- The direction of rotation depends on the discharge power density.



Andreas Pflug & Michael Vergöhl (2019).

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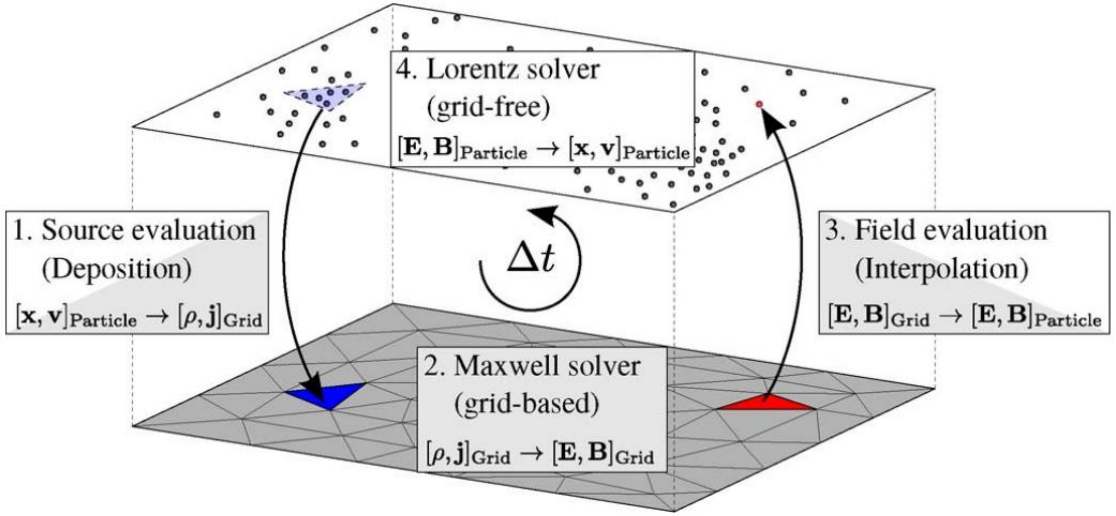
Particle-in-cell (PIC) Method

(simulations done using open-source code, PICLas)

- The PIC method describes the electromagnetic interaction between charged particles in a plasma. Particle tracking and electromagnetic fields (Eulerian) are coupled in PIC.
- **Particle Solver** - particle push (motion) determined by Newton's laws of motion and Lorentz force
  - calculates charge and current density due to the particles
- **Field solver** – **Electrostatic** PIC (Poisson's equation) or **Electromagnetic** PIC (Maxwell's equation)
  – The field solver calculates the Electric (E) & Magnetic (B) fields at **grid points**



Physics of Fluids 31, 072006 (2019)

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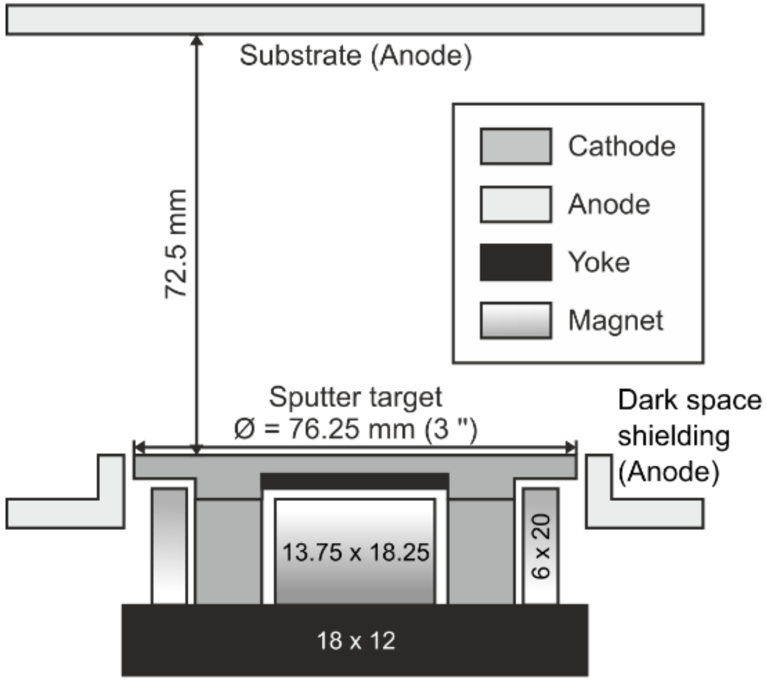
PIC-MCC simulations – Problem formulation

(simulations done using open-source code, PICLas)

- Electrostatic 3D PIC model with a constant background magnetic field considered here.
- Background Ar gas density >> Ar+ & e- density. Particle collisions modelled using the Monte Carlo Collision (MCC) model.
- Total Discharge current = 5 mA, Total Power =1.5W
- Discharge voltage = -(250 to 300) V.
- Neumann BC at the gap and Dirichlet BC at all other boundaries
- Secondary electron emission yield = 0.13
- Magnetic remanence =1.4 T



