Simulation of Plasma Processes for Mikroelectronics Fabrication

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Plasma Processing in Mikroelectronics Fabrication

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Plasma Processing I

Of all process steps employed during the manufacturing of a microelectronic circuit, more than 40 % are plasma based:

- Plasma etching (PE, RIE, MERIE ...)
- Plasma enhanced CVD (PECVD)
- Sputtering / Ionized physical vapor deposition (IPVD)
- Plasma oxidation
- Plasma ashing / plasma cleaning

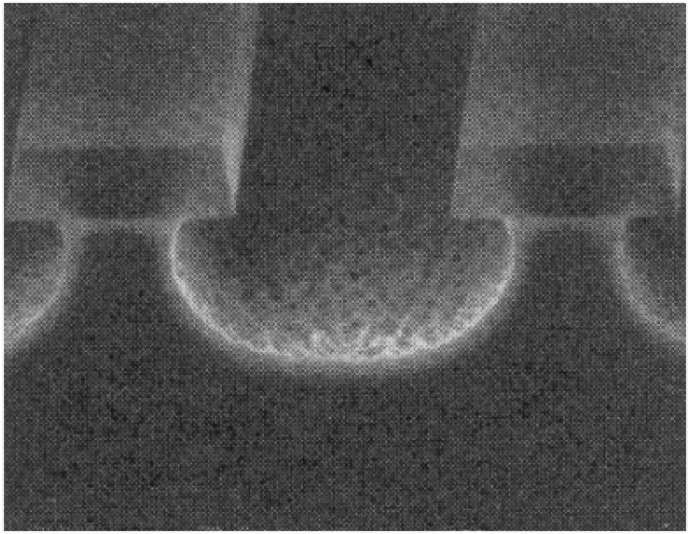
Plasma processes have unique features:

- Non-equilibrium chemistry
- Directionality and anisotropicity
- High flexibility and controllability

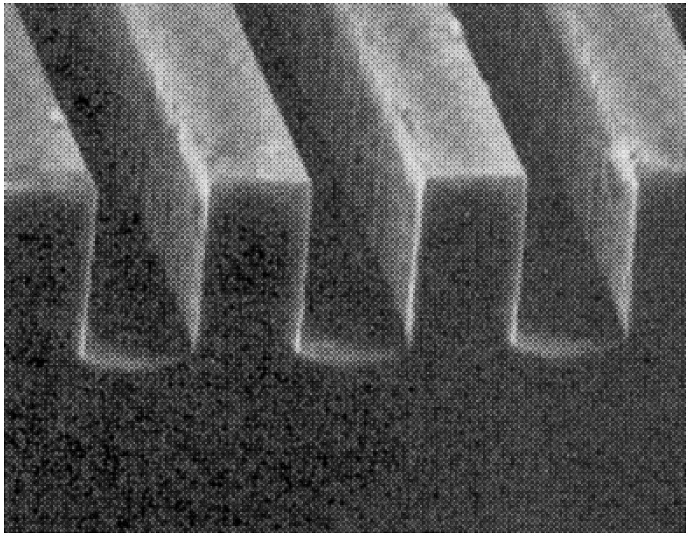
For microelectronics, plasma processes are indispensable!

Plasma Processing II

Adjusting the bias voltage can change the etch characteristics:
(Etching of GaAs with BCl_3/Cl_2, Agarwala et al., 1999)



U_{bias} = 0 V



U_{bias} = 100 V

Plasma processes have „more knobs to turn“

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Plasma Processing III

The increasing demands of the microelectronic industry pose a continuous challenge for the methods of plasma processing:

- Smaller device structures (0.1 µ and below)
- Larger wafer areas (300 mm)
- New materials (low k, high e, Cu, Ti ...)
- More complex processes
- Environmental issues

Simulation methods can help in several ways:

- Provide insight and understanding
- Can assist in process optimization
- May form the basis of process control

Necessary for simulation: A physical process model

Modeling of Process Plasmas

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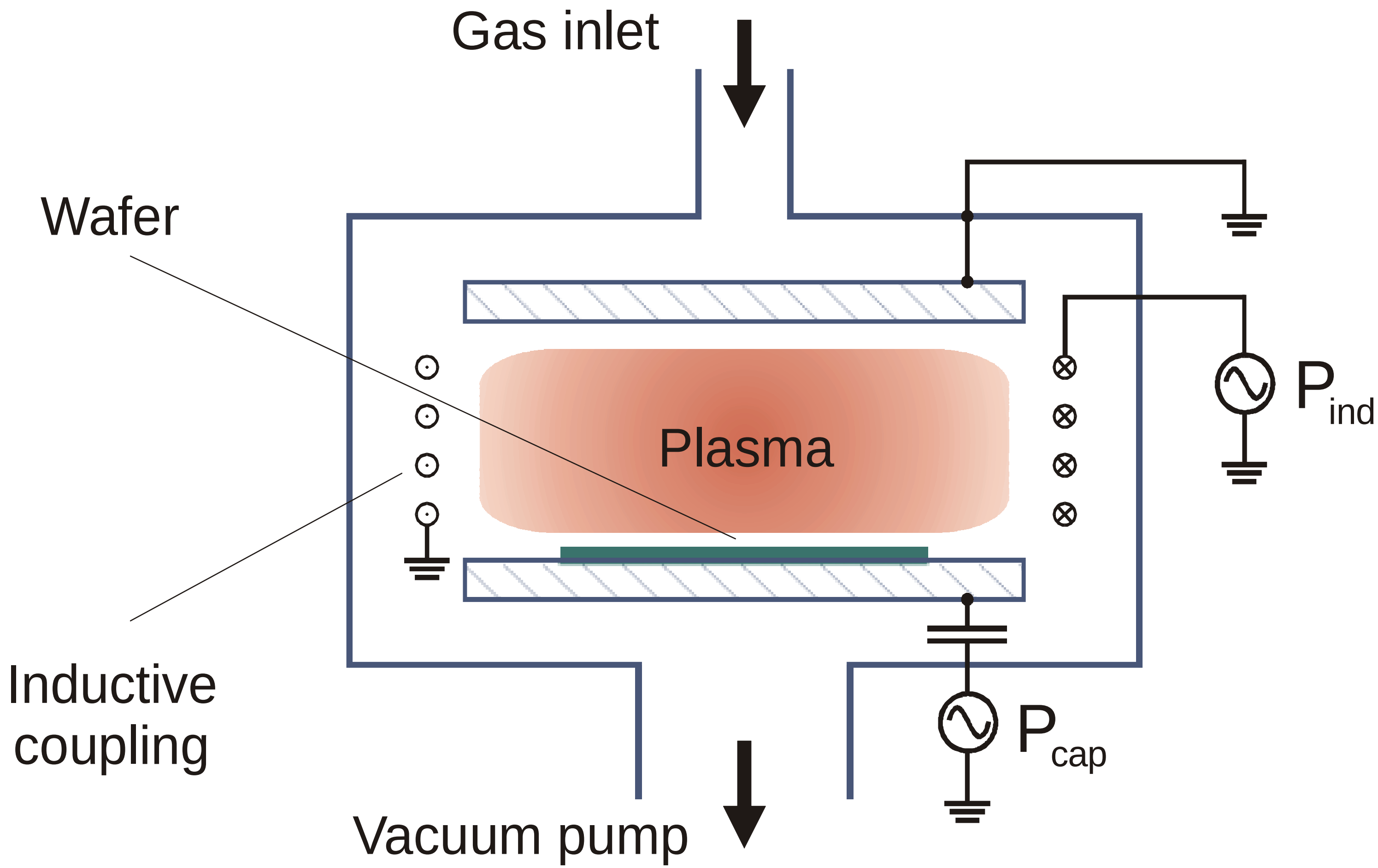
Scope of Plasma Modeling I



