POLITECNICO DI MILANO

Plasma Reactor Model

Maurizio Rondanini, Carlo Cavallotti

Dip. Chimica, Materiali e Ingegneria Chimica "G. Natta" – Politecnico di Milano

Aim and Approach

- Aim: model of LE-PECVD reactor that can link operating parameters to:
  - Local gas phase composition (ions and radical)
  - Flux of gas phase species to surface
  - Growth rate and mean surface composition
- Approach:
  - solution of Maxwell + mass conservation + momentum conservation + energy balance equations
  - Validation of model through comparison with experimental data
- Literature status: no detailed model with accurate experimental validation

Features of the Model

2 D plasma discharge model

2D Electronic density, electric field

Gas phase composition

Ions + radicals

2 D model of gas phase and surface chemistry model

Surface fluxes

Growth Rates

Reaction rates

Literature + Polimi

UniMib

Gas phase and surface

kinetic mechanism of elementary reactions

Model of a DC Discharge in a Magnetic Field

Plasma sustained by Ar discharge, SiH_4 and H_2 introduced in upper chamber → Ar plasma well characterized experimentally (Langmuir probe + Hiden in situ mass spectrometer)

Plasma discharge model initially tested through simulation of Ar discharge in 2D

$$\nabla^2 V = \frac{q_e}{\varepsilon}\left(n_e - n_i\right)$$

$$\nabla \bullet \left(n_e \vec{v}_e\right) = R_e$$

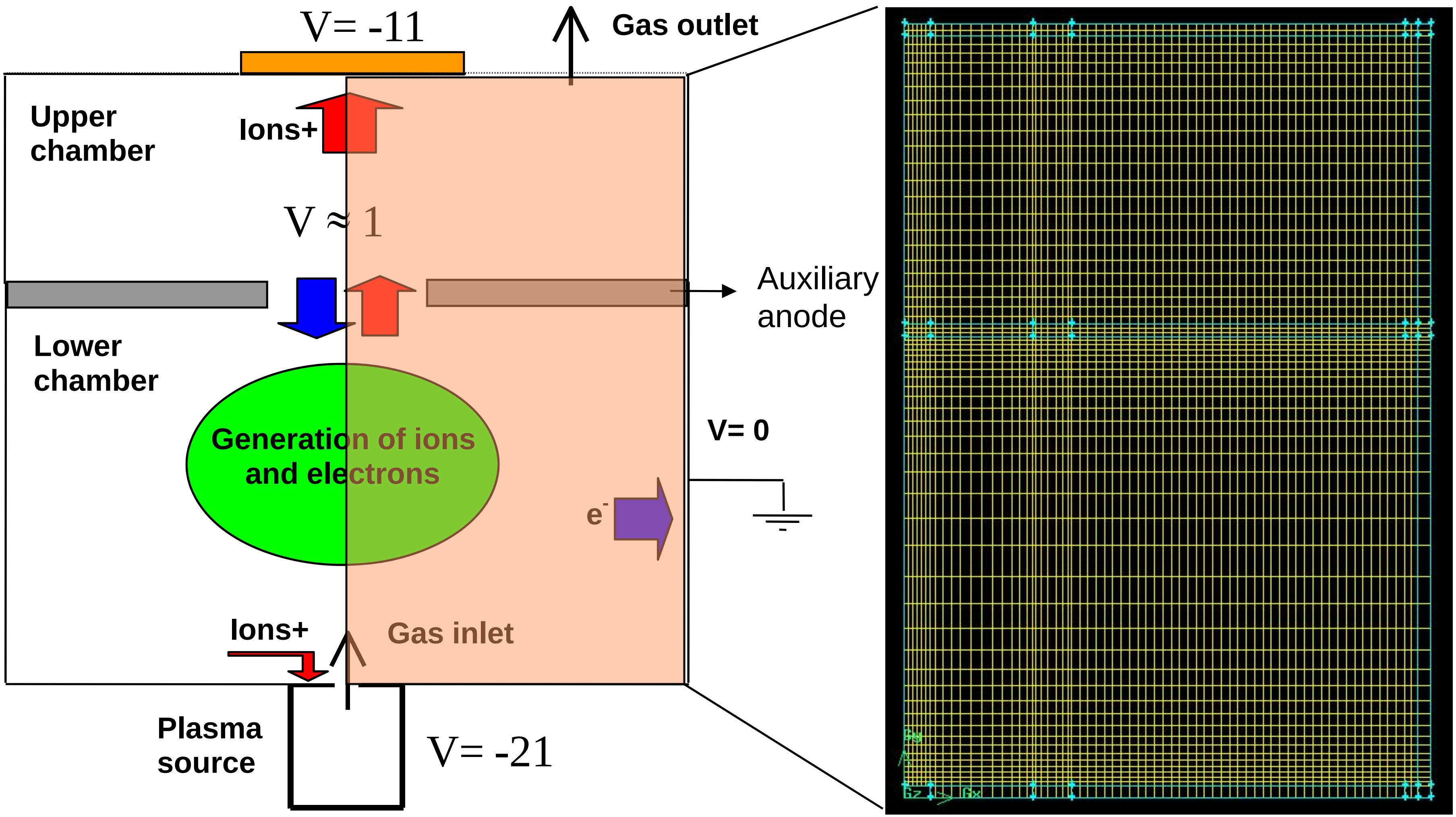
$$\nabla \bullet \left(n_i \vec{v}_i\right) = R_i$$