Schematic of DC Magnetron geometry

PIC-MCC simulations – Problem formulation

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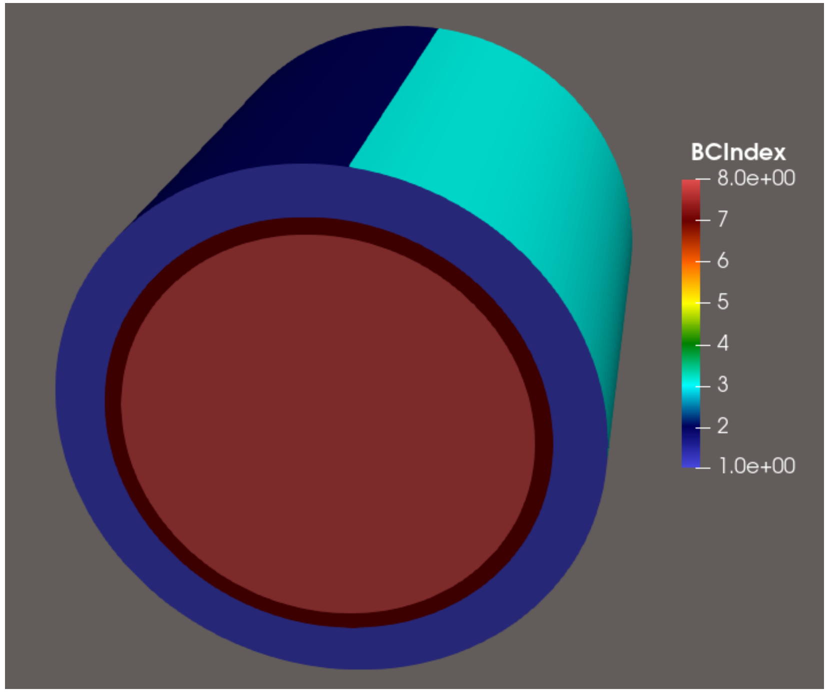
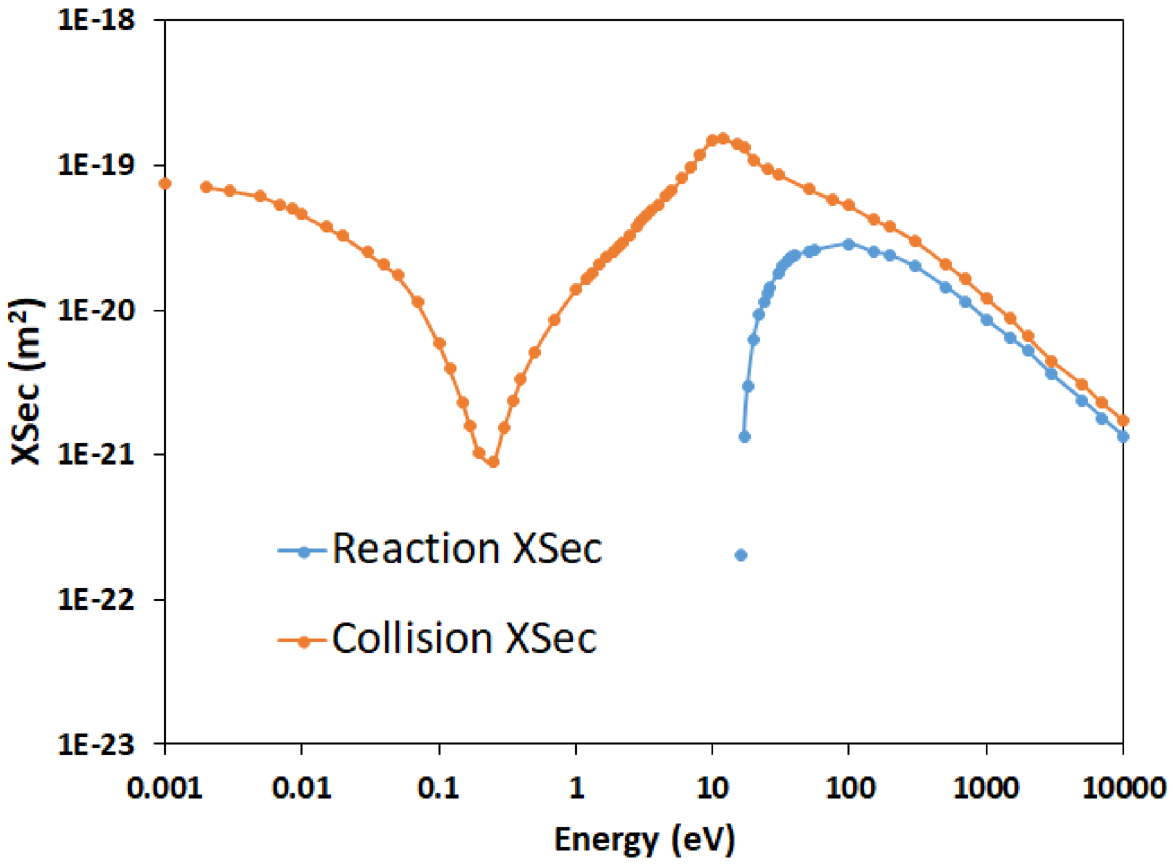
- Secondary electron emission yield = 0.13
- Magnetic remanence =1.4 T (1.11×10^6 A/m)



Representative computational domain considered for the 3D PIC-MCC simulations

Reaction framework & cross sections



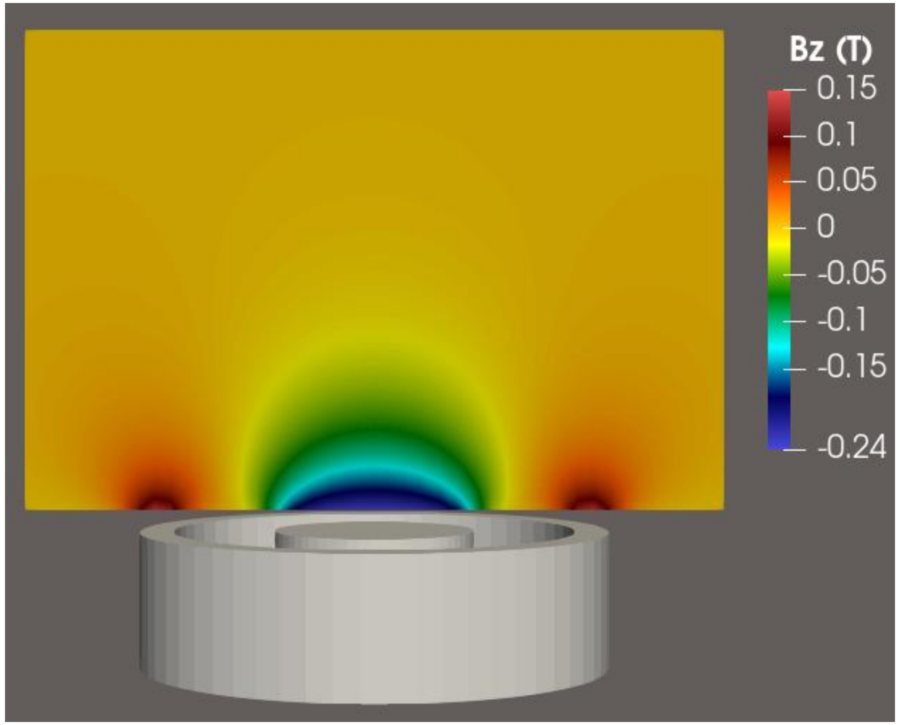
Electron Impact Ionization: $e^- + Ar \rightarrow Ar^+ + 2e^-$

