

Simulation-driven Engineering of Plasma Equipment for Material Applications, Gas Conversion, and Space Applications in COMSOL

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with great support from:

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PlasmaSolve

Since 2016, providing **consultancy service** for plasma technology development.

Expert in introducing **meaningful Industry 4.0** components into plasma technologies.

Subject matter expertise in plasma coating, ion sources, and plasma gas conversion.

Trusted by some of the most influential stakeholders in the industry.

Using COMSOL + own software product "MatSight" launched in 2024 (non-competing)



Department of Plasma Physics and Technology

Department head: Petr Vašina

Research groups at the department:

- > [Applied Plasmachemistry](#)
- > [Deposition of Thin films and Nanostructures](#)
- > [Didactics of Physic](#)
- > [Optics for Thin films and Solid surfaces](#)
- > [Plasma Diagnostics and Modelling](#)
- > [Plasma Nanotechnologies and Bioapplications](#)

Head: Tomáš Hoder

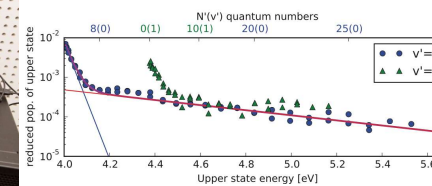
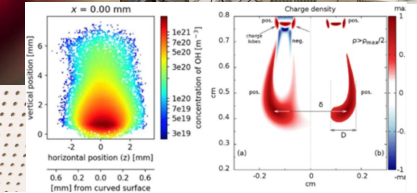
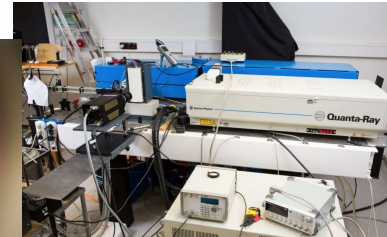
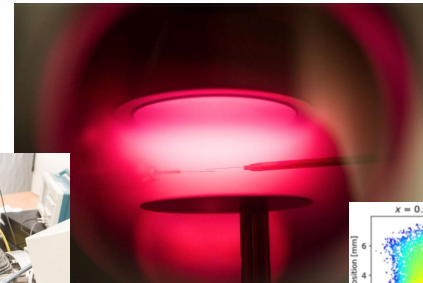
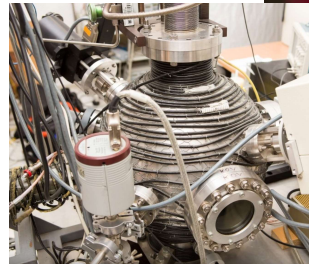
Zdeněk Bonaventura
Adam Obrusník
Zdeněk Navrátil
Vít Kudrle
Lucia Potočňáková
Pavel Dvořák
Martina Mrkvičková
Nima Bolouki

and
9 PhD students

Project director: Mirko Černák

Research programmes of the project:

- Discharge physics
- Plasma surface treatment
- Thin film deposition
- Plasma modified surface analysis
- Research and development of plasma generators
- Technology transfer



Contents

- What kind of medium is plasma?
- Where does humanity use plasma?
- What makes plasma simulation difficult? And how does COMSOL make it easier?

Case studies:

1. Optimizing a plasma reactor for solar-grade silicon production.
2. Simulating a hollow-cathode reactor for architectural glass applications.
3. Understanding the effect of waveforms on the plasma distribution.
4. Simulating gas flow in an MPD plasma thruster.

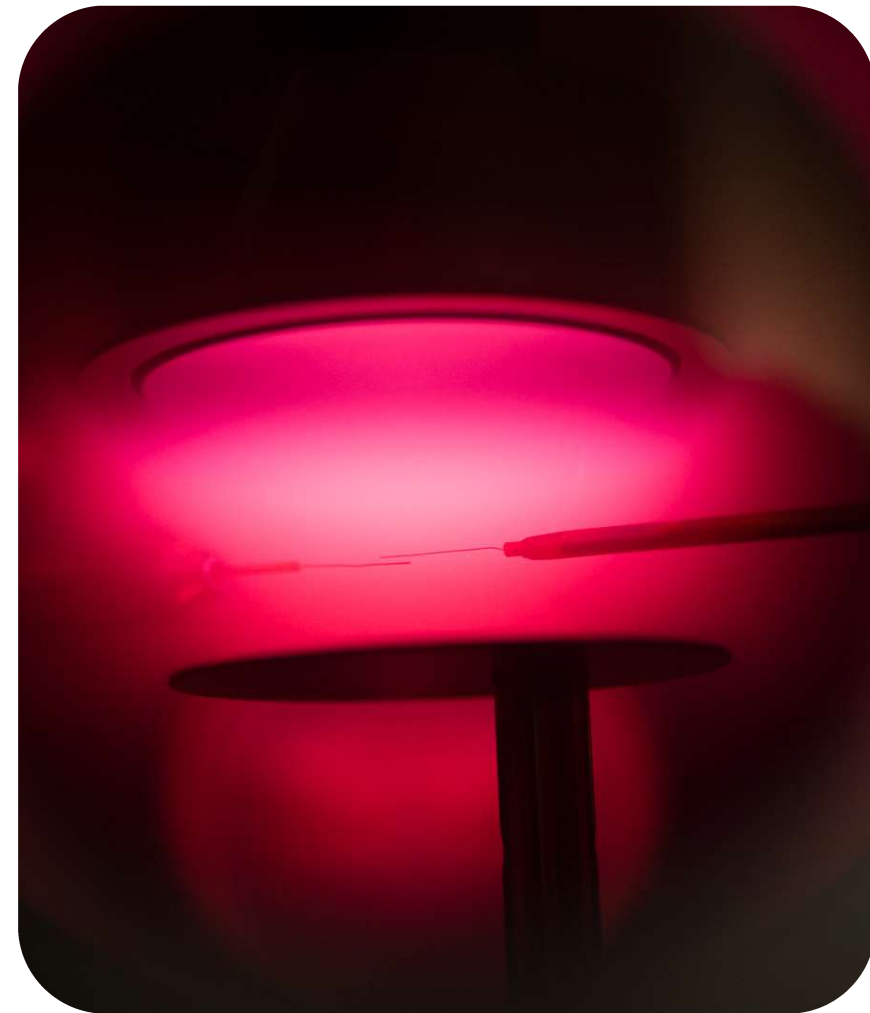
What is plasma?

Plasma

- Fourth state of matter...
- Gas with some/all atoms ionized, e.g. **Ar⁺ and e⁻**
- Electrically, partial ionization makes plasma a **lossy medium with complex ϵ** that depends on its properties.
- Further **ionization is caused primarily by electrons**.
- **Plasma is quasineutral** - density of positive and negative charge carriers is *nearly equal in most of the volume*.

Two fundamental plasma types

- **Equilibrium** - fusion plasmas, some arc discharges, stars. All particles are in thermodynamics equilibrium, Maxwell energy distribution
- **Non-equilibrium** - all other human-made plasmas. Light and heavy particles can maintain different temperatures and exotic energy distribution functions



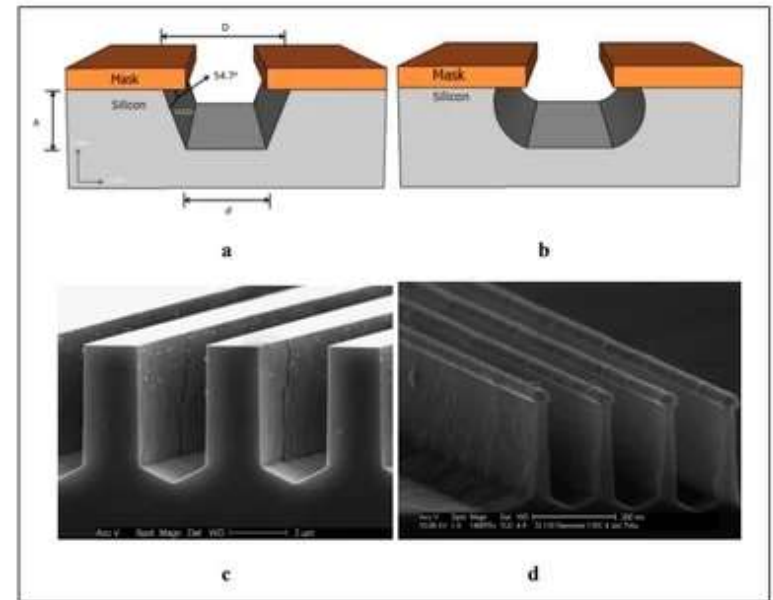
Where do we use plasma?

Plasma applications

Plasma is everywhere 😊

Plasma applications

Plasma is everywhere 😊



A&C- Anisotropic etching

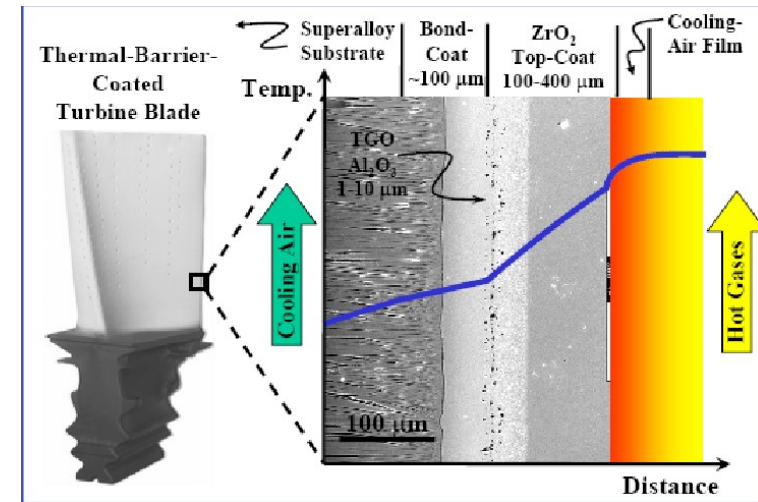
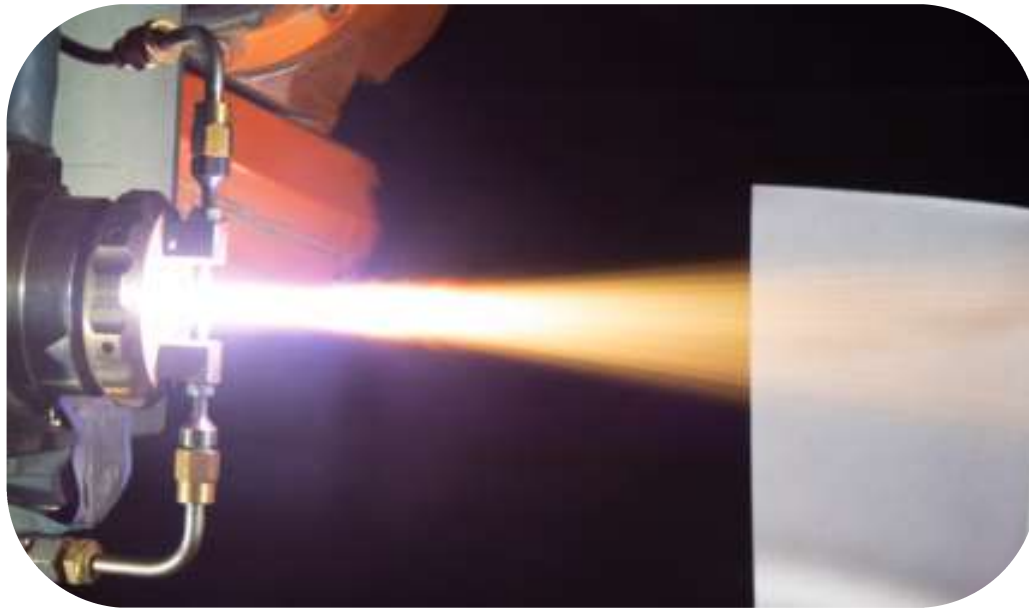
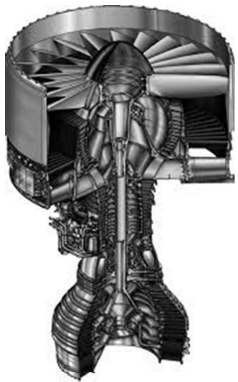
B&D Isotropic etching

(Avinash P. Navak . Logeeswaran VJ and M. Saif Islam, Univ. of California, Davis)

Wafer processing **in semiconductor industry** (dry etch, deposition).

Plasma applications

Plasma is everywhere ☺



Plasma sprayed barrier **coatings in turbines** for aerospace and energy sectors.

Plasma applications

Plasma is everywhere 😊



In modern buildings, nearly **all architectural glass is plasma-coated with low-e coatings.**
Solar panels are processed in similar large-area plasma coaters.

Plasma applications

Plasma is everywhere 😊



In a car, everything is plasma-treated.

ICU: pistons, cylinders for friction, oil bath for anti-corrosion, plastics and textiles for hydrophobicity, windows for anti reflection, decorative components for metallic look.

BEV: All of the above + battery anodes and battery contacts.

Plasma applications

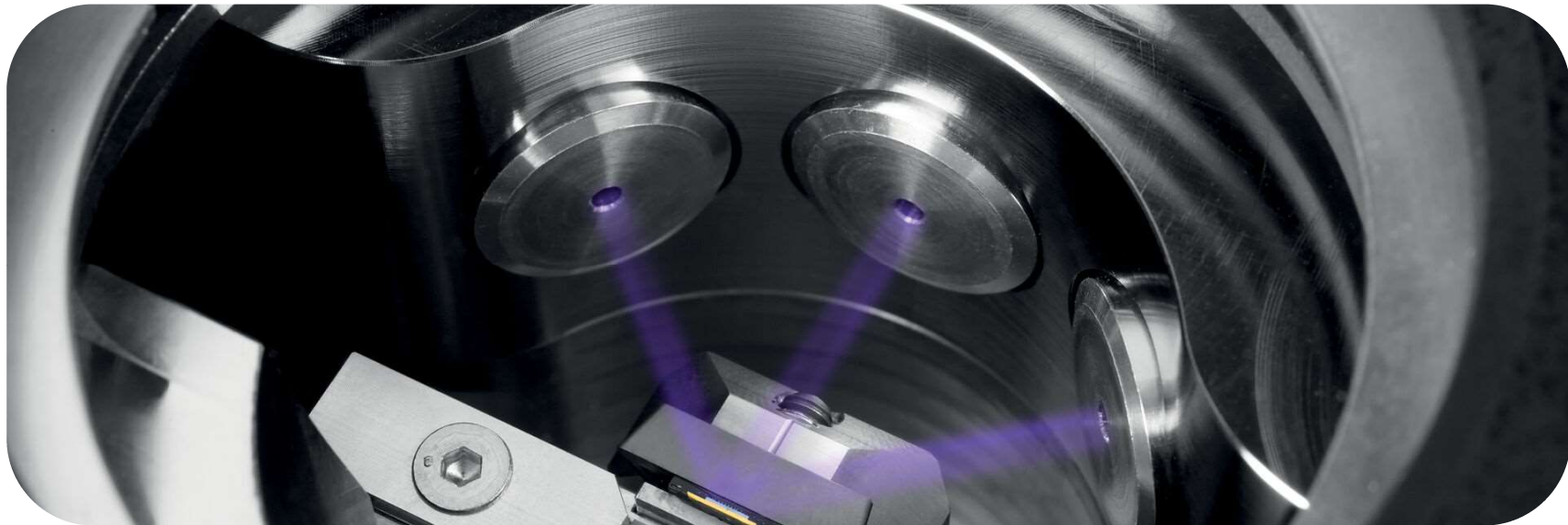
Plasma is everywhere 😊



Most plastics are porous - **plasma barrier SiOx coatings** now a standard on all food packaging.

Plasma applications

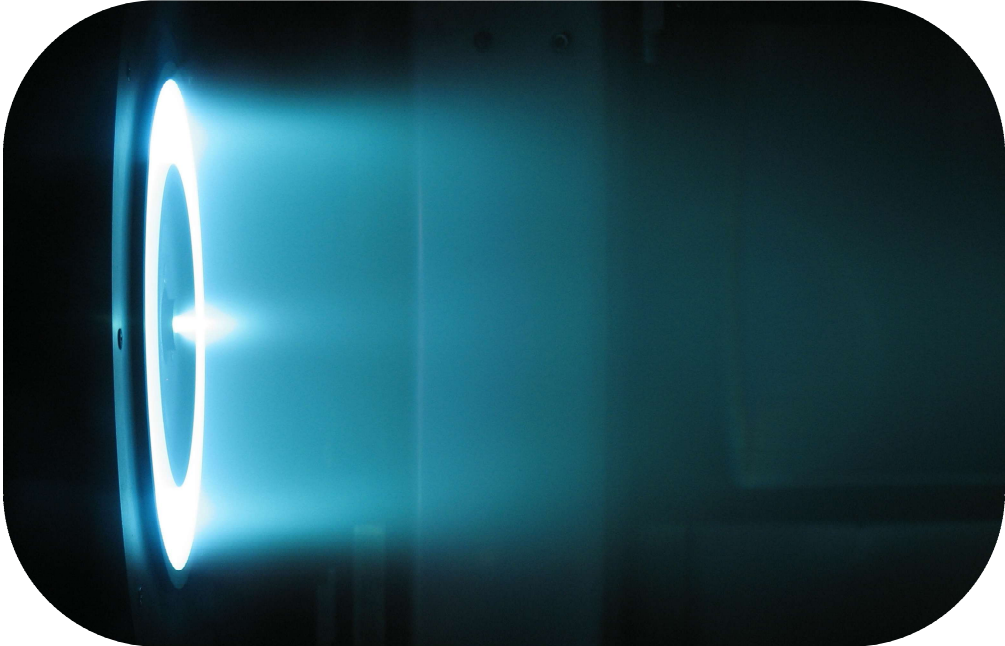
Plasma is everywhere 😊



Plasma-produced **ion beams** are a standard in nanostructure diagnostics, becoming standard in nanoscale manufacturing too (qubits, etc.)

Plasma applications

Plasma is everywhere 😊



Satellite electric propulsion - Hall thrusters and Gridded Ion Engines used since the 80s. Starlink equipped with argon Hall thrusters.

What makes plasma such a pain to simulate?

And how does COMSOL make it easier?