$$v \bullet \nabla C_{in} = D_{in} \nabla^2 C_{in} + R_{in}$$

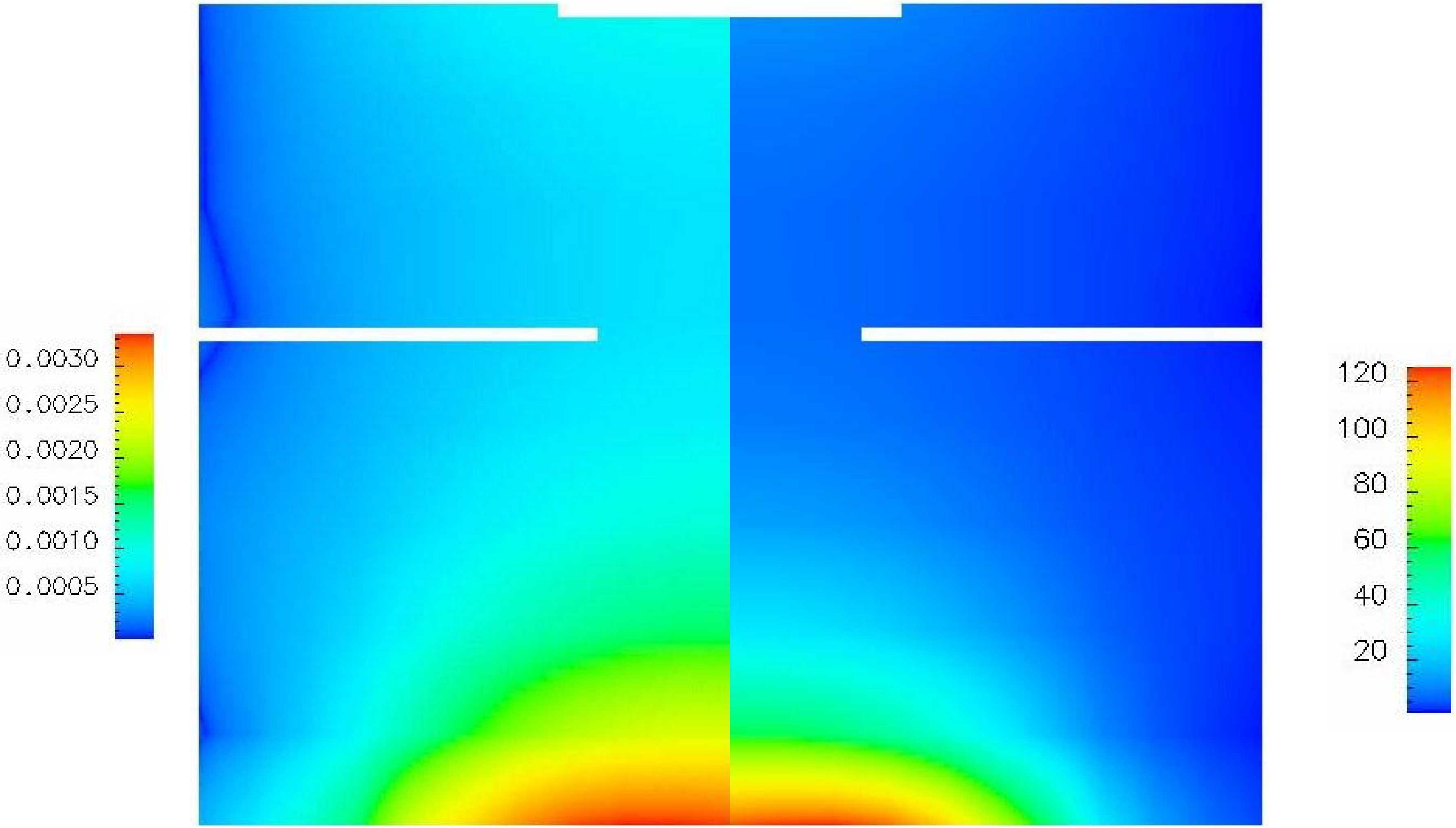
Magnetic field confinement effect

$$\mathrm{v}_{\mathrm{i}\perp} n_i = -D_{i\perp} \nabla n_i + \frac{z_i e m_{ij} \nu_{ij}}{z_i^2 m^2 \omega^2 + m_{ij}^2 \nu_{ij}^2} \mathbf{E}$$