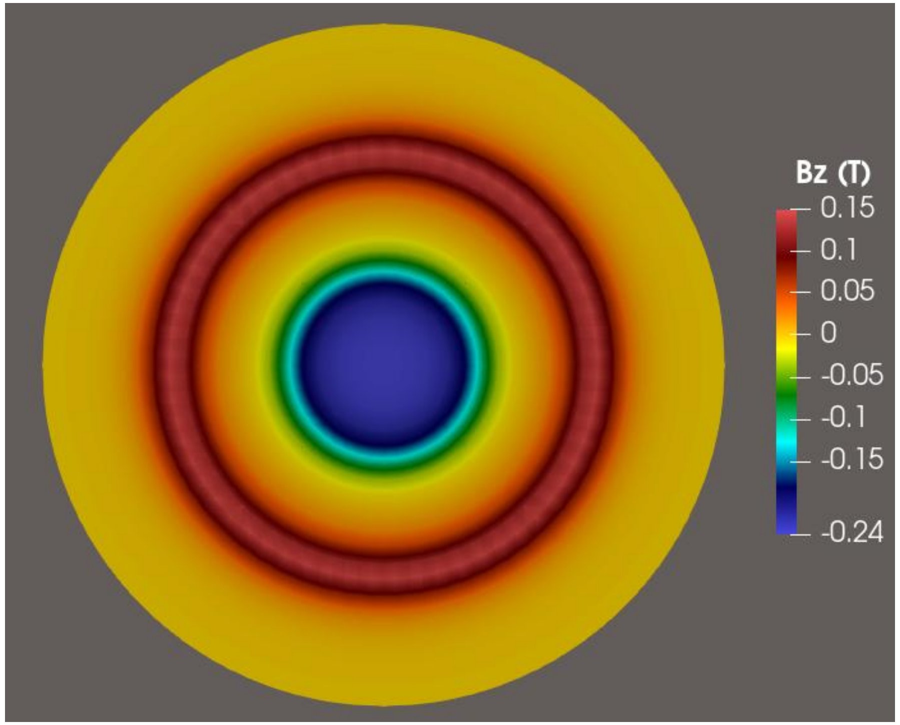
Wall Secondary Electrons : Ar^+ + Target → Ar + Target + e^-

Electron Impact Excitation: $e^- + Ar \rightarrow Ar^* + e^-$

Charge Exchange Collision: $Ar^+ + Ar \rightarrow Ar + Ar^+$

Background Magnetic Field for the PIC Simulations



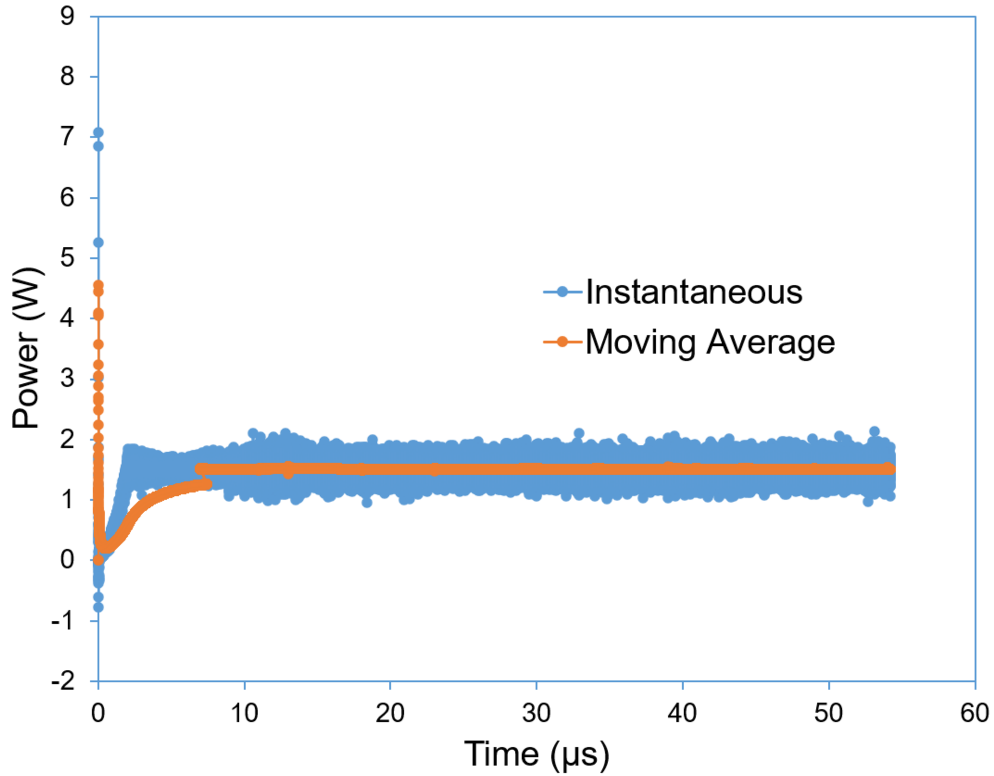


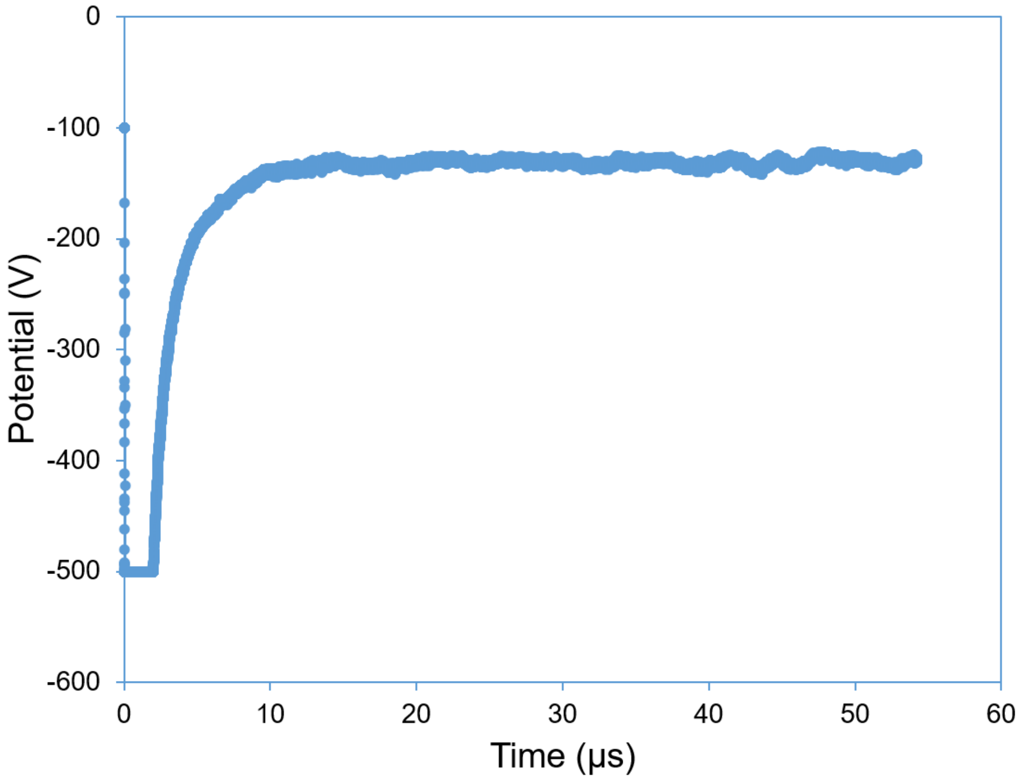
Fixed Power Controller Scheme

(Variation of power and voltage versus time)

