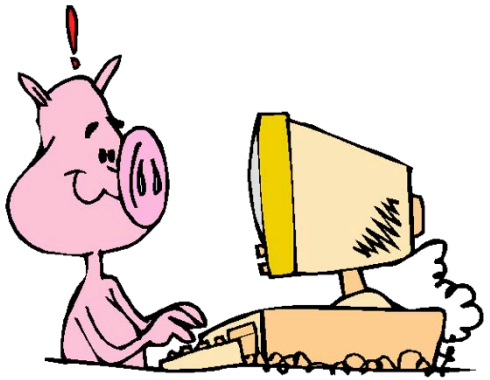
Modeling of plasmas

Annemie Bogaerts

Department of Chemistry,
University of Antwerp (UA),
Research group PLASMANT
Belgium
Annemie.Bogaerts@uantwerpen.be



19th EU Summer School "Low Temperature Plasma Physics"
Bad Honnef, October 5, 2014

Contents

1. General overview of plasma models
   - Explanation of different models
   - Advantages and disadvantages

2. Examples of some models
   for various applications
   + Typical results

1. General overview of plasma models

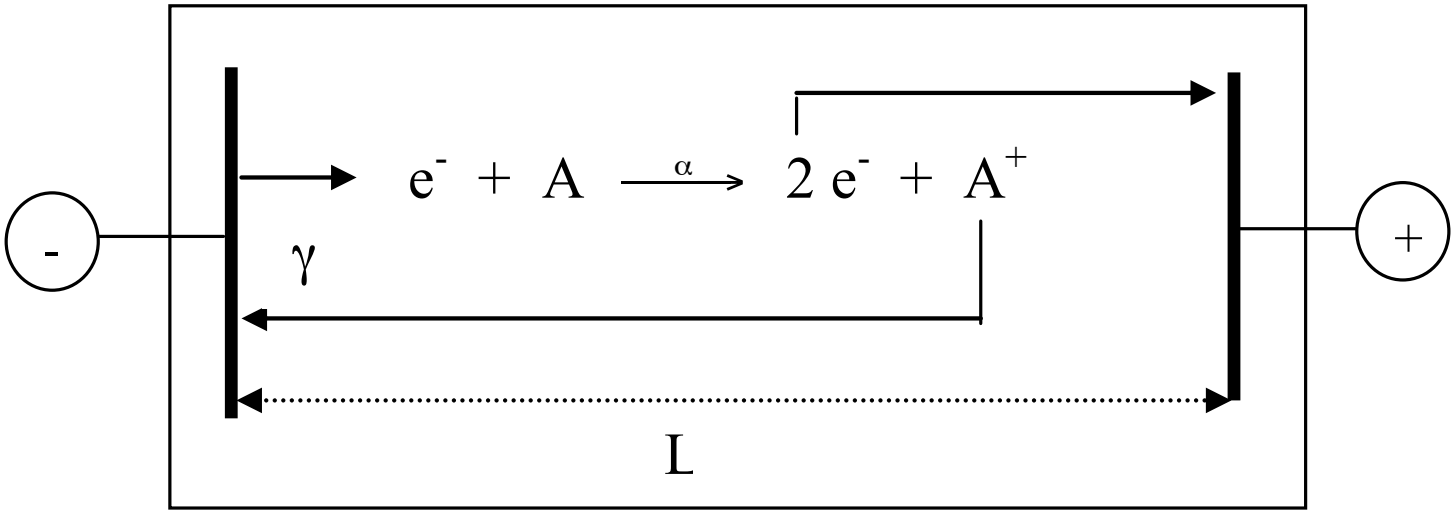
A. Analytical model

Principle:

Simple analytical formulas,

valid for specific range of conditions

e.g.: Condition for self-sustaining discharge:



α = 1st Townsend coefficient (ionization)

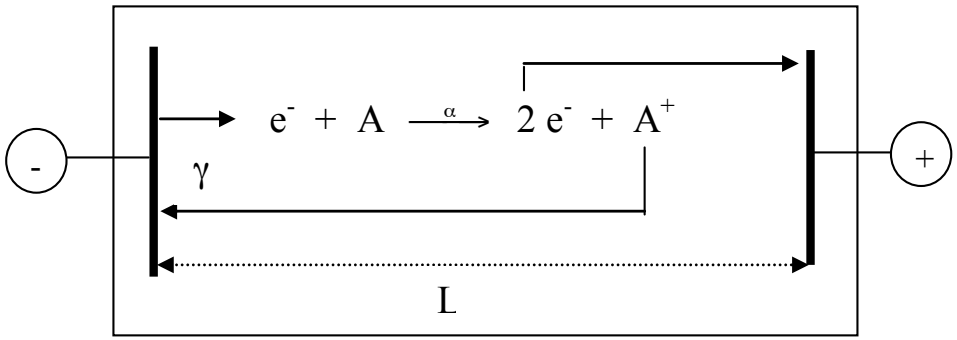
γ = 2nd Townsend coefficient (sec. e^- emission)

A. Analytical model (cont)

Electron multiplication in plasma, by electron impact ionisation:

Balance equation: $\frac{dN_e}{dx} = \alpha N_e$

Solution: $N_e = N_{e,0} \exp\left(\int \alpha \, dx\right)$



At cathode: $N_{e,0}$

At anode: $N_e = N_{e,0} \exp(\alpha L)$

Hence: for 1 electron at cathode: exp(αL) electrons at anode

→ Hence formed in plasma: exp(αL) – 1

Number of electrons formed = number of ions formed

Secondary electron emission: γ

Number of sec.electrons formed by these ions: γ * (exp(αL) – 1)

→ Condition "self-sustaining discharge": γ * (exp(αL) – 1) = 1

$\rightarrow \alpha L = \ln\left(1 + \frac{1}{\gamma}\right)$

A. Analytical model (cont)

Advantage: Simple, fast

Disadvantage: Approximation, limited validity

B. 0D chemical kinetics model
Also called: Global model

Principle:

Rate equations (balance equations) for all species,

based on production/loss by chemical reactions:

$$\frac{\partial n_i}{\partial t} = \mathrm{Rprod}_i - \mathrm{Rloss}_i$$

$$\mathrm{Rprod}/\mathrm{Rloss} = k_{2B}\, n_1 n_2 \quad (\mathrm{or}: k_{3B}\, n_1 n_2 n_3,\ \mathrm{or}: A\, n_1)$$

Electron impact reaction rates:

From Boltzmann solver (→ Look-up tables: k(ε))

+ Electron energy balance equation (→ ε)

B. 0D chemical kinetics model (cont)

Advantage:

Simple, fast (detailed chemistry)

Disadvantage:

Approximation: No transport (assumes plasma = uniform)

However: based on gas flow velocity:

can deduce spatial behavior from temporal behavior

(equivalence batch reactor – plug flow reactor)

B. 0D chemical kinetics model (cont)

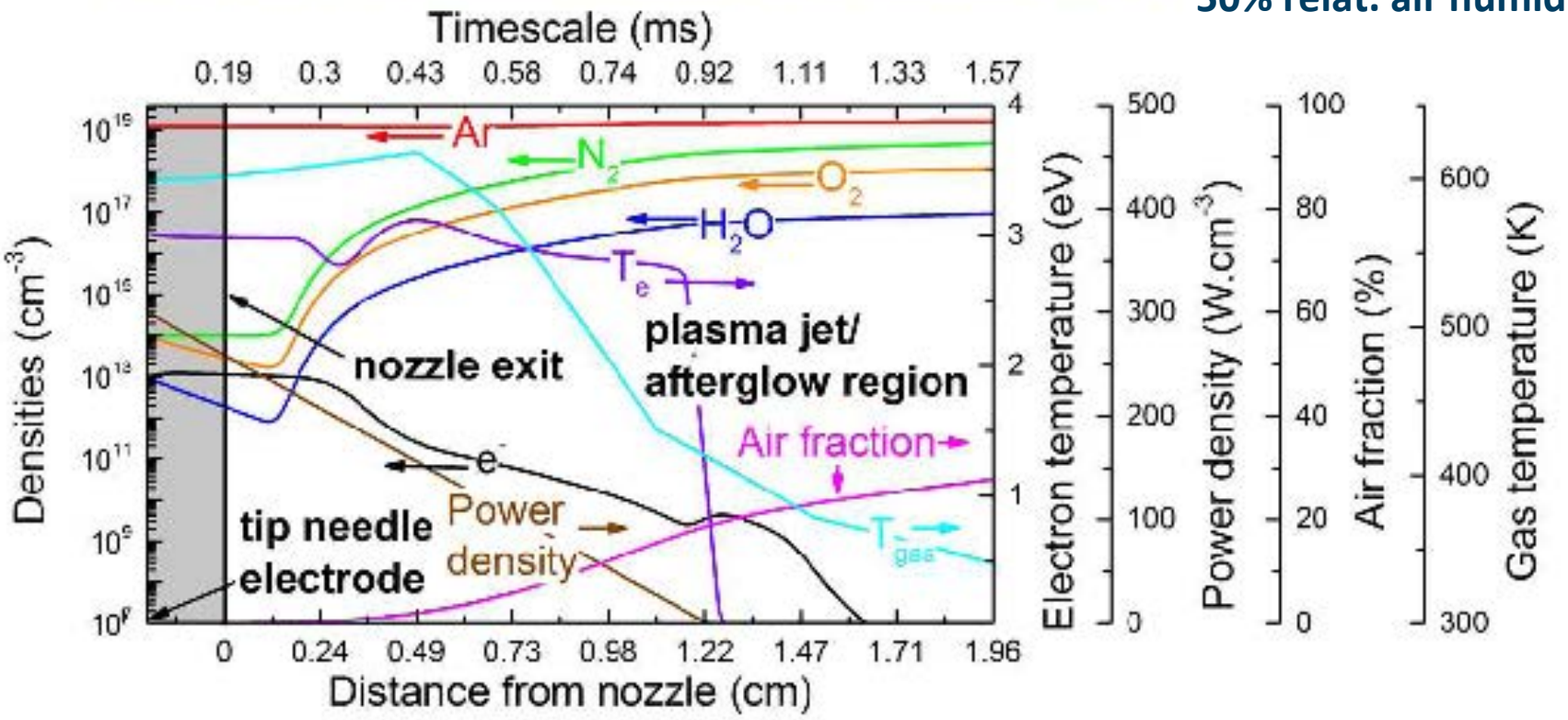
Example: Plasma jet

Plasma jet TU/e

(2 slm Ar gas feed,

6.5 W,

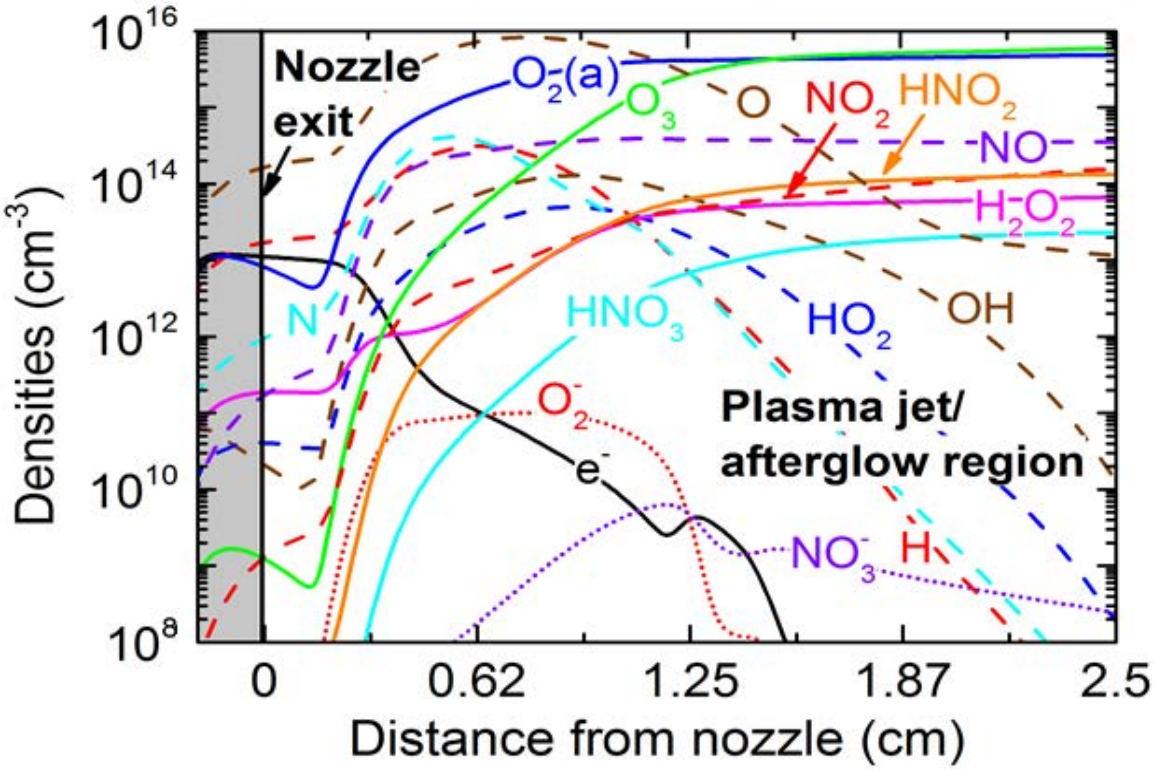
50% relat. air humidity)



W. Van Gaens and A. Bogaerts, *J. Phys. D: Appl. Phys.* 46, 275201 (2013)

B. 0D chemical kinetics model (cont)

Example: Plasma jet



Plasma jet TU/e

(2 slm Ar gas feed,

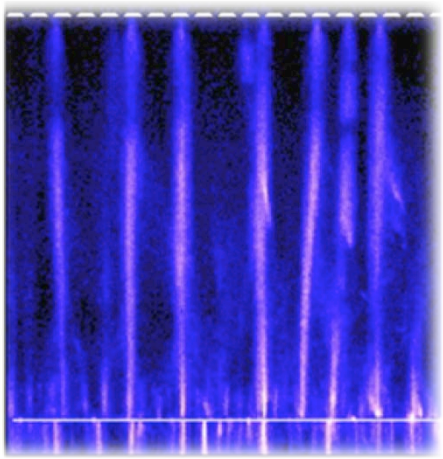
6.5 W, 50% relat. air humidity)