Integration Domain



Magnetic Field Intensity and Confinement ratio

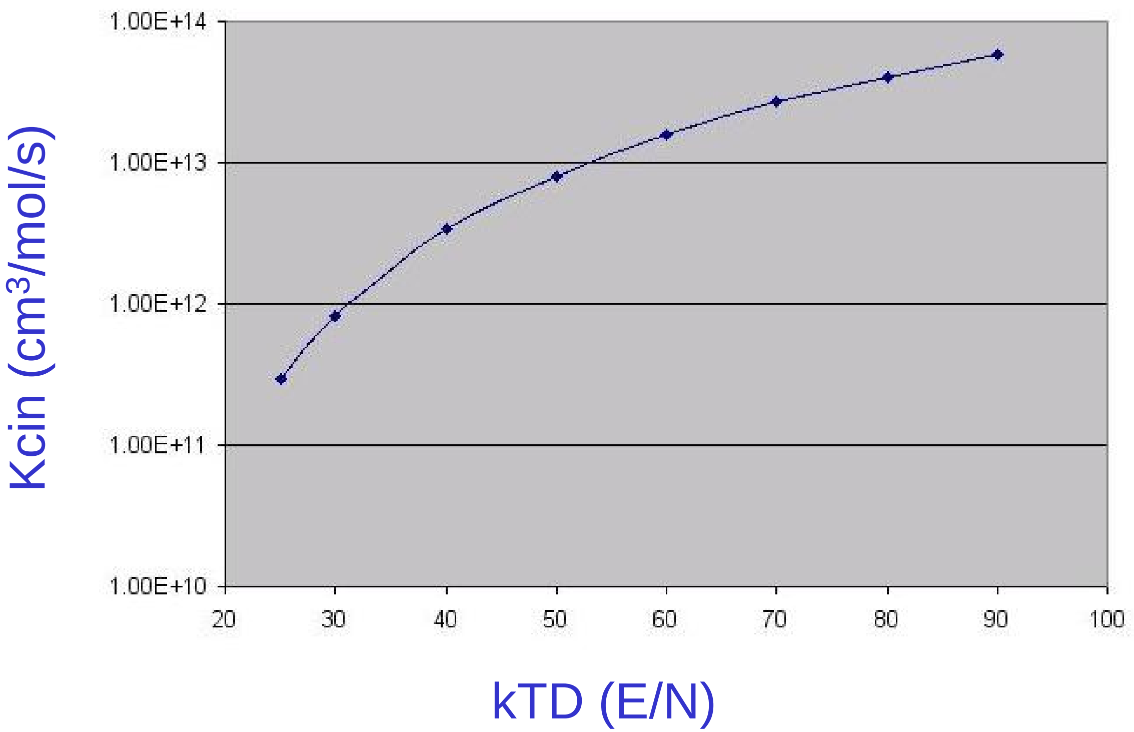


ratio between axial and radial electron diffusion coefficient

Ionization Rate Constants

Ar + el → Ar+ + 2el $r_j = k_j\left(T_e\right) n_e C_i \quad k_j\left(T_e\right) = \int_0^\infty \sqrt{\frac{2\varepsilon}{m_e}} f\left(\varepsilon, T_e\right)\sigma\left(\varepsilon\right) d\varepsilon$

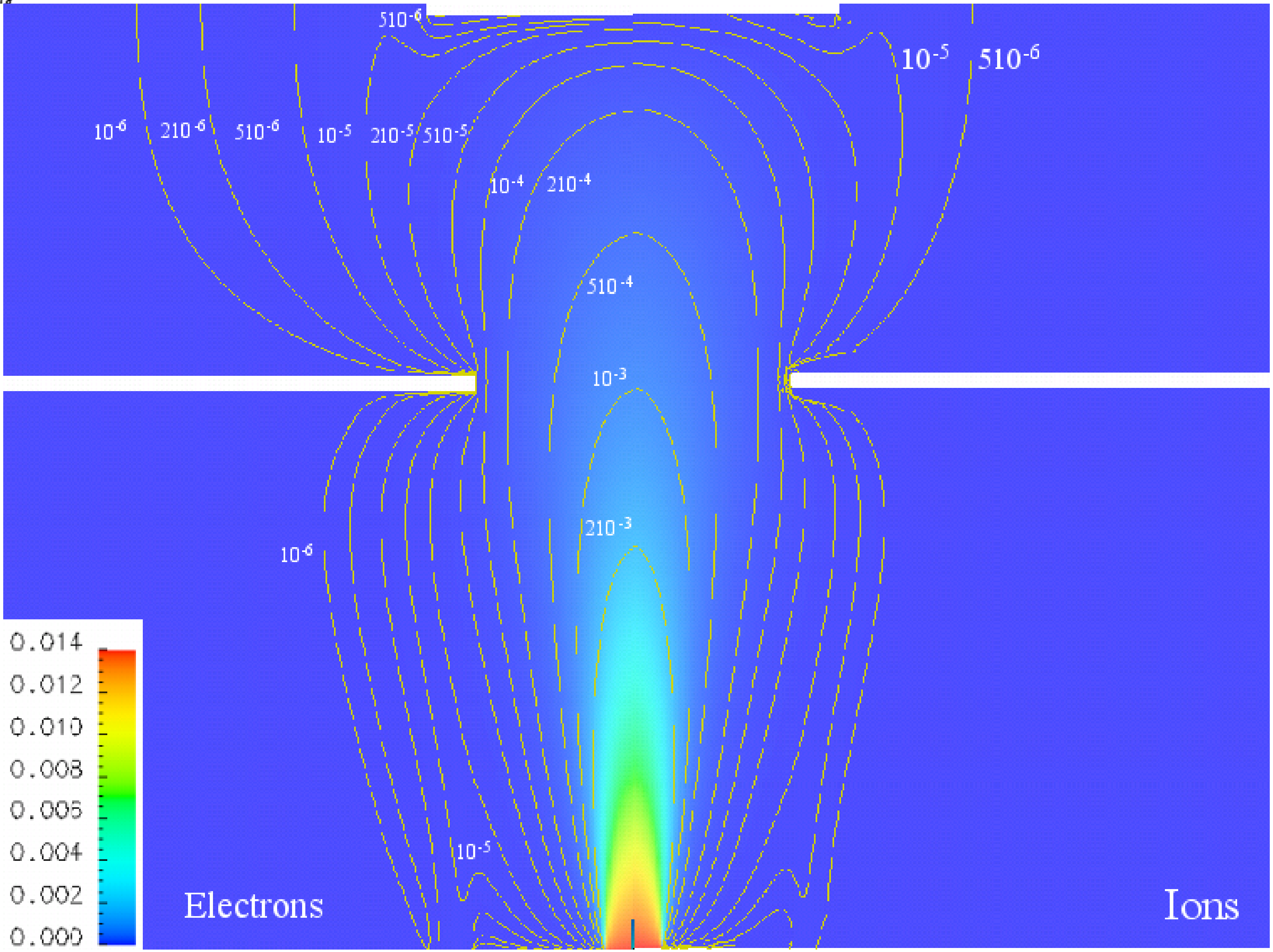
Electron energy distribution function calculated solving the Boltzmann equation as a function of Pressure and Electric field (Daria Ricci, Istituto dei Plasmi, Mi)