Plasma reactor with inductive and capacitive coupling

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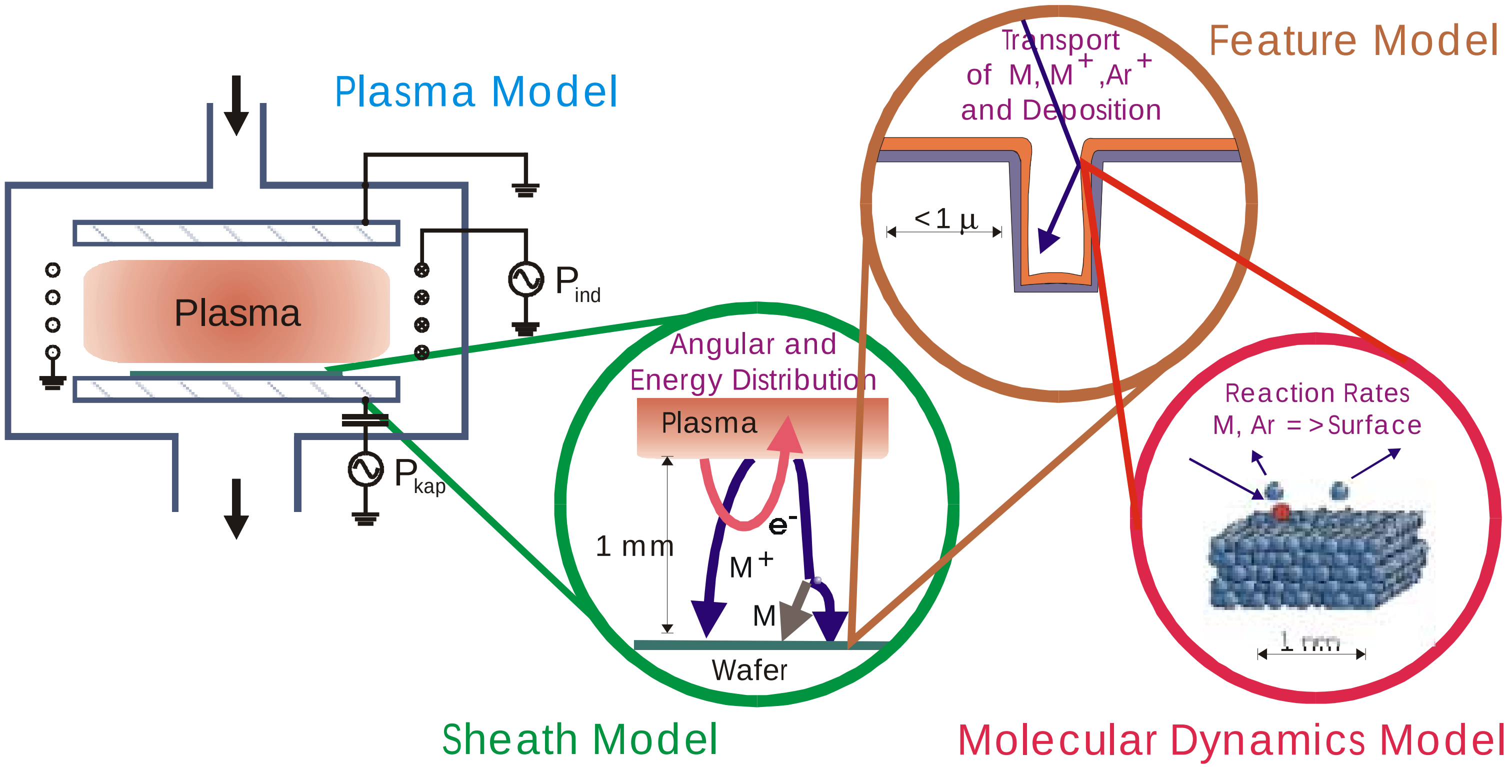
Scope of Plasma Modeling II



Plasma processes include phenomena on many different scales:

Necessary for simulation: A hierarchy of models

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Scope of Plasma Modeling III

In order to make meaningful contributions to the development of a VLSI process, simulation tools must

- be numerically stable and computationally efficient
- account for realistic process conditions
- make physically accurate predictions

Only if **all important mechanisms** on **all scales** are adequately understood and modeled, these requirements can be met!

Scope of this presentation:

- Detailed description of the boundary sheath model
- Outline of the feature scale simulation (Hansen/Kersch)
- Description of a pilot application (Hansen/Kersch. authors)

A Model of the Plasma Boundary Sheath

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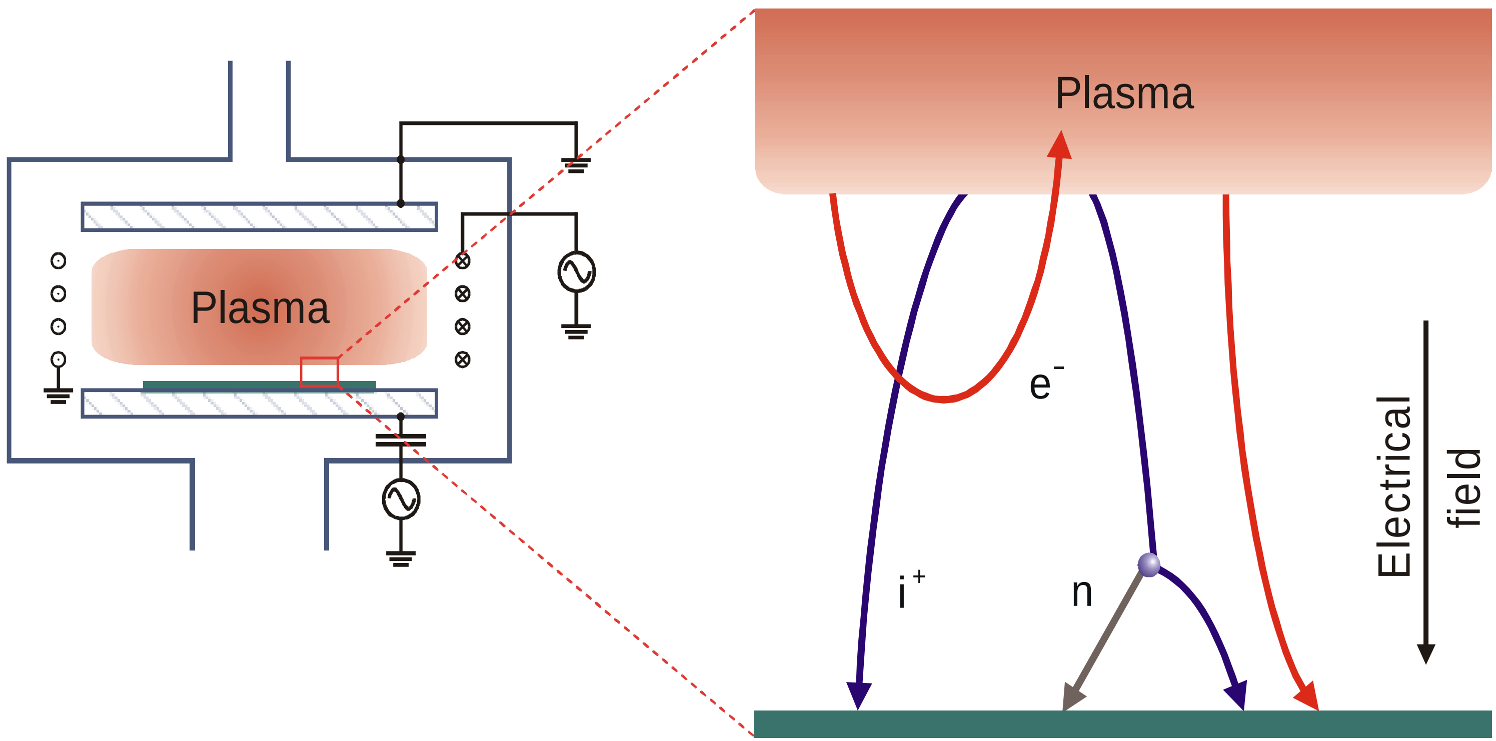
Scope of the Sheath Model I

Processes in a plasma boundary sheath:



Reactor scale: < 1 m

Sheath scale: 1 mm

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Scope of the Sheath Model II

Goal: Efficient calculation of the electrical field in the sheath and the energy and angle distribution of the wafer-incident particles:

- Arbitrarily many species of (positive) ions and neutrals.
- Elastic and charge exchange ion/neutral collisions.
- Externally applied bias fields, not necessarily sinusoidal.

Our approach: A hybrid boundary sheath model which couples a self-consistent fluid model to a one-particle Monte Carlo code:

- The fluid dynamic part solves the macroscopic equations of motion together with Poisson's equation.
- The Monte-Carlo code follows the trajectories of a large set of ions (and possibly neutrals) in the calculated field.
- A statistical evaluation of the trajectories yields the energy and angle distribution of the particles incident on the wafer.

Fluid-Dynamic Model I

Equations of motion, coupled to Poisson's equation:

Electrons

$$\begin{cases} \dfrac{\partial n_e}{\partial t} + \dfrac{\partial}{\partial x}(n_e v_e) = 0 \\[2ex] \dfrac{\partial v_e}{\partial t} + v_e \dfrac{\partial v_e}{\partial x} = -\dfrac{e}{m_e} E - \dfrac{T_e}{m_e} \dfrac{1}{n_e} \dfrac{\partial n_e}{\partial x} - \nu_e v_e \end{cases}$$

Ions (α=1..N)

$$\begin{cases} \dfrac{\partial n_\alpha}{\partial t} + \dfrac{\partial}{\partial x}(n_\alpha v_\alpha) = 0 \\[2ex] \dfrac{\partial v_\alpha}{\partial t} + v_\alpha \dfrac{\partial v_\alpha}{\partial x} = \dfrac{q_\alpha}{m_\alpha} E - \dfrac{T_\alpha}{m_\alpha} \dfrac{1}{n_\alpha} \dfrac{\partial n_\alpha}{\partial x} - \nu_\alpha v_\alpha \end{cases}$$

Electrical field

$$\varepsilon_0 \frac{\partial E}{\partial x} = \sum_\alpha q_\alpha n_\alpha - e n_e$$

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Fluid-Dynamic Model II

Assumptions which are already embodied in the equations:

- Only electrons, positive ions and neutrals are present, negative ions do not enter the sheath.
- The sheath thickness is small against the reactor scale.
- The momentum loss of the ions due to collisions with neutrals can be described by an effective friction term.
- Ionization and recombination in the sheath are negligible.
- Electrons and ions have constant kinetic temperature.

Further simplifications which must be implemented separately:

- The frequency of the (possibly inharmonic) RF modulation lies between the plasma frequencies, $w_{pi} << w_{RF} << w_{pe}$.
- The thickness of the boundary sheath is much larger than the electron Debye length, $H >> l_D$.