- O, O_3, O_2(a), OH, H_2O_2
- NO, NO_2, HNO_2, HNO_3
- O ↓ at longer distance
- O_3 , O_2(a) ↑ at longer distance
- OH dimerizes into H_2O_2 (~ 1.2 cm)
- Cluster formation important in ion chemistry
- O_2^- and NO_3^- : relatively low (ppb) levels

W. Van Gaens and A. Bogaerts, *J. Phys. D: Appl. Phys.* 46, 275201 (2013)

B. 0D chemical kinetics model (cont)

Example: DBD reactor: filamentary character

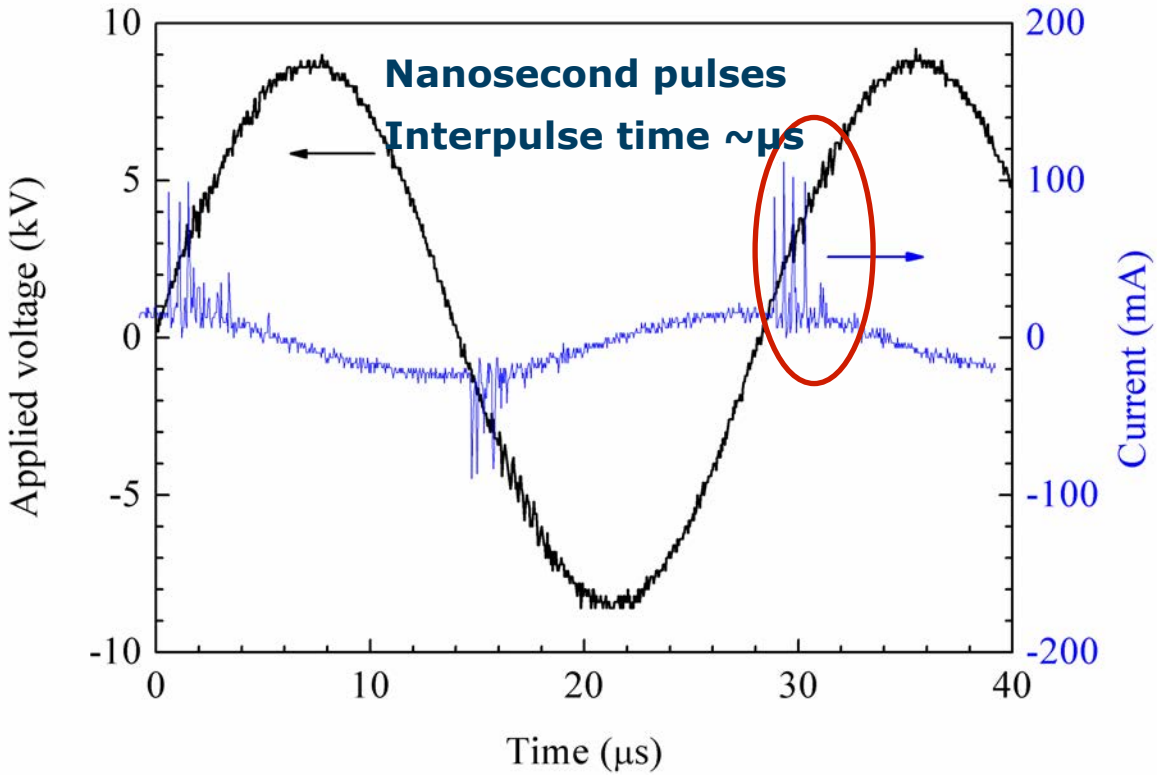


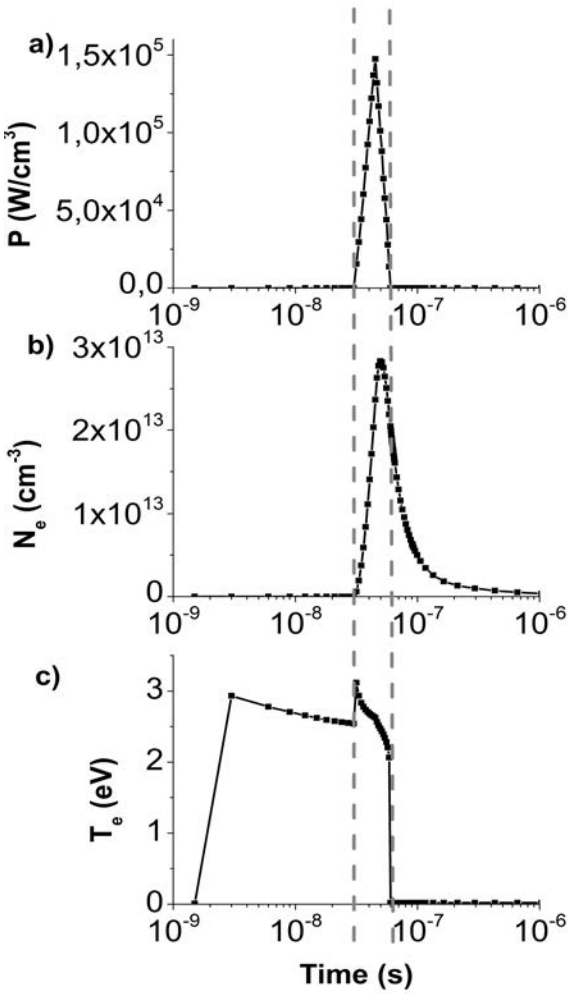
Reactor length + gas flow → residence time

(correlation spatial – temporal behavior)

B. 0D chemical kinetics model (cont)

Example: DBD reactor: filamentary character





1 microdischarge pulse + afterglow

- T_e ~ 2-3 eV

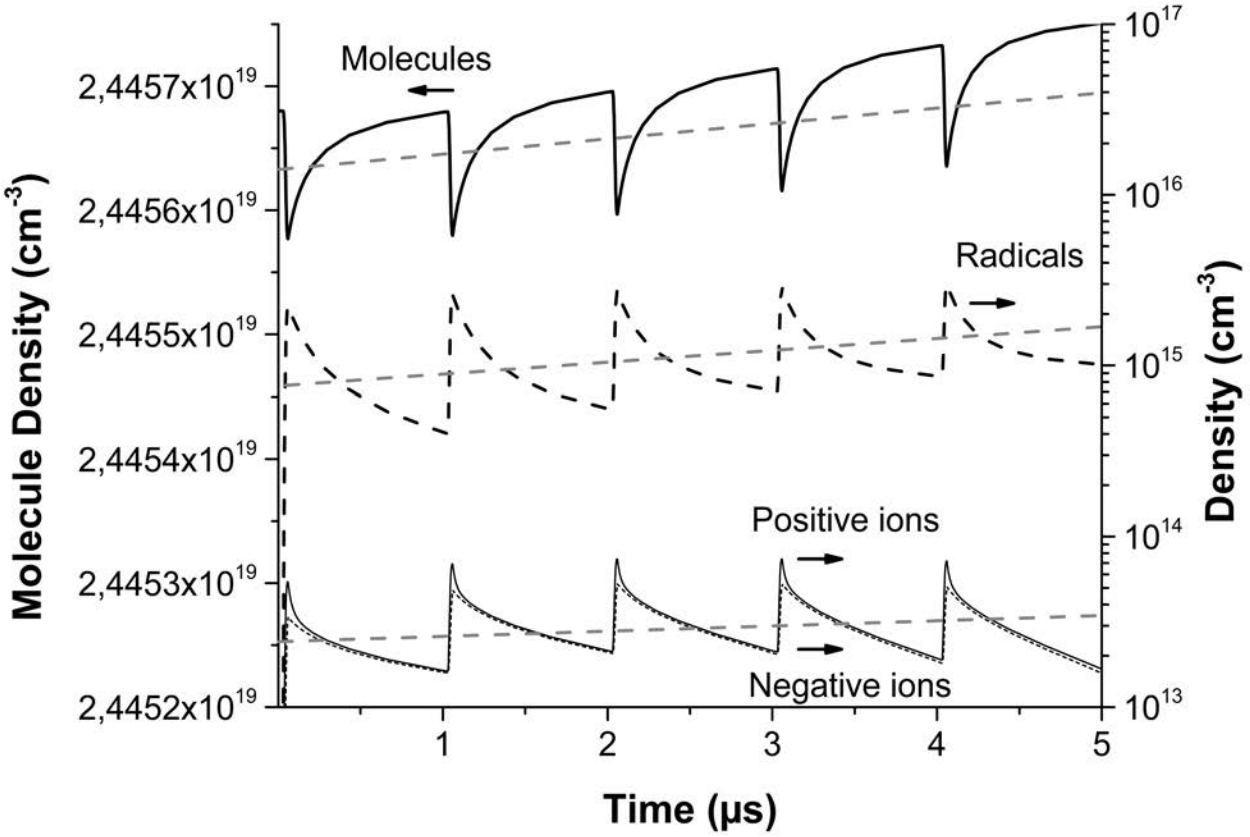
(30 ns) - N_e ~ 10^{13} cm^{-3}

B. 0D chemical kinetics model (cont)

Example: DBD reactor: filamentary character

5 consecutive pulses: species pass through several filaments

(as function of distance, or function of residence time)



C. Fluid model: 1D or 2D

Principle:

Moment equations of Boltzmann equation:

Conservation of mass, momentum, energy

Continuity equations (for all species i):

$$\frac{\partial n_i(z,r)}{\partial t} + \vec{\nabla} \cdot \vec{j}_i(z,r) = \mathrm{Rprod}_i(z,r) - \mathrm{Rloss}_i(z,r)$$

Momentum equation: often drift-diffusion approximation:

→ Transport equations

(drift-diffusion for charged species; diffusion for neutrals):

$$\vec{j}_i(z,r) = \left[\pm \mu_i n_i(z,r) \vec{E}(z,r) \right] - D_i \vec{\nabla} n_i(z,r)$$

C. Fluid model (cont.)

Electron energy balance equation:

$$\frac{\partial\, n_e\, \varepsilon}{\partial\, t} + \overline{\nabla} \cdot \overline{j_w} = -e\, \overline{j_w} \cdot \overline{E} + \sum_i k_i\, n_e\, N_g\, \Delta\varepsilon_i$$

$$\overline{j_w} = \frac{5}{3} \mu_e\, n_e\, \varepsilon\, \overline{E} - \frac{5}{3} D_e\, \overline{\nabla}\, n_e\, \varepsilon$$

Ions, neutrals: assumed T_g

Advantage: Simple, fast (detailed chemistry)

Coupling to Poisson equation for self-consistent E-field

$$\nabla^2 V + \frac{e}{\varepsilon_0}\left(n_{X^+} - n_{X^-} - n_e \right) = 0 \quad | \quad \overline{E} = -\overline{\nabla}\, V$$

Disadvantage:

Approximation (assumes species gain more or less same amount of energy from E-field as they lose by collisions

D. Boltzmann model

Principle:

Full solution of Boltzmann transport equation

(terms with E-gain, E-loss)

$$f_j(r,v,t): \quad \frac{\partial f_j}{\partial t} + \bar{v} \bullet \bar{\nabla}_r f_j + \bar{a} \bullet \bar{\nabla}_v f_j = C_{el}(f_j) + C_{inel}(f_j)$$

Advantage: **Accounts for non-equilibrium behavior**

Disadvantage: **Mathematically complex**

→ **Typically only used for electron behavior**

(e.g., 2-term approximation): e.g., BOLSIG+

E. Monte Carlo model

Principle:

- Treats particles on lowest microscopic level
- For every particle – during successive time-steps:

  * trajectory by Newton's laws:

$$z = z_0 + v_{z_0}\Delta t + \frac{qE_{ax}}{2m}(\Delta t)^2 \qquad v_z = v_{z_0} + \frac{qE_{ax}}{m}\Delta t$$

$$x = x_0 + v_{x_0}\Delta t + \frac{qE_{rad}\cos(\alpha)}{2m}(\Delta t)^2 \qquad v_x = v_{x_0} + \frac{qE_{rad}\cos(\alpha)}{m}\Delta t$$

$$y = y_0 + v_{y_0}\Delta t + \frac{qE_{rad}\sin(\alpha)}{2m}(\Delta t)^2 \qquad v_y = v_{y_0} + \frac{qE_{rad}\sin(\alpha)}{m}\Delta t$$

  * collisions by random numbers

E. Monte Carlo model (cont)

- **Probability of collision:** $\mathrm{Prob}_{coll} = 1 - \exp\left(-\Delta s \Sigma(n\sigma_{coll}(E))\right)$

→ **Compare with RN (0 - 1): If Prob < RN => no collision**
If Prob > RN => collision

- **Kind of collision: partial collision prob. + compare with RN**

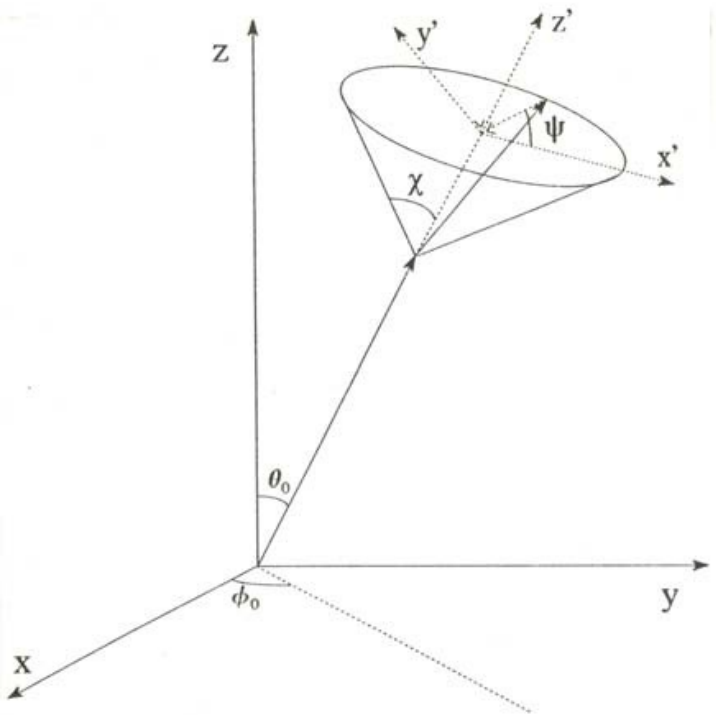
E. Monte Carlo model (cont)

- **New energy + direction: scattering formulas + RN, e.g.:**

  - after ionization: $E_{prim} = (E_0 - E_{ion})*RN$; $E_{sec} = E_0 - E_{ion} - E_{prim}$

or: $$RN = \frac{\int_0^{E_{prim}} \sigma_{ion,diff}(E_0, \varepsilon)\, d\varepsilon}{\sigma_{ion}(E_0)}$$