Kinetic constant fitted as:

$$k_{cin} = 1.0^{12} E^{1.677} \exp(-E / 26.1)$$

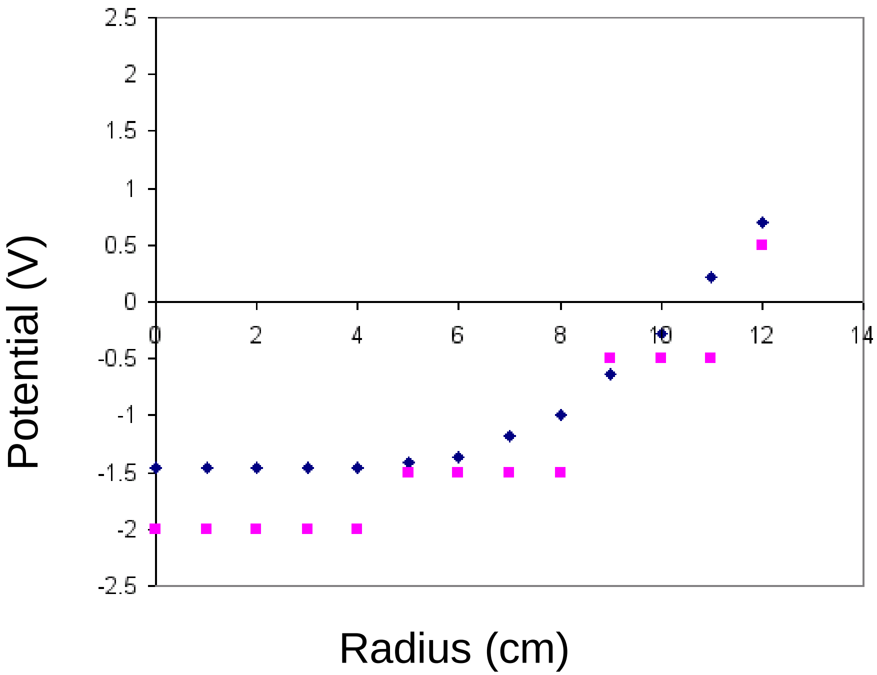
Electron and Ion Mole Fractions

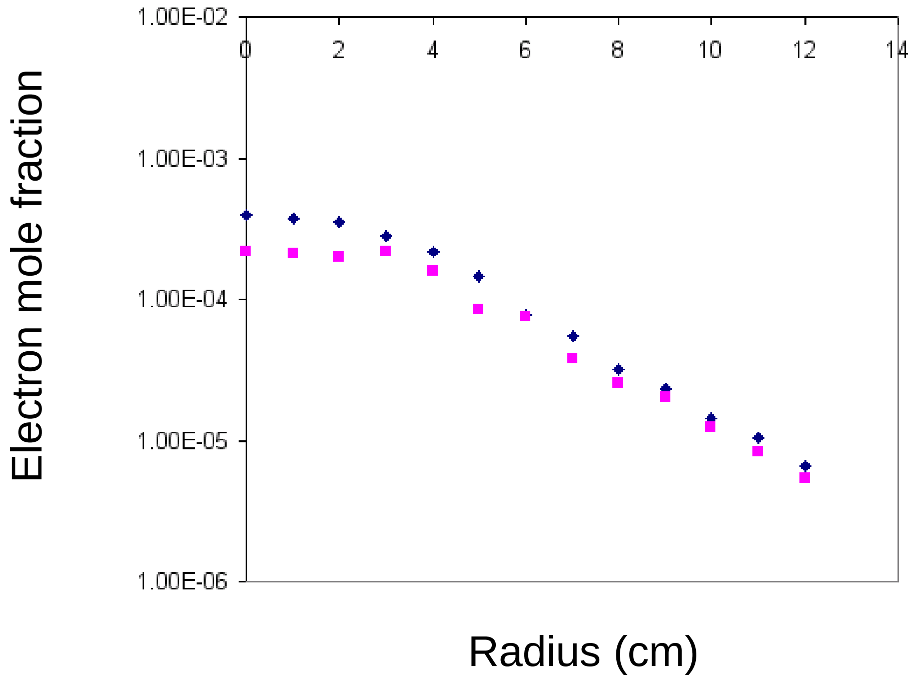


Electron Density = Electron mole fraction x 2.4 10^{20} m^{-3}

Comparison with experimental data

Exp data measured through Langmuir probe in front of the susceptor along the reactor radius (T. Moiseev and D. Chrastina, L-Ness, Politecnico di Milano)