Difficulties with plasma simulation

There are a few properties that make plasma difficult to model:

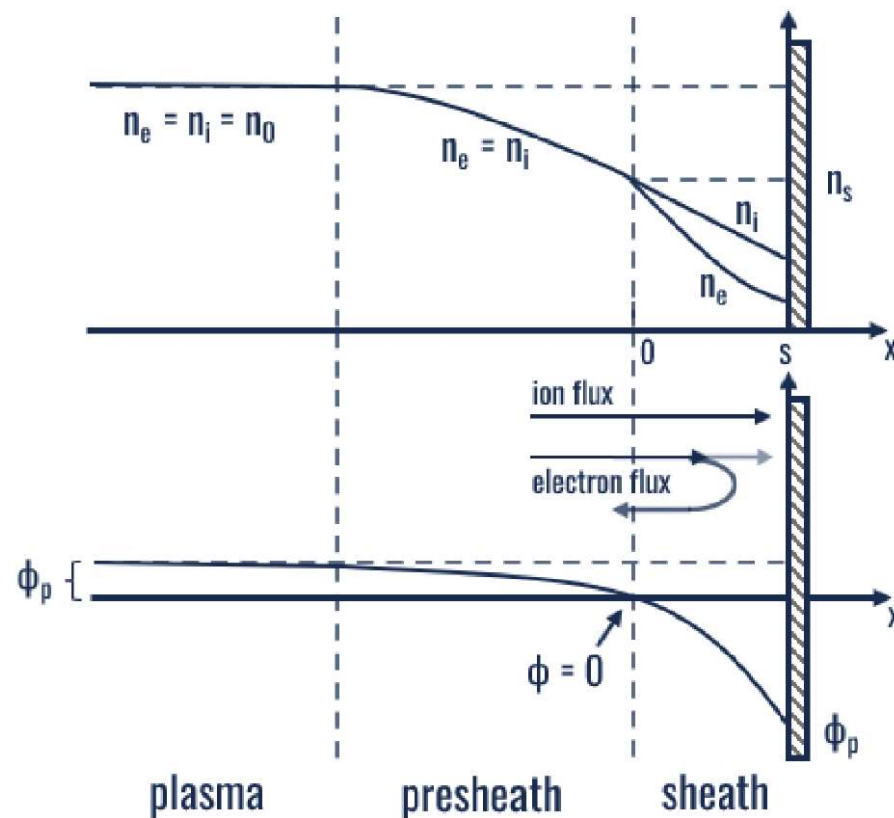
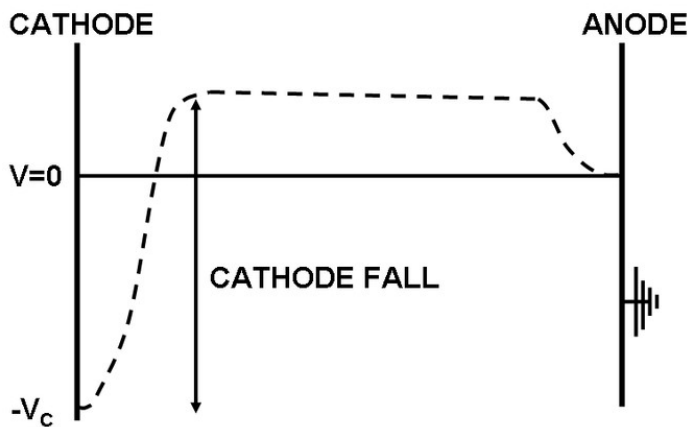
1. It is a dielectric medium with a **complex tensor dielectric function**.
2. Particles (electrons, ions, neutral gas) undergo diffusion and drift according to **complex tensor mobility which depends on the local energy**
3. **Each particle species has a very different mobility** (viscosity) but not different enough to consider either of them infinitely fast.
4. There are **large gradients of quantities** - orders of magnitude drop over a millimeter.
5. Particles undergo different reactions, the rates of which **depend on local electron and gas temperature**.
6. Different regimes between different regions - **some plasma regions are reaction-dominated, others are transport-dominated** and the boundary between those is fuzzy

Difficulties with plasma simulation

Possibly the **main pain behind plasma simulation** is the *imperfect quasineutrality*:

- In the plasma "bulk" $n_{el} = 0.99999 n_{ion}$
- In the plasma "sheath" $n_{el} \gg n_{ion}$ or $n_{ion} \gg n_{el}$

You solve for two quantities with a large magnitude and the interesting stuff could happen at the N^{th} decimal digit!



Difficulties with plasma simulation

So how bad can it be? Let's talk numbers!

$$n_{el} = 1.0000000 \cdot 10^{17} \text{ m}^{-3}$$

$$n_{el} = 1.00 \cdot 10^{12} \text{ m}^{-3}$$

$$n_{ion} = 1.0000764 \cdot 10^{17} \text{ m}^{-3}$$

$$n_{ion} = 1.00 \cdot 10^{17} \text{ m}^{-3}$$

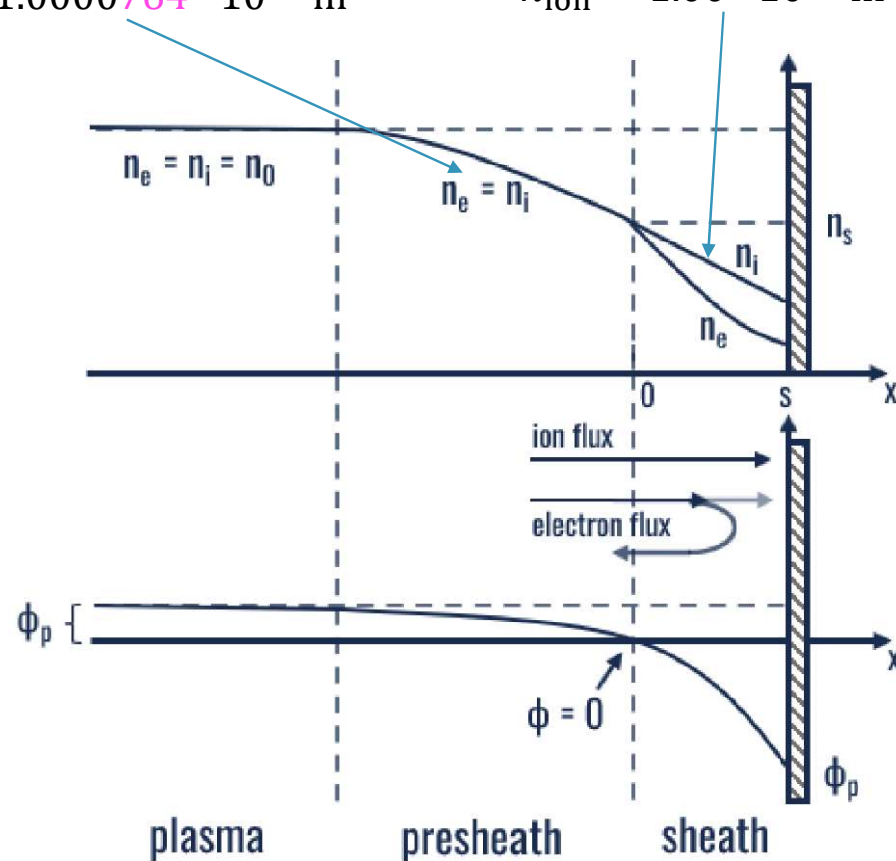
Bulk electron density, up to 10^{20} drops to sheath electron density, as low as 10^{12} . Bulk ion density same as electrons but drops less.

Furthermore, you have to solve for both n_{ion} and n_{el} with very high accuracy, because they are coupled through the Poisson equation

$$\Delta V = - \frac{q(n_{ion} - n_{el})}{\epsilon_0}$$

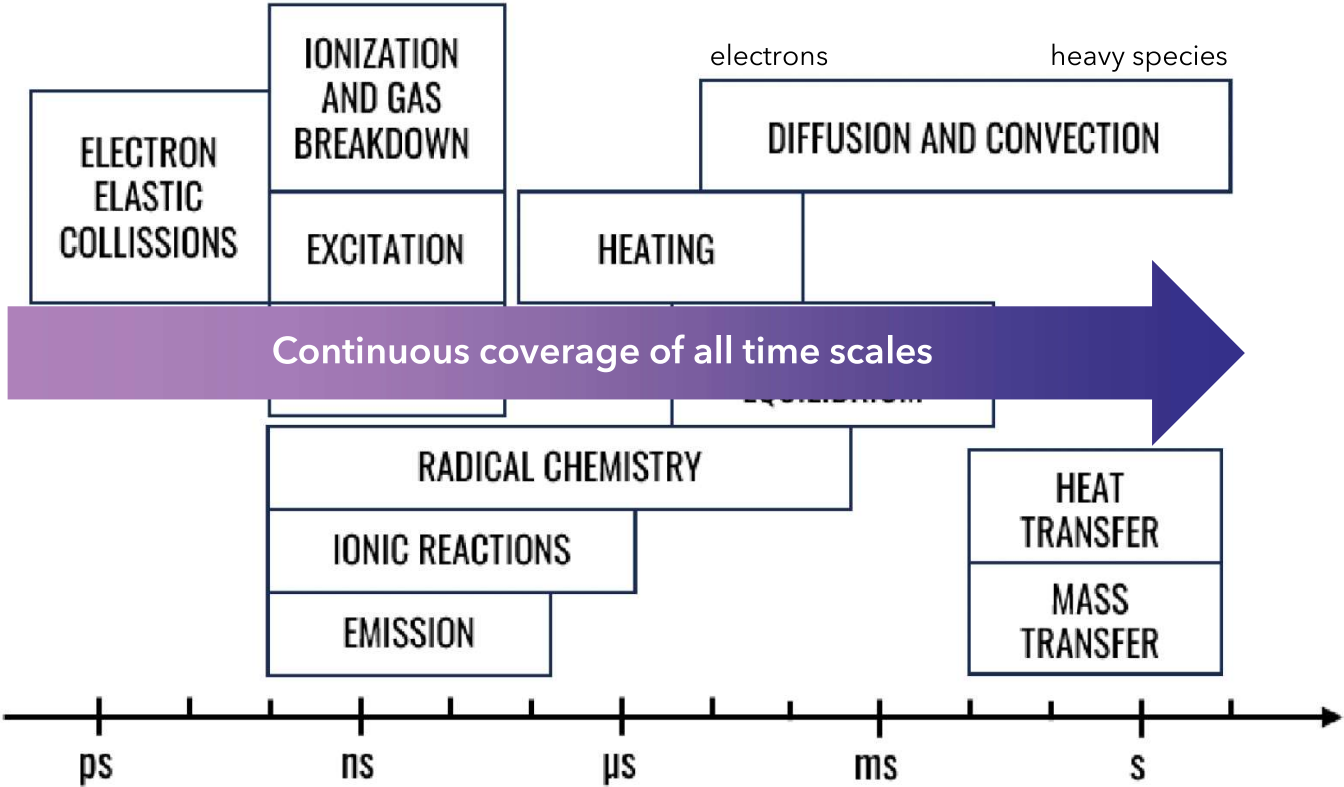
You could re-parametrize the system and solve for charge density $n_{ion} - n_{el}$ but even this quantity varies from 0.00001 to 10000...

This forces ridiculously high relative tolerance on your independent variables (charged species densities).



Multiple time scales in a plasma

We are facing processes happening at completely different time scales. And we need to explicitly resolve all.



The shortest time scale is sub-nanoseconds (electron dynamics).

Does this imply that the simulation time step has to be a nanosecond?

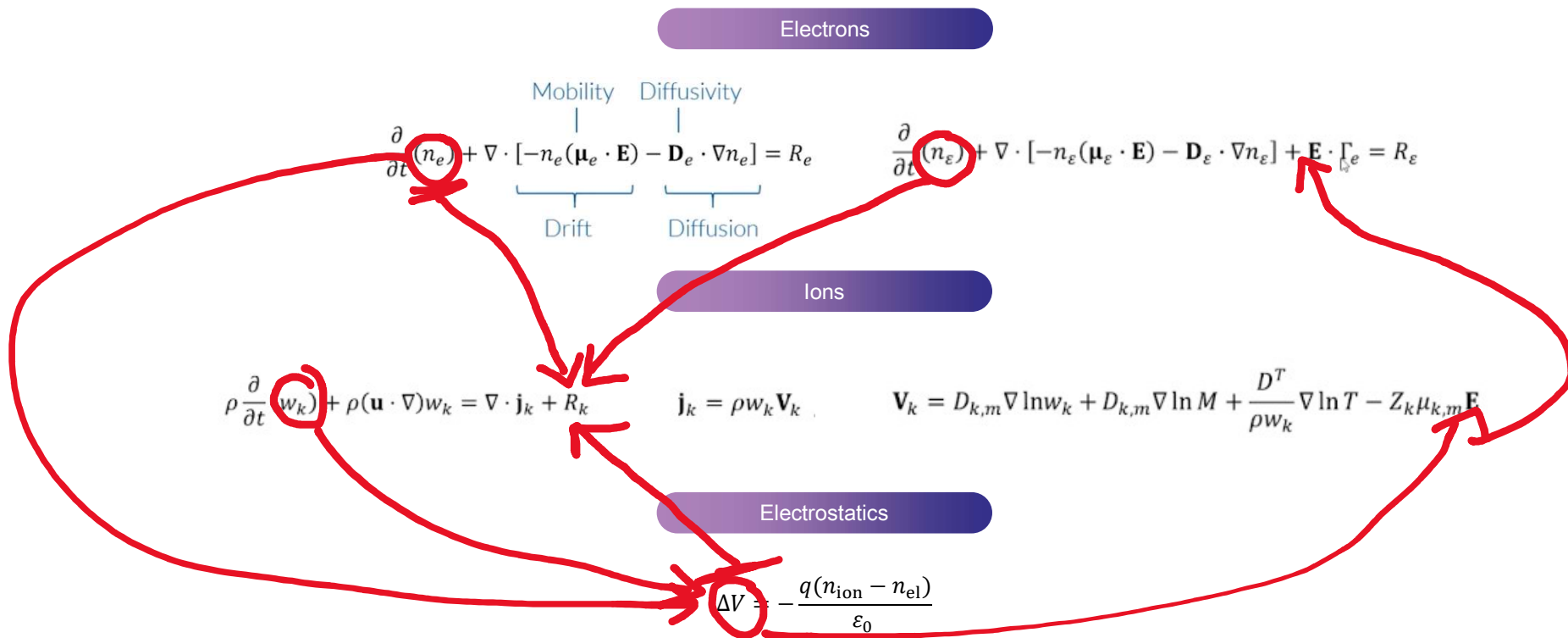
So you need over a billion time steps to reach steady-state?

Yes, if you are most simulation tools...

... but COMSOL engineers are creative 😊

Why COMSOL's Plasma Module?

- COMSOL's Plasma Module is the best there is for **fluid plasma simulation**.
- **Fluid plasma simulation** = all components (electrons, ions, neutrals) treated as immiscible fluids with certain transport properties. interaction between species happens through source terms and also highly non-linear transport properties.



Why COMSOL's Plasma Module?

What is COMSOL's special salt when it comes to plasma sim?

- 1. Logarithmic formulation for density equations** - solving for $\ln(n_{eI})$ instead of n_{eI} . This solves the problem of quantities varying over many orders of magnitude, even if it makes computation of matrix residuals much more tricky.
- 2. Fully-coupled solver** for electrons and ions - the nanosecond and microsecond features need to be resolved but as the system approaches steady-state and potential V is not changing anymore, solver time steps can be arbitrarily high!
- 3. Easy coupling** to other multi-physics interfaces

So what type of challenges have we been using COMSOL for?

Case studies

Case study: Optimizing a Plasma Reactor for Solar Grade Silicon (SGS) Production



Optimizing a Plasma Reactor for SGS Production

Here, we aim to optimize a metallurgical process which generates Si out of SiO_2 powders using plasma.

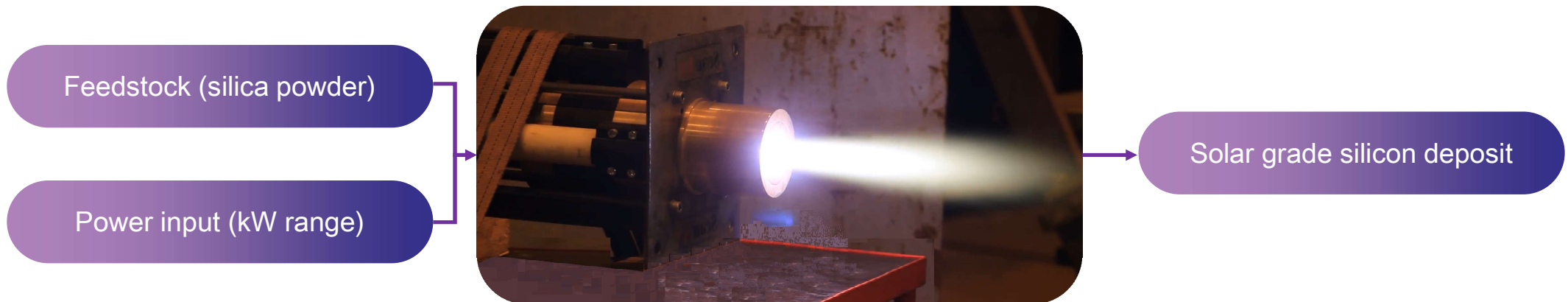
We are motivated to identify the key drivers behind the system's energy efficiency and maximize the amount of material synthesised per unit power.

Due to the exotic nature, it is not apparent whether the plasma is an equilibrium one or a non-equilibrium one.

Understanding the energy efficiency and distribution of reacting mixture is the big task for the model(s).