Fluid-Dynamic Model III

Electrons follow the field instantaneously

$$\left.\begin{aligned} \frac{T_e}{e}\frac{\partial n_e}{\partial x} + nE = 0 \\ \varepsilon_0 \frac{\partial E}{\partial x} = e(n_i - n_e) \end{aligned}\right\} \rightarrow E = -\frac{T_e}{e\lambda_D}\Xi_0 - \frac{T_e}{e}\Xi_1 \frac{1}{n_i}\frac{\partial n_i}{\partial x}$$

The ions see the average field $\langle E \rangle = -\frac{T_e}{e\lambda_D}\Gamma_0 - \frac{T_e}{e}\Gamma_1 \frac{1}{n_i}\frac{\partial n_i}{\partial x}$

$$n_\alpha v_\alpha = -\Psi_\alpha$$

$$v_\alpha \frac{\partial v_\alpha}{\partial x} = \frac{q_\alpha}{m_\alpha}\langle E \rangle - \frac{T_\alpha}{m_\alpha}\frac{1}{n_\alpha}\frac{\partial n_\alpha}{\partial x} - \nu_\alpha v_\alpha$$

Transformation into $q = \int n_i \, dx$ yields the sheath equation

$$\left(\frac{T_\alpha}{m_\alpha} - \left(\frac{\Psi_\alpha}{n_\alpha}\right)^2\right)\frac{n}{n_\alpha}\frac{\partial n_\alpha}{\partial q} + \frac{q_\alpha T_e}{e m_\alpha}\Gamma_1 \frac{\partial n}{\partial q} = \frac{\Psi_\alpha}{n_\alpha}\nu_\alpha - \frac{q_\alpha T_e}{e m_\alpha \lambda_D}\Gamma_0$$

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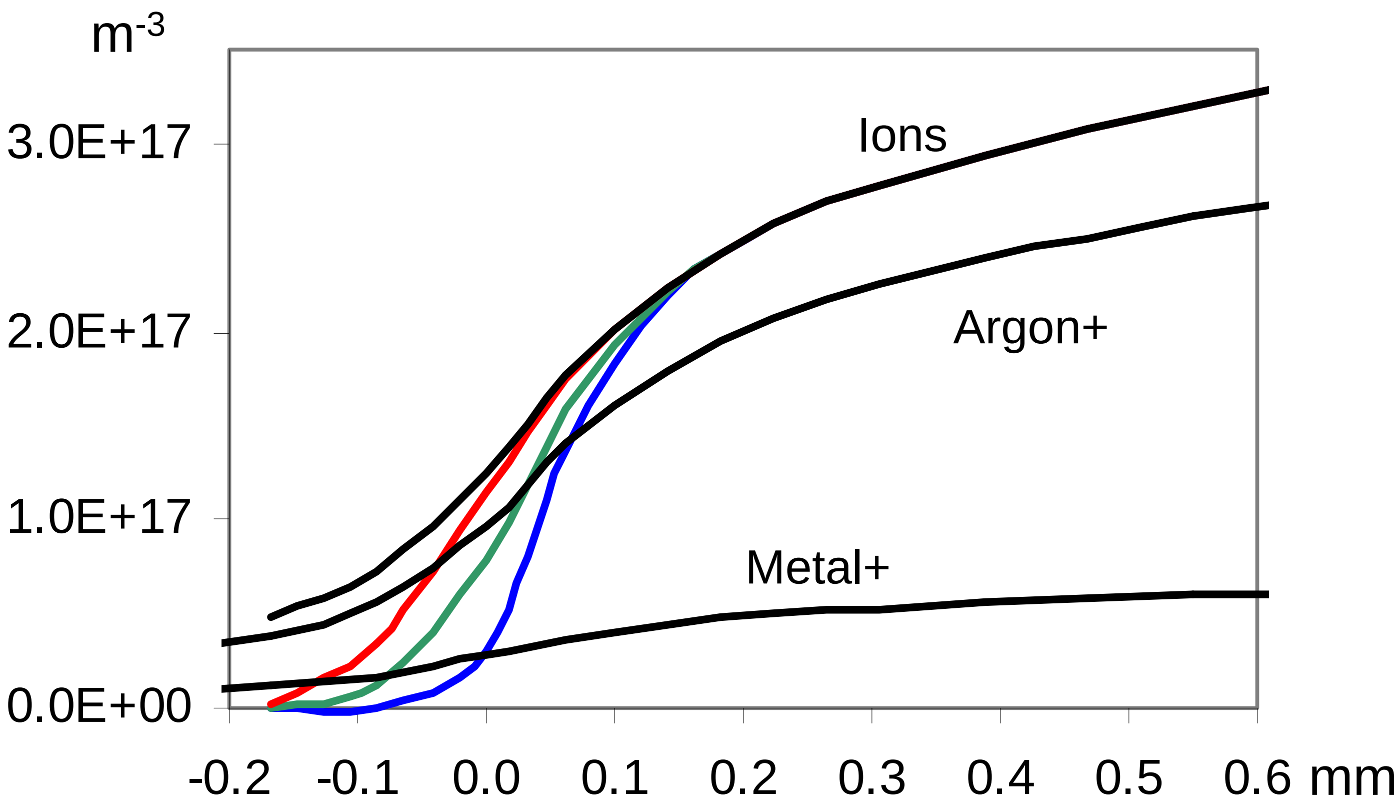
Fluid-Dynamic Model IV

Typical results of the fluid-dynamical model:



Electron and ion densities an argon-metal plasma

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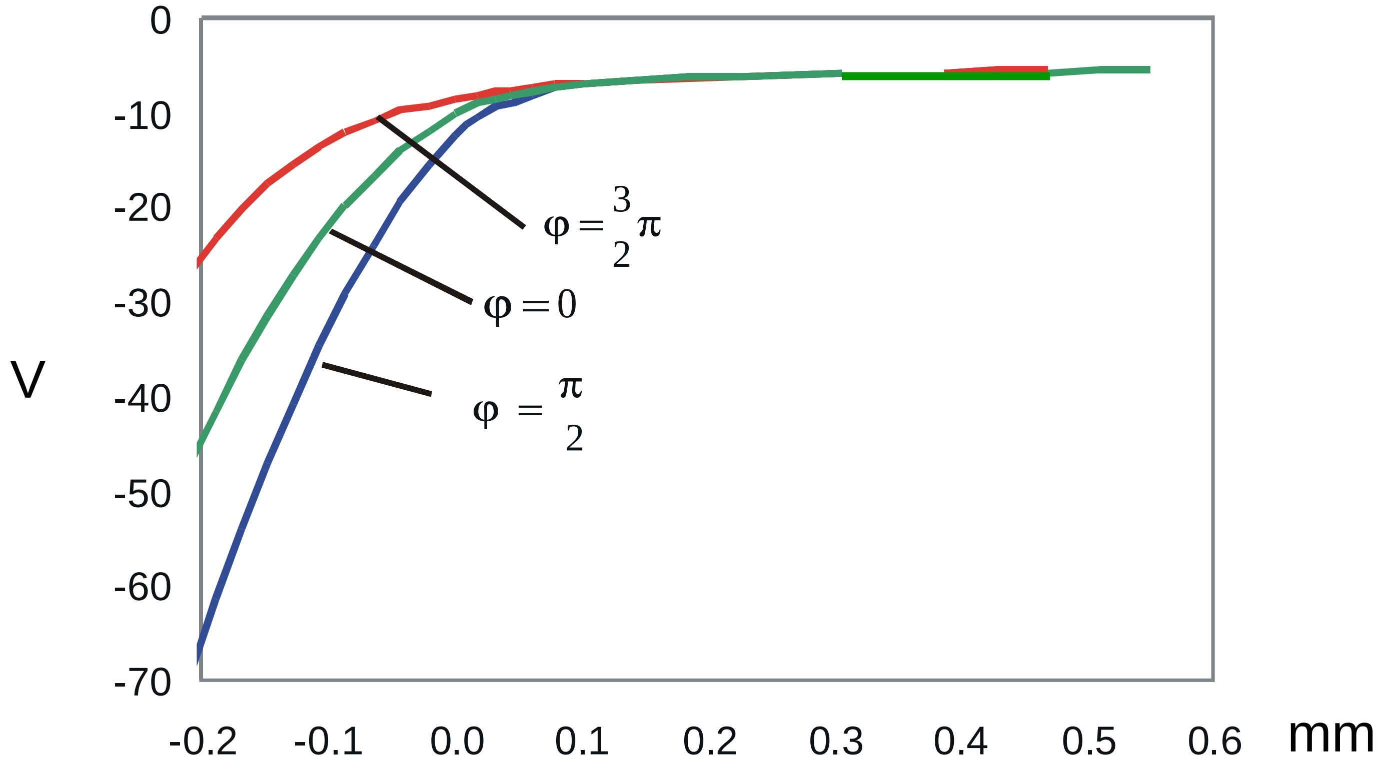
Fluid-Dynamic Model V

Typical results of the fluid-dynamical model:



Potential distribution at different phase angles

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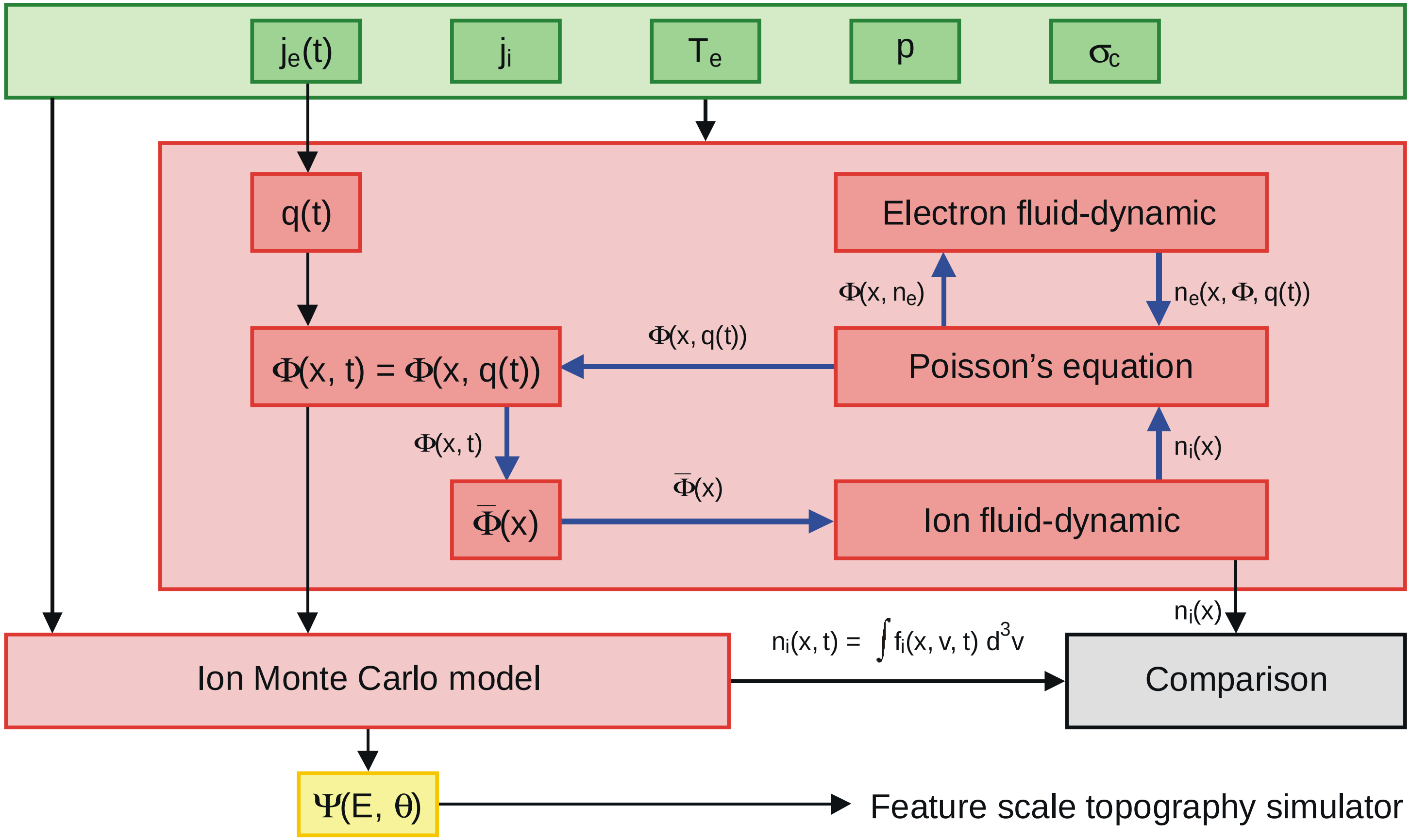
Monte-Carlo Model

The one-particle Monte Carlo simulation follows the trajectory of the ions (and possibly neutrals) in the electrical field E(x,t)

- One spatial and three velocity coordinates (x, v_x, v_y, v_z)
- Consideration of the relevant ion neutral collisions:
  - Resonant charge exchange
  - Elastic hard sphere interactions
  - Langevin-enhanced elastic collisions
- The Monte-Carlo collision cross sections are chosen compatible to the fluid dynamic transport parameters.
- The statistical evaluation of a sufficient number of ion trajectories yields the energy and angle distributions.
- The distribution of the energetic neutrals is calculated on the basis of a linearized Boltzmann equation.

Hybrid Sheath Model



The hybrid boundary sheath model is as accurate as a fully self-consistent particle-in-cell calculation, but **considerably faster**.

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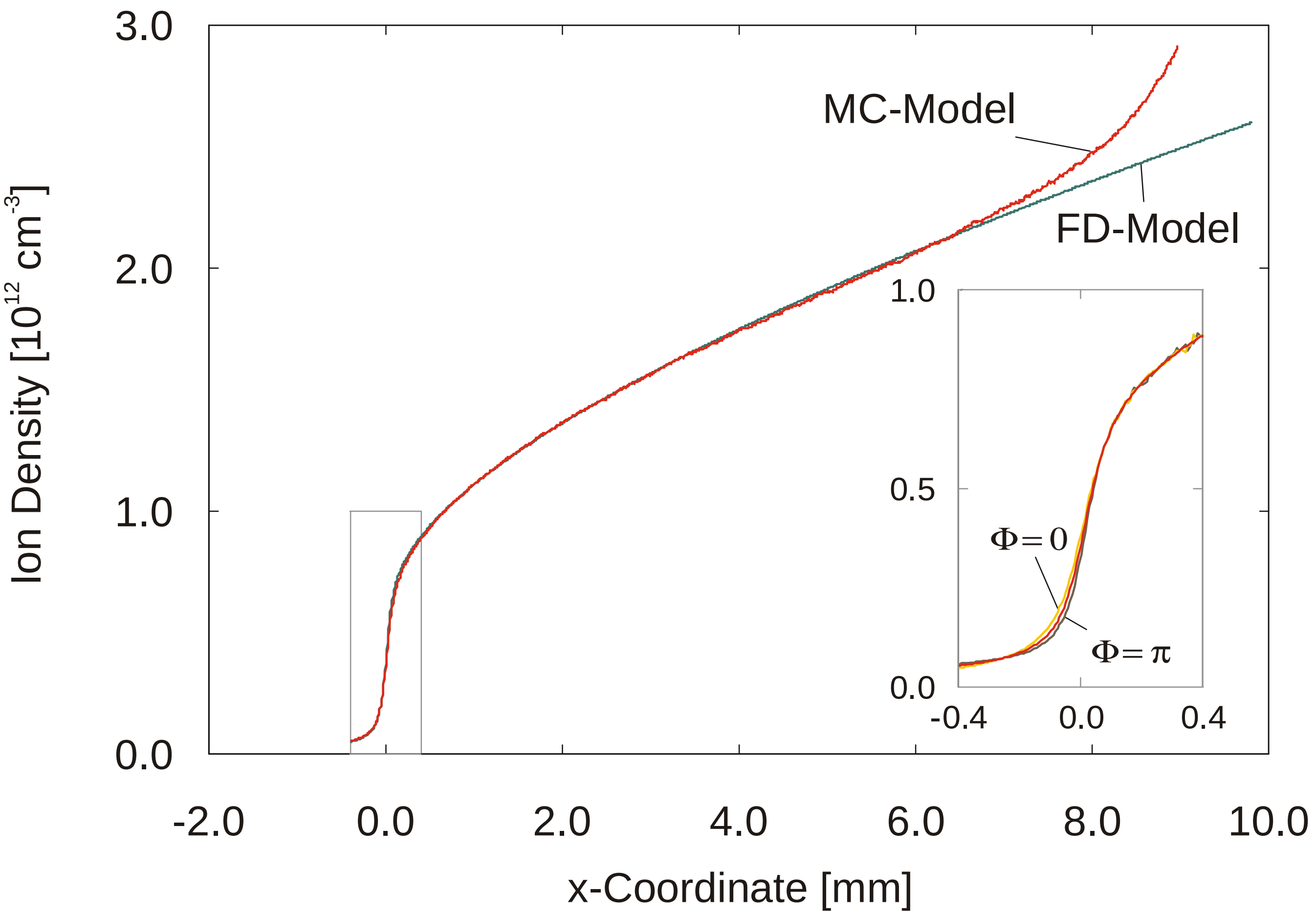
Fluid Dynamic vs. Monte Carlo