- Fix power by adaptively changing the potential difference at the target. A constant voltage would lead to incorrect power-voltage relationship as plasma discharge is a dynamic process.

(Ar gas pressure = 280 mPa, Target Power=1.5W)



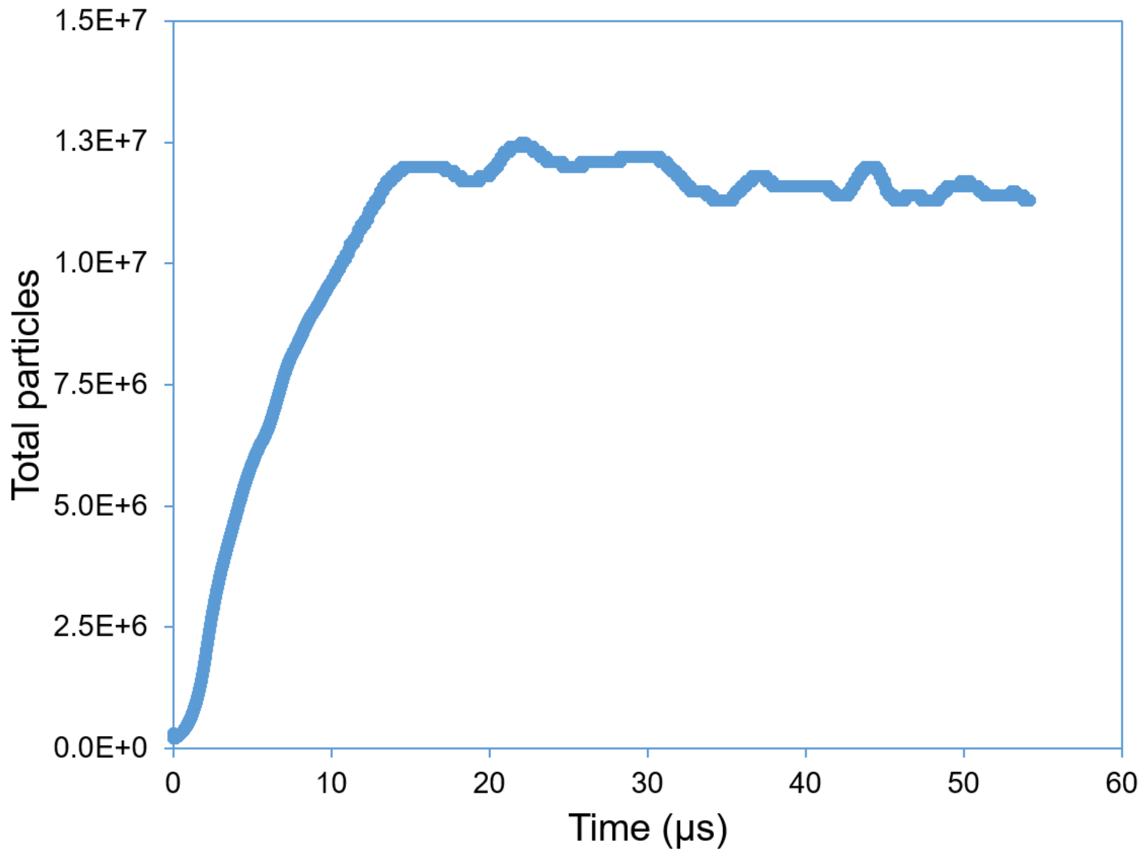


Fixed Power Controller Scheme

(Evolution of number of particles in the domain)

- Fix power by adaptively changing the potential difference at the target. A constant voltage would lead to incorrect power-voltage relationship as plasma discharge is a dynamic process.

(Ar gas pressure = 280 mPa, Target Power=1.5W)