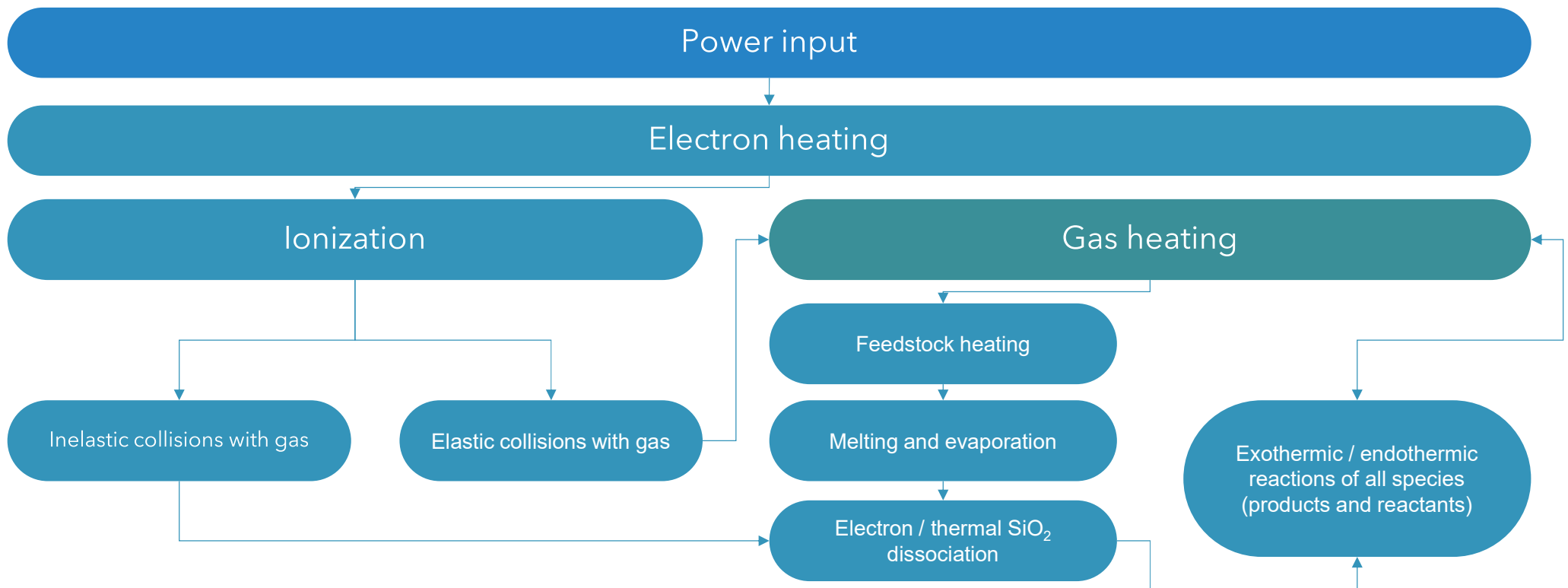
Optimizing a Plasma Reactor for SGS Production

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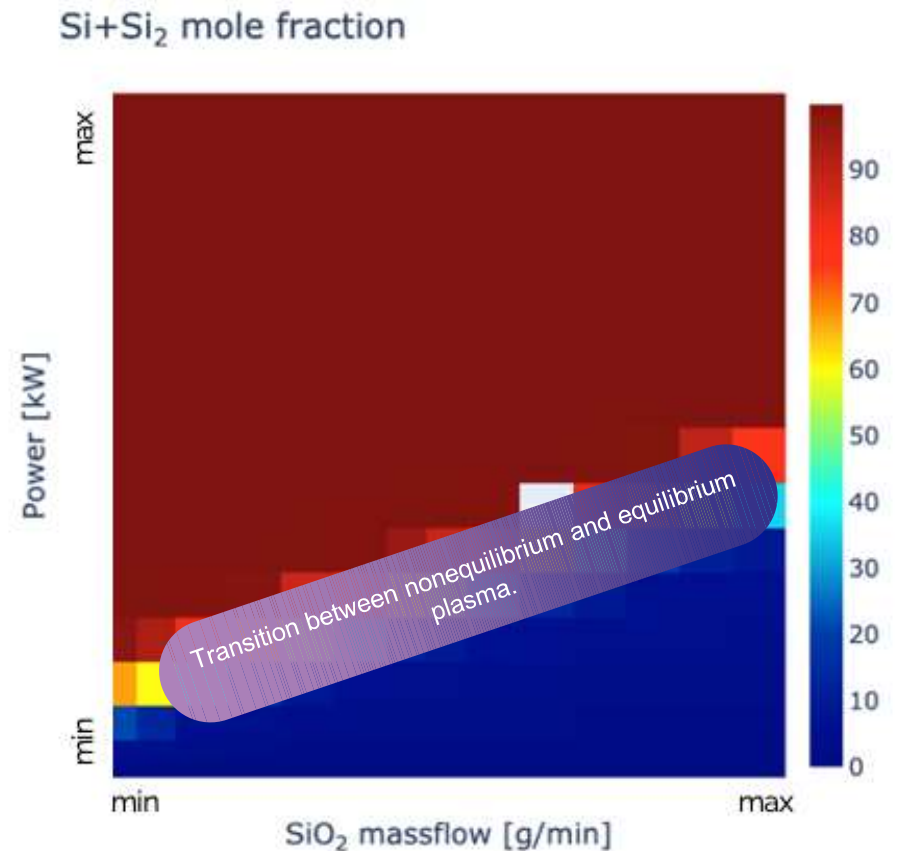
Understanding the Energy Pathways

- Engineering question - how to maximize the power efficiency?
- Scientific question - what are sinks and sources for the energy inputted to the plasma?



Optimizing a plasma reactor for SGS production

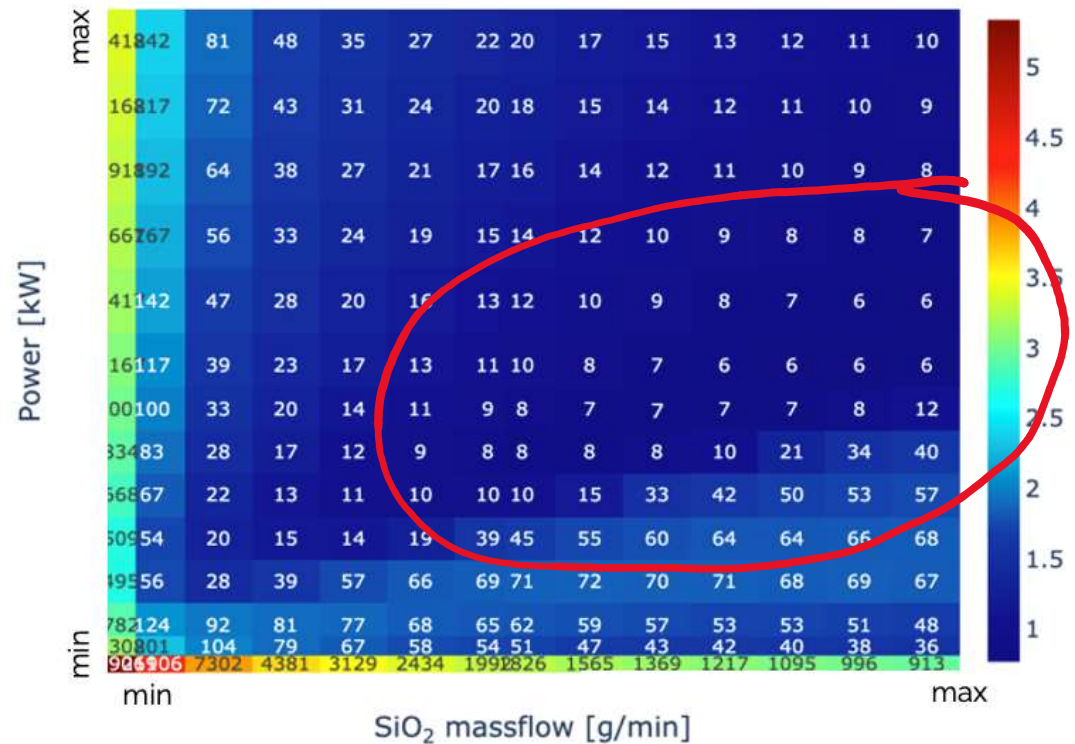
- First, we perform a high-level energy analysis - probing the region of approx 10 - 100 kW and up to 1 kg/min feedstock flow rate.
- By building an ODE-based "global plasma model" and taking into account all the possible reactions of the carrier gas, electrons, silica- and silicon-derived species, we can **quantify the concentration of the species of interest in the system.**
- The global model is volume-averaged but takes into account all the important plasma dynamics and reaction kinetics (>3000 reactions, >100 species)
- **With the help of the global model, we can sweep the parametric space of the system, looking for the point of optimum process efficiency.**



Optimizing a plasma reactor for SGS production

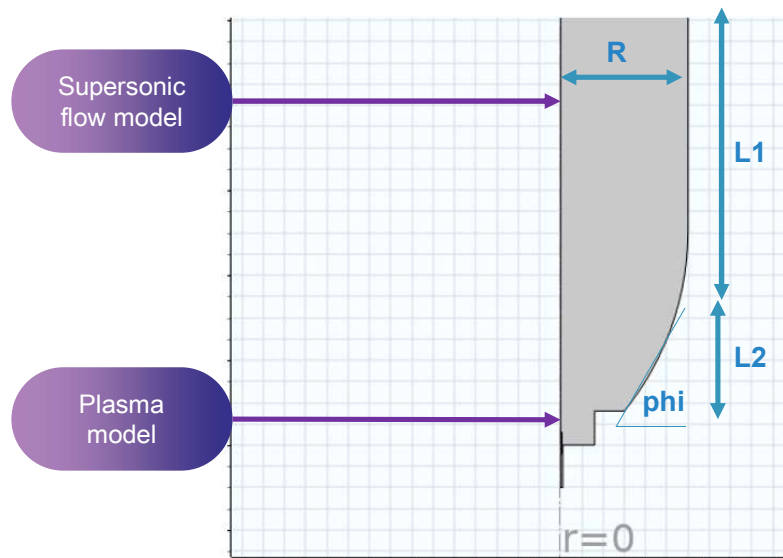
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Si+Si₂ energy cost [kWh/kg] (color in log10)



But how do we achieve this in an actual industrial furnace?

Optimizing a plasma reactor for SGS production

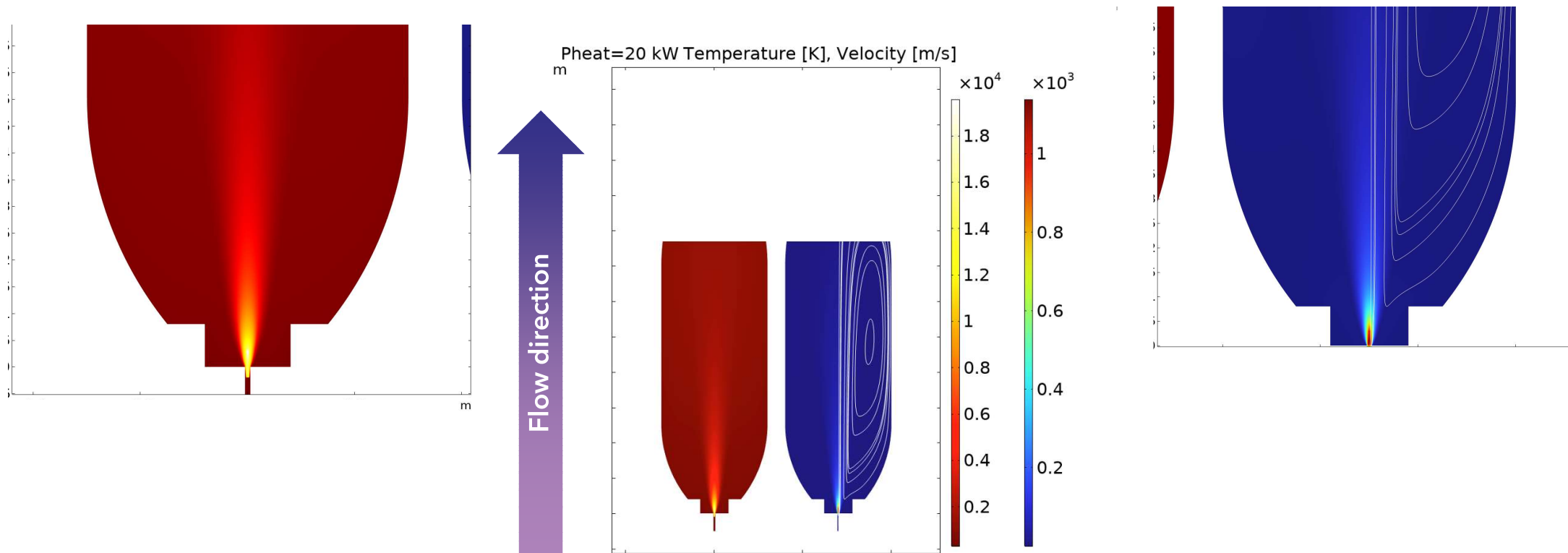


- In plasmas near the atmospheric pressure, advection is one of the main drivers behind species transport.
- For that reason, **the first step in understanding atm. plasmas is understanding how the plasma interacts with the flow.**
- Typically, we want to suppress re-circulation of products back into the plasma region.
- In this high-power setup, the Mach number exceeds 1.0, so we had to **couple the plasma model to the new HMNF (high-Mach number flow) interface.**

Plasma temperature and flow velocity

Temperature and velocity in the plasma zone are in the expected range $T \approx 20\,000\text{ K}$, $Ma \approx 3 \Rightarrow$ **equilibrium window**

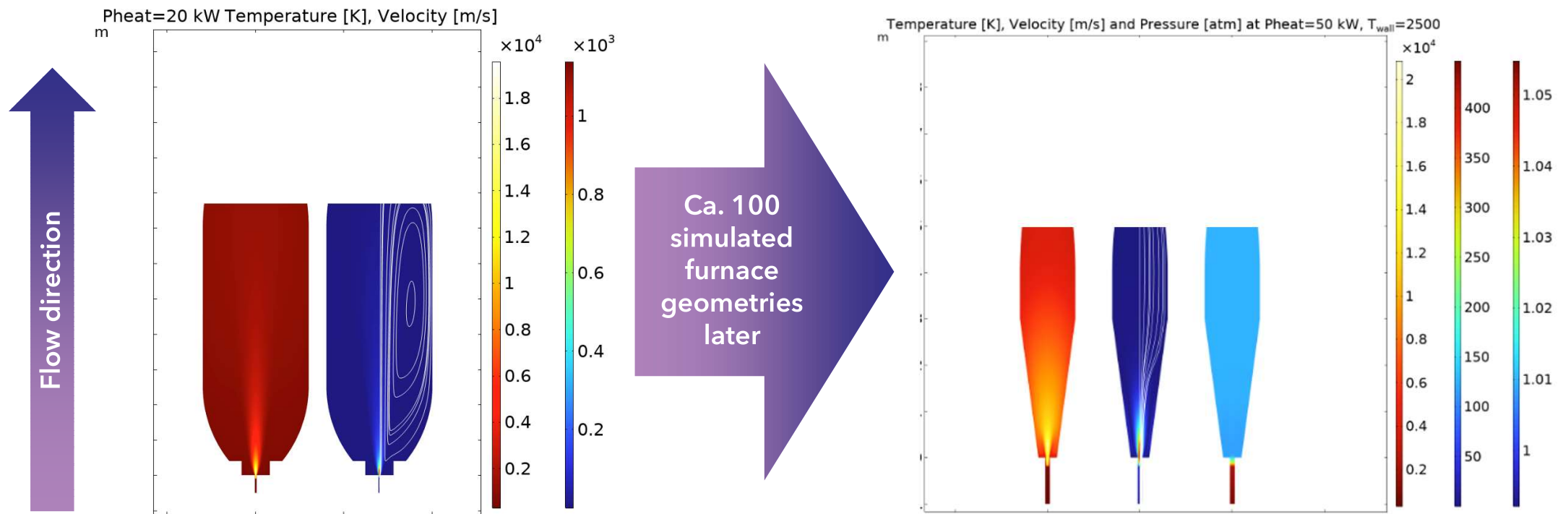
However, substantial re-circulation present, which causes species re-introduction \Rightarrow **need to optimize gas flow**



Plasma temperature and flow velocity

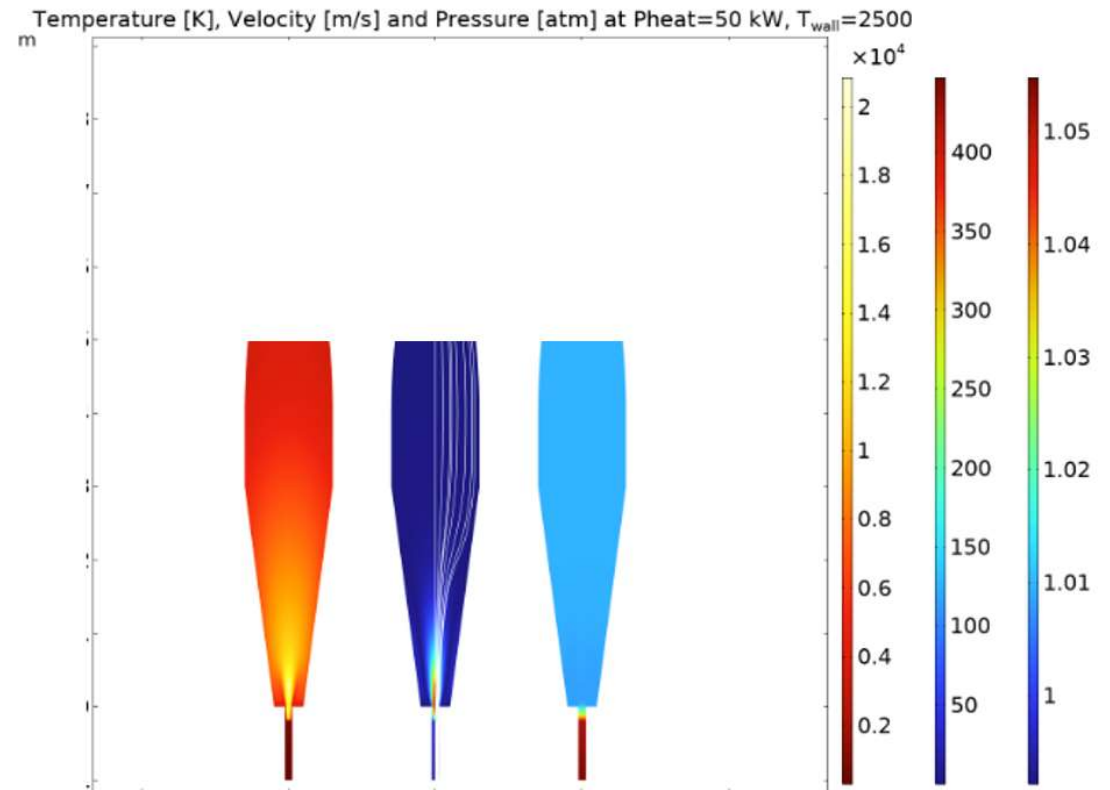
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Optimizing reactive flow re-circulation

- The main power of the combined flow+plasma model is that it allows us to rapidly test different modifications of the furnace geometry and their impact on the re-circulation patterns.
- It turns out that the downstream flow is not affected by plasma dynamics notably. So **modifications to the downstream region do not affect the upstream flow so much.**
- Apparently, we need to think outside the box to make the plasma flow patterns more uniform.
- This is possible only if we permit a **radical re-design of the furnace geometry**. In this case, the hot plasma zone gets much closer to the furnace wall.
- We did solve the latter challenge with COMSOL, but that is proprietary ☺.