  - after excitation: $E = E - E_{excit}$



- scattering angles (χ, ψ):

$$\cos\chi = 1 - \frac{2\,RN}{1 + 8\,\varepsilon\,(1 - RN)} \quad ; \quad \psi = 2\pi\,RN$$

- new angles (θ, φ):

$$\begin{pmatrix} \sin(\theta)\cos(\varphi) \\ \sin(\theta)\sin(\varphi) \\ \cos(\theta) \end{pmatrix} = \begin{pmatrix} \cos(\theta_0)\cos(\varphi_0) & -\sin(\varphi_0) & \sin(\theta_0)\cos(\varphi_0) \\ \cos(\theta_0)\sin(\varphi_0) & \cos(\varphi_0) & \sin(\theta_0)\sin(\varphi_0) \\ -\sin(\theta_0) & 0 & \cos(\theta_0) \end{pmatrix} x \begin{pmatrix} \sin(\chi)\cos(\psi) \\ \sin(\chi)\sin(\psi) \\ \cos(\chi) \end{pmatrix}$$

E. Monte Carlo model (cont)

Advantage:

Accurate (non-equilibrium behavior) + simple

Can be applied for all species

Disadvantage:

Long calculation time + not self-consistent

In practice: used for electrons (in hybrid model)

Or for species in sheath (detailed behavior, e.g., EDF)

F. Particle-in-cell / Monte Carlo model

Principle:

- Similar to MC model (Newtons' laws, random numbers)
- But at every time-step: calculation of electric field from positions of charged particles (Poisson equation)

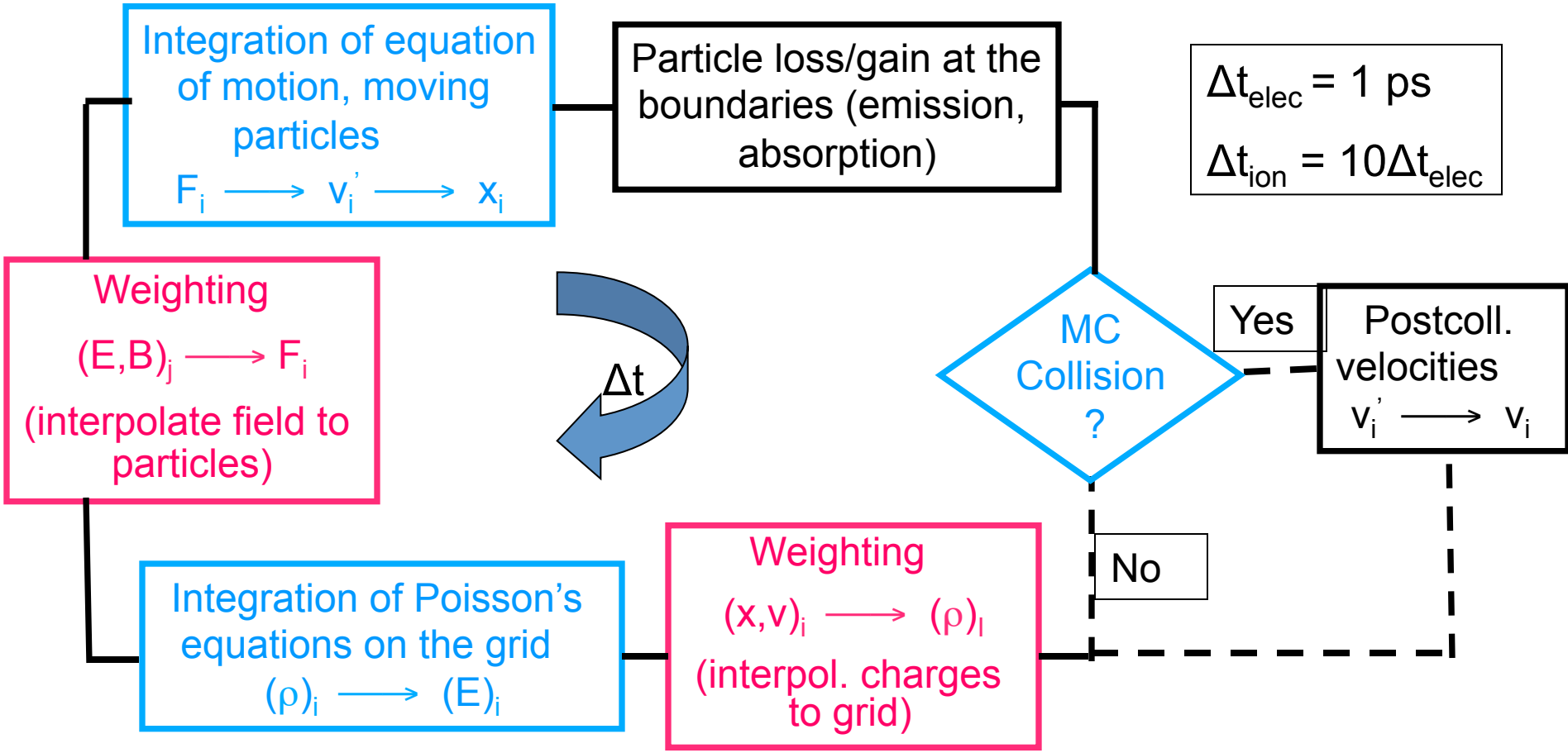
Advantage: Accurate + self-consistent

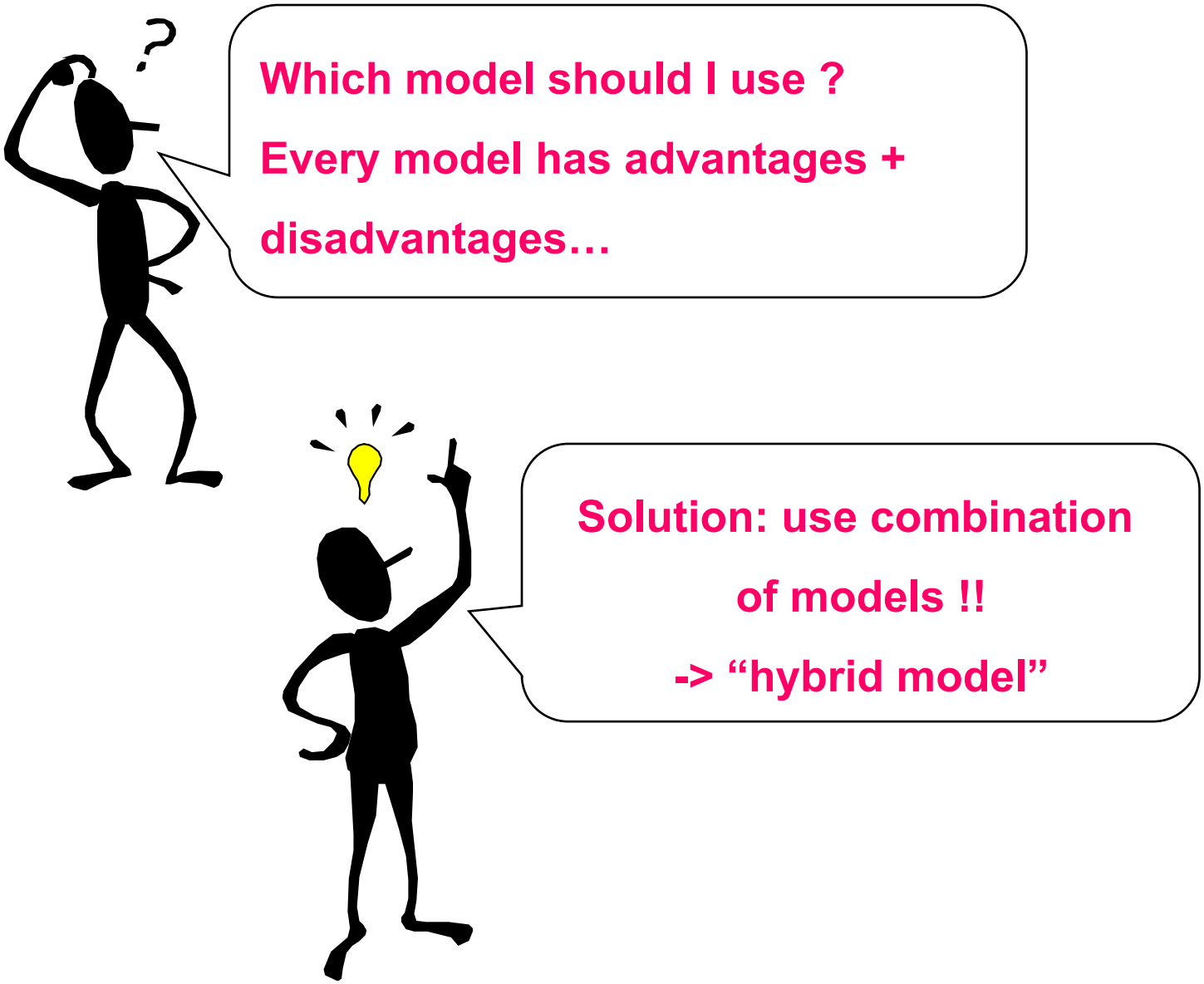
Disadvantage: Even longer calculation time

Principle of PIC-MC (cycle):

Real plasma particles: replaced by superparticles

1 superparticle = W real particles (W = weight, e.g. 2×10^7)




Which model should I use ?
Every model has advantages +
disadvantages…
Solution: use combination
of models !!
-> “hybrid model”

G. Hybrid model

Principle:

Because some species = fluid-like, others = particle-like:

→ Combination of above models, e.g.:

- Monte Carlo for fast (non-equilibrium) species
- Fluid model for slow (equilibrium) species + E-field
- (transfer from fast to slow group: if $(E_k + E_p) <$ threshold)

Advantage:

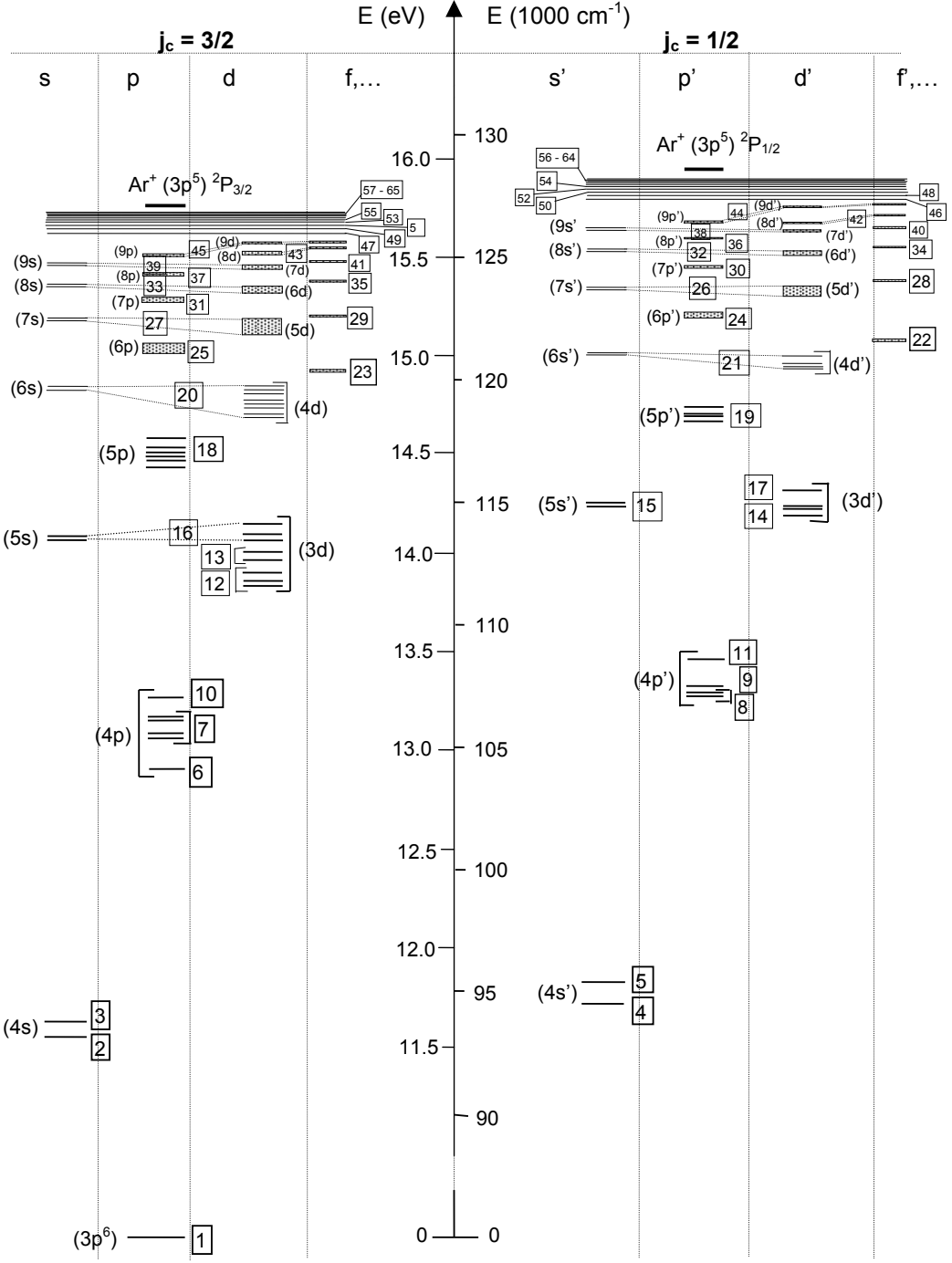
- Combines the advantages + avoids the disadvantages
- Accurate + self-consistent + reduced calculation time

Disadvantage: /

H. Collisional-radiative model (for excited levels)

Example: Ar: 65 Ar levels (individual or group of levels)

Energy level scheme for Ar* CR model



H. Collisional-radiative model (for excited levels)

For each level: continuity equation (balance equation):

$$\frac{\partial n_{Ar^*}}{\partial t} - D_{Ar^*}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial n_{Ar^*}}{\partial r}\right) - D_{Ar^*}\frac{\partial^2 n_{Ar^*}}{\partial z^2} = R_{prod} - R_{loss}$$

Production + loss processes for each level:

* electron, Ar ion + Ar atom impact excitation, de-excitation, ionization
* electron-ion three-body recombination, radiative recombination
* radiative decay
* Hornbeck-Molnar associative ionization (for Ar* levels with E > 14.7 eV)

Additional processes for 4s levels:

* Ar* - Ar* collisions -> (associative) ionization
* Penning ionization of sputtered atoms
* three-body collisions with Ar atoms
* radiation trapping of resonant radiation

I. Model for plasma-surface interactions: Molecular Dynamics simulations

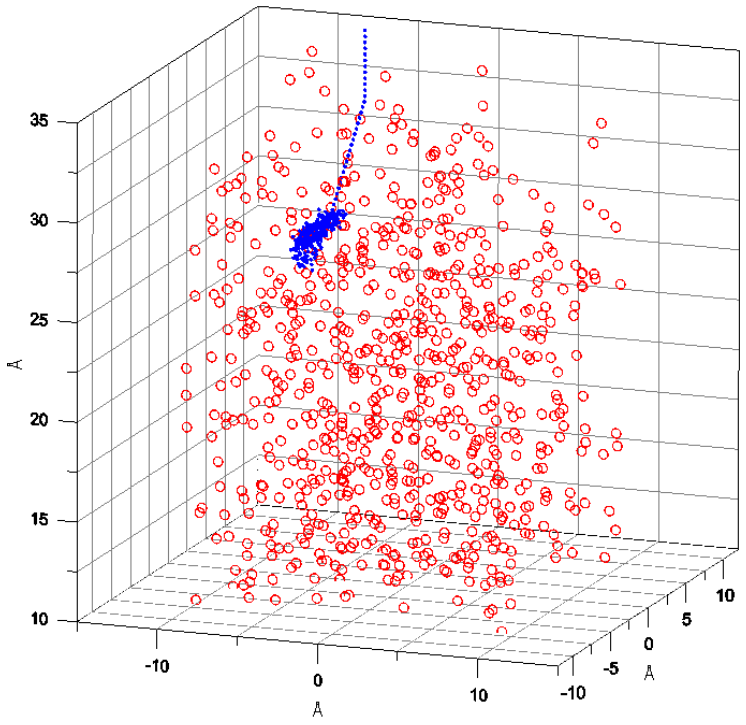
- **Newton's laws:** Calc. of position + velocities of atoms, by interatomic interaction potentials

$$\bar{F} = -\bar{\nabla} U$$

$$\bar{a} = \bar{F} / m$$

$$\bar{v} = \bar{v}_0 + \bar{a}\,\Delta t$$

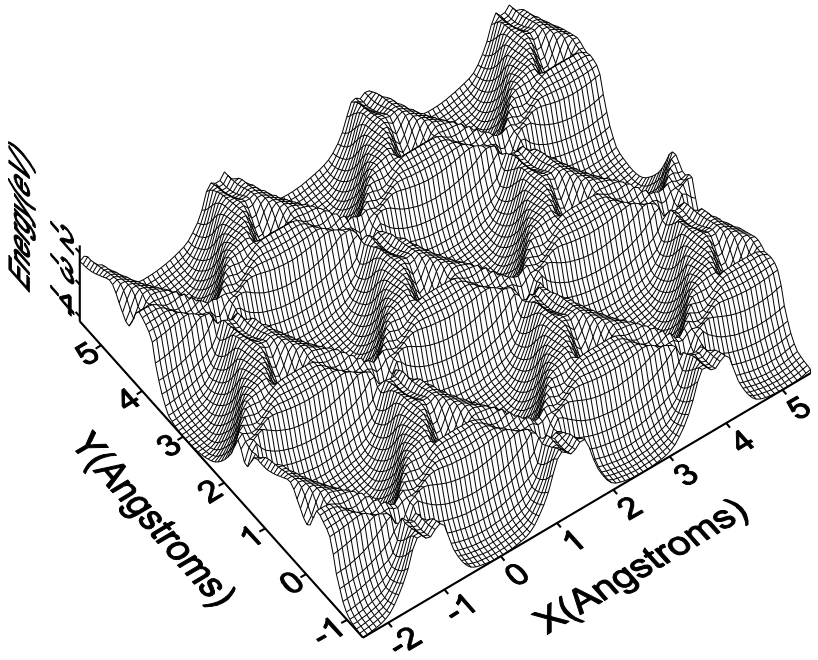
$$\bar{r} = \bar{r}_0 + \bar{v}_0\,\Delta t + \frac{1}{2}\bar{a}\,(\Delta t)^2$$



Time-integrated trajectory of impacting C-atom on amorphous C substrate

I. Model for plasma-surface interactions: Molecular Dynamics simulations (cont)

- **Interaction potential: empirical potential (parameters)**



Potential energy surface for impacting H-atom on diamond {111} surface

I. Model for plasma-surface interactions: Molecular Dynamics simulations (cont)

E.g.: C-films: Brenner interaction potential

- Binding energy: sum of binding energies between atoms *i* and *j* :

$$U_{system} = \sum_i \sum_{j>i} \left[V_R(r_{ij}) - \overline{b_{ij}} V_A(r_{ij}) \right]$$

- Repulsive (V_R) and attractive (V_A) terms:

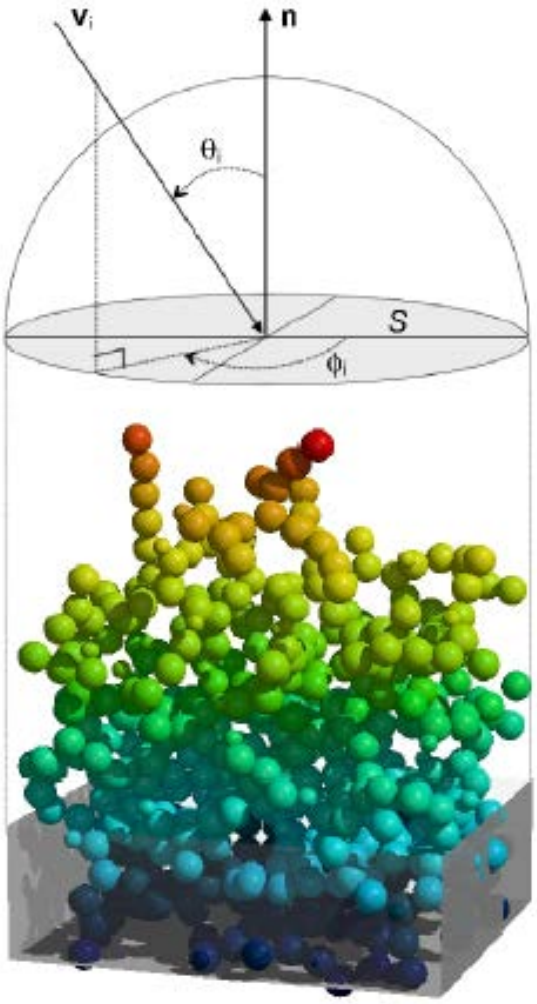
$$\begin{cases} V_R(r_{ij}) = f_{ij}(r_{ij}) A_{ij} \exp(-\lambda_{ij} r_{ij}) \\ V_A(r_{ij}) = f_{ij}(r_{ij}) B_{ij} \exp(-\mu_{ij} r_{ij}) \end{cases}$$

- 'Many-body' chemistry: binding order function b_{ij}

  b_{ij} = f(local binding topology)

I. Model for plasma-surface interactions: Molecular Dynamics simulations (cont)

- Semi-infinite surface:
  periodic ±{x,y} boundaries
- Time scale ~ ns (Δt ~ 0.1-1 fs)
  Length scale ~ nm
- Initialisation of the simulation:
  - Define substrate
  - Particle impacts
    - » Film growth: sequentially
    - » Reaction mechanisms
    - » Random orientation + {x,y} position above surface
  - Bottom layers fixed
  - Heat dissipation by heat bath



I. Model for plasma-surface interactions: Molecular Dynamics simulations (cont)

Advantage:

- Very accurate + deterministic (self-consistent)

Disadvantage:

Long calculation time…

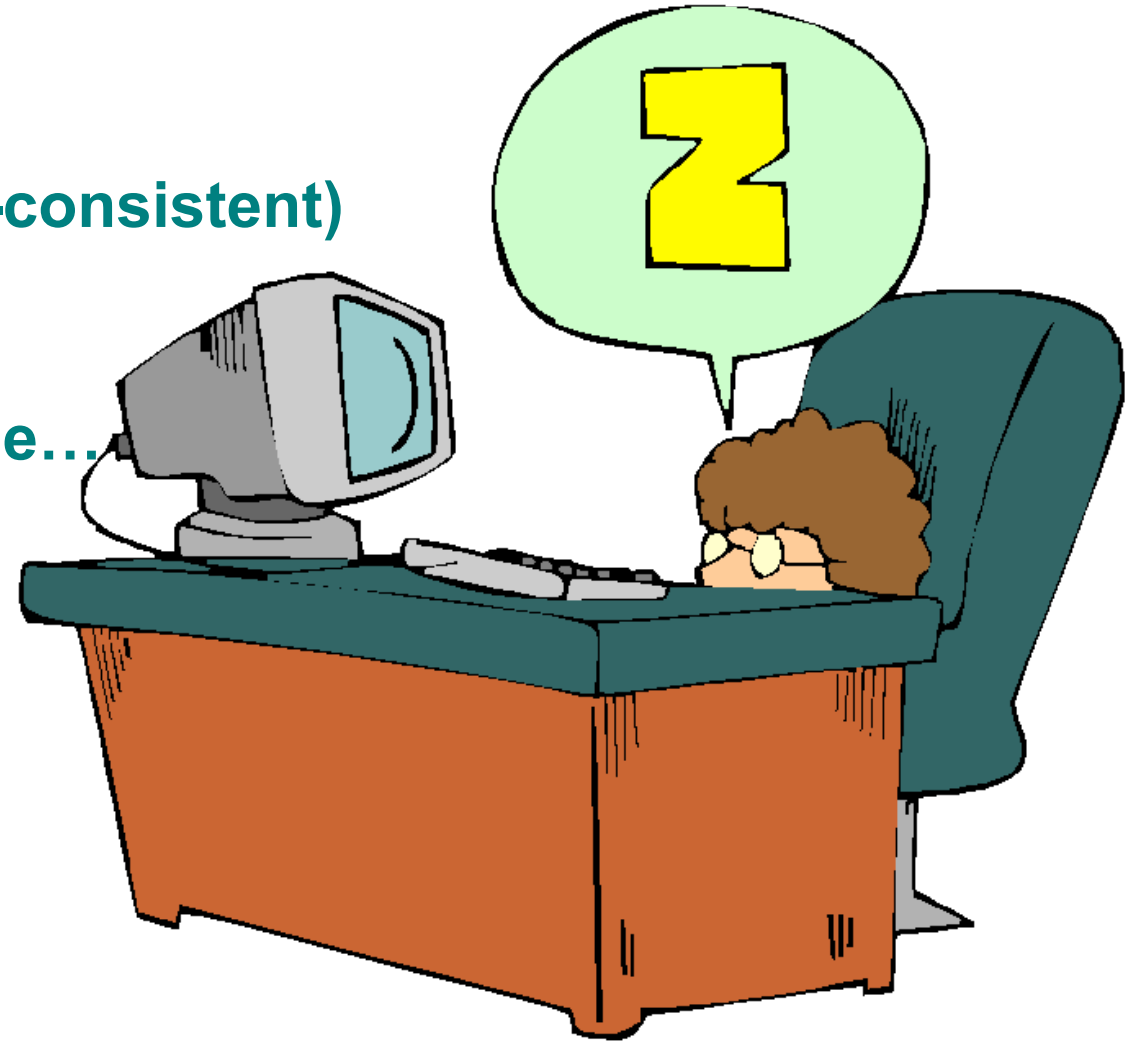
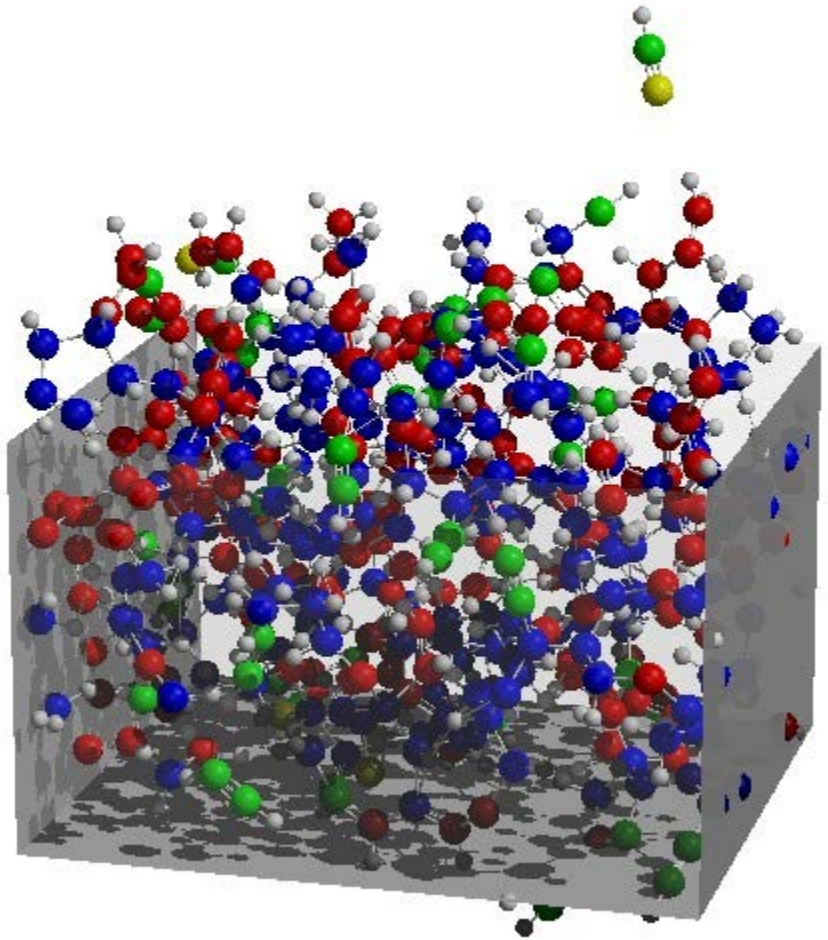


Illustration of MD simulations for film deposition
(diamond like carbon)

- 5-fold coordinated C-atom
- 4-fold coordinated C-atom
- 3-fold coordinated C-atom
- 2-fold coordinated C-atom
- 1-fold coordinated C-atom
- H-atom



Result: Calculated microscopic structure of the film

- 5-fold coordinated C-atom
- 4-fold coordinated C-atom
- 3-fold coordinated C-atom
- 2-fold coordinated C-atom
- 1-fold coordinated C-atom
- H-atom