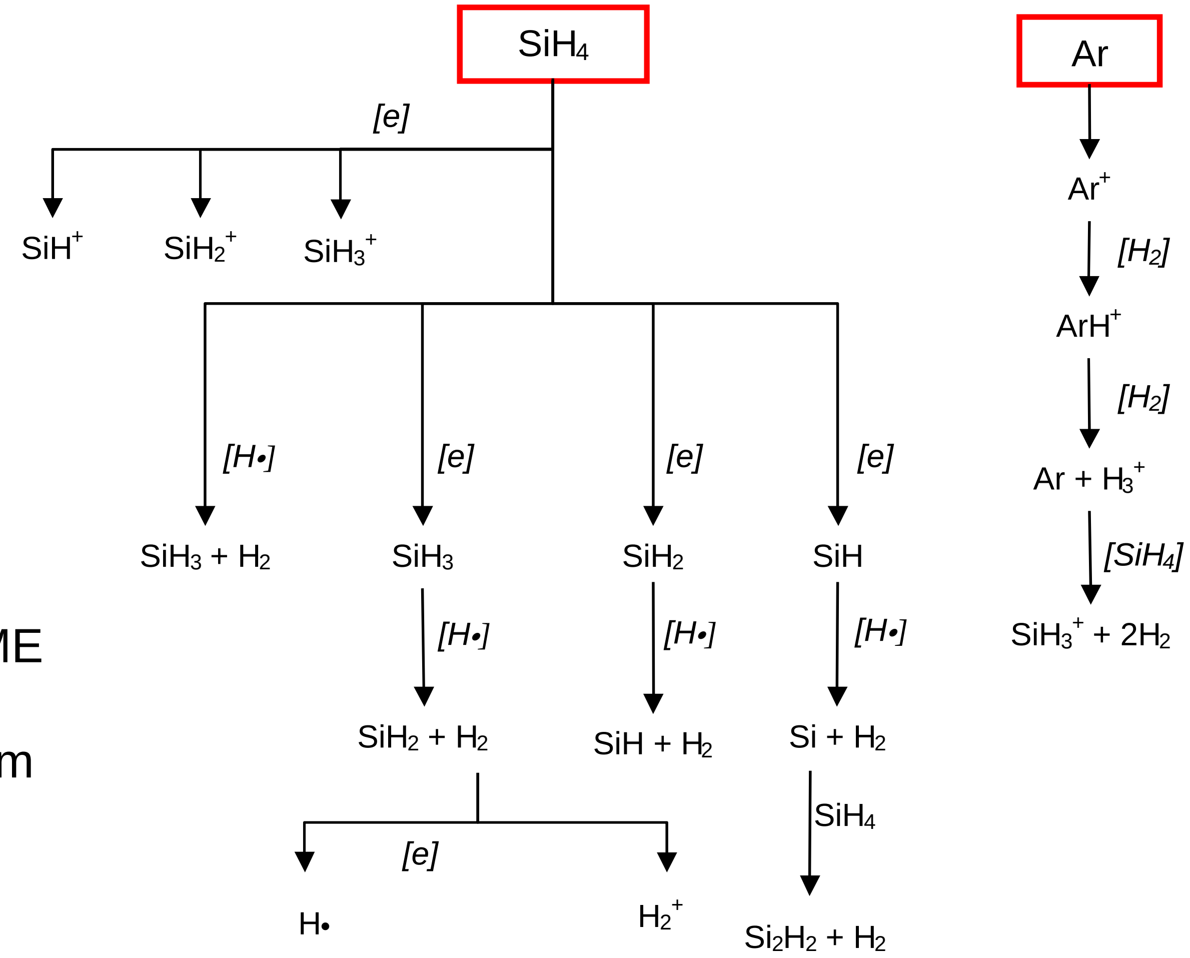




Electron Density = Electron mole fraction x 2.4 10^{20} m^{-3}

Modeling nc Silicon deposition – gas phase chemistry

SiH_4/H_2 introduced in the upper chamber through an injection ring
Ionic and radical species diffusion modeled using ambipolar theory (allows decoupling from Poisson equation)



- Gas phase reactivity from literature + ab initio RRKM/ME estimation
- Surface reactivity partly from literature, but mostly from UNIMB calculations

Chemistry Model

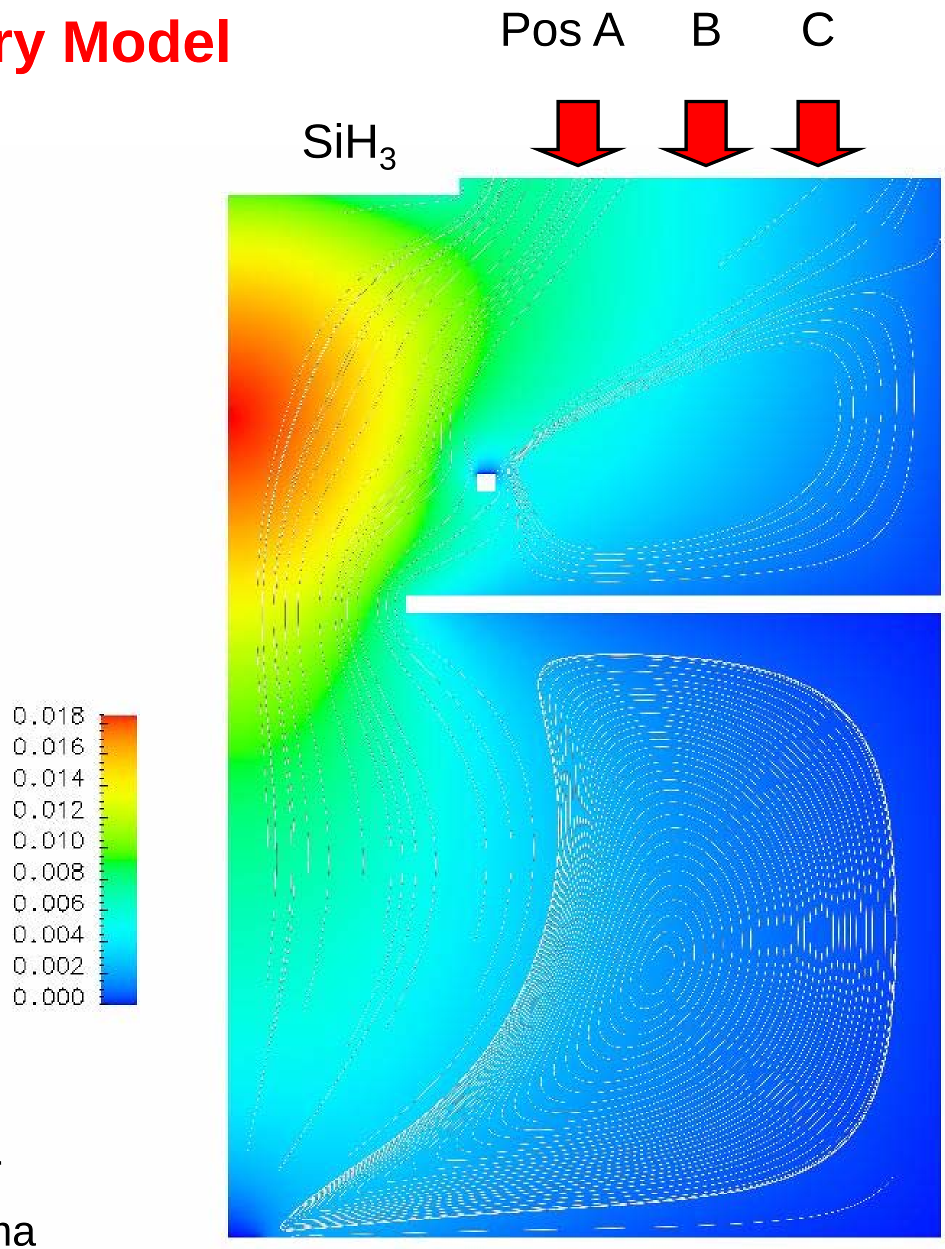
$$\nabla \bullet \left(n_i \vec{v}_i \right) = R_i$$