Ion densities of the fluid model and the Monte Carlo model

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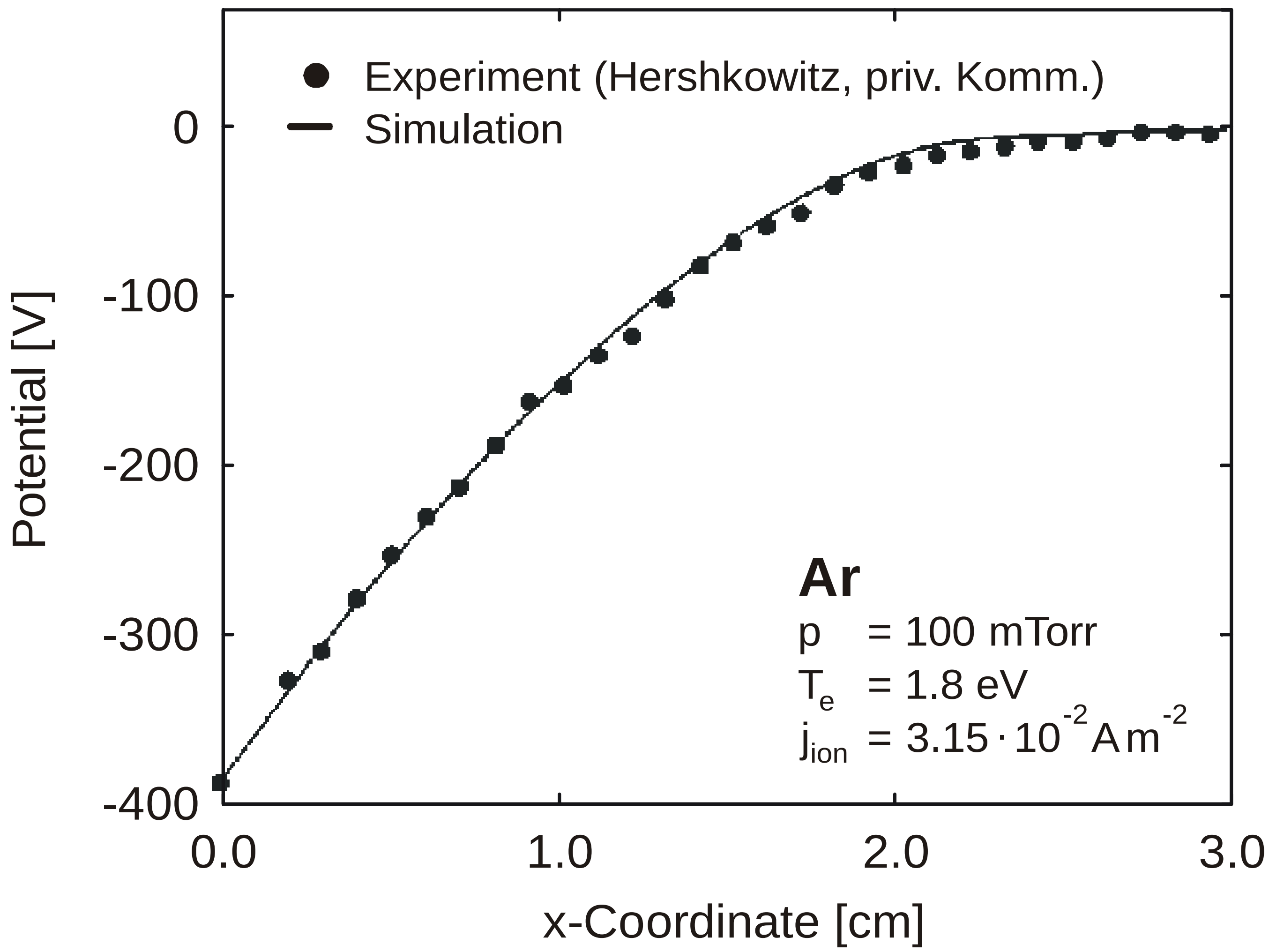
Simulation vs. Experiment I



Electrical Potential (100 mTorr Argon, DC)

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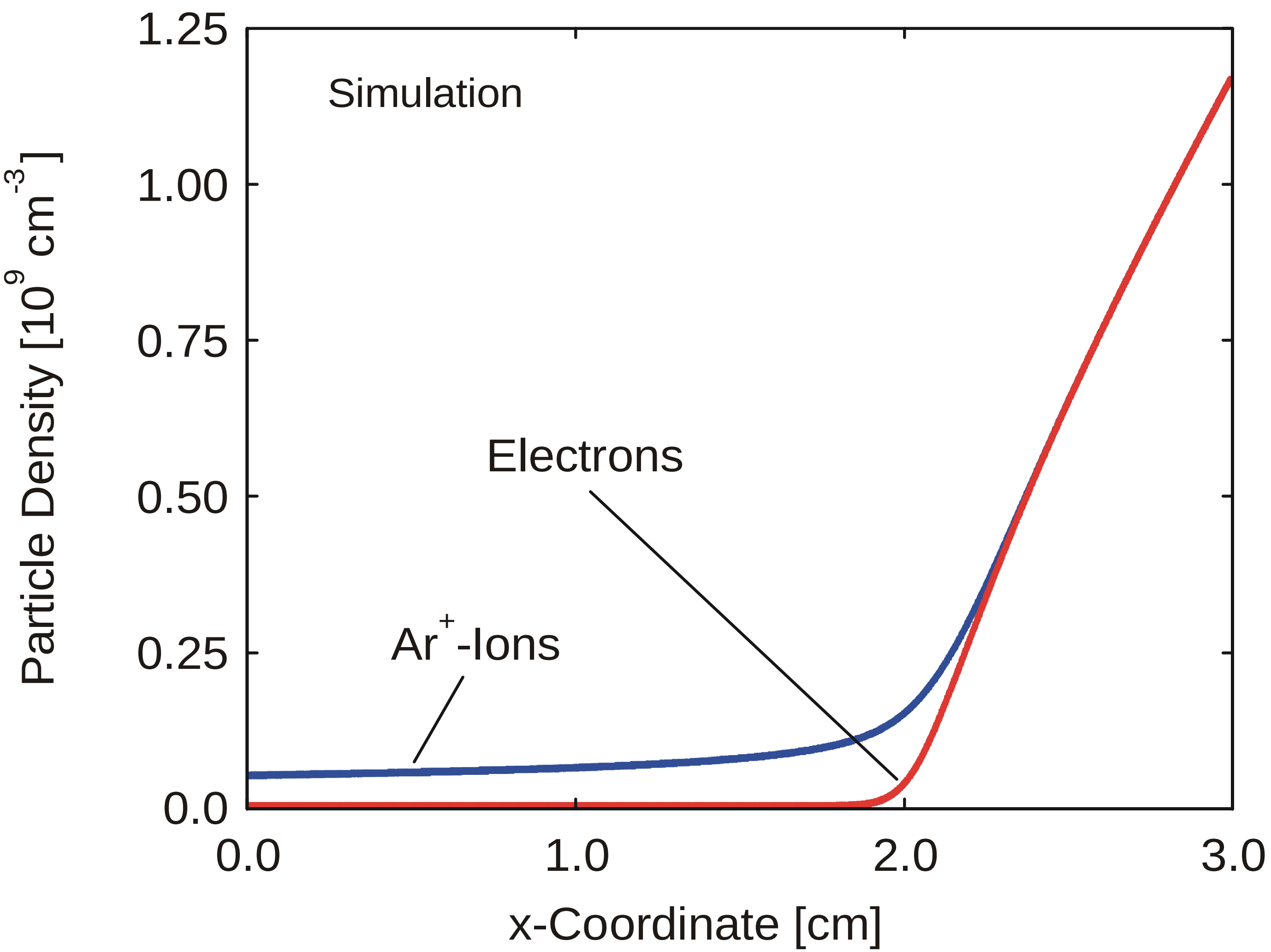
Simulation vs. Experiment II



Electron and ion densities (100 mTorr Argon, DC)

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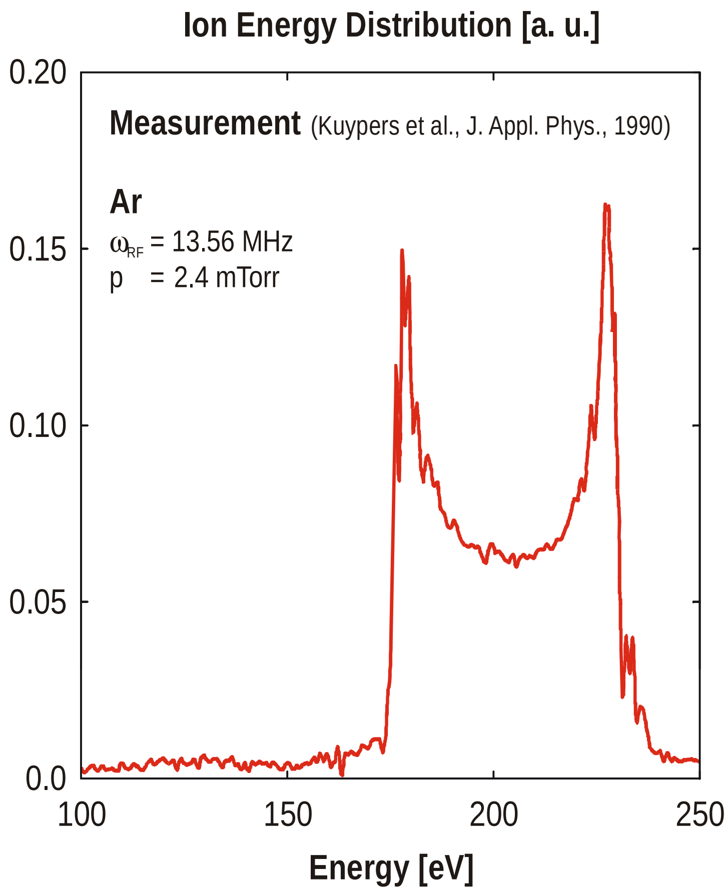
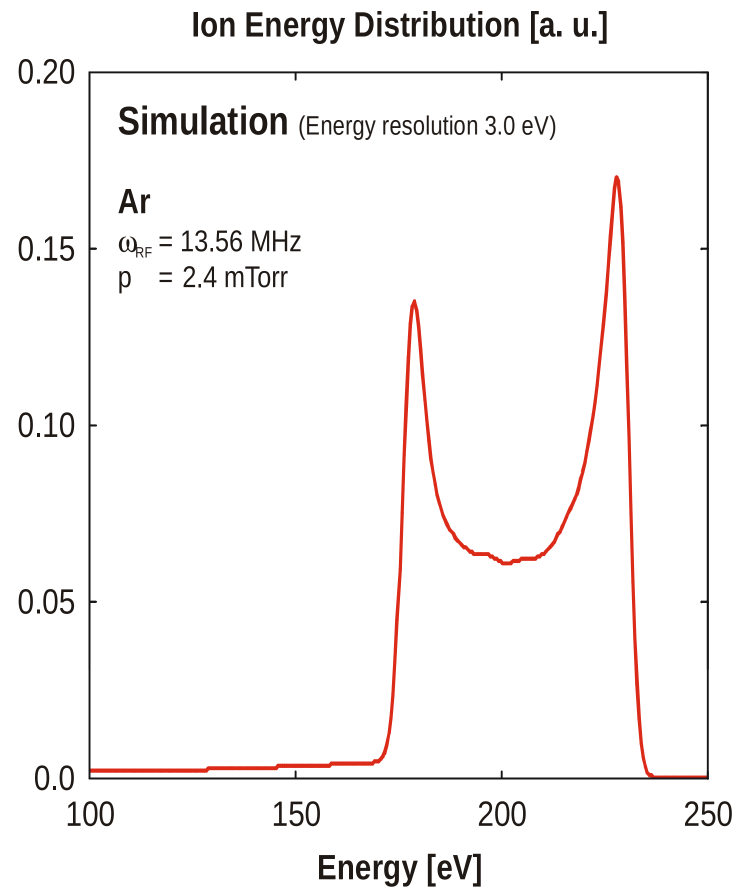
Simulation vs. Experiment III