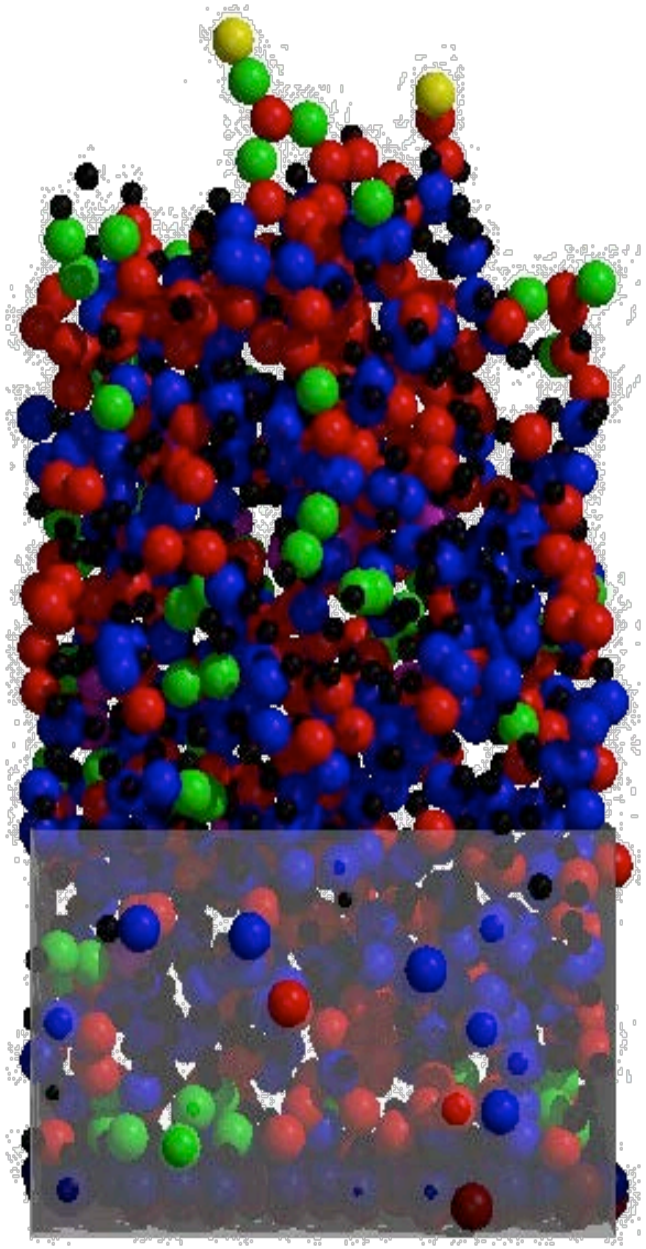


Illustration of MD simulations for plasma catalysis

CH_3 radicals on Ni catalyst surface

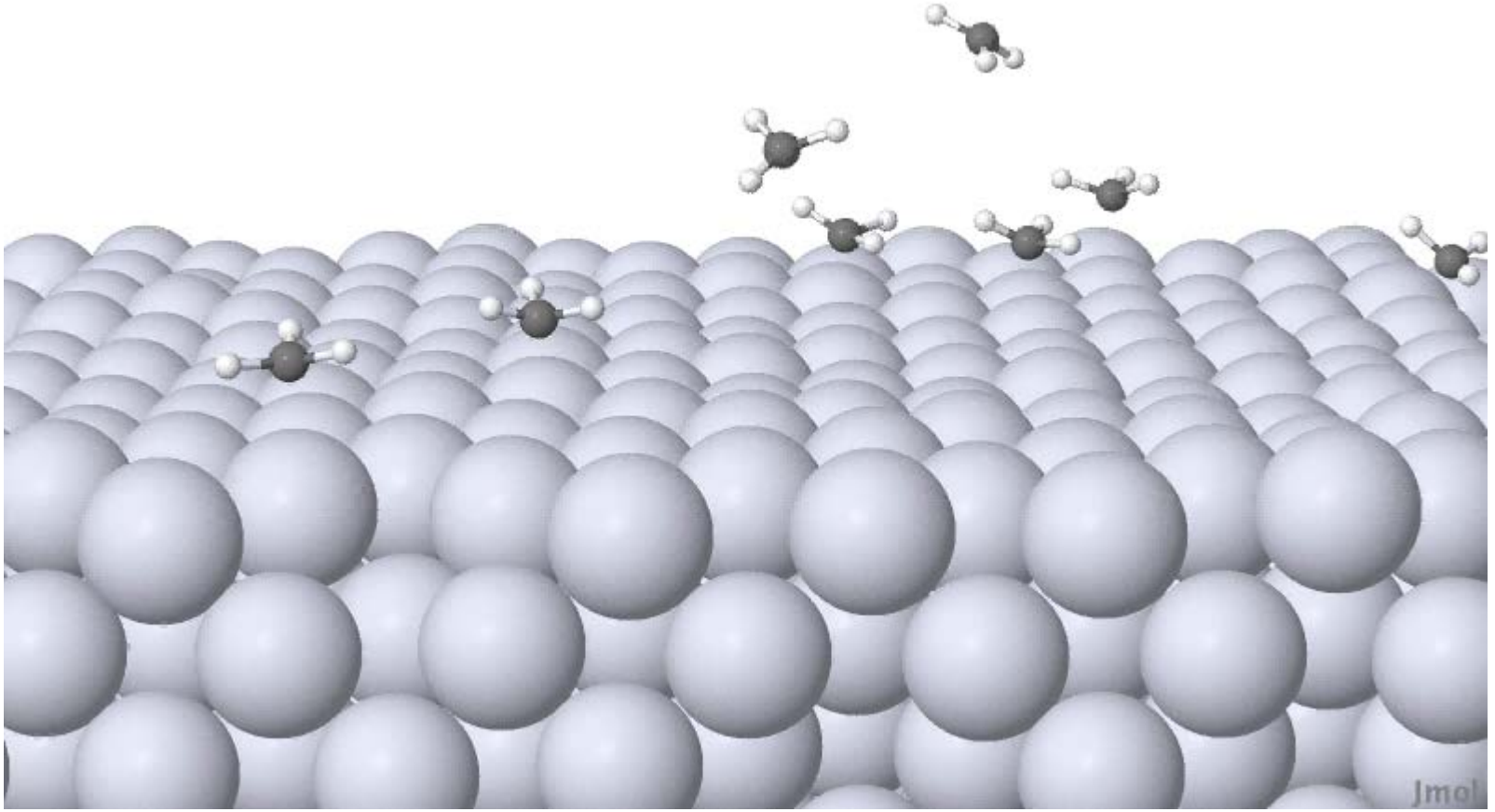


Illustration of MD simulations for carbon nanotube growth

Mechanism of cap formation of single walled carbon nanotube on Ni nanoparticle

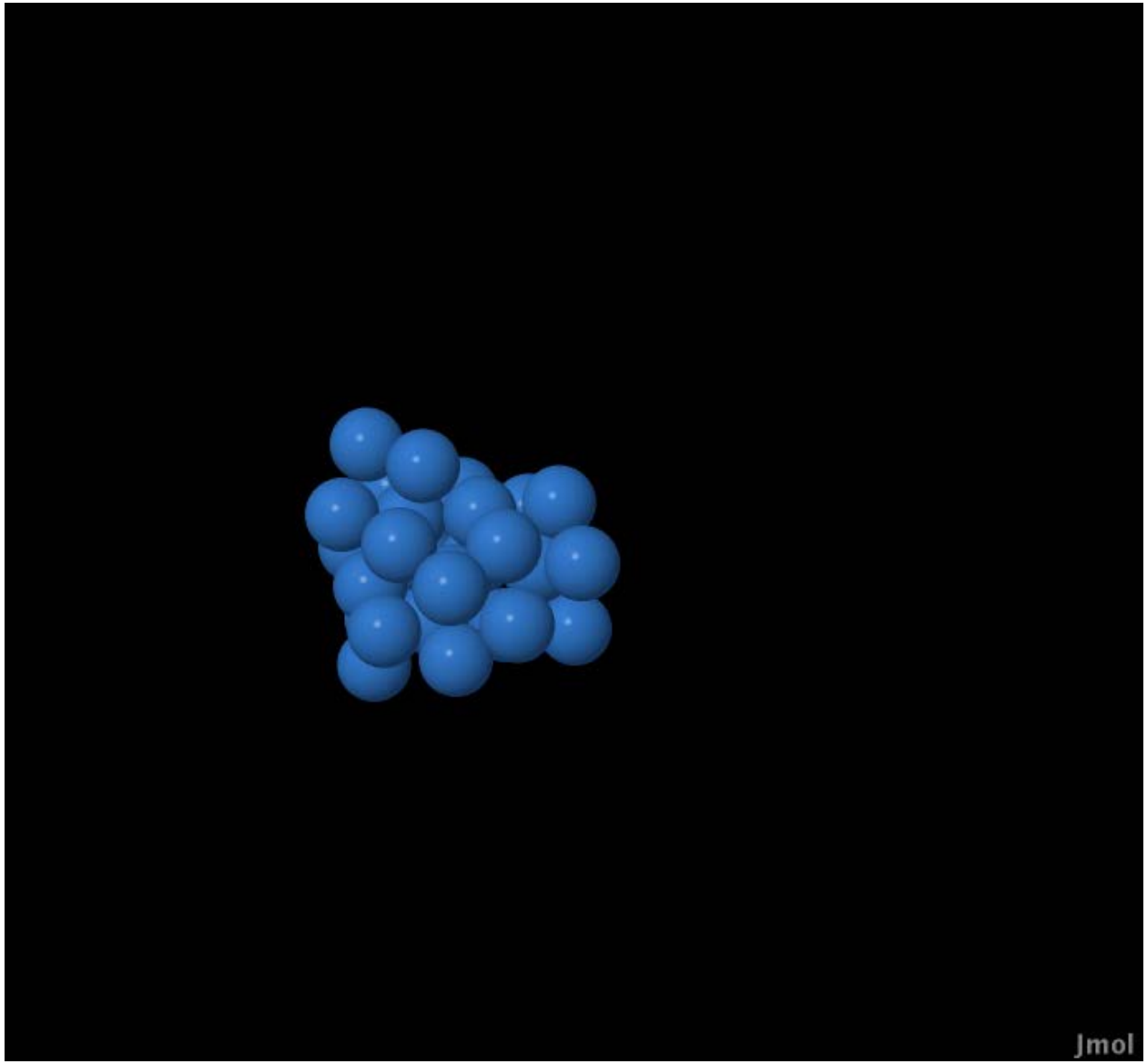
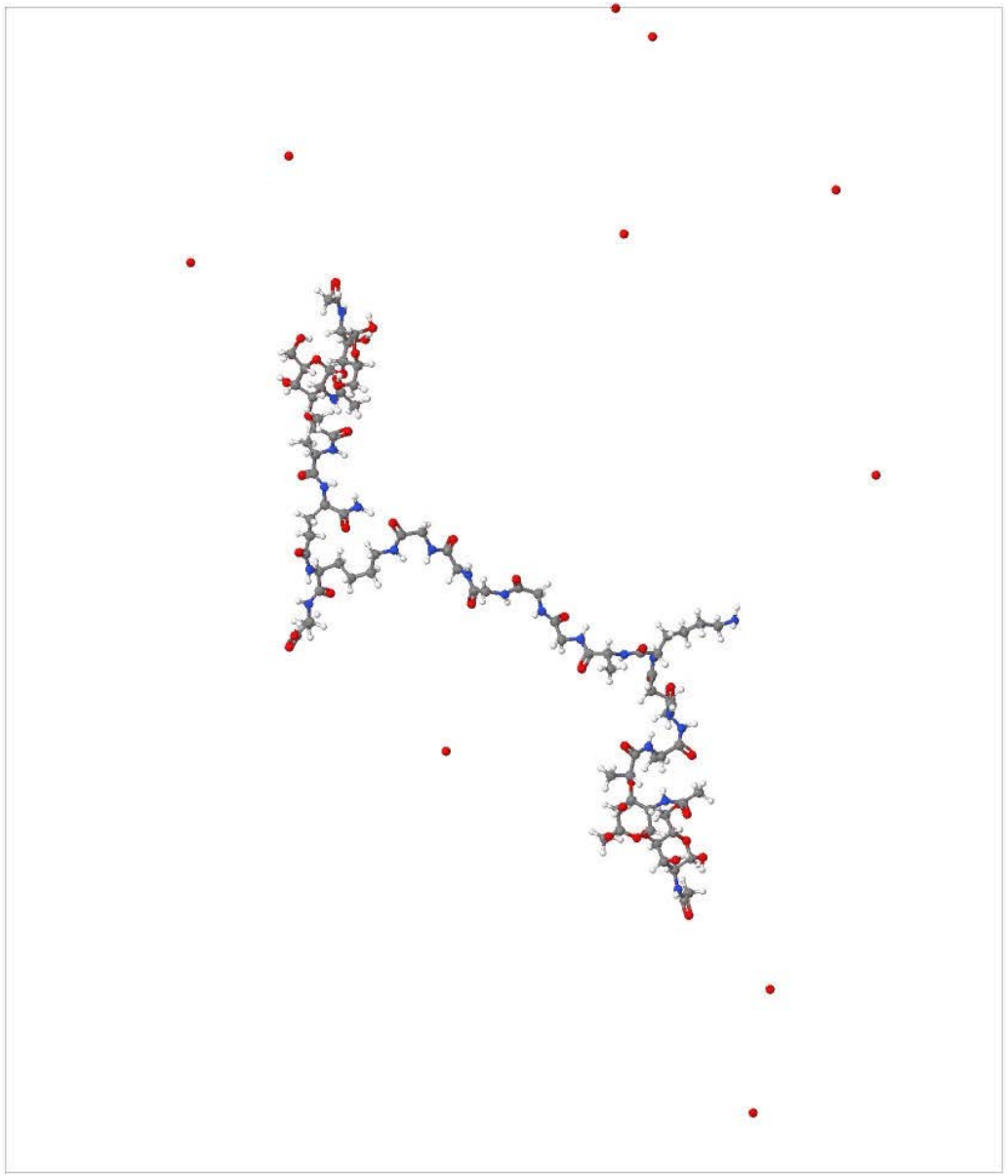


Illustration of MD simulations for plasma medicine

Breaking of peptidoglycan
(~ bacterial cell wall damage)
upon impact of O radicals