$$v \bullet \nabla C_{in} = D_{in} \nabla^2 C_{in} + R_{in}$$

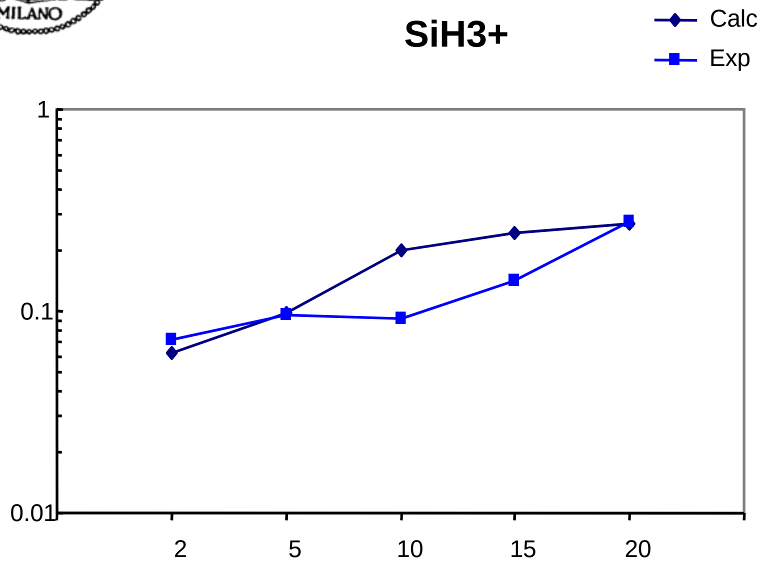
$$\mathrm{v}_{i\perp} n_i = -D_{i\perp} \nabla n_i + \frac{z_i e m_{ij} \nu_{ij}}{z_i^2 m^2 \omega^2 + m_{ij}^2 \nu_{ij}^2} \mathbf{E}$$

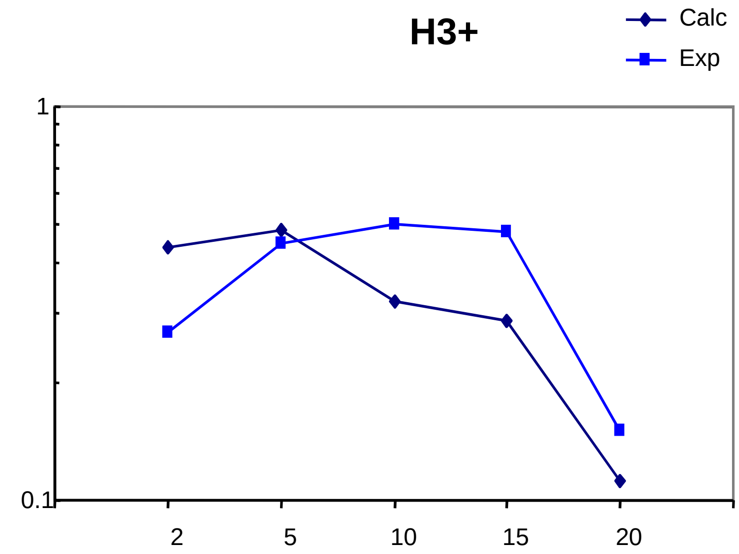
+ momentum balance (Navier Stokes) and energy balance (Fourier)

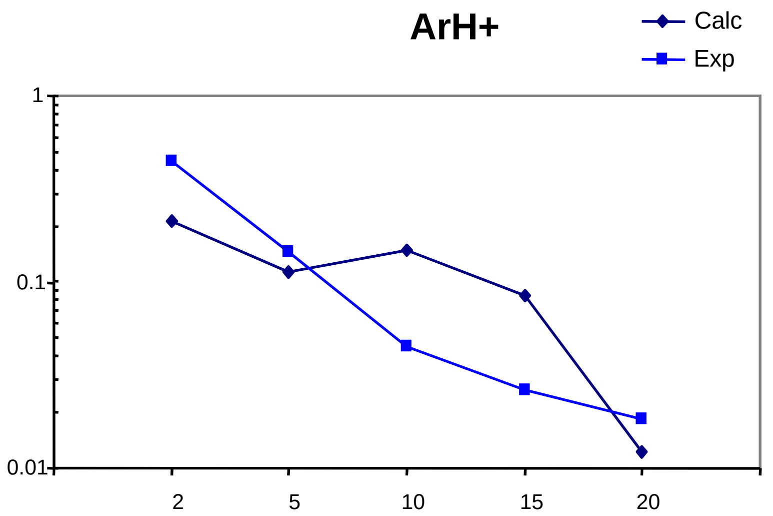
Assumption that the mass spectrometer perturbs the eedf in front of the orifice so that there is a volume where electronic reactions are not active. Non reactive volume fitted over exp ArH+ / H_3+ ratio measured for Ar/H_2 plasma