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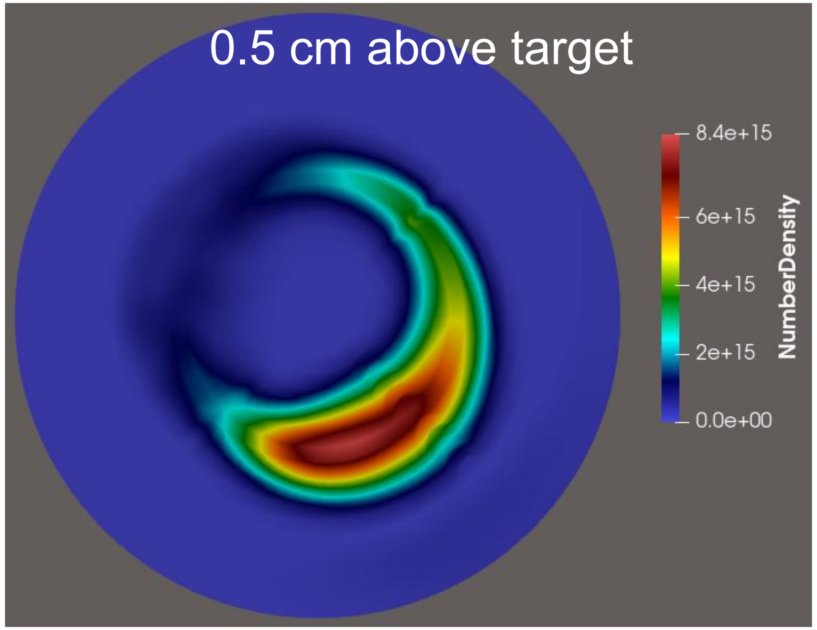
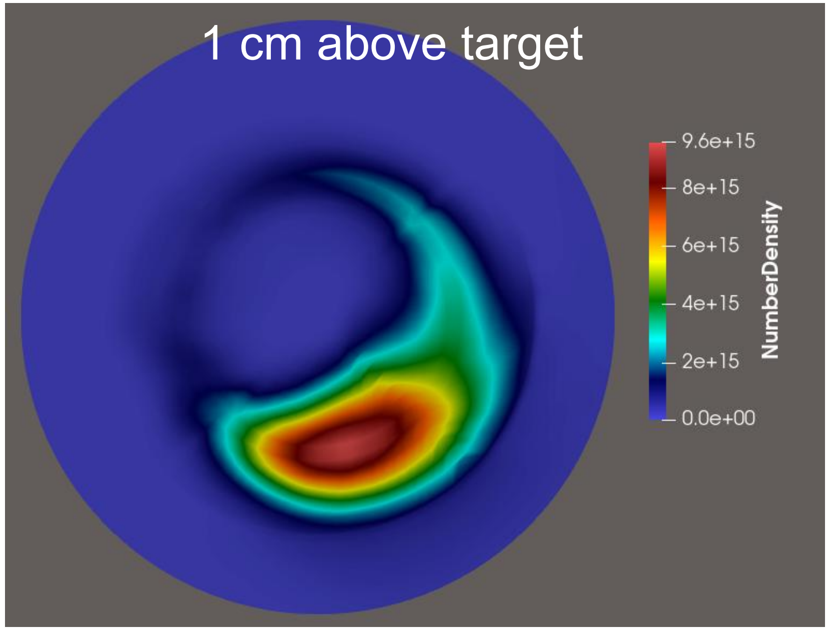
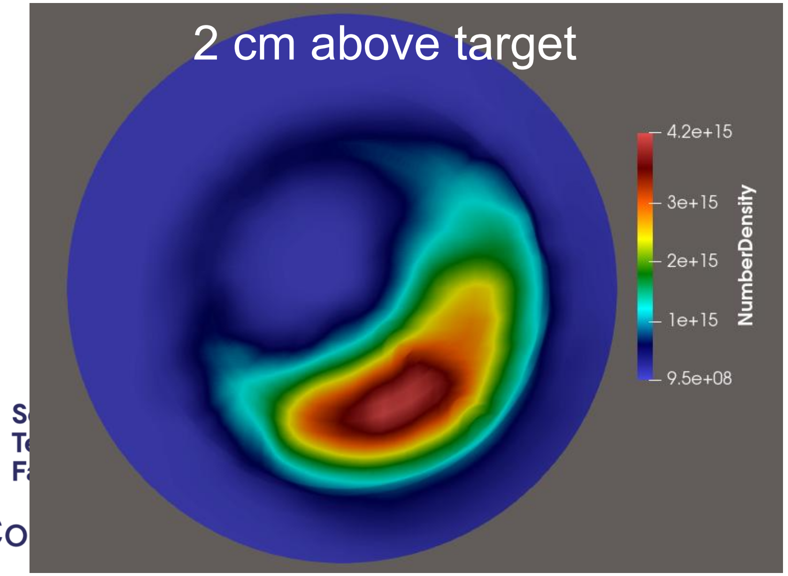
Spokes at different locations above the target

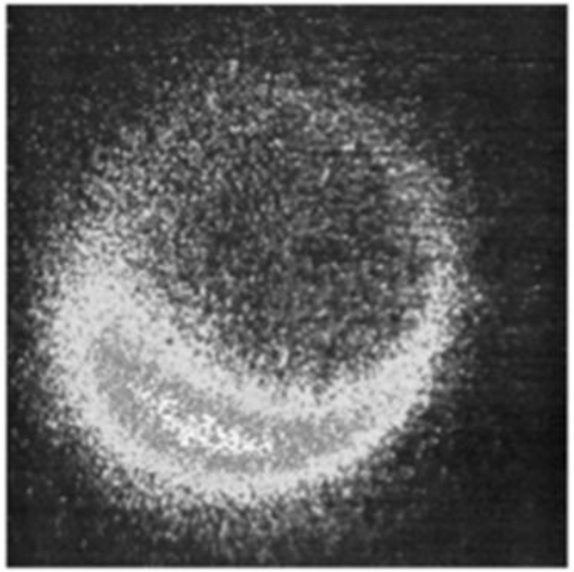
(Ar gas pressure = 280 mPa)