Conclusions from the analysis

Energy Efficiency

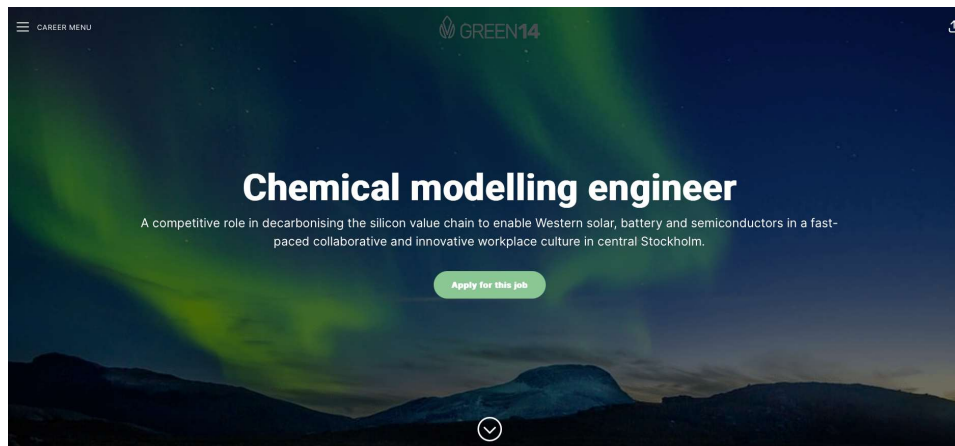
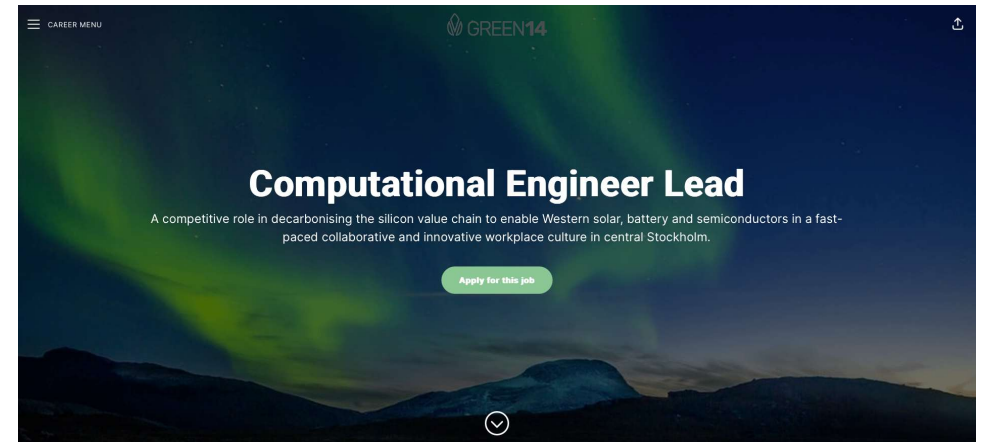
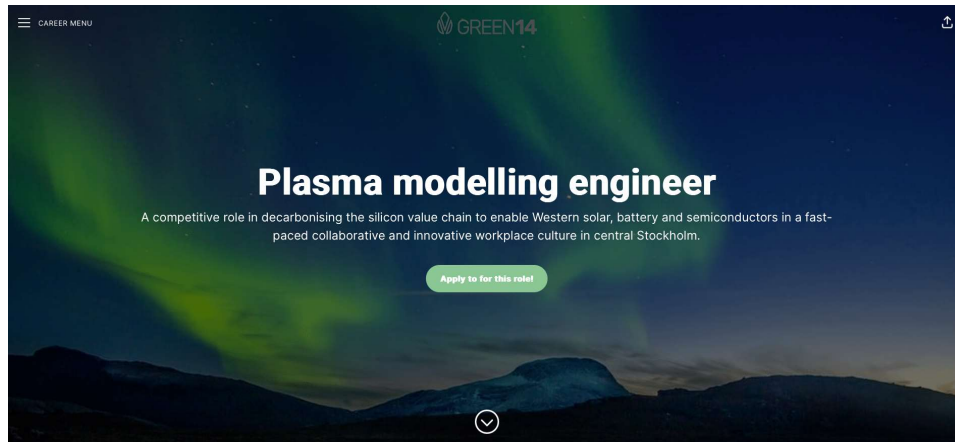
- There are various energy flow channels and they all need to be included in order to get the correct picture of the process
- Maximum energy efficiency is achieved at the tricky boundary between equilibrium and non-equilibrium plasma.

Flow dynamics

- The high-Mach number flow dynamics behaves in a non-intuitive way, at least for a plasma engineer 😊.
- The combined CFD+plasma simulation helped us optimize the furnace geometry so that gas recirculation is almost entirely suppressed.

The simulation (1) helped us identify the ideal working point for the technology regarding energy efficiency and (2) acted as the main engineering tool for optimizing the flow.

Green14 Job Opportunities



Go to <https://green14.com> > Careers to learn about the openings in this deep tech start-up

Case study: Modeling the PlasmaMAX™ PECVD Technology



Plasma
Technology
Solutions

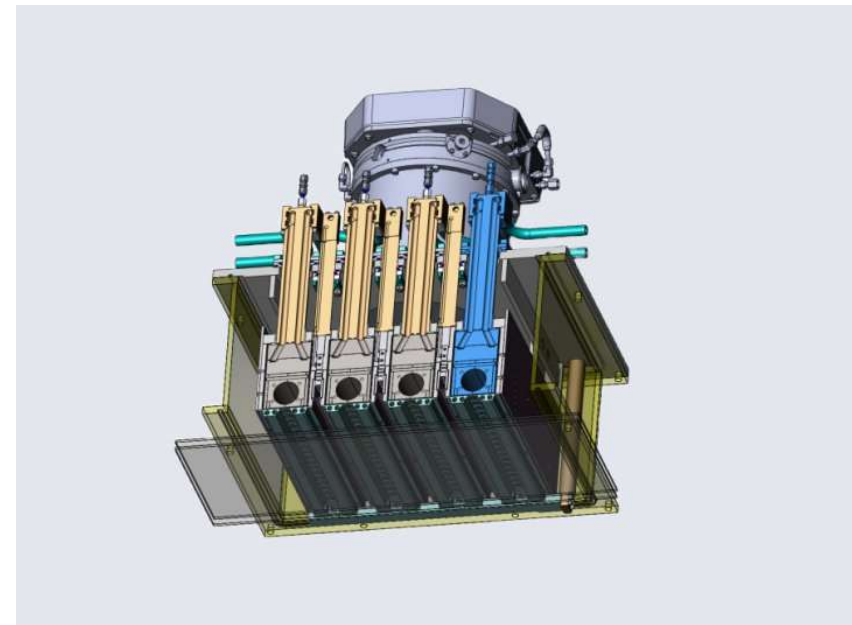


Modeling the PlasmaMAX™

- PlasmaMAX™ is a highly scalable PECVD technology for fast growth of oxides (10x faster over standard PVD)
- The original application were architectural glass coatings, but nowadays also used for barrier coatings, protective coatings, or high-tech battery coatings.



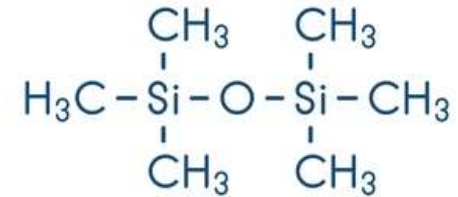
<https://www.agc-plasma.com>



M-era.net MIST (Reference Number: project8261)

Modeling the PlasmaMAX™

- Similar to the SGS case study, the PECVD process is highly driven by the advective transport.
- The oxide films are grown in plasma from complex organic precursors.
- However in this case, the system has a **highly non-local behavior** - the chemical species which cause SiOx film growth are produced quite far from the deposition zone.
- In the ideal case, we would need a model that does:
 1. Full plasma dynamics in 3D
 2. High-Mach number gas flow in 3D
 3. Advection-diffusion-reaction equation in 3D for 62 species

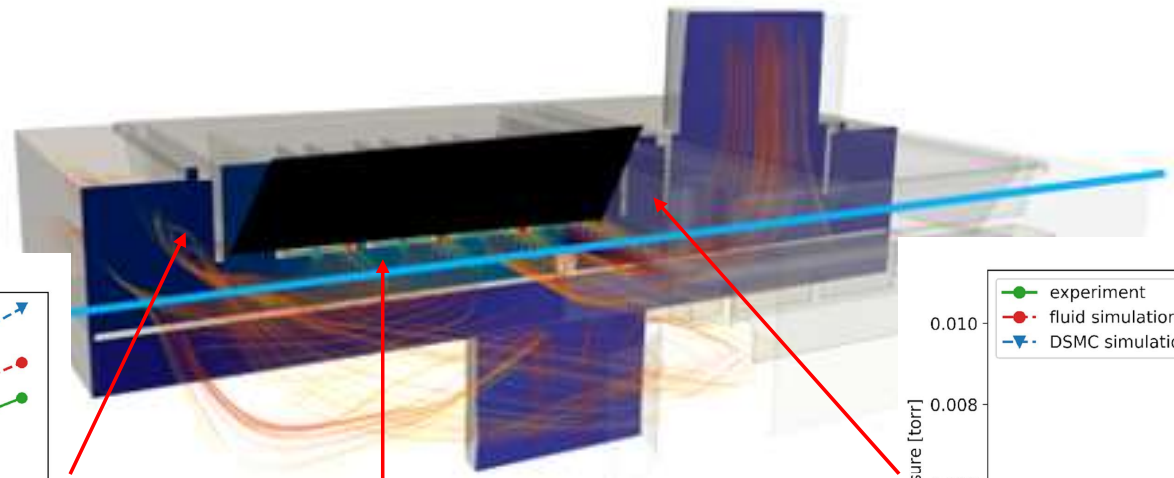


hexamethyldisiloxane

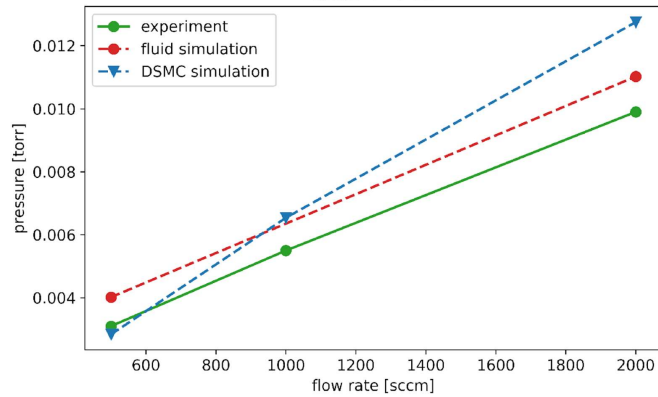
This is simply not attainable considering any reasonable amount of processing power and memory.

Modeling the PlasmaMAX™

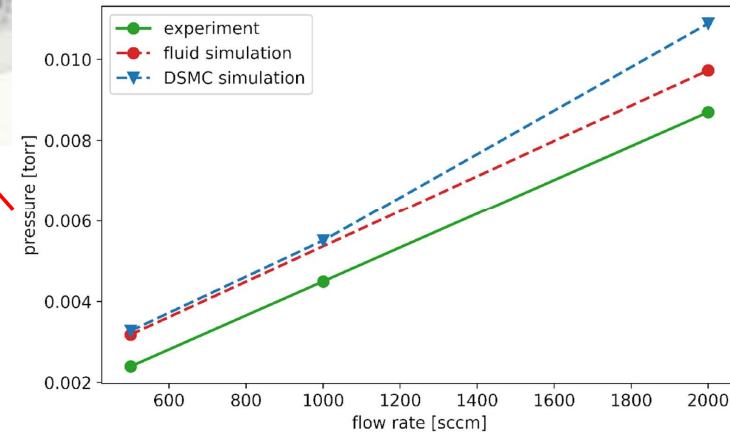
- Gas flow simulation gave us insight into the transport of the precursor.
- It highlighted the asymmetry in the flow and made us aware of the importance of the pressure gauge position in the system.
- On the scientific level, we confirmed a very good match between DSMC and density-based fluid model, the latter of which should not work ☺ on such low pressures (5-100 Pa)



CASE 4 - PVD



CASE 4 - PUMP

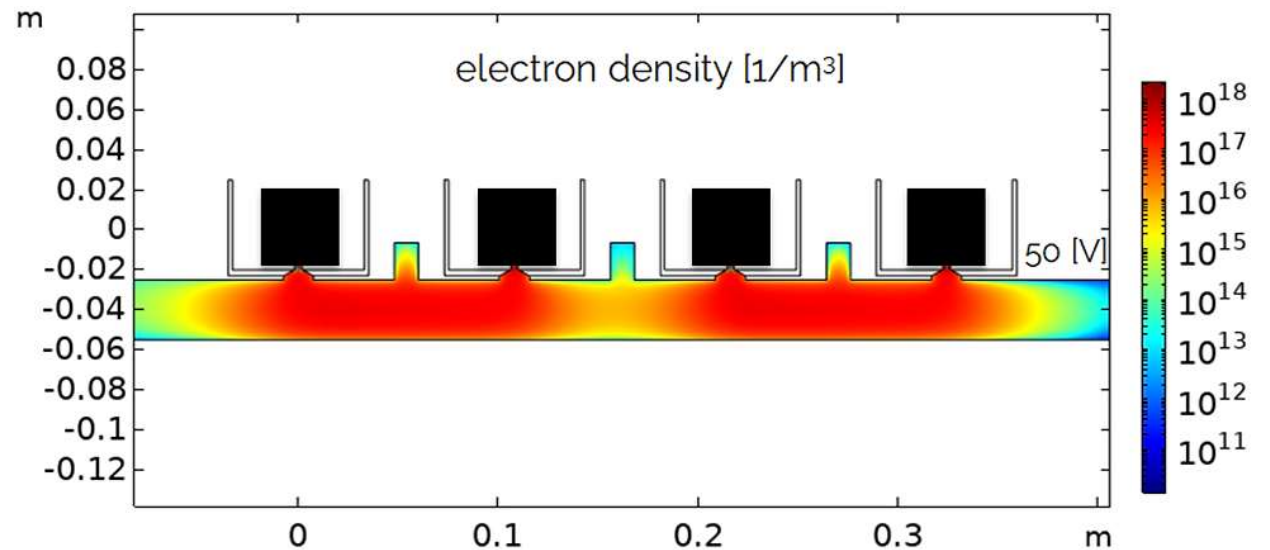


$$p_{\text{COATING}} = 1.5 \cdot p_{\text{PUMP}}$$

$$p_{\text{COATING}} = 1.2 \cdot p_{\text{PVD}}$$

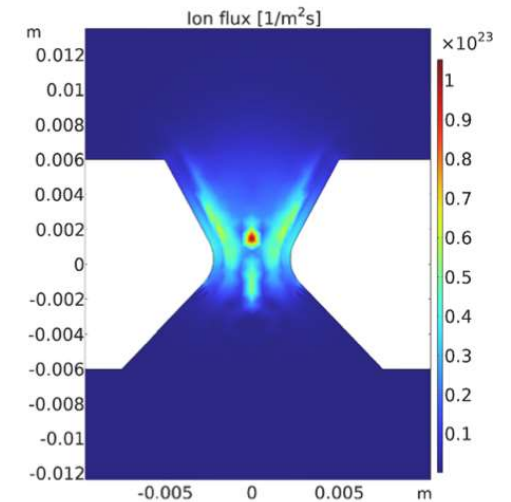
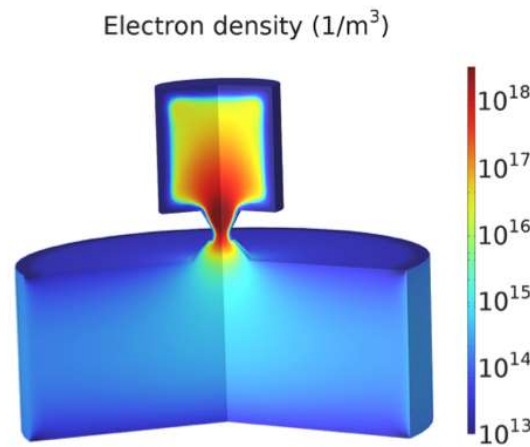
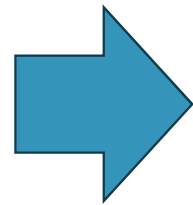
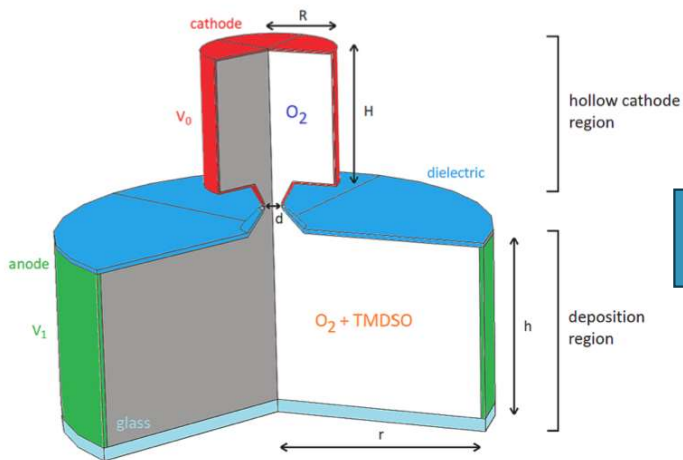
Modeling the PlasmaMAX™

- We also performed plasma dynamics simulations in 2D slices through the system.
- These were done in simplified chemistry of **argon and oxygen**, complex precursor was not considered.
- Computation time per one DoE is on the order of 1-3 hours.
- We got the information about lateral plasma distribution and learned how it can be controlled.



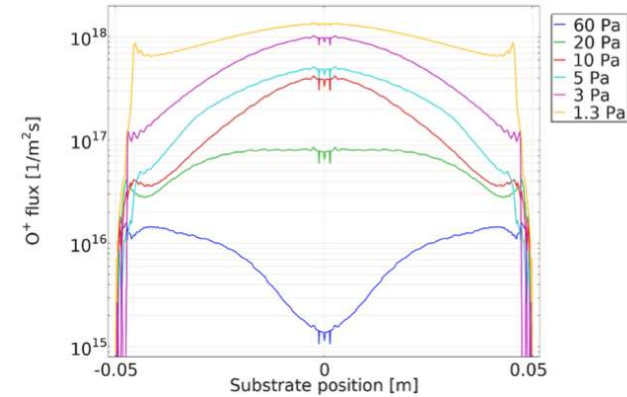
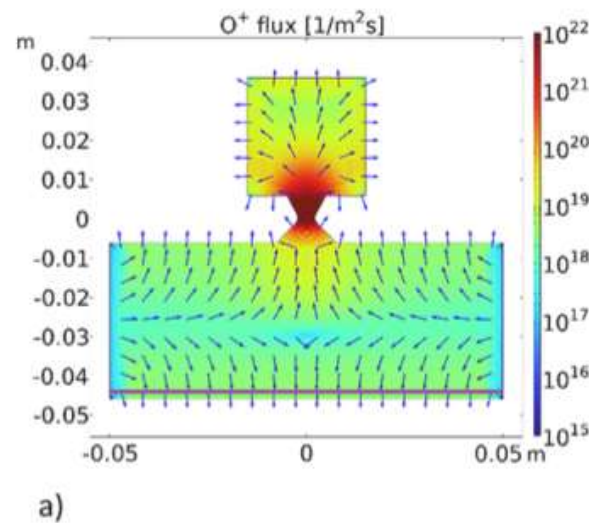
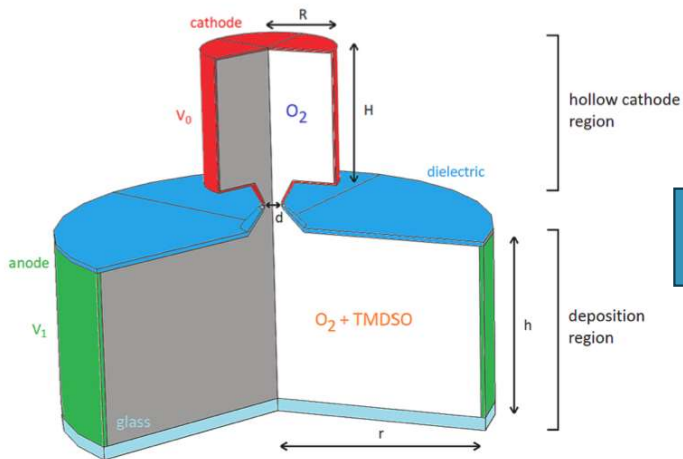
Modeling the PlasmaMAX™

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- We also did a “zoomed-in” simulation in a surrogate geometry to understand how the plasma is generated inside the hollow cathode and **why the ejection nozzle of the plasma source is being eroded**.