2. Examples of models for various applications

A. Fluid model: for DBD in CH_4/CO_2 or CH_4/O_2
   Greenhouse gas conversion (plasma chemistry)

B. PIC-MC model: for magnetron discharge

C. MC model for electrons: for magnetron discharge

D. Hybrid model: for glow discharge with sputtering

E. Hybrid model: for ICP etch reactor

A. Fluid model for DBD in CH_4/CO_2 or CH_4/O_2 Greenhouse gas conversion

Global warming ~ greenhouse gases

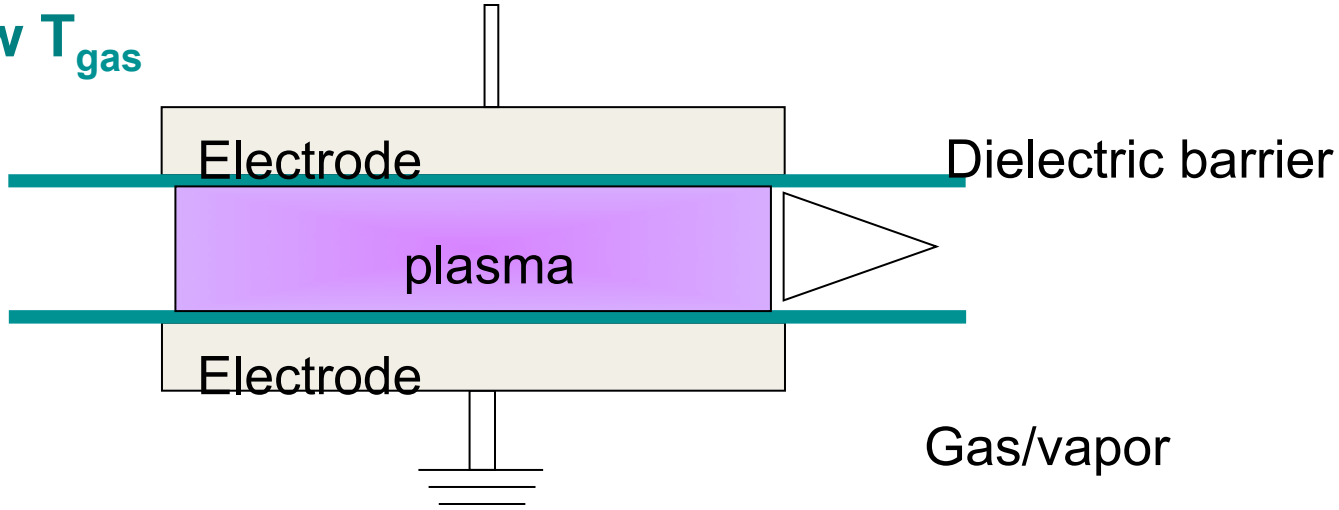
→ conversion into value-added chemicals

However: greenhouse gases = inert

→ Classical processes: high T, p

DBD reactor = very useful: $T_e >> T_{gas}$

Enables reactions that would thermodynamically not occur at low T_{gas}



Fluid model (DBD in CH_4/CO_2 or CH_4/O_2: greenhouse gas conversion)

Plasma chemistry

75 species (same for CH_4/CO_2, CH_4/O_2):

Molecules	Charged species	Radicals
CH_4	CH_5^+, CH_4^+, CH_3^+, CH_2^+, CH^+, C^+	CH_3, CH_2, CH, C
C_2H_6, C_2H_4, C_2H_2, C_3H_8, C_3H_6, C_4H_2 H_2	$C_2H_6^+$, $C_2H_5^+$, $C_2H_4^+$, $C_2H_3^+$, $C_2H_2^+$, C_2H^+, C_2^+ H_3^+, H_2^+, H^+, H^-	C_2H_5, C_2H_3, C_2H, C_2, C_3H_7, C_3H_5 H
O_3, O_2	O_4^+, O_2^+, O^+, O_4^-, O_3^-, O_2^-, O^-	O
CO_2, CO	CO_2^+, CO^+	
H_2O, H_2O_2	H_3O^+, H_2O^+, OH^+, OH^-	OH, HO_2
CH_2O, CH_3OH, C_2H_5OH, CH_3CHO, CH_2CO, CH_3OOH, C_2H_5OOH	Electrons	CHO, CH_2OH, CH_3O, C_2H_5O, C_2HO, CH_3CO, CH_2CHO, CH_3O_2, $C_2H_5O_2$

Fluid model (DBD in CH_4/CO_2 or CH_4/O_2: greenhouse gas conversion)

Plasma chemistry

1088 reactions taken into account:

165 Electron-neutral collisions

(ionization, excitation, dissociation,…)

e.g.: $e^- + CH_4 \rightarrow e^- + CH_3 + H$

50 Electron-ion recombination reactions

e.g.: $e^- + O_2^+ \rightarrow O + O$

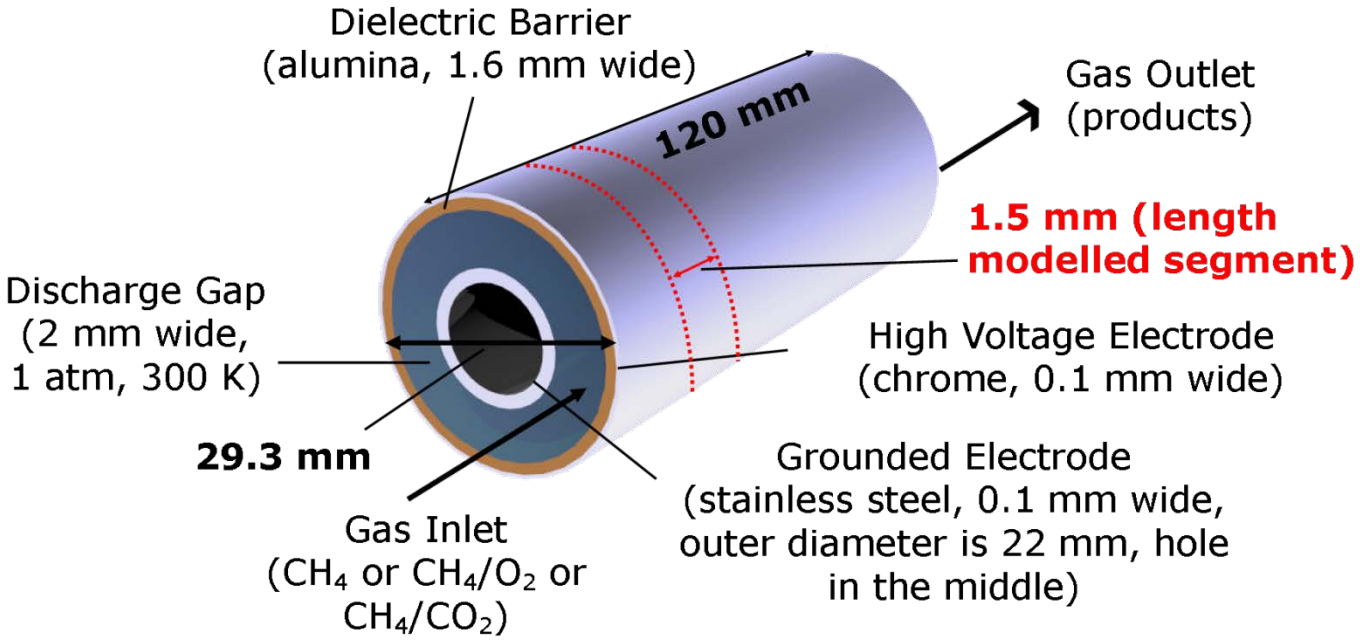
873 Ion/neutral chemical reactions

e.g.: $CH_3 + OH\ (+M) \rightarrow CH_3OH\ (+M)$

$CH_4^+ + CH_4 \rightarrow CH_5^+ + CH_3$

Fluid model (DBD in CH_4/CO_2 or CH_4/O_2: greenhouse gas conversion)

Reactor setup and conditions



Operating conditions: 5 kV, 10 kHz

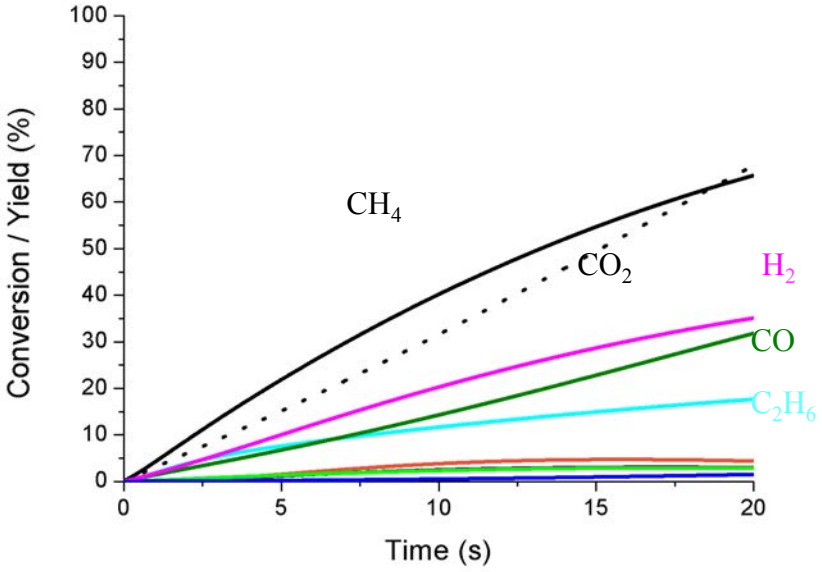
Gas fractions:

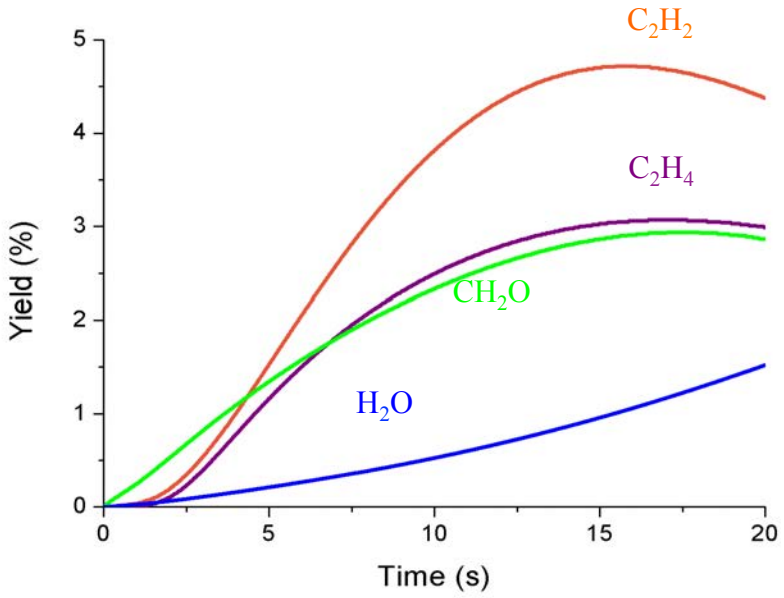
- **Pure CH_4**
- **CH_4/CO_2 (90/10 – 70/30 – 50/50 – 30/70 – 10/90)**
- **CH_4/O_2 (90/10 – 70/30)**

Fluid model (DBD in CH_4/CO_2 or CH_4/O_2: greenhouse gas conversion)

Calculated conversion, yields

CH_4/CO_2 = 70/30



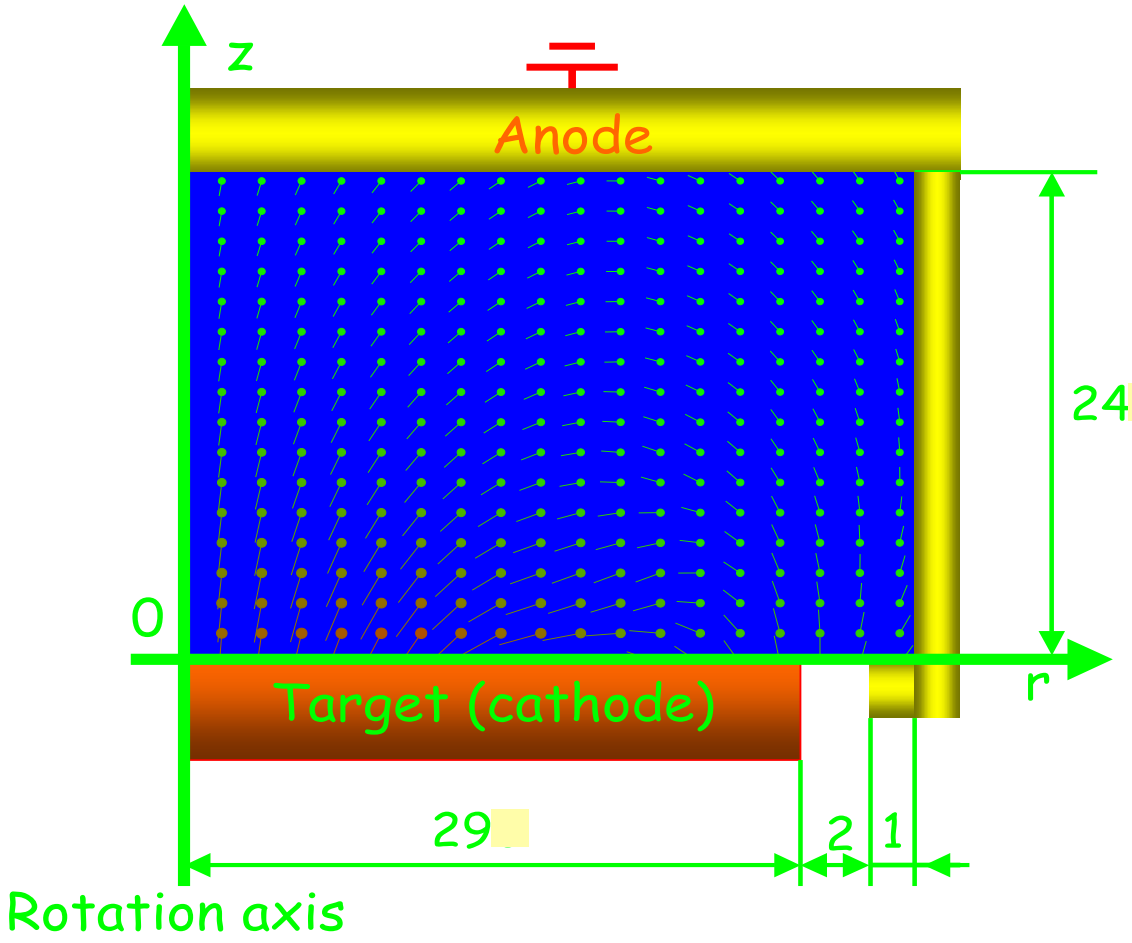


- **65 % of both CO_2 and CH_4 converted after 20s**
- **Formation of syngas (H_2/CO ~ 1.5/1)**
- **Formation of C_xH_y**
- **Formation of CH_2O (~ 3%) and H_2O (~1,5 %)**