High speed camera



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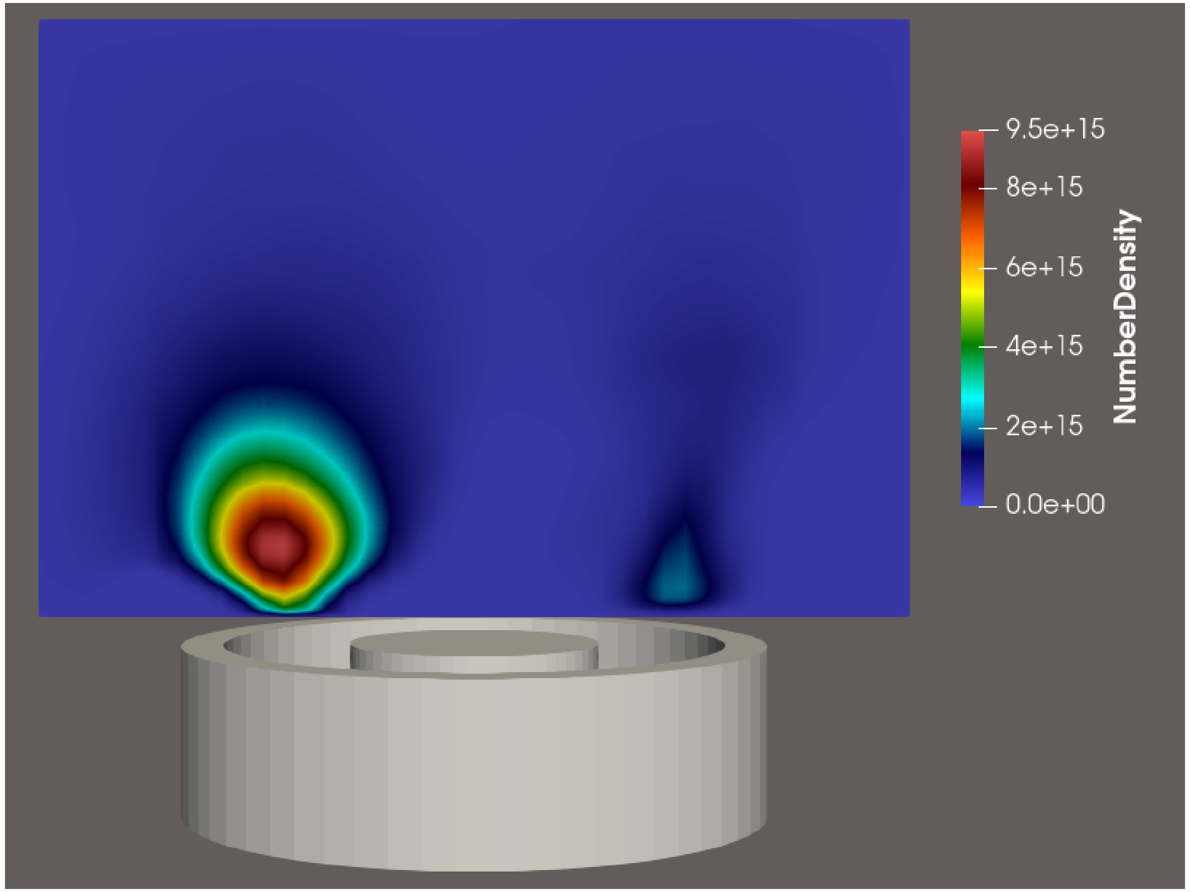
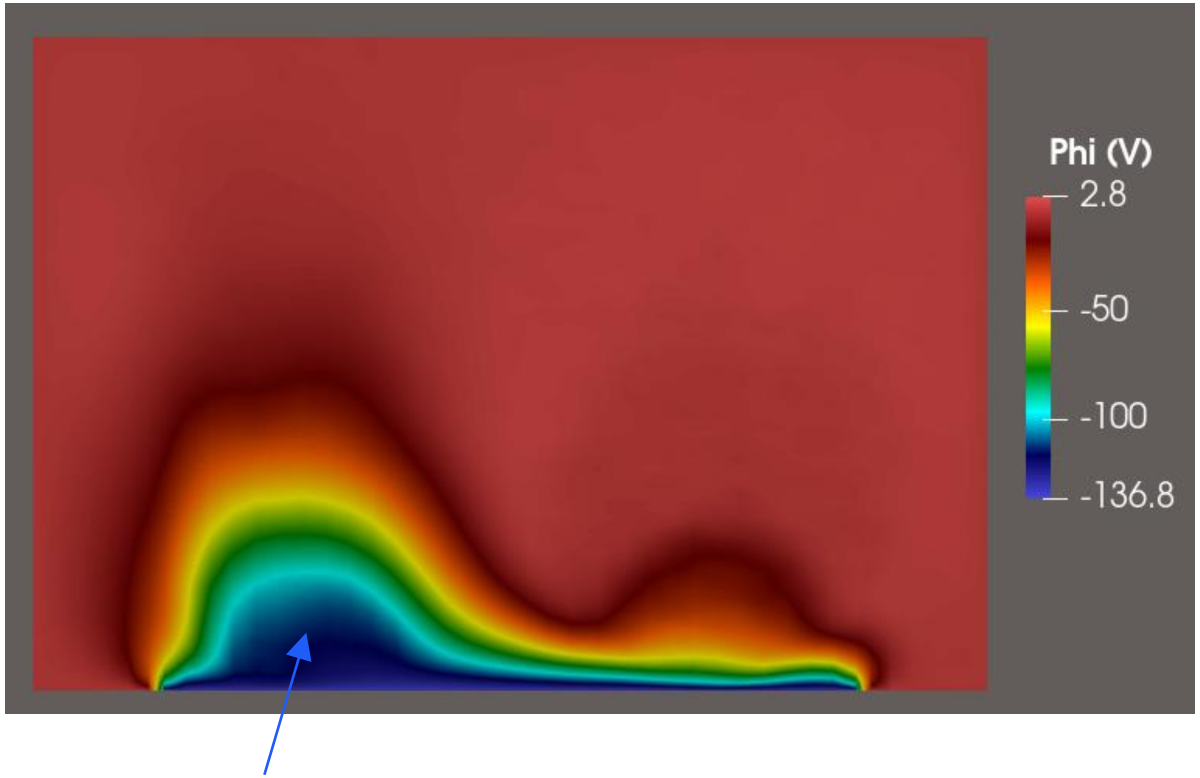
Plasma Potential Distribution in the Domain

(Ar gas pressure = 280 mPa)

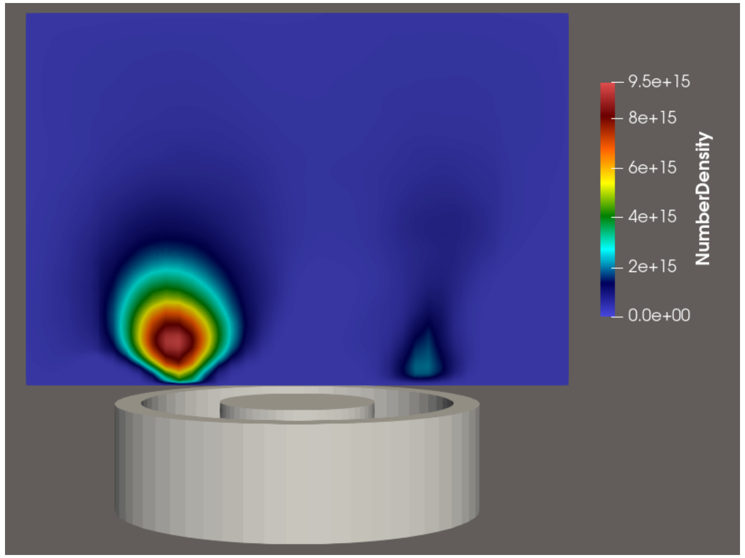


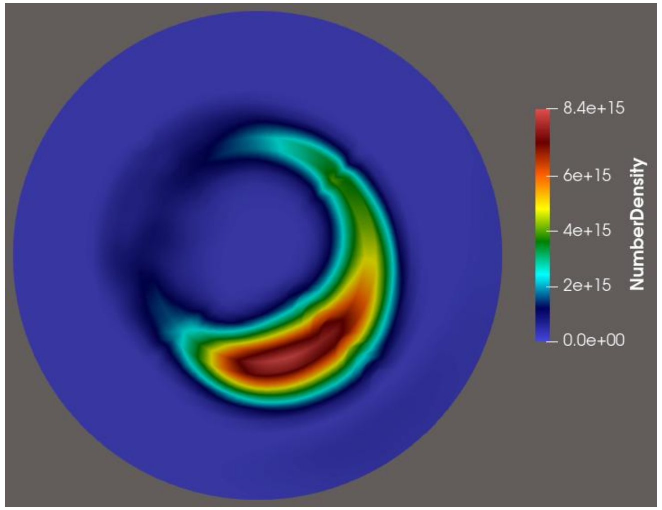


Local plasma potential rises sharply by several tens of volts in regions of high ionisation zones (spokes).