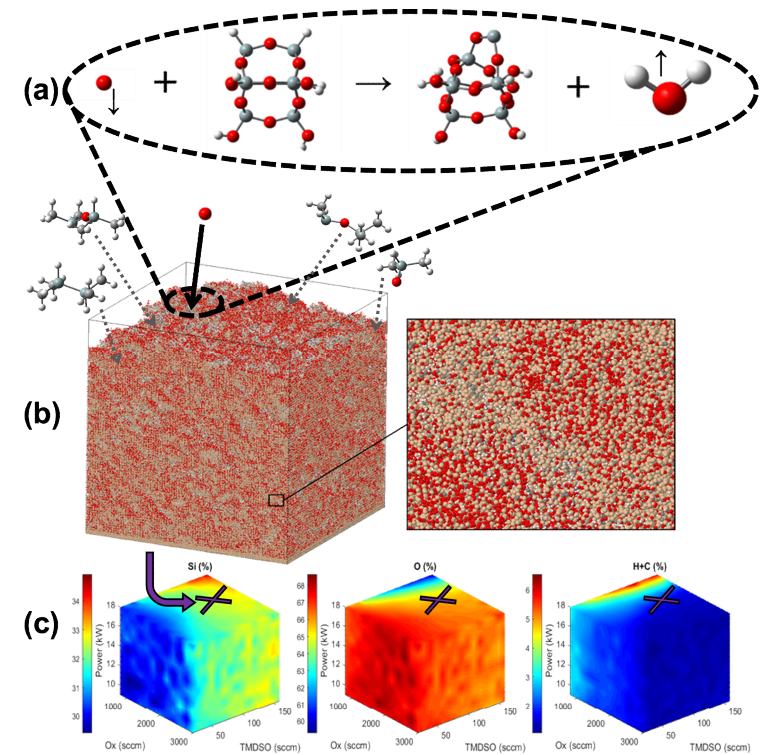
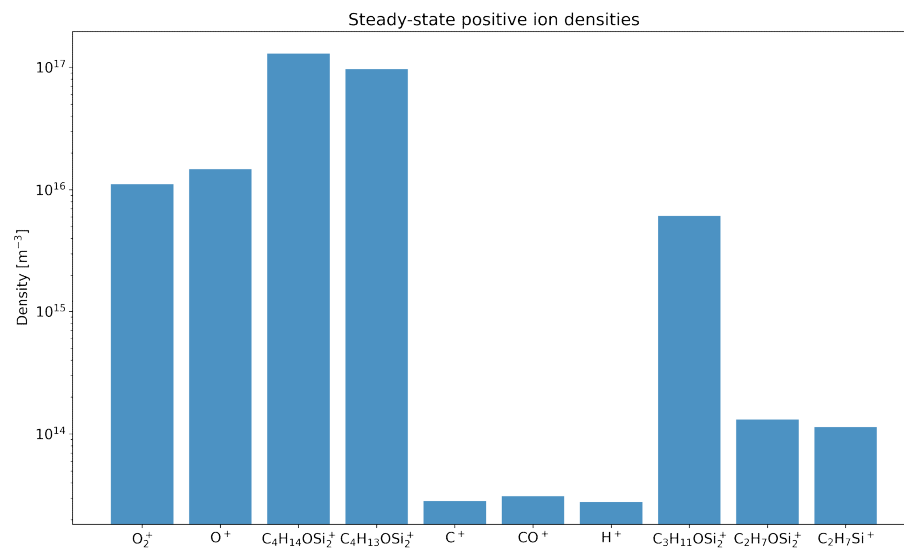
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- The models also helped us understand and **optimize the oxygen ion bombardment** in the system.



Modeling the PlasmaMAX™

- Ultimately, to understand the chemistry and growth, we coupled COMSOL to PlasmaSolve's MatSight Global Model software again.
- The Global Model of the process solves **balance and transport equations for 62 species and 617 plasma-chemical reactions.**
- **Atomistic film growth was modeled using the NASCAM** software, which relies on kinetic Monte-Carlo. That would not be doable in current COMSOL versions but the coupling was smooth.



Case study: Understanding the effect of power waveform on the plasma behavior and distribution



Problem specification

This simulation challenge relates to vacuum plasma coating equipment (PVD sputter coater).

The equipment operates at high vacuum pressures of 0.3 - 0.6 Pa.

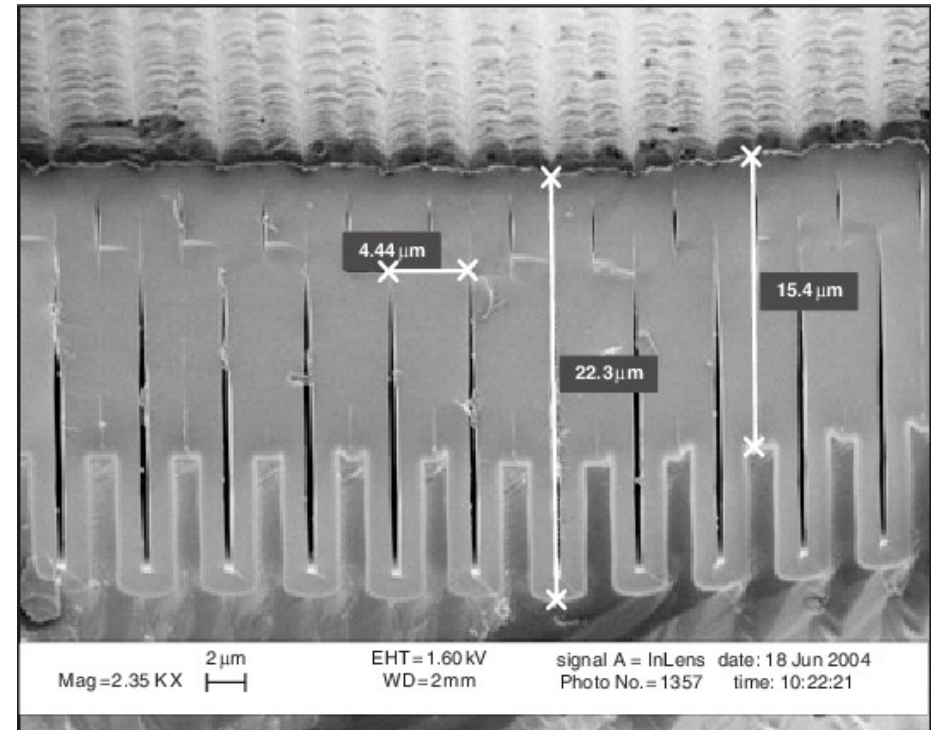
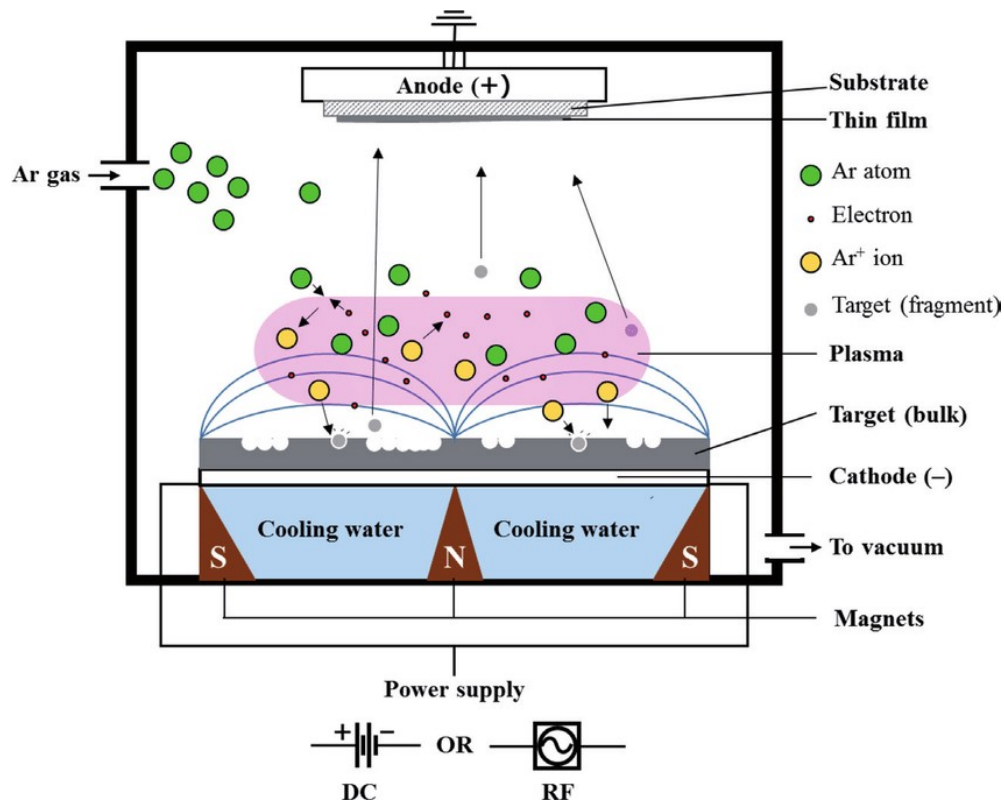
It is a magnetron-sputtering-based equipment - solid metal cathode is converted to gaseous metal, which is deposited together with some reactive gas onto a substrate.

The application is deposition of SiN semiconductor components.

We want to understand how different voltage waveforms on the cathodes affect the plasma behavior and material growth conditions.

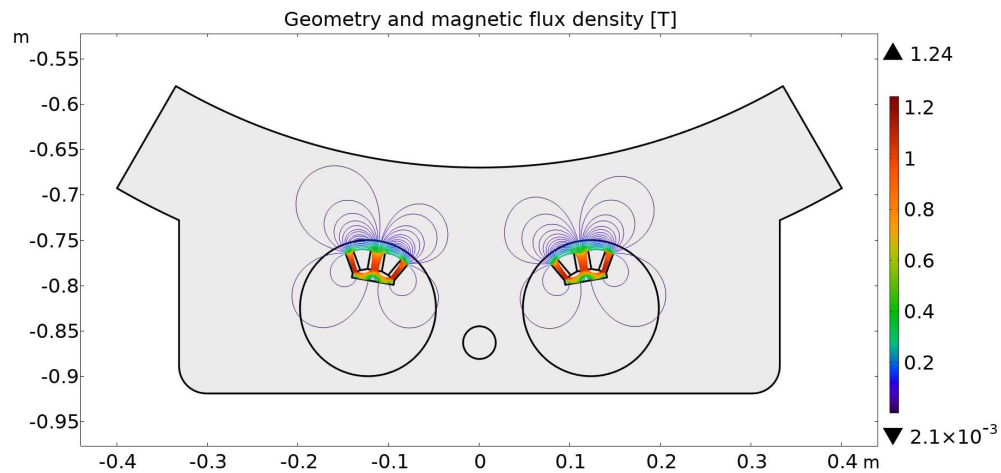
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The application is deposition of SiN semiconductor components.



Equipment layout

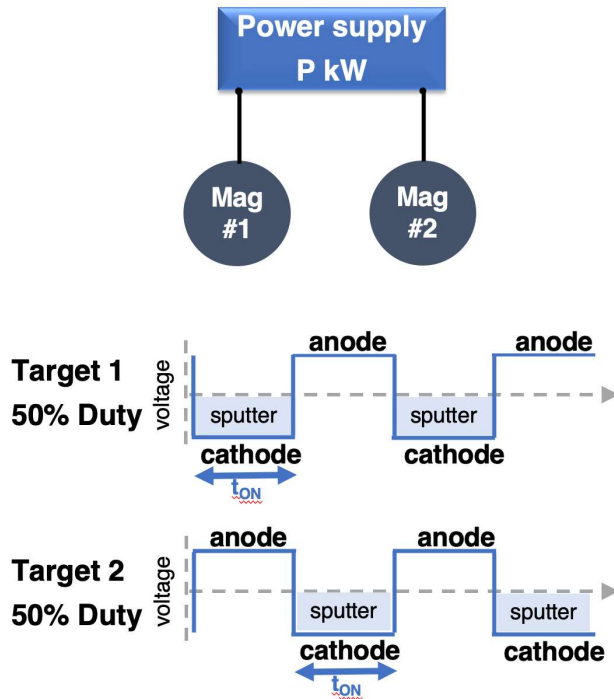
- **Drum coater** with dual cathodes
- **Mirror-configuration** of the magnetic field
- Supports **BP square** and **DRP waveforms**
- **Anode count and position** can be varied
- **Cathodes floating** relative to grounded walls and drum.



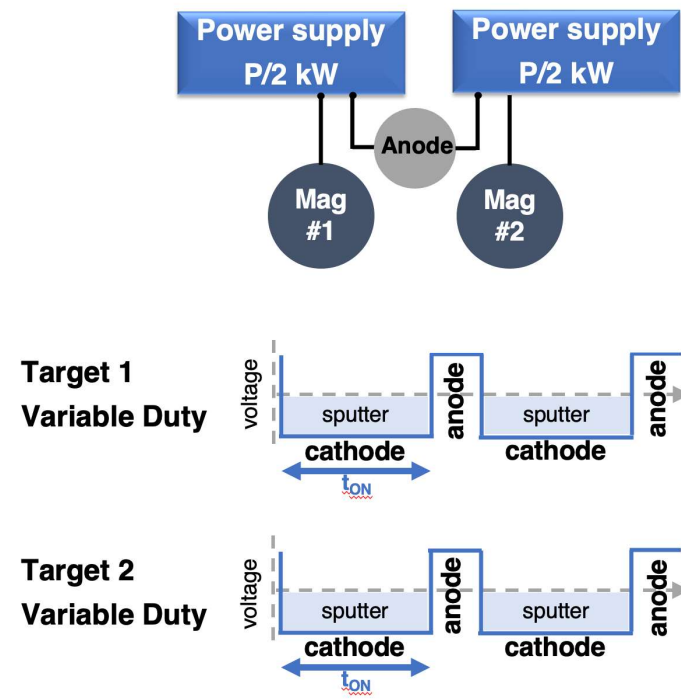
Problem specification

Question 1: What impact does the MF-waveform have on the coating process?

Bi-polar pulsing (BP)



Dynamic reverse pulsing (DRP®)

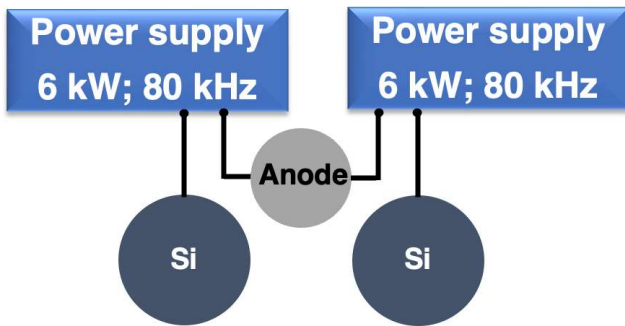


Problem specification

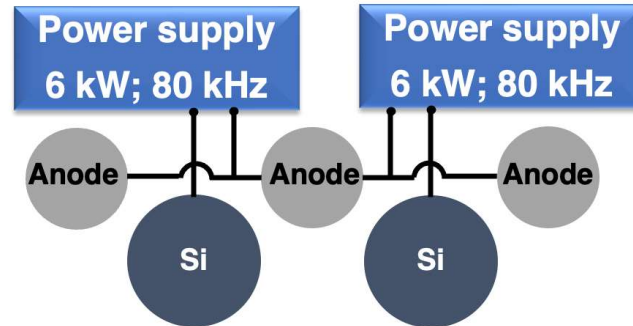
Question 2: DRP-powered processes are sensitive to anode position, what are the phenomena driving this, can we simulate them?