Ion energy distribution (2.4 mTorr Argon / 13.56 MHz)

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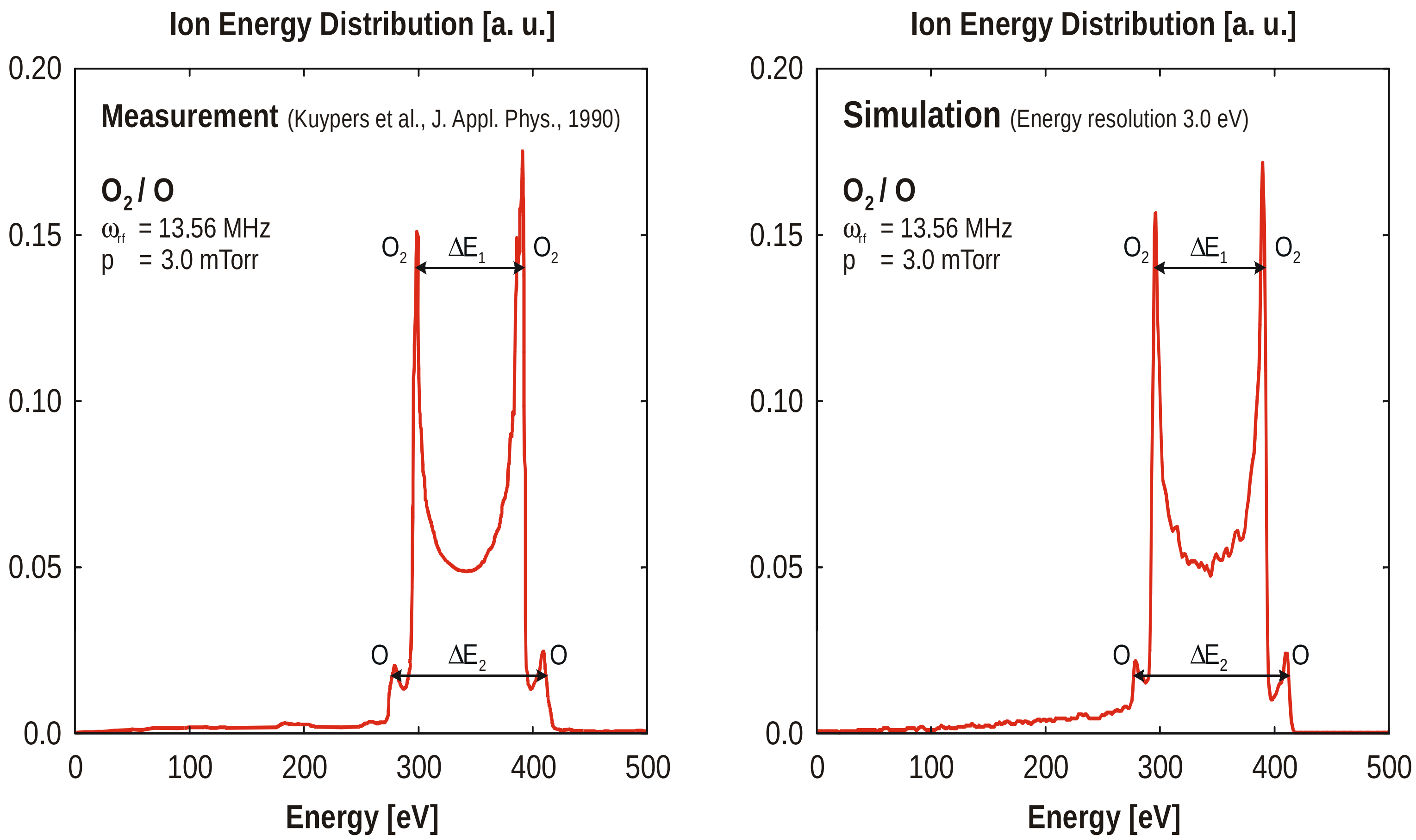
Simulation vs. Experiment IV



Ion energy distribution (3.0 mTorr Oxygen / 13.56 MHz)

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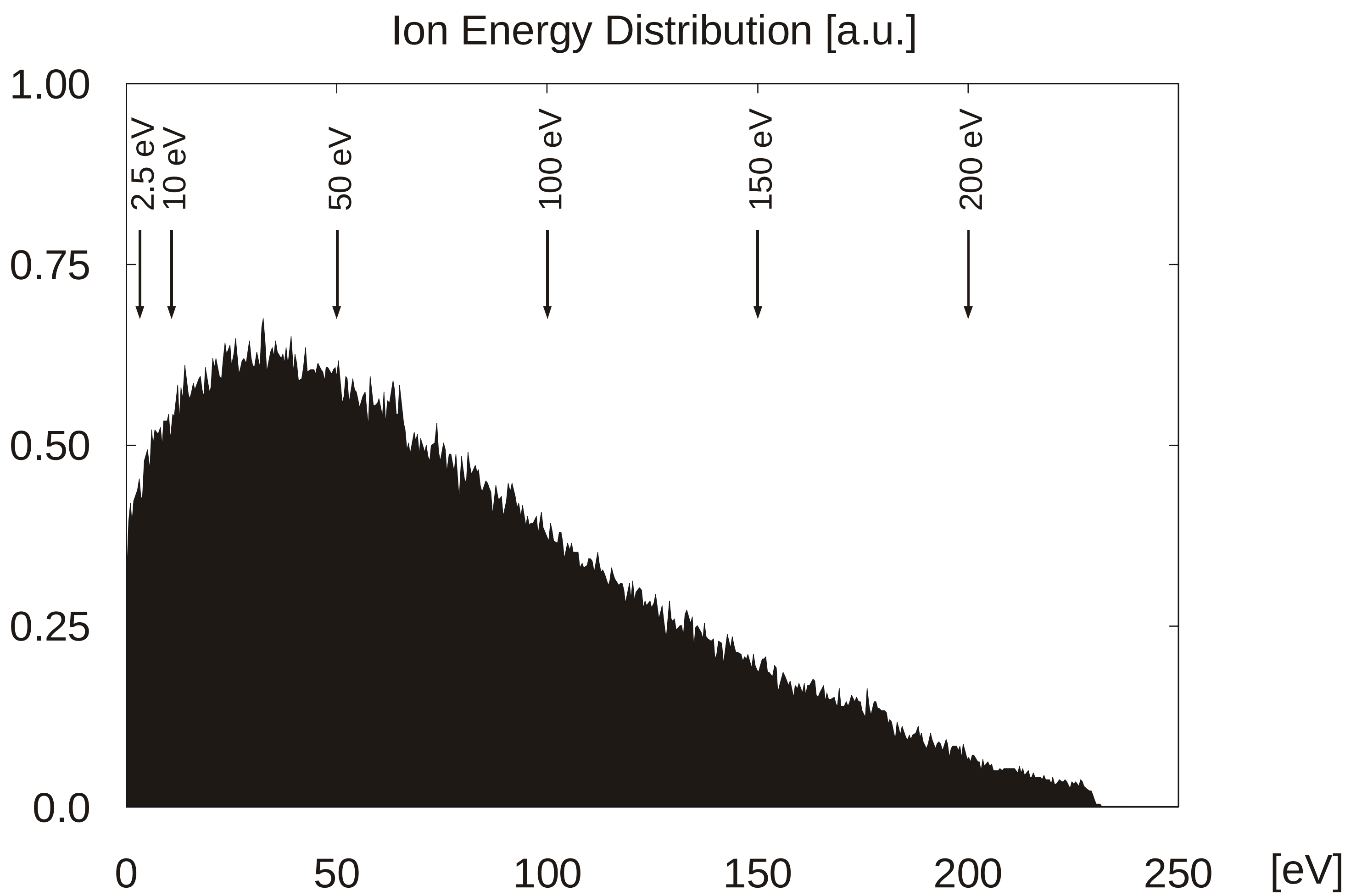
Model Predictions I