Fluid model (DBD in CH_4/CO_2 or CH_4/O_2: greenhouse gas conversion)

B. PIC-MC model: for magnetron discharge

Reactor geometry + Magnetic field



Br_{max} = 300 – 1100 G

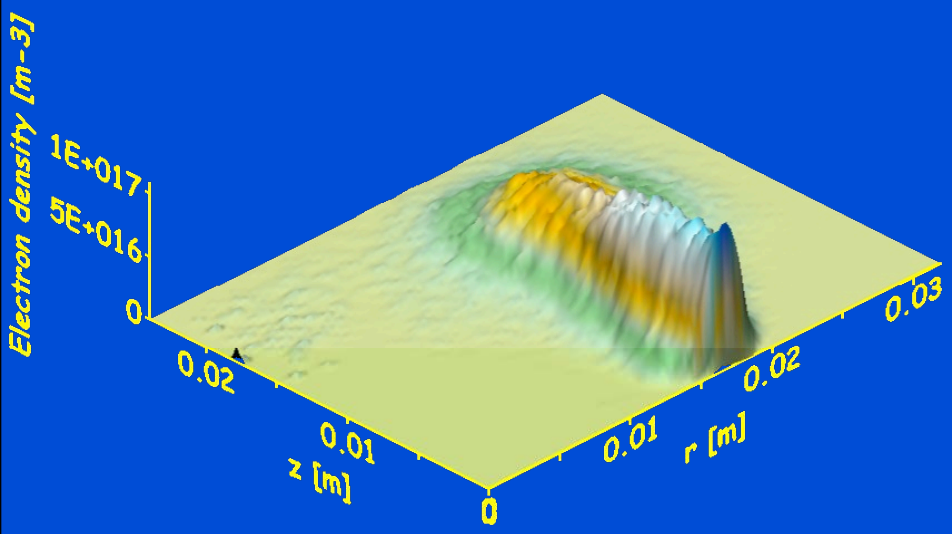
Vext = -400 V

p = 4 - 30 mtorr

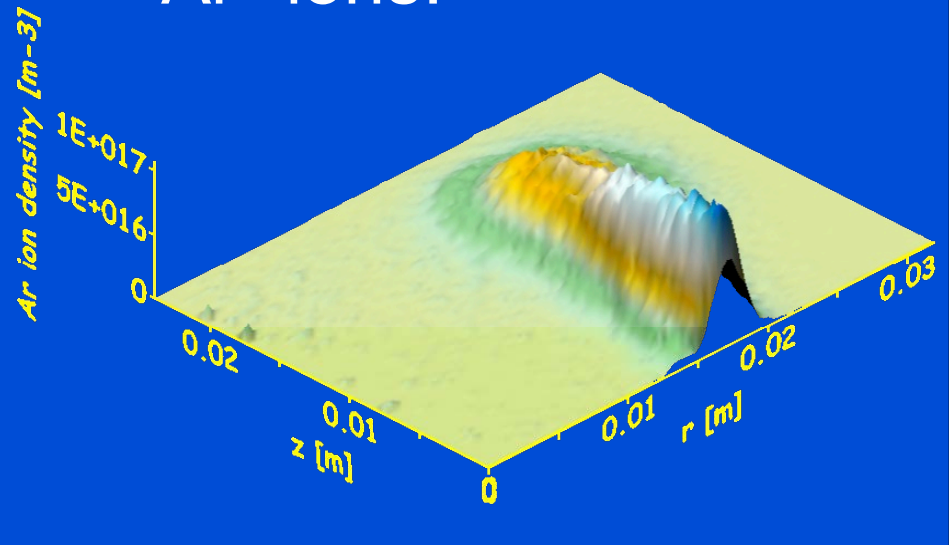
Argon

Calculated Electron and Ar^+ Ion Density

Electrons:



Ar^+ ions:

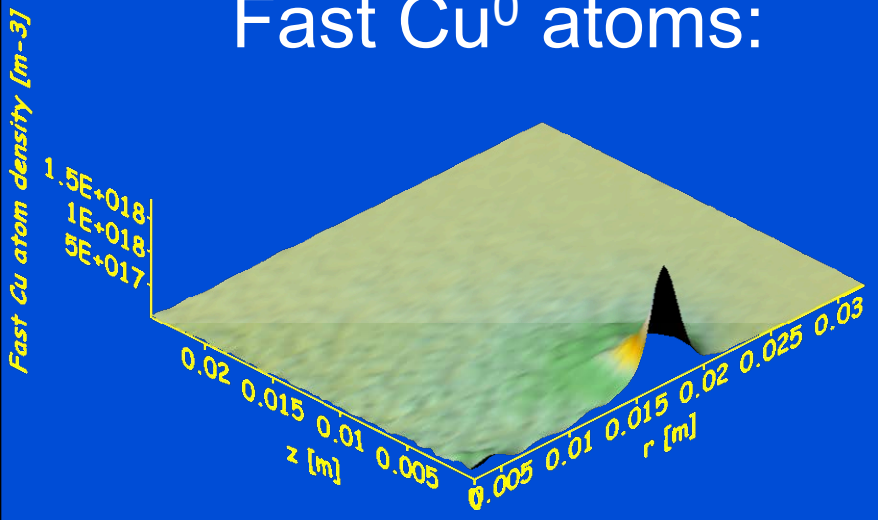


Maximum ~ 10^{17} m^{-3}
at r = 1.85 cm (maximum B_r)

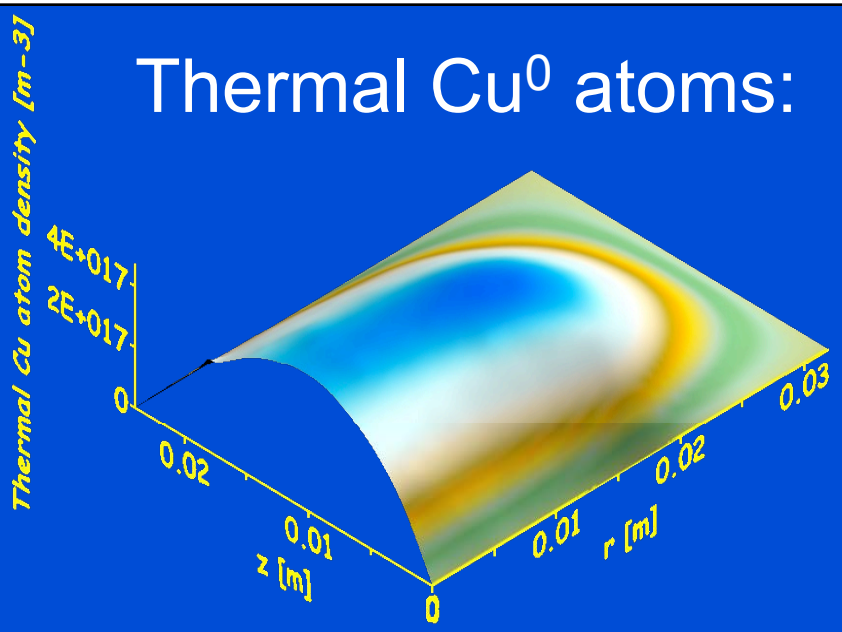
PIC-MC model (magnetron discharge)

Fast Cu Atom Density and Thermal Cu atom density

Fast Cu^0 atoms:



Thermal Cu^0 atoms:

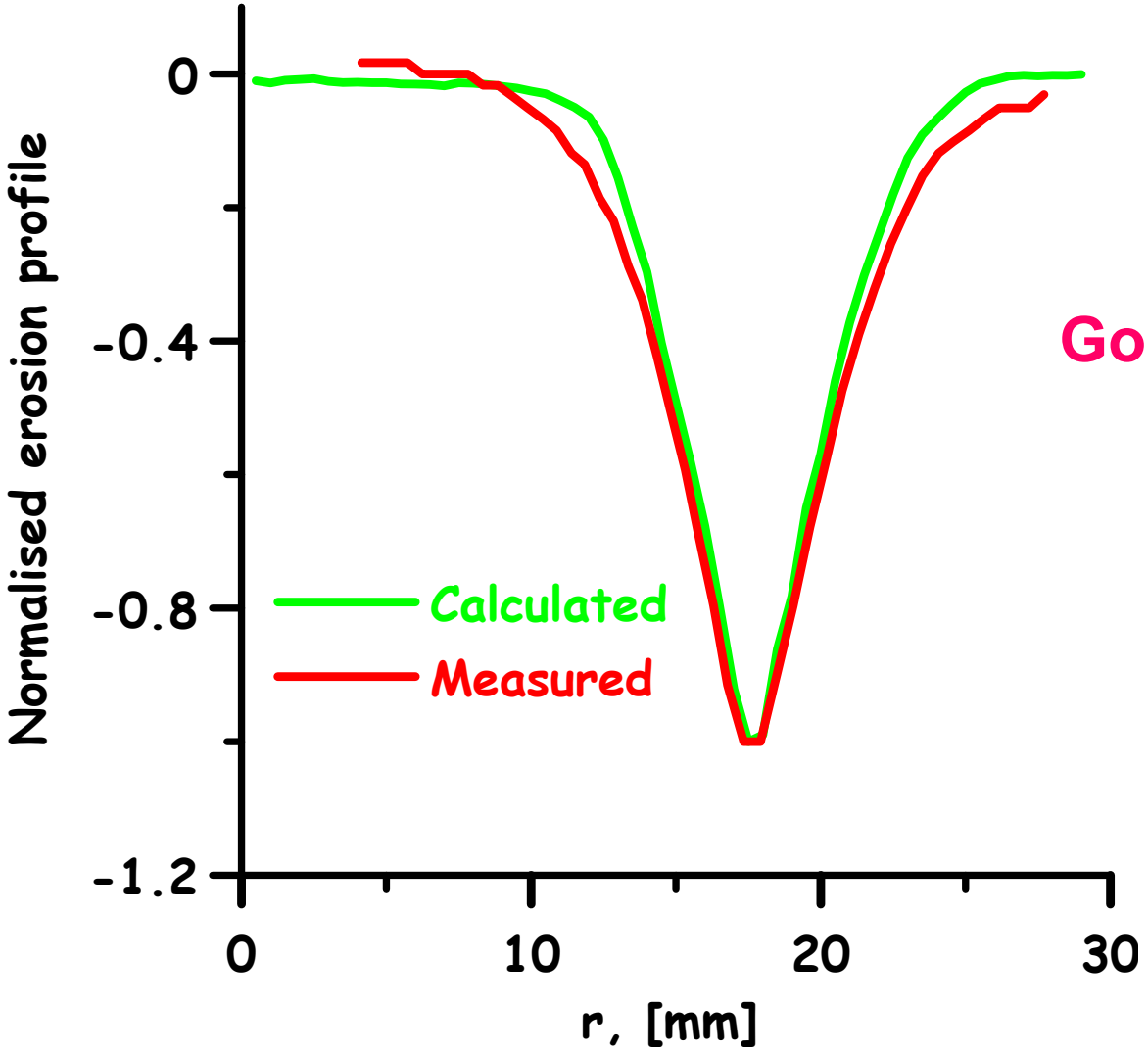


Concentrated near cathode
Max ~ 10^{18} m^{-3}

Broad distribution
Max ~ $4x10^{17}$ m^{-3}

PIC-MC model (magnetron discharge)