Dynamic reverse pulsing (DRP®)

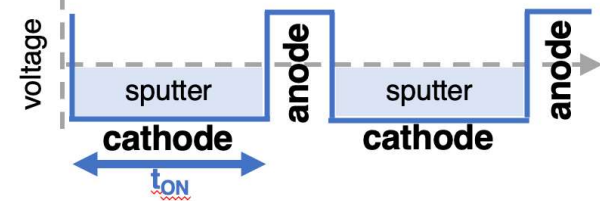
1 anode cathode



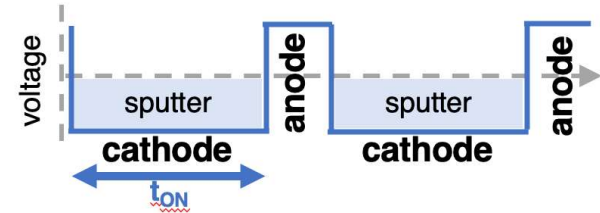
3 anode cathode



Target 1
80% Duty

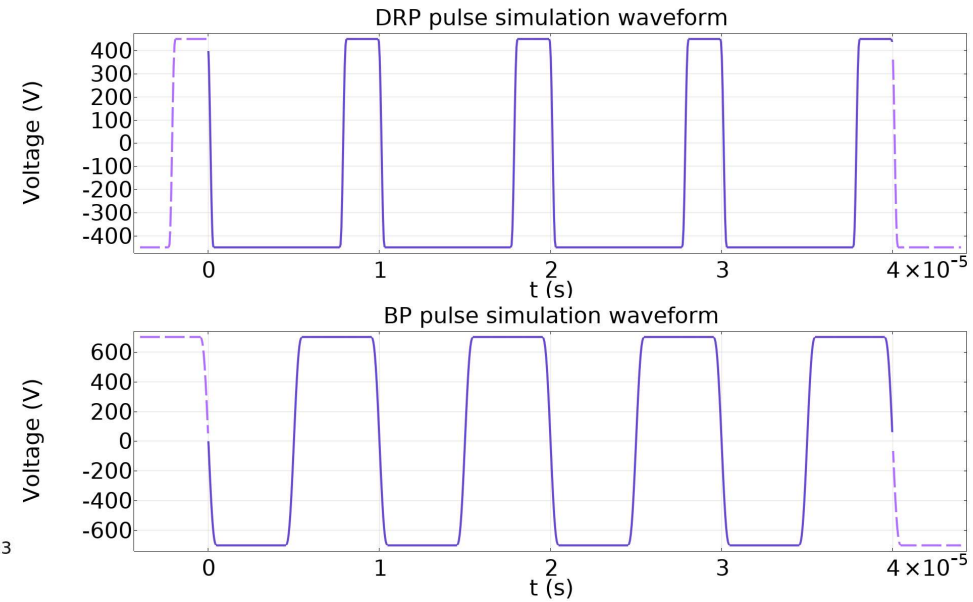
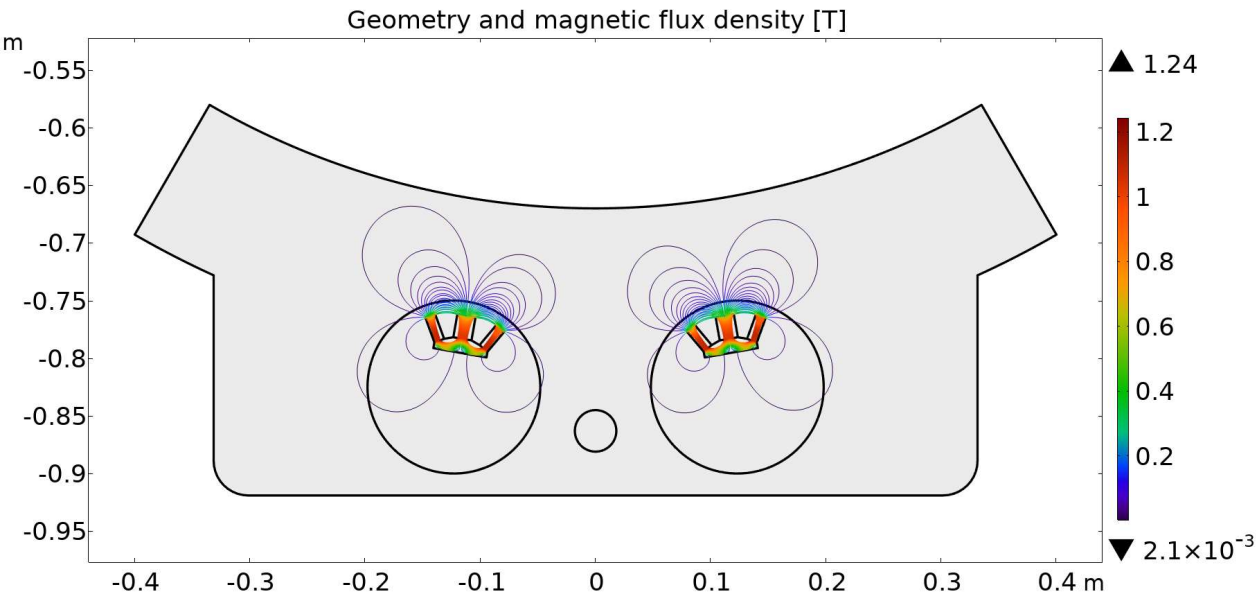


Target 2
80% Duty



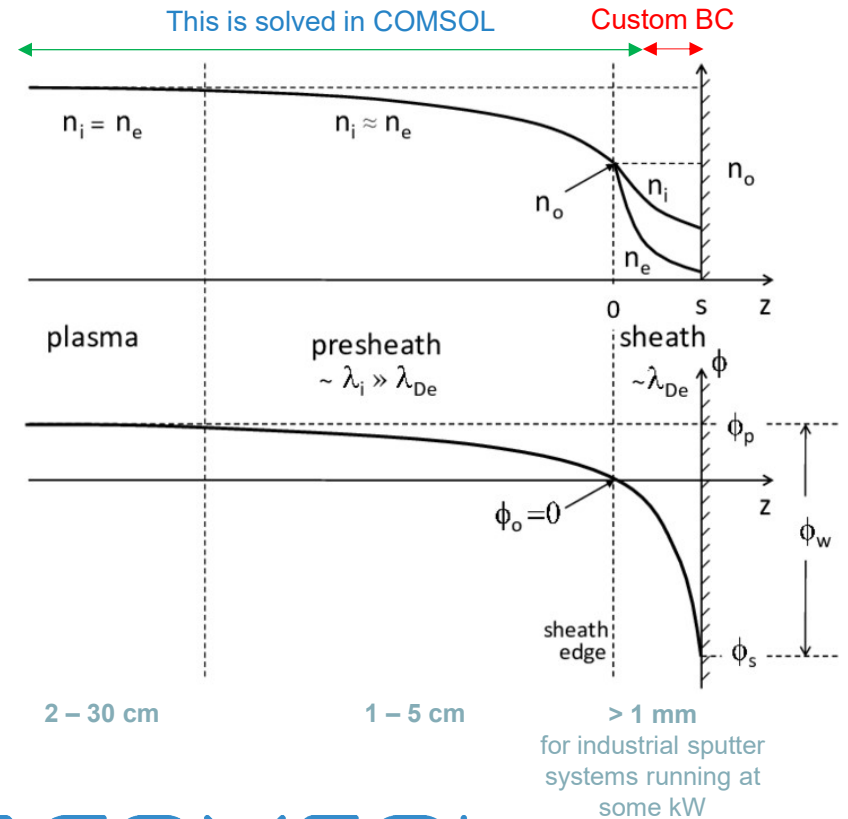
Equipment virtual representation

- Problem simulated in **2D geometry** - horizontal slice through the coater
- **Realistic voltage profiles applied** between the cathodes and the anode => current computed from the model (validation quantity)
- **3D coater simulation is feasible** but slower and requires more assumptions



Numerical model

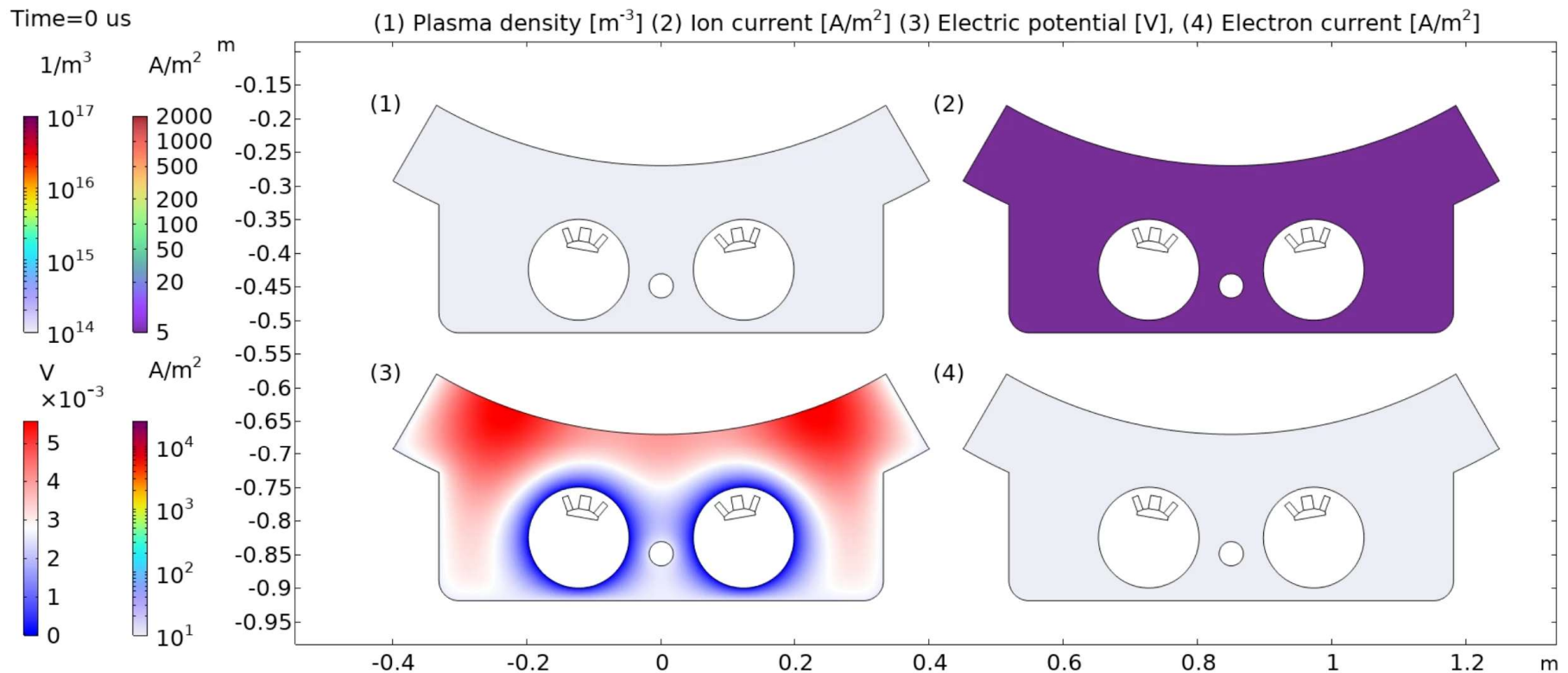
- To understand the plasma as a whole, we need to use a **full plasma model**, that actually resolves the distribution of ions, electrons and other species.
- Our **hybrid plasma model** is mostly based on the drift-diffusion approximation but contains special boundary conditions that are "trained" on kinetic algorithms (particle-in-cell, test-particle Monte-Carlo).
- Technical solution:** coupling between PlasmaSolve's MatSight (kinetic component) and COMSOL Multiphysics (fluid component).
- The innovative **solution is over 100x faster compared to competing particle-in-cell solvers.**



Comparing BP and DRP Plasma

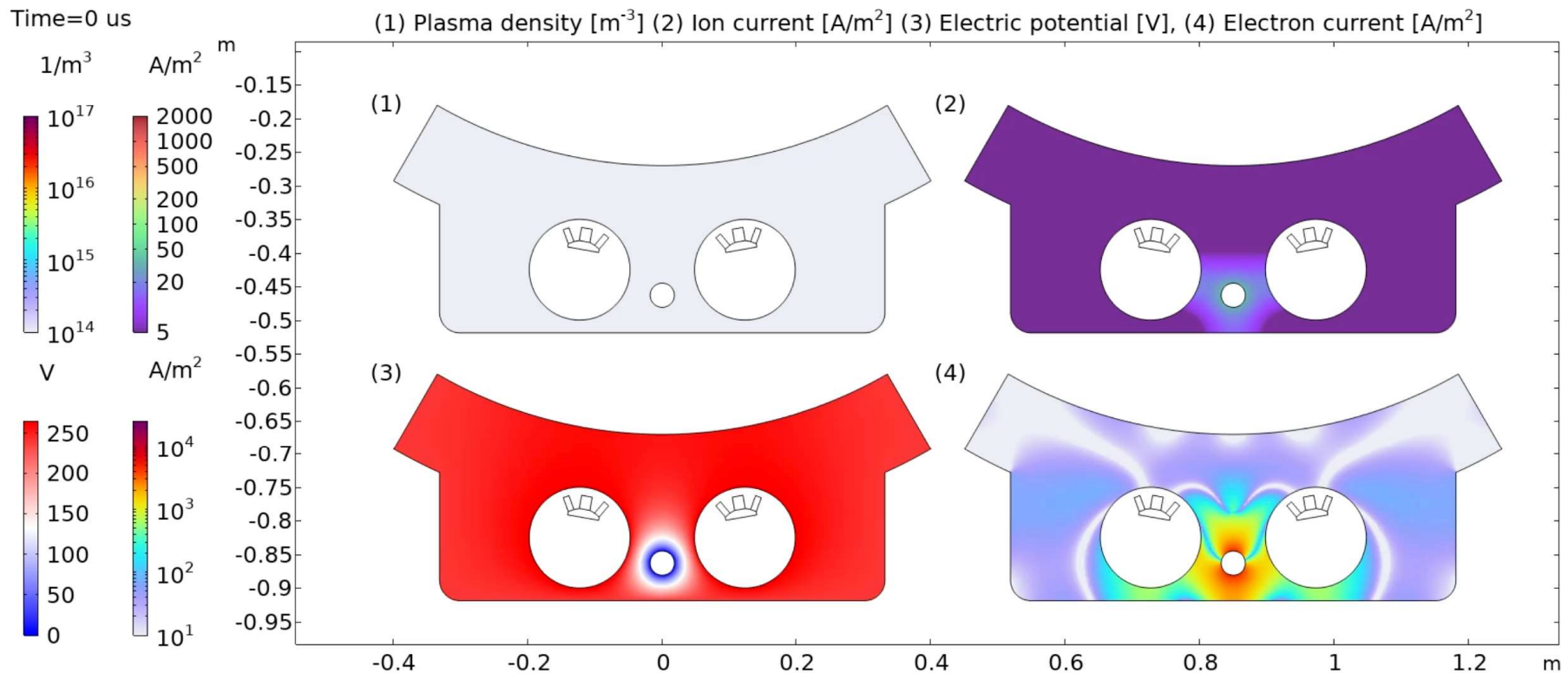
Comparing BP and DRP at 80 kHz

- In **bipolar pulsing**, the plasma alternates between cathodes
- Ion current **heats the substrate in the mid-point** between the cathodes



Comparing BP and DRP at 80 kHz

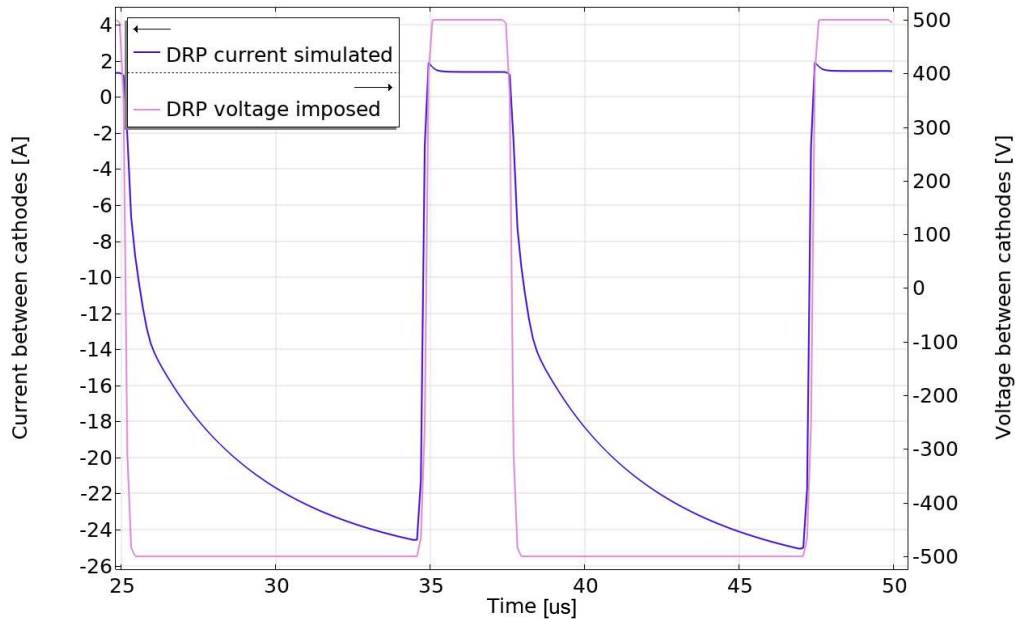
- In **dynamic reverse pulsing**, the plasma varies in time and the anode is an active and important part.
- Ion current **heats the substrate only during the positive phase** of the pulse => ability to tune the energy dose



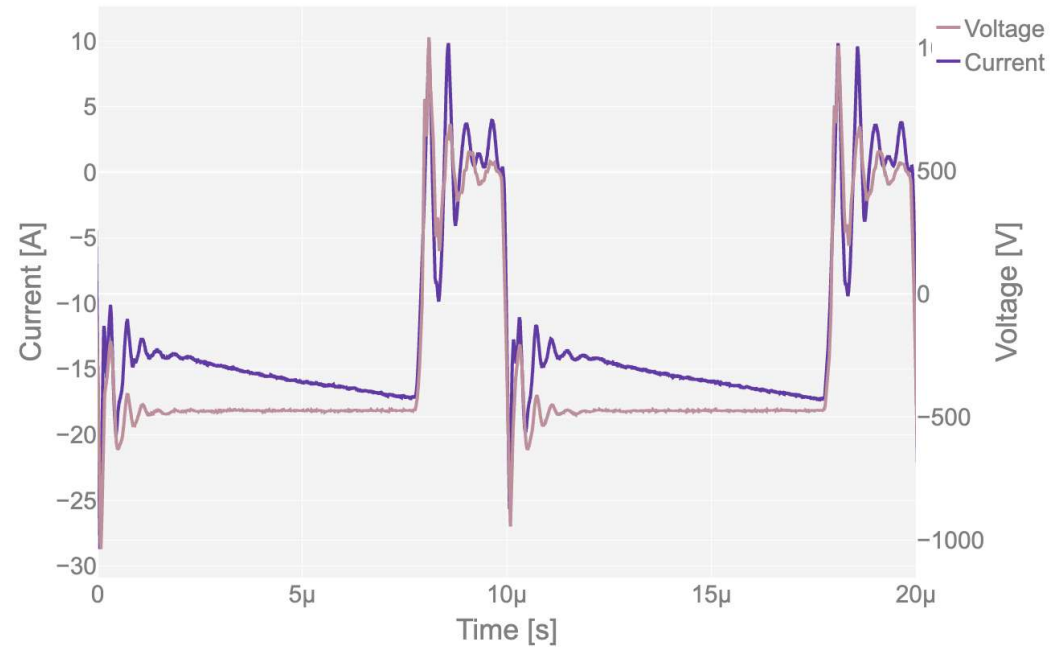
Validating IV readings in the DRP mode

- Model predicts **somewhat slower current rise which leads to a higher peak-current** compared to experiment
- Model computes the correct plasma conductivity (voltage is imposed, power/current computed)