Ion energy distribution (300 mTorr Argon / 13.56 MHz)

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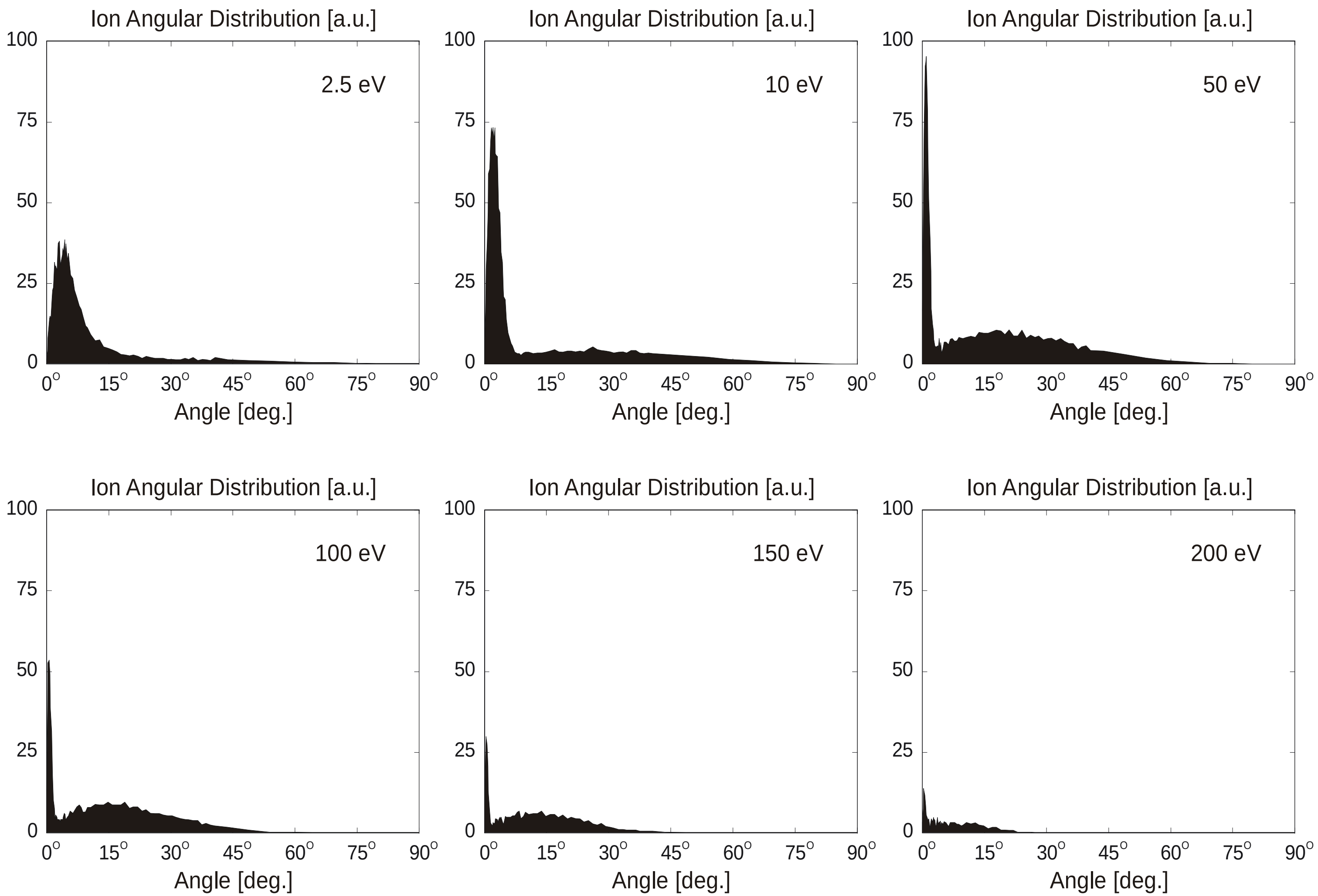
Model Predictions II



Angle distribution at different energies (300 mTorr / 13.56 MHz)

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Application:
Ionized Physical Vapor Deposition

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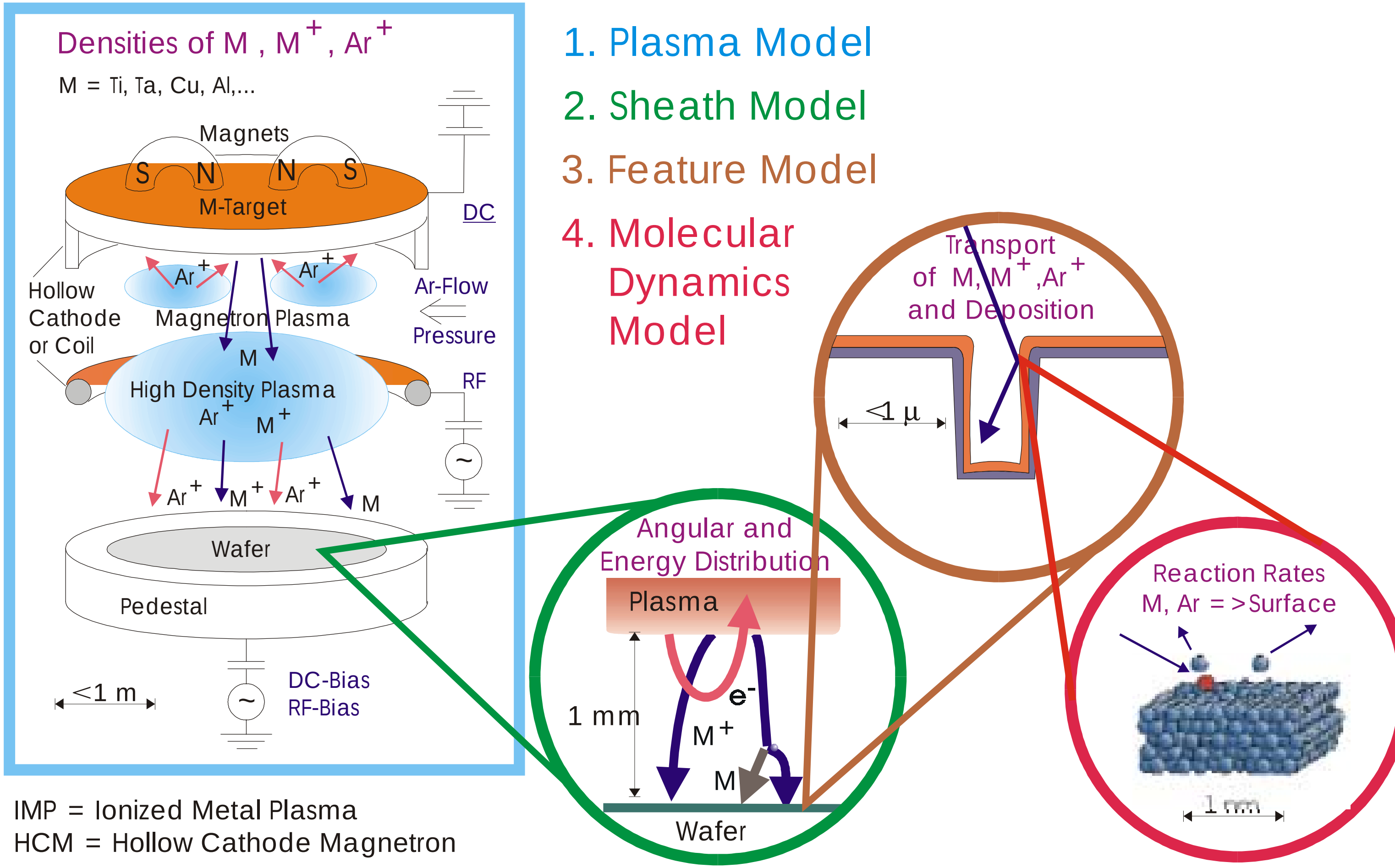
Ionized Physical Vapor Deposition I