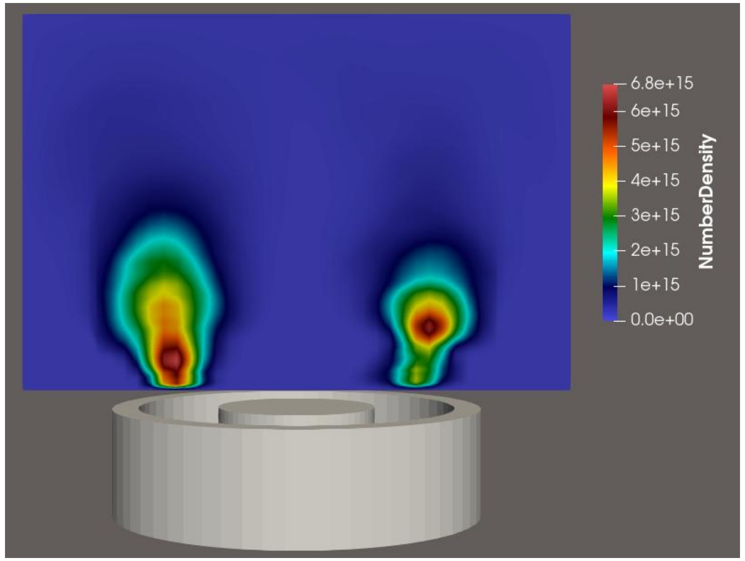
Effect of Operating Pressure on Plasma Discharge