simulation



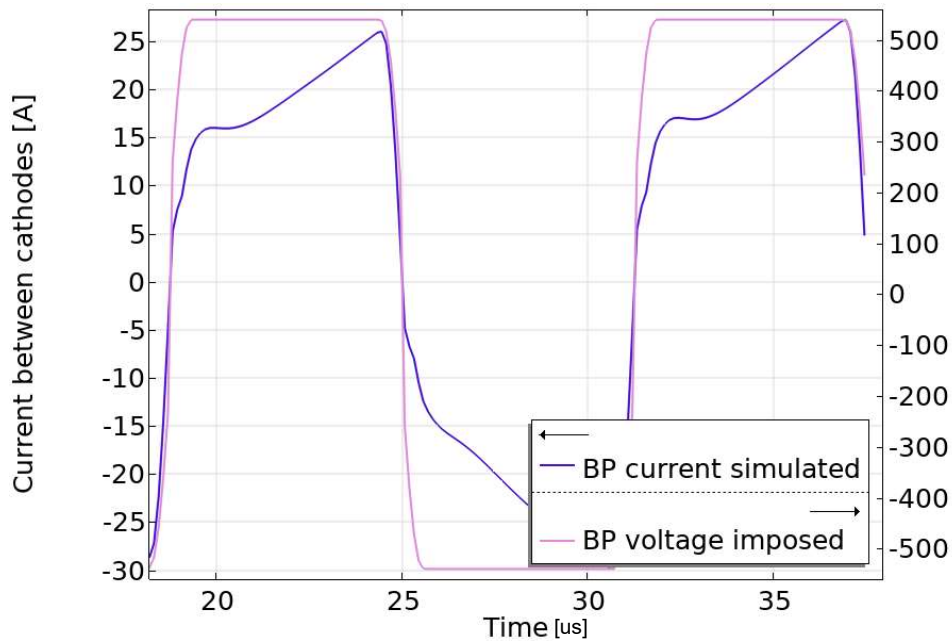
measured



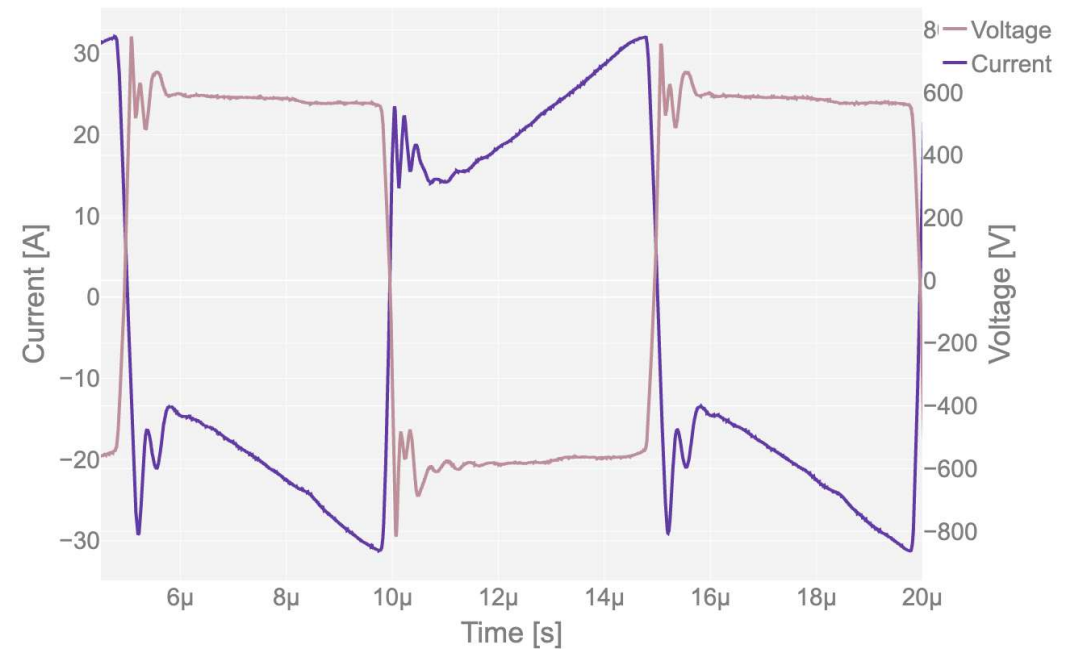
Validating IV readings in the BP mode

- The model **predicts correct shape and magnitude of current response** => indicates correct physics
- Model computes the correct plasma conductivity (voltage is imposed, power/current computed)

simulation



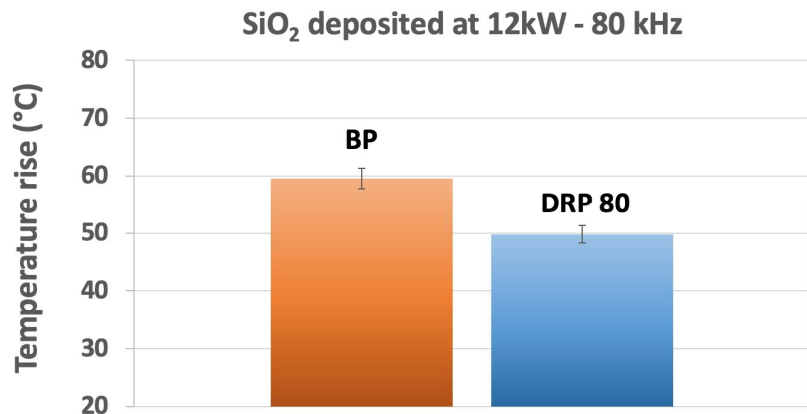
measured



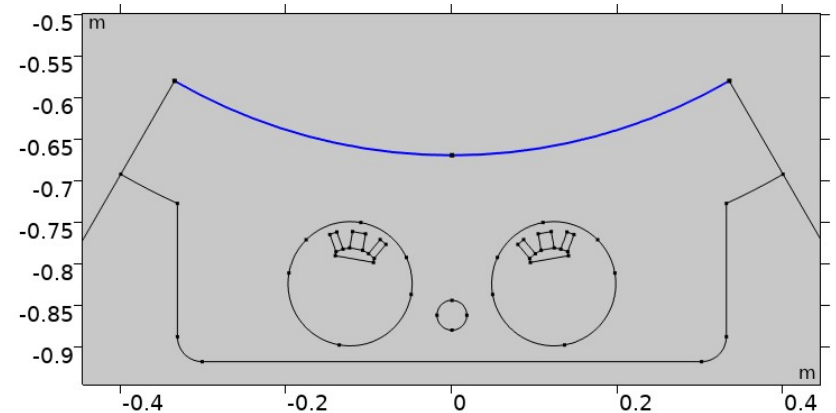
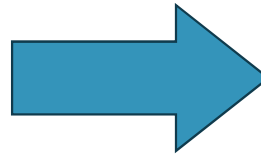
Question 1: How does the waveform affect the process?

Substrate heating in BP and DRP

- Experimentally, differences have been observed between DRP-grown and BP-grown coatings
- These have been correlated with a **change in substrate temperature**, significantly and systematically higher in BP.
- Can the model explain why that is?



Experimentally observed

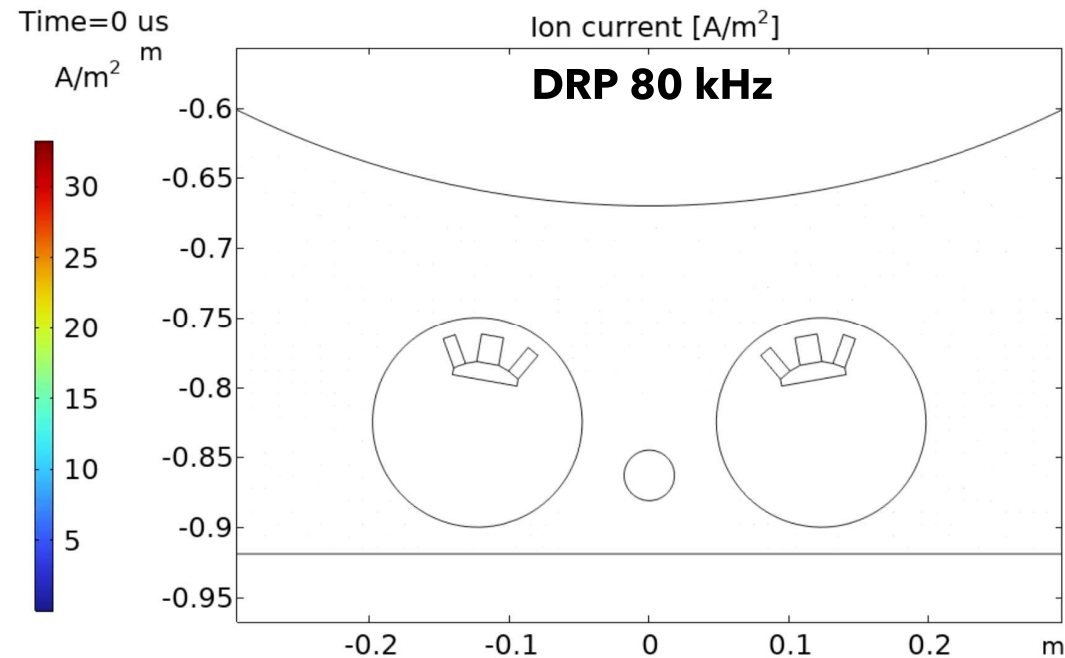
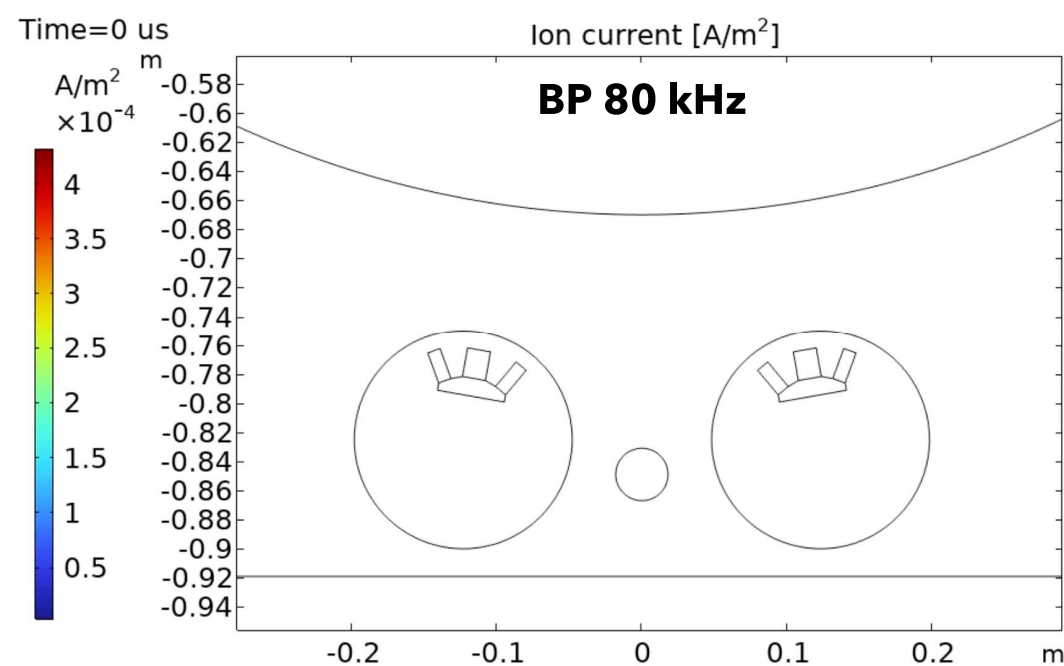


Deposited energy is proportional to the ion current bombarding the substrate.

Substrate heating in BP and DRP

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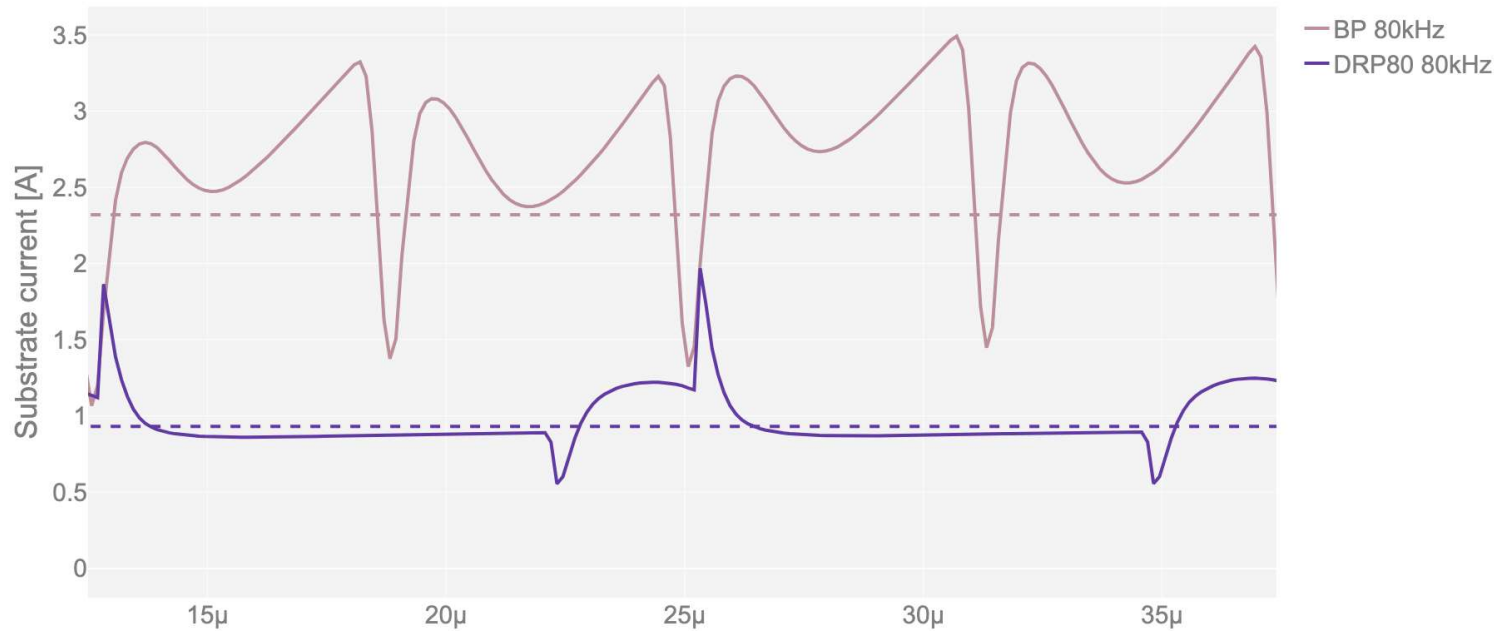
The BP waveform provides more intense ion bombardment and substrate heating



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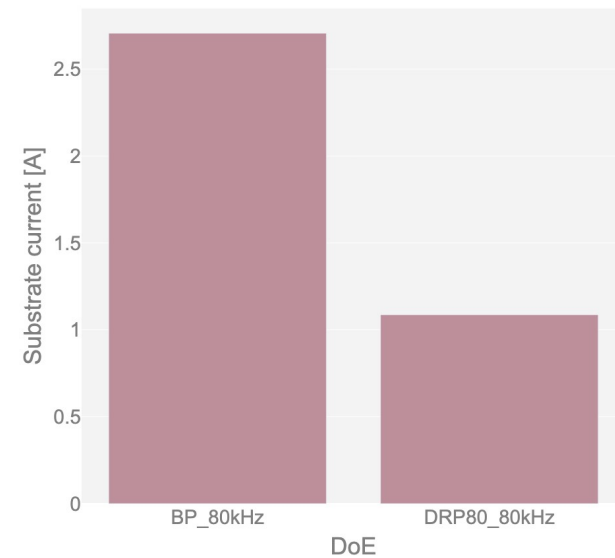
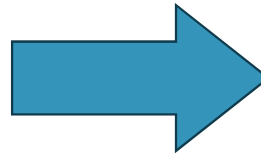
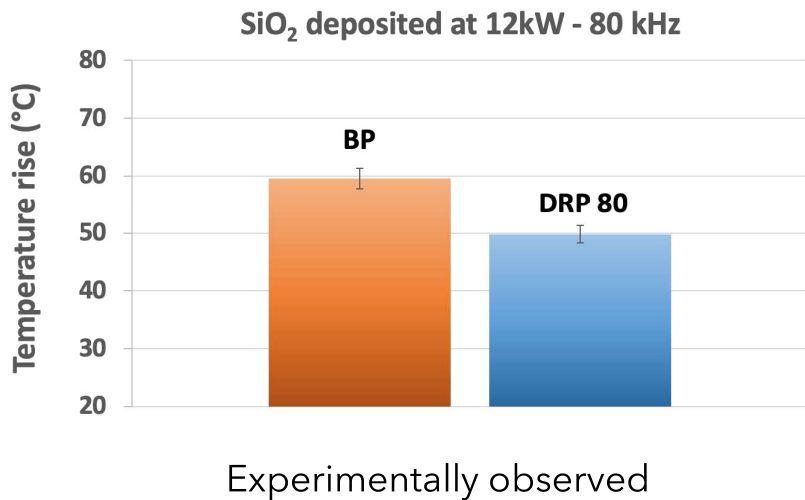
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Substrate heating in BP and DRP

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The BP waveform provides more intense ion bombardment and substrate heating



Question 2: What effect does the anode play in DRP?

Anode effects in DRP processes

- The demo equipment has 3 anode slots and anode position can be changed.
- Even in the default positions, experiment suggested that there is a **change in deposition rate when 3 anodes are installed instead of 1** - what is the reason for that?

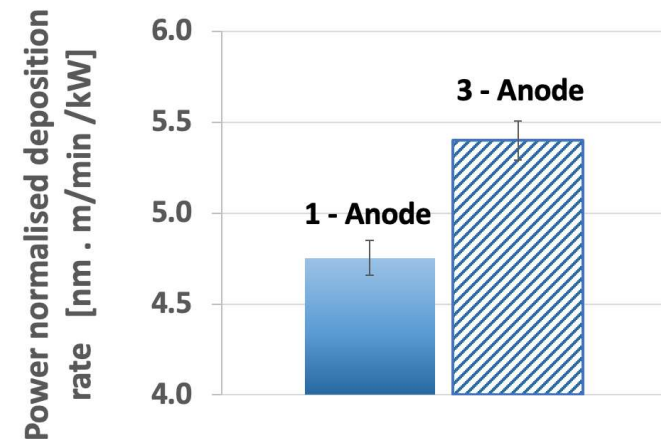
Analysis:

- The total amount of Si sputtered from the target that can be deposited depends only on IV: $\int_{\text{target}} \Gamma_M \sim V^{\frac{1}{2}} \cdot I$
- The total amount of Si arriving at the substrate also depends on the relative orientation of the racetrack and substrate, so

$$\int_{\text{substrate}} \Gamma_M \sim \beta \cdot V^{\frac{1}{2}} \cdot I \text{ where } \beta \text{ is a geometrical factor}$$

So the real question is - do the anodes affect the position of the plasma on in any way?