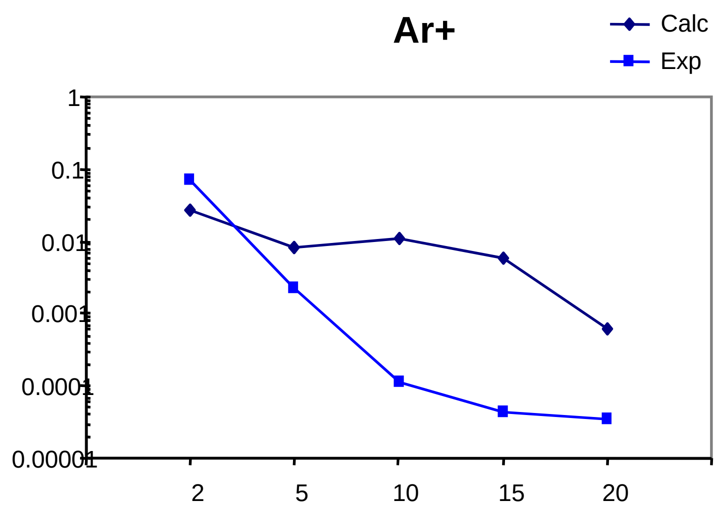


Results – position B

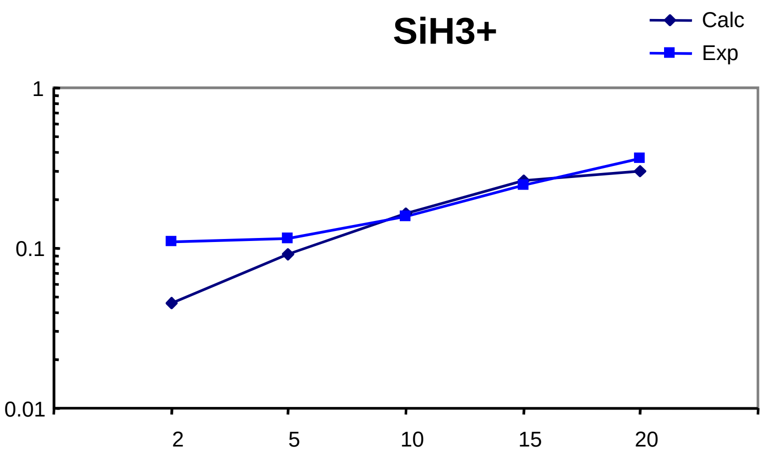


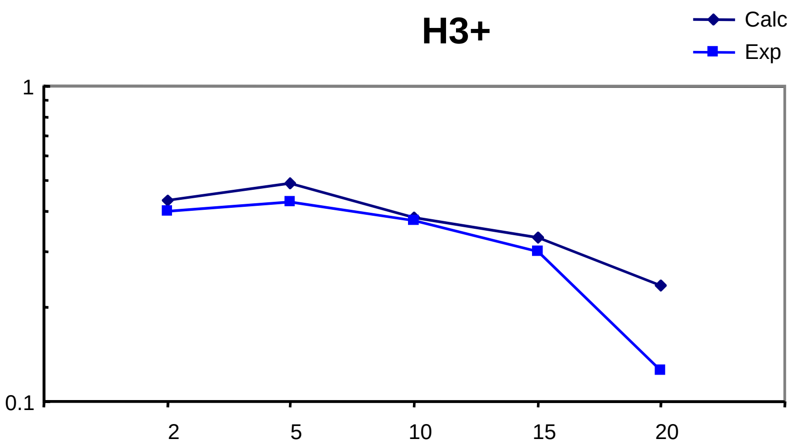


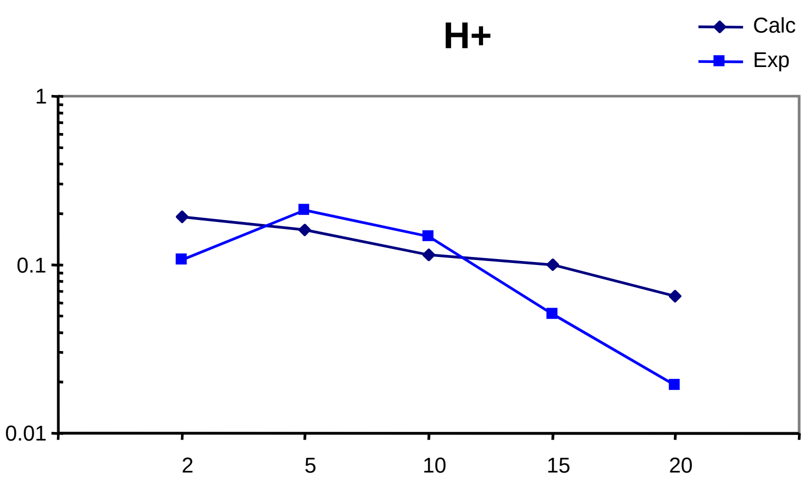


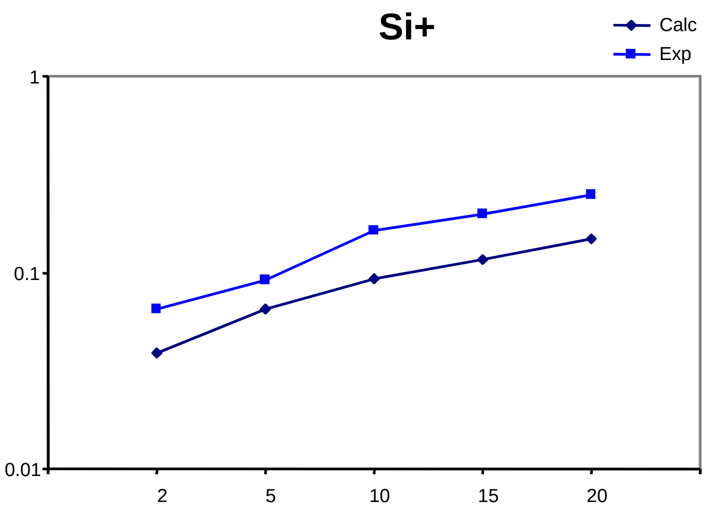


Results – position C

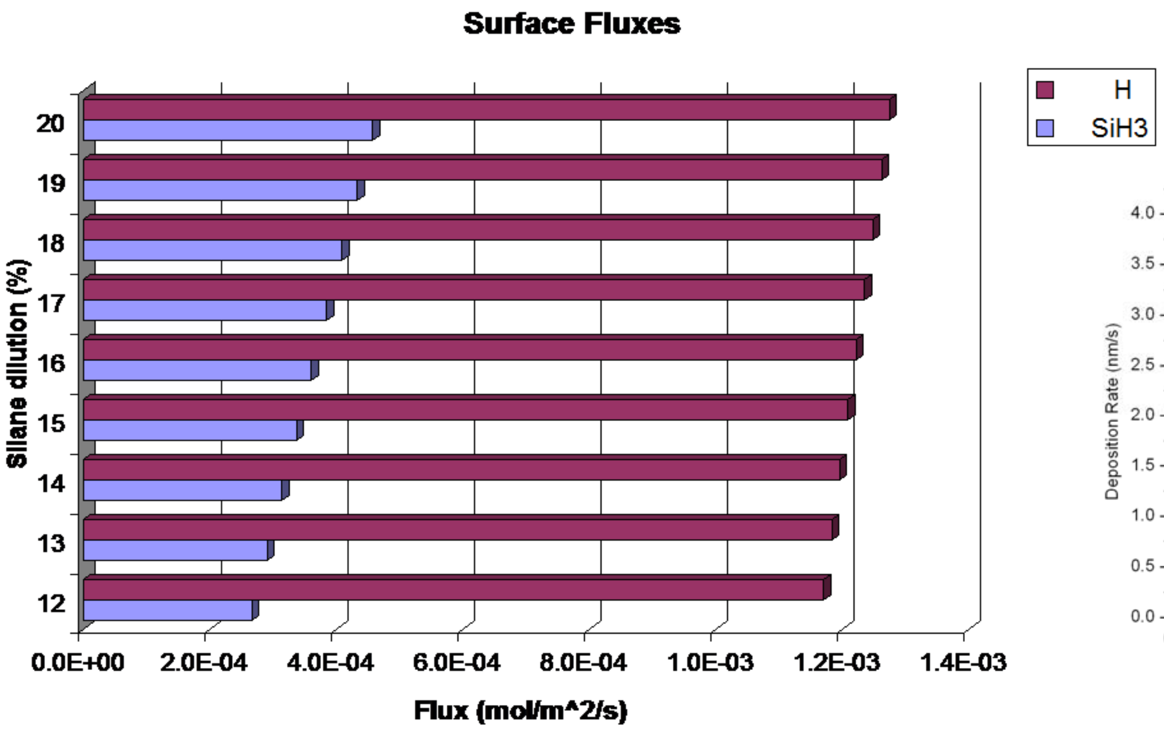


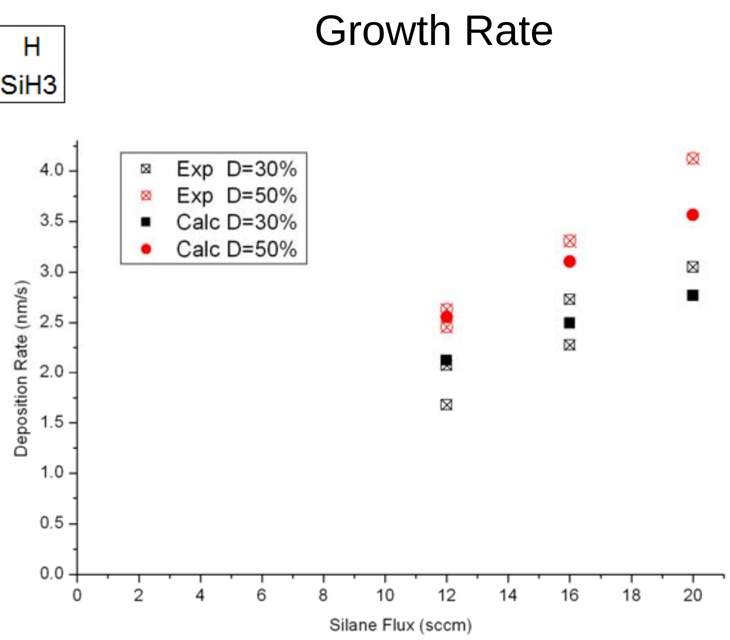






Model Predictions for other partners





→ Inputs for atomistic model of surface growth (UNIMIB) and indications for L-Ness about relation between growth rate, gas phase composition and surface quality

Summary (from the project objectives standpoint)

- New model of plasma discharge, home made FEM code, in very good agreement with experimental data Langmuir Probe data
- New model of plasma chemistry, home made FEM code, in very good agreement for the prediction of local gas phase composition with experimental measurements
- Part of Input for simulations taken from partner UNIMIB
- Output of simulations used by UNIMIB for surface modeling and by L-Ness to interpret growth conditions
- Task 1.3 (Plasma reactor modeling in LEPECVD) and Task 1.6 (Modeling of the deposition process, with UNIMIB) fully accomplished

Conclusions (scientific standpoint)

- High electron density due to confining magnetic field
- High decomposition of Silane determined by extremely high reactivity of this system (much higher than that found in higher pressure capacitive plasmas)
- LE-PECVD, by decoupling ion flux from plasma density, allows to grow in a region characterized by an extremely high flux of SiHx and H radicals
- Increasing the hydrogen content leads to an increase of the H/Si flux to the surface (higher atomic hydrogen flux, increase of relative abundance of slightly hydrogenated SiHx radicals
- Surprisingly, surface mostly covered by H during growth, high sticking on H covered surface allows high growth rates anyway