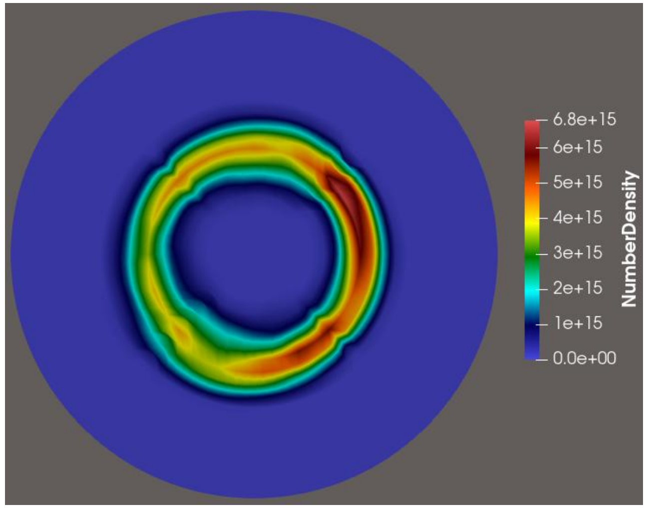
280 mPa





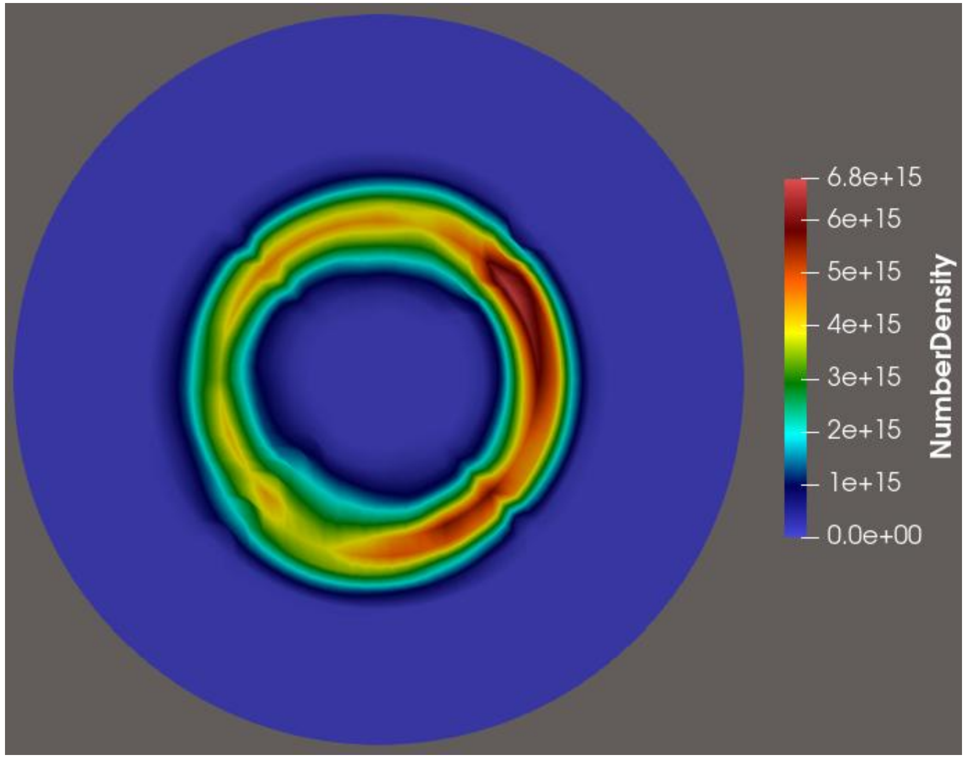
1700 mPa

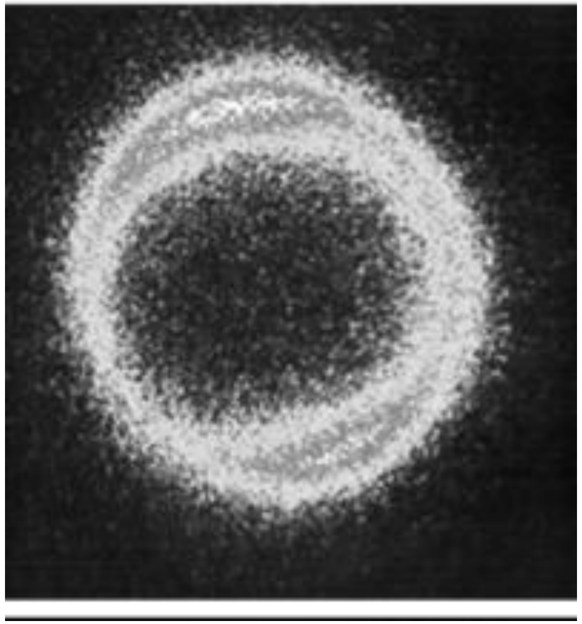




Comparison of Spokes at Higher Pressures

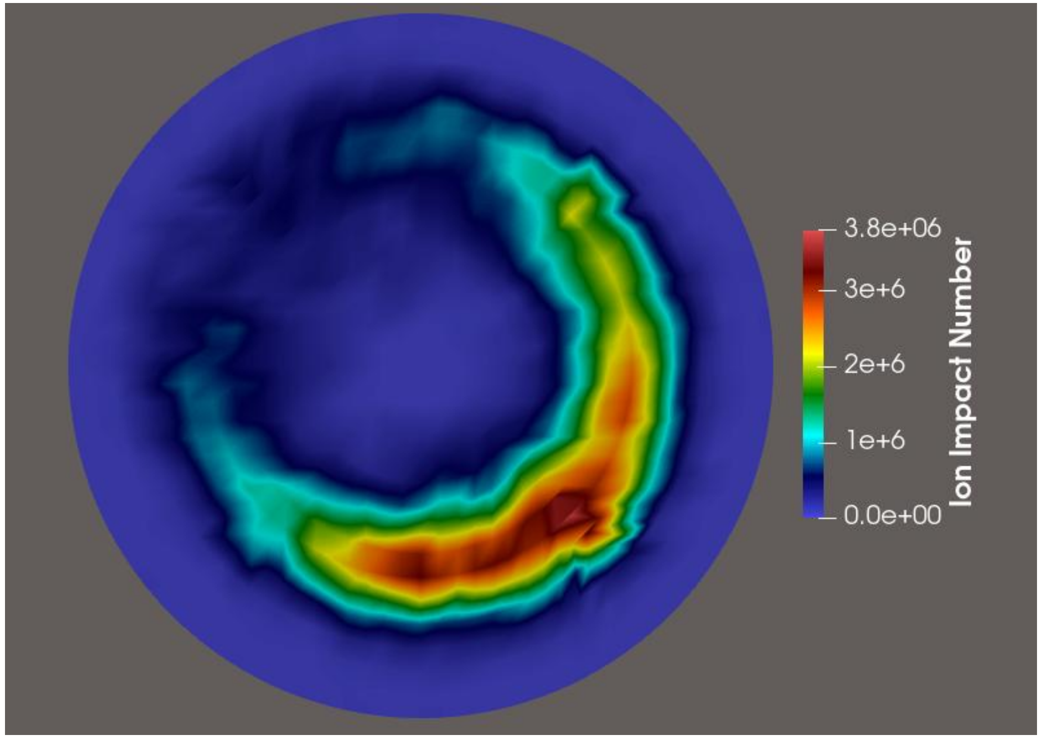
(Ar gas pressure = **1700 mPa**)

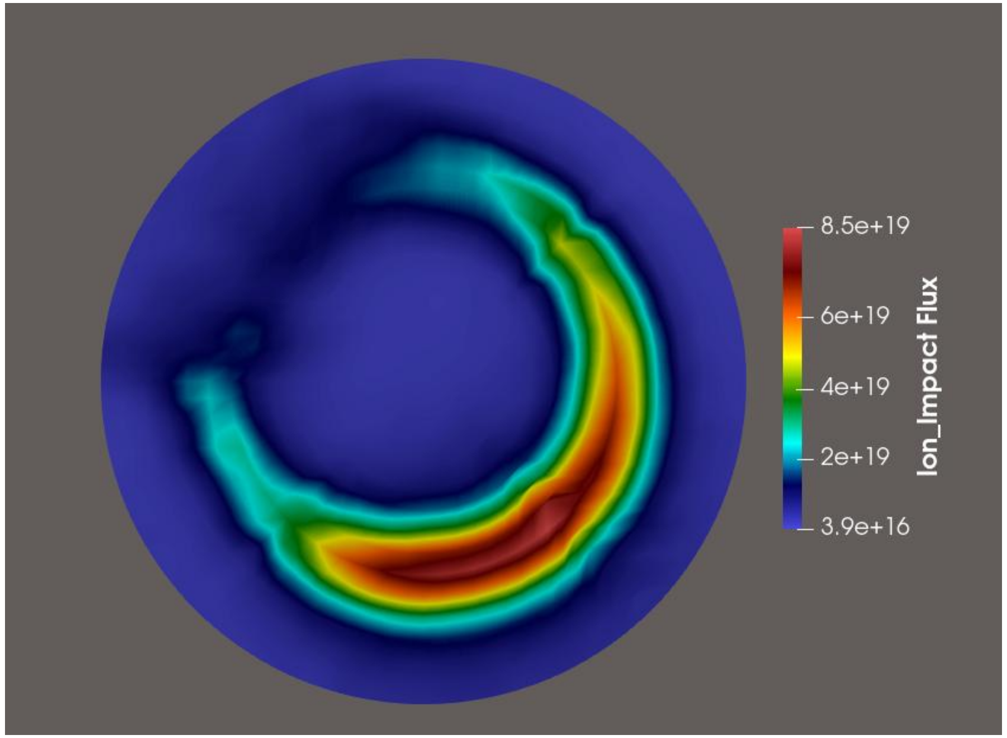




Ion impact rate Patterns at the Target

(Ar gas pressure = 280 mPa)





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Summary

- PIC models customised for DC Magnetron simulations at different operating conditions.
- Qualitative validation for the plasma discharge/ spokes obtained from the simulations.
- Parametric studies being carried out & testing the sensitivity of different parameters on the plasma discharge.
- Challenges due to uncertainties in the values of SEE, geometry and B field.

Future Outlook: Improvements to Plasma Discharge & Sputtering Transport Models

- Switch from a PIC-MCC to PIC-DSMC model for the plasma discharge.
- Models need to account for gas heating and local rarefaction.
- Addition of more reactions, charge exchange models, reactive sputtering models.
- Scaling strategies from low power densities to more realistic power densities.

- Couple plasma discharge to a DSMC model with realistic collision models.
- Knudsen number in the transition regime
- Track the transport of sputtered particles from target to the substrate.

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Thank you

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