Silicon nitride - DRP 80 - 12 kW - 50 kHz



Anode effects in DRP processes

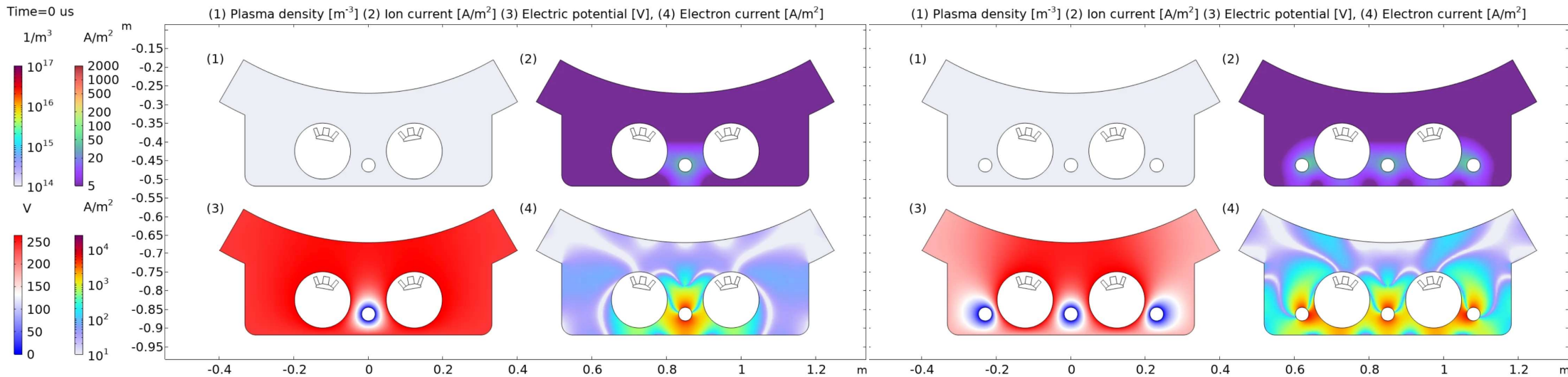
Additional outer anodes actually “shape” the plasma in front of the sputter cathodes.

Plasma is more “spread out” for the 3-anode config!

Mechanism: Outer anodes attract some electrons. Due to ambipolar diffusion, the whole plasma moves with them

1 anode config

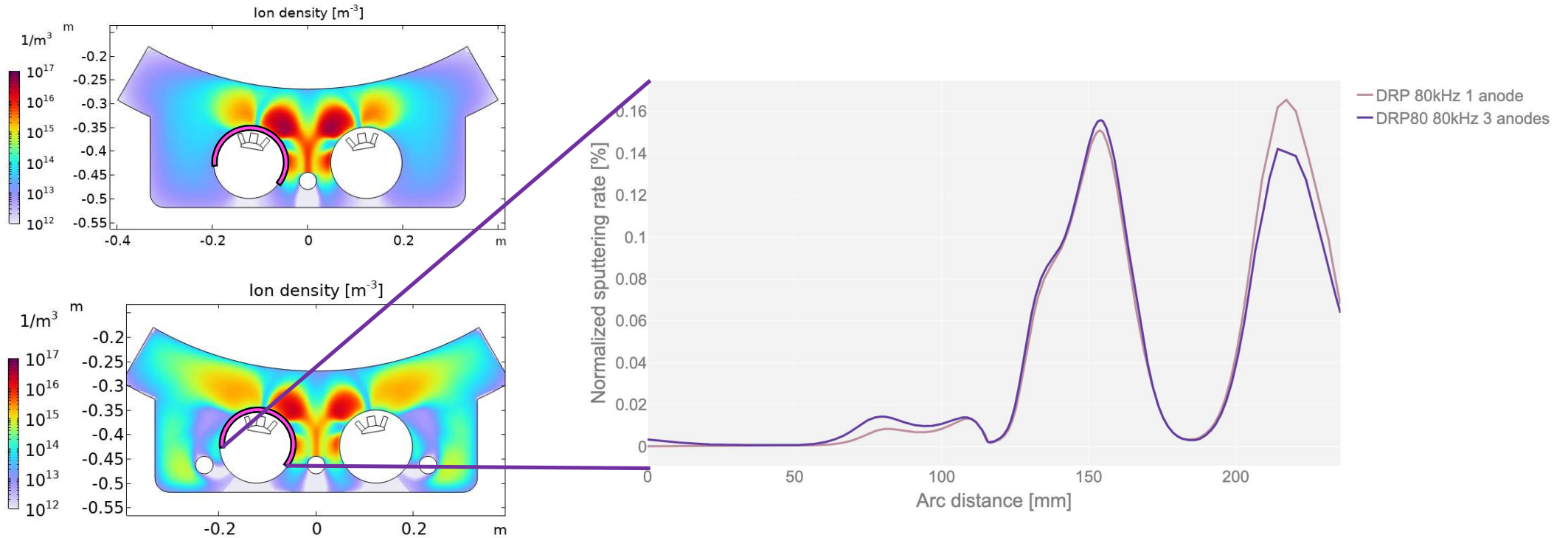
3 anode config



Anode effects in DRP processes

We can also look at the erosion and see that the outer anodes are certainly helping.

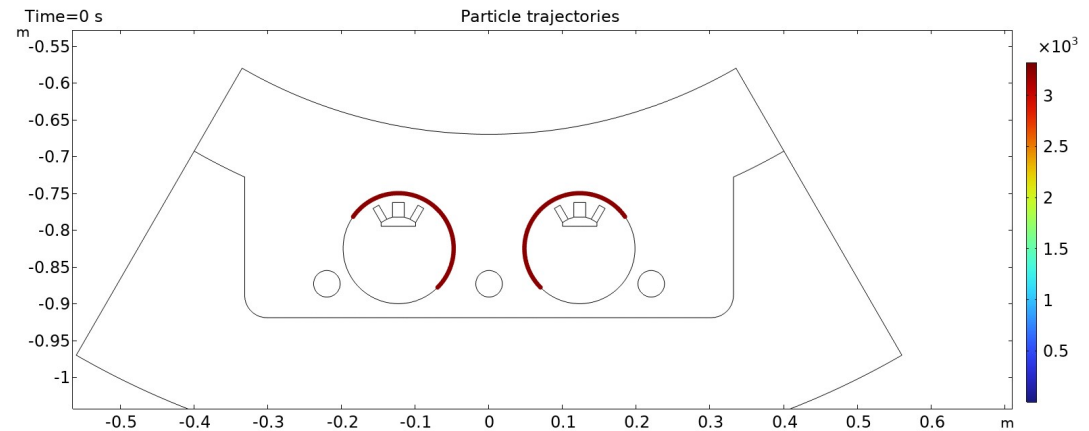
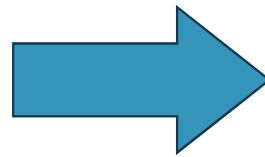
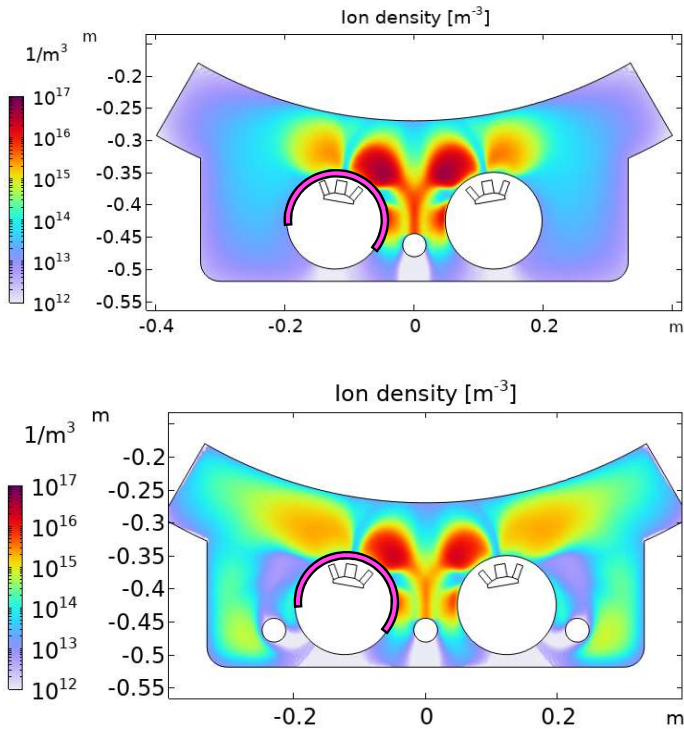
But is this enough to cause a significant change in the deposition rate?



Anode effects in DRP processes

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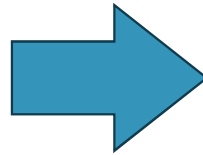
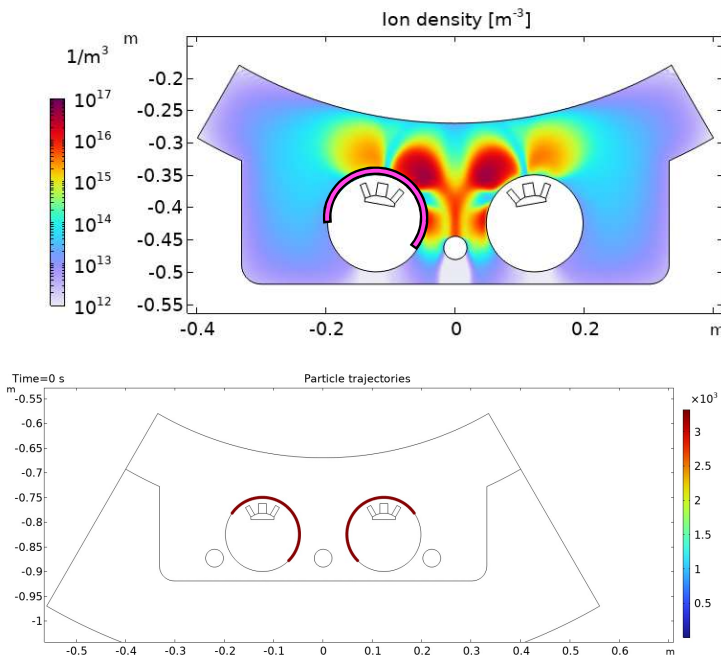


For both setups, we can trace metal atoms according to the local erosion rate and assess **what percentage of all sputtered atoms makes it to the substrate?**

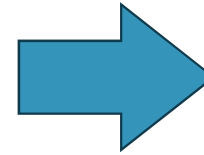
Anode effects in DRP processes

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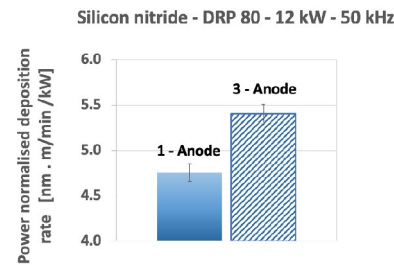
But is this enough to cause a significant change in the deposition rate?



The percentage of particles deposited on the substrate is
33.4% for 1 anode
35.7% for 3 anodes



According to the model, the 3anode setup should deposit **+7% more material per unit time per unit power**



Consistent with experimental observations.

Conclusions from the analysis

Waveform impact on the process

- **Qualitatively different plasma dynamics** for BP and DRP waveforms.
- Whether an application requires **low-energy or high-energy growth should affect the choice of power supply waveform.**
- **DRP probably offers greater flexibility** by tuning the duration of the positive pulse.

Anode effect in DRP

- **Anodes are a powerful driver** for the plasma distribution in DRP.
- By placing additional outer anodes next to the cathodes, the total **deposition rate per unit power** can be boosted significantly (+7%).
- Models show that there is **potential for further improvement** (parasitic plasma) - to be confirmed.

The simulation (1) provided quantities which are difficult to obtain by measurement and (2) opened avenues for further process optimization, that may not even be achievable experimentally.



Case study: MP2S thruster project

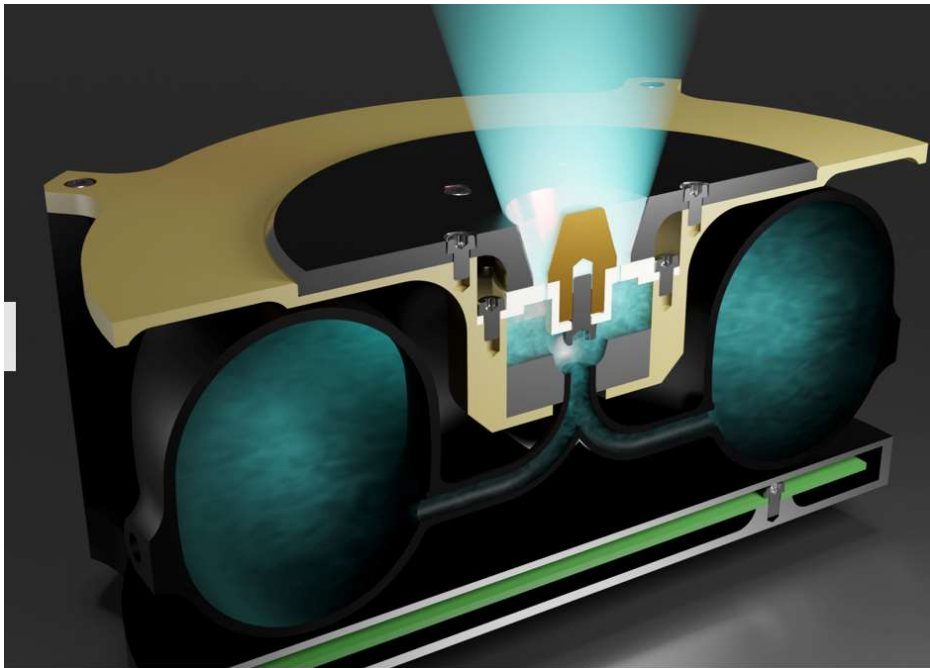


PlasmaSolve



MP2S thuster project

This project proposes an **innovative pulsed magnetoplasmadynamic thruster** (MPDT) for satellites.



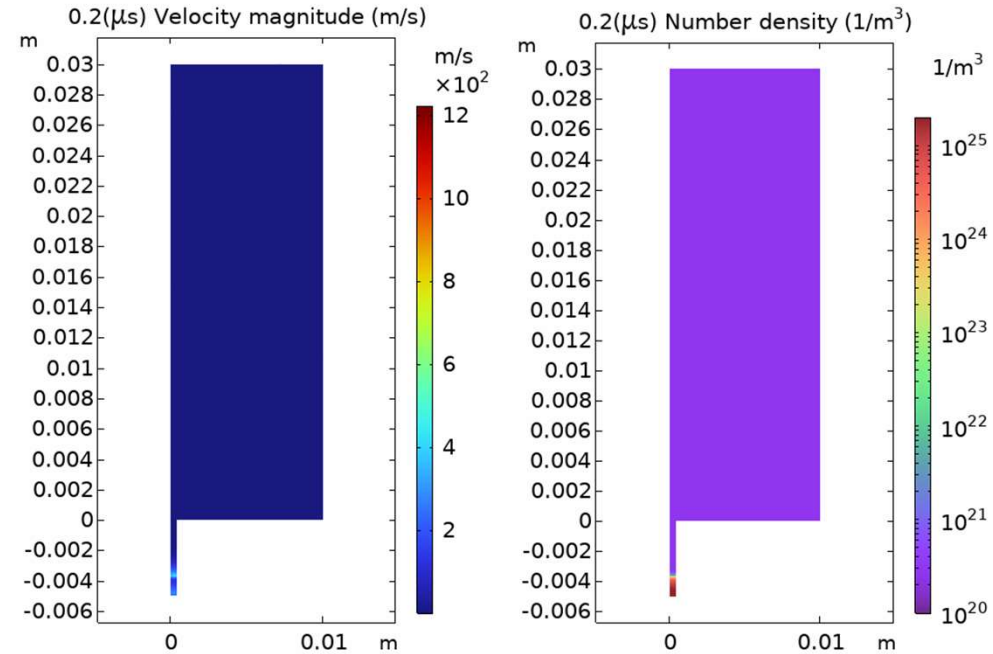
The principle is to accelerate plasma with a magnetic field which is created by an electric discharge between two electrodes. This discharge has an energy of several Joules.

The **main innovation of this technology lies in the pulsed operating of the thruster**, which allows to modulate the thrust generated simply by controlling the frequency of the pulses.”

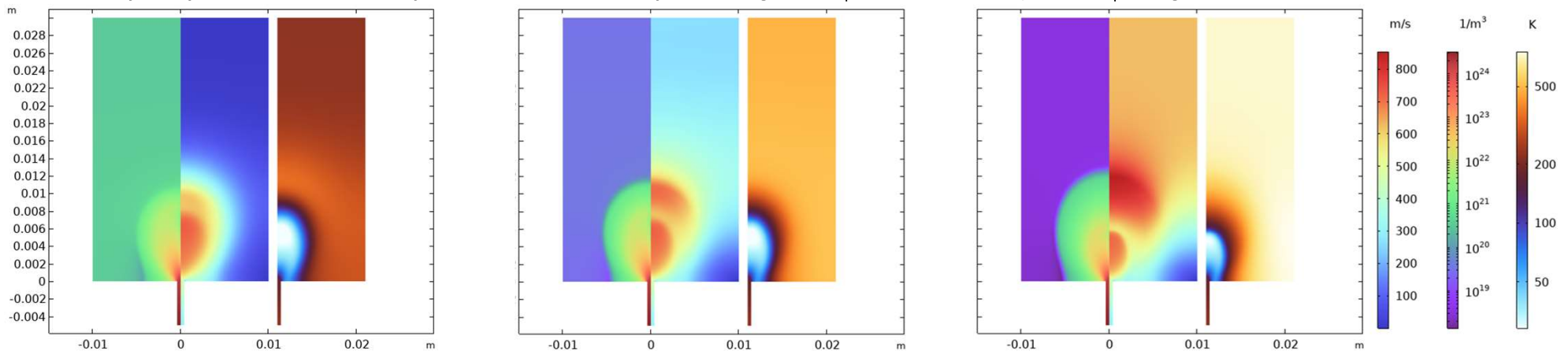
The valve permits to inject just the amount of gas that will be ionized in the discharge chamber at each pulse. But the valve behavior and performance is an unknown...

MP2S Vacuum Expansion

- Quite a fresh project, we started with HMNF flow simulations.
- HMNF model now being coupled to plasma simulation, which is a challenge 😊.



Sensitivity study: (Left) Number density [1/m³], (Middle) Velocity [m/s], (Right) Temperature [K] at 20 μs after opening the valve



$\Delta p = 99\,999.00\text{ Pa}$

$\Delta p = 99\,999.90\text{ Pa}$

$\Delta p = 99\,999.99\text{ Pa}$

Summary and Bottomline

Summary and Bottomline

PlasmaSolve has been supporting customers from **diverse fields where plasma is crucial**.

In most project, our consultancy is heavily centered on **physics and chemistry simulation**.

COMSOL Multiphysics has been a stable and irreplaceable tool on our belt for the past few years and it will remain so.

COMSOL's Plasma Module has some unique features, that makes it **stand above all the other mainstream simulation libraries**, when it comes to plasma sims.

The Multiphysics aspect is equally important - industrial plasma systems almost always require coupling plasma calculation to the flow, chemistry, thermal balance, or particle tracing.

PlasmaSolve

obrusnik@plasmasolve.com