1. Plasma Model
2. Sheath Model
3. Feature Model
4. Molecular Dynamics Model



IMP = Ionized Metal Plasma
HCM = Hollow Cathode Magnetron

U. Hansen and F. Kersch, to appear in Phys. Rev. B.

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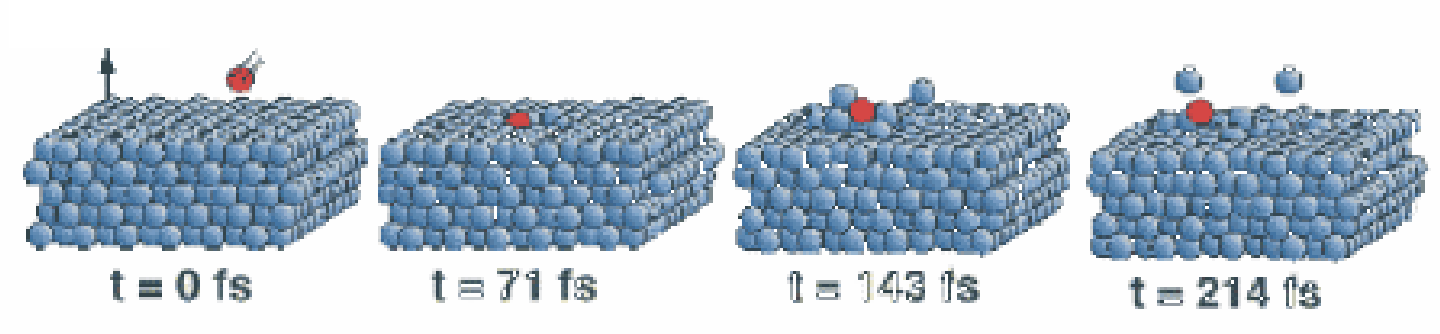
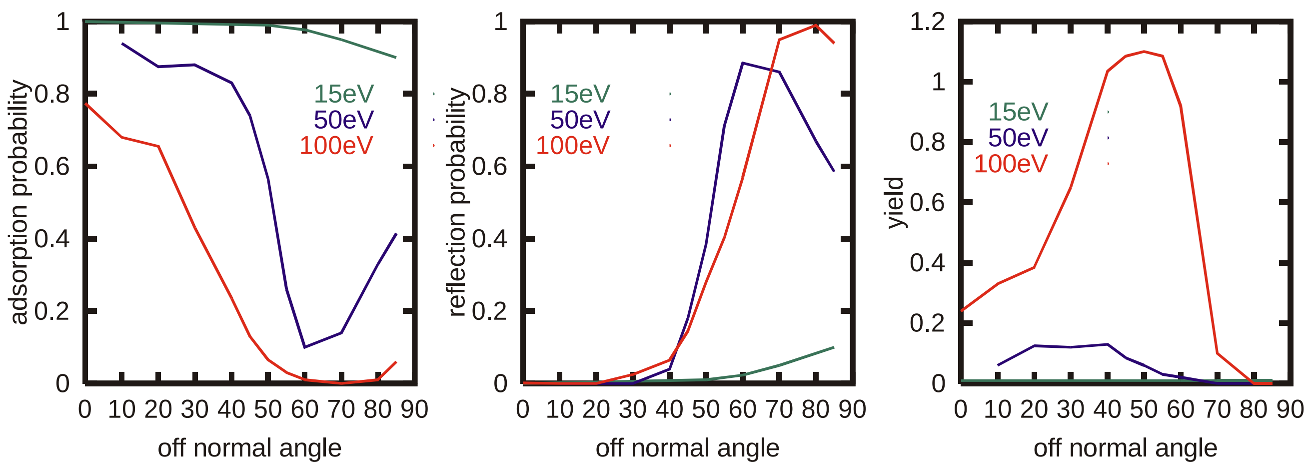
Ionized Physical Vapor Deposition II

Example: M-atom hits M (111)-surface (100eV, 45º off-normal)



Reaction rates from the statistical analysis of trajectories:



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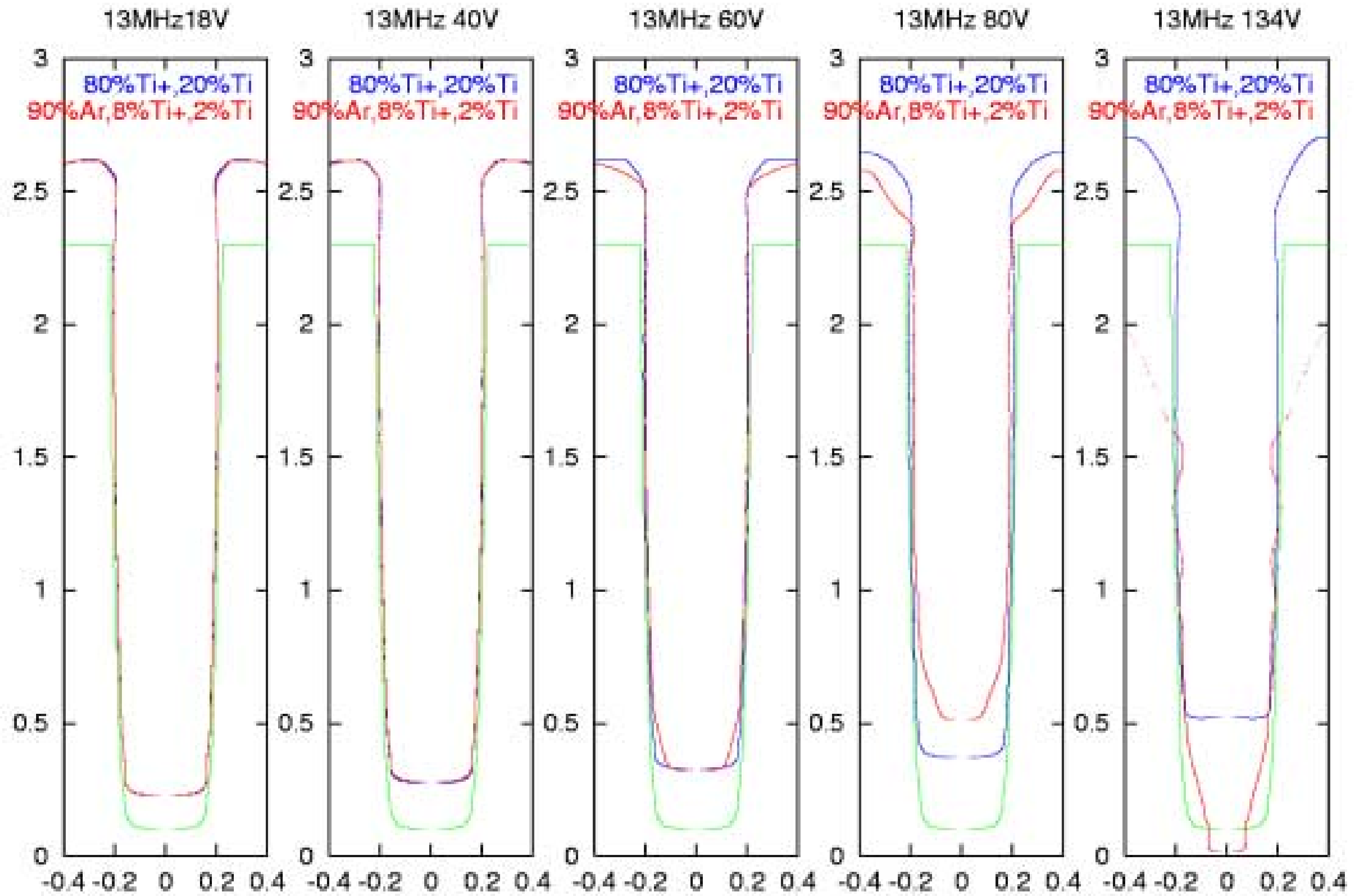
Ionized Physical Vapor Deposition III



Example of a systematic parameter study (DC bias, flux ratio)

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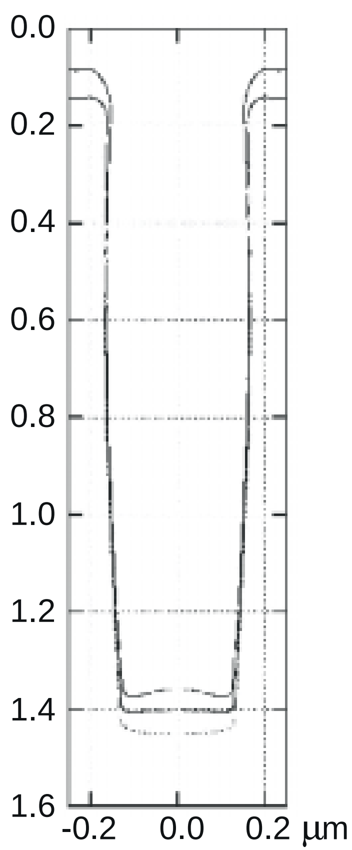
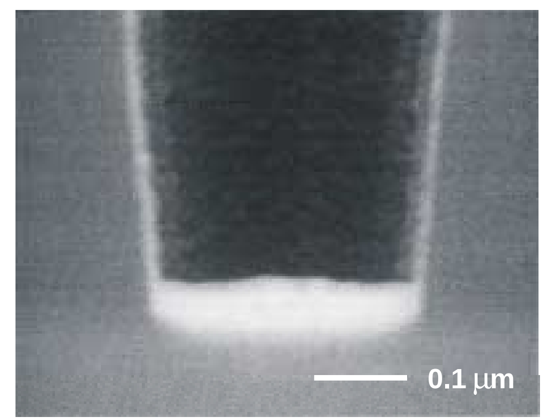
Ionized Physical Vapor Deposition IV

Comparison of simulation and experiment:



Simulation

TEM-Scan



Detail

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Summary and Conclusion

Summary and Conclusions

Presented: An approach capable of explaining and predicting essential process features in plasma-based VLSI fabrication:

- **A fluid dynamic sheath model solves self-consistently the equations of motion together with Poisson's equation.**
- **A subsequent Monte-Carlo run records the trajectories of plasma particles and builds the energy/angle distribution.**
- **The results are fed into a feature scale simulator based on molecular- dynamics calculations (Kersch/Hansen).**

Advantages of the approach:

- **Mathematical consistency and numerical efficiency**
- **Physical accuracy on all relevant scales (µm to m)**

Conclusion: Physics-based modeling and simulation can make meaningful contributions in the development of a VLSI process.