Erosion profile: Calculated - Measured

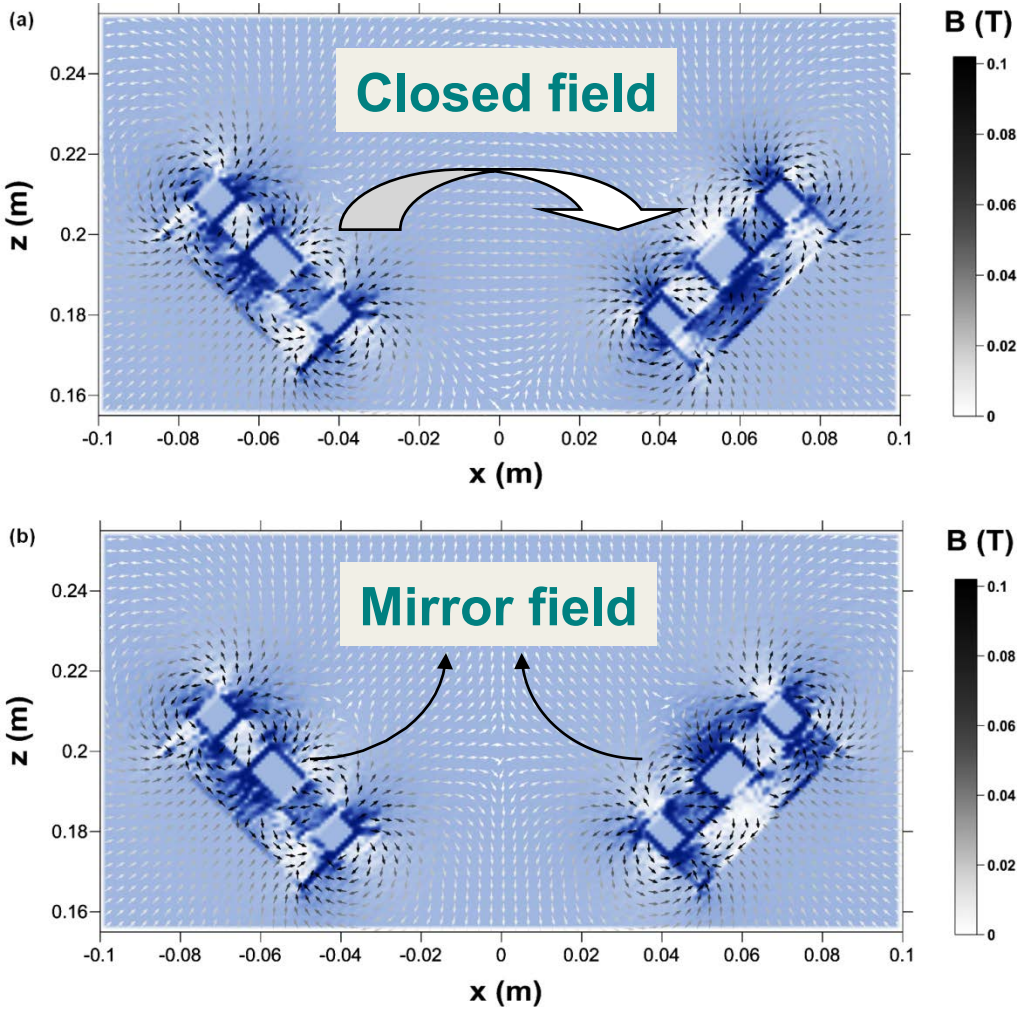


Good agreement

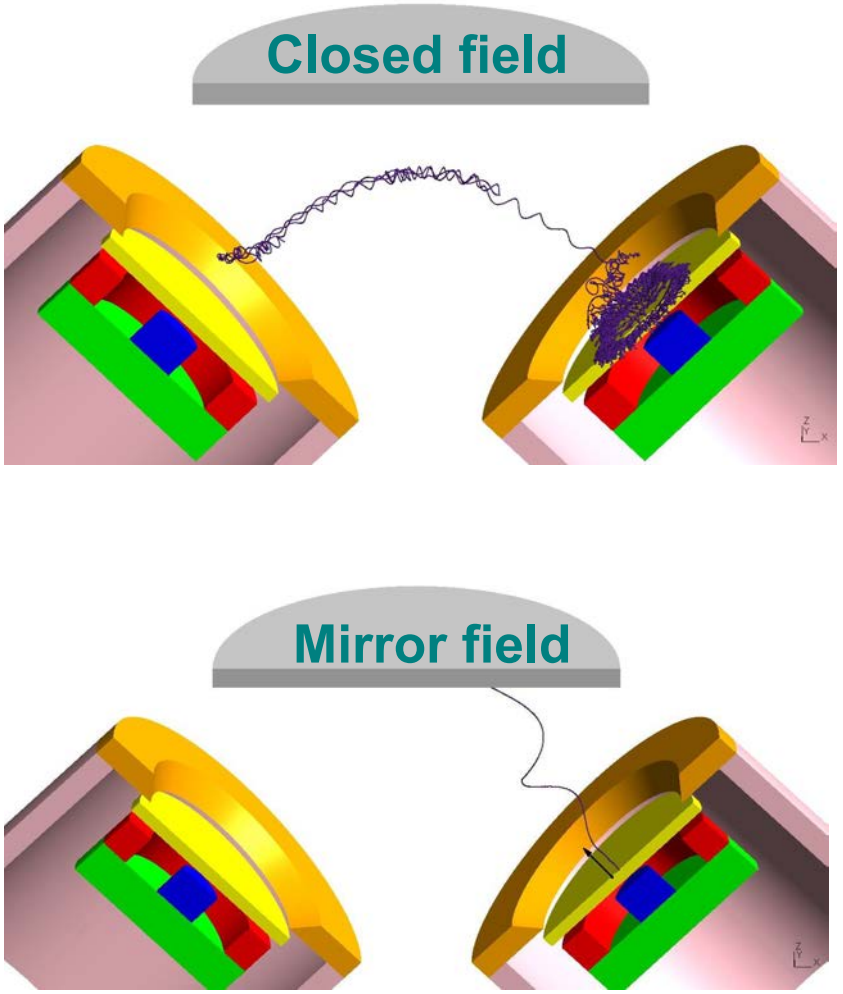
PIC-MC model (magnetron discharge)

C. MC model for electrons: dual magnetron discharge

Magnetic field



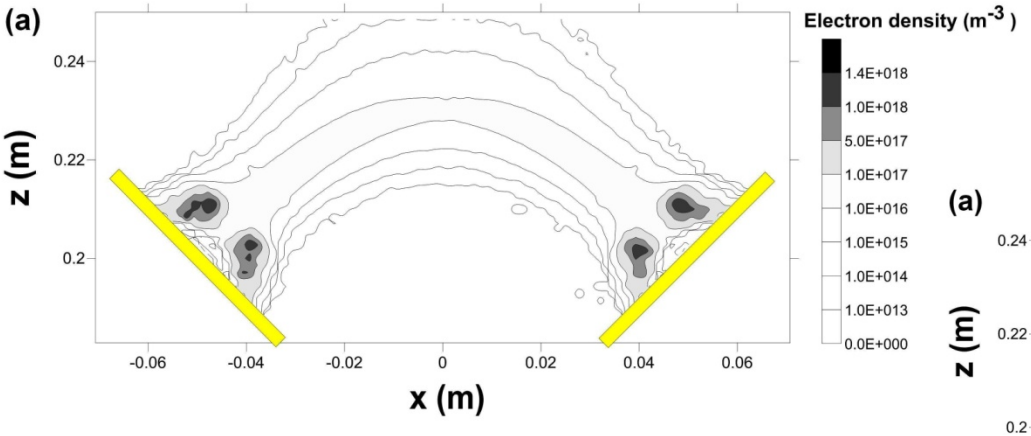
Single electron trajectory

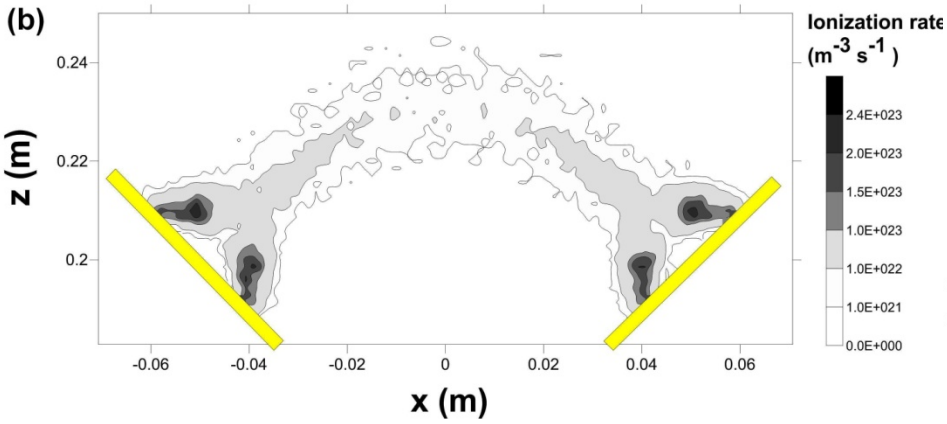


MC model for electrons (dual magnetron discharge)

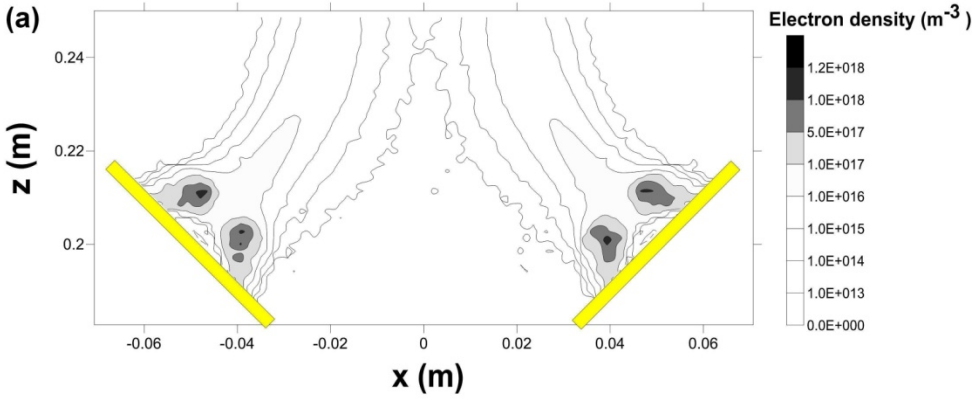
Calculated electron density – ionization rate

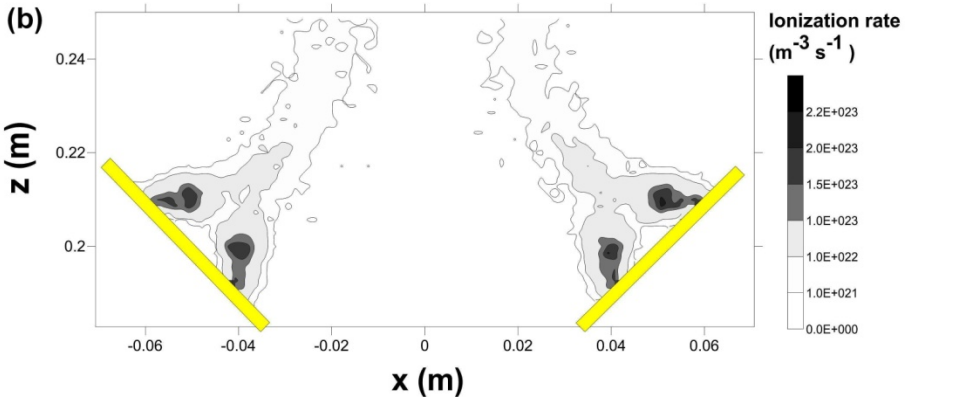
Closed field:





Mirror field:





MC model for electrons (dual magnetron discharge)

Comparison MC vs PIC-MC model

MC =

- **faster (minutes to 1 hour vs. several weeks for PIC)**
- **complex geometries possible**

But: not self-consistent:

- Input B needed (e.g., from

Gmsh (http://www.geuz.org/gmsh/)

& GetDP (http://www.geuz.org/getdp/)

- Input E needed (e.g., from PIC-MC model)

MC model for electrons (dual magnetron discharge)

D. Hybrid model for GD plasma with sputtering

Combination of different models for various species

Species:	Model used:
Ar^0 atoms	no model (assumed thermalized) or: heat conduction equation
electrons	MC for fast electrons fluid for slow electrons
Ar^+ ions	fluid (with electrons + Poisson) MC in sheath
Ar^0_f fast atoms	MC in sheath
Ar* excited atoms	collisional-radiative model
Cu^0 atoms	thermalization after sputtering: MC
Cu^*, $Cu^{+(*)}$, Cu^{++}	collisional-radiative model
Cu^+ ions	MC in sheath

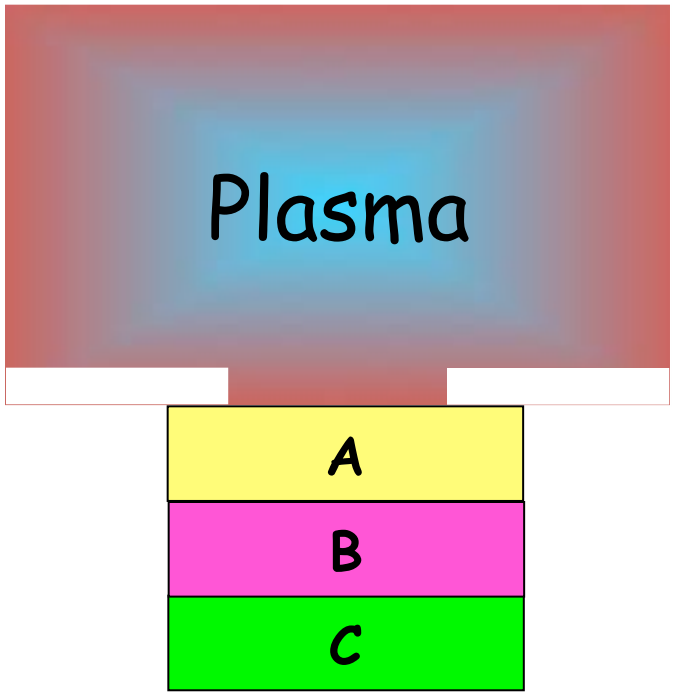
Application: Analysis of solid materials:

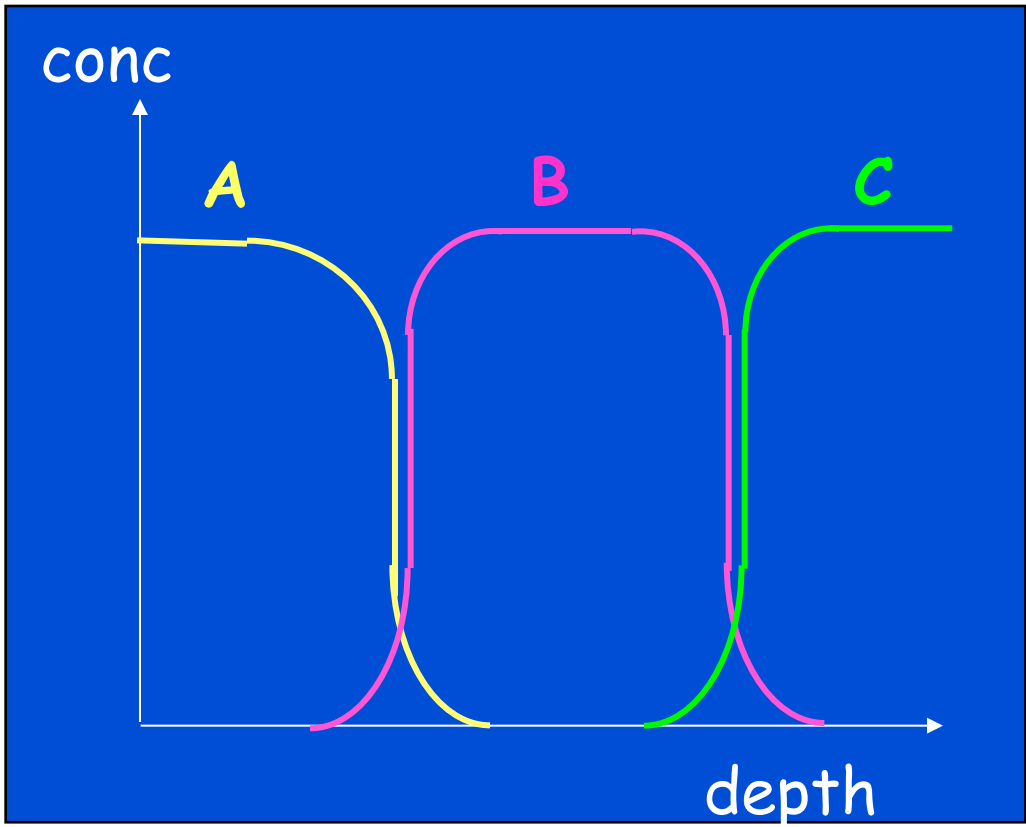
Sample to be analyzed = cathode of GD

Sputtering → Excitation, ionization in plasma → OES, MS

E.g.: Depth profiling:

Concentr as f(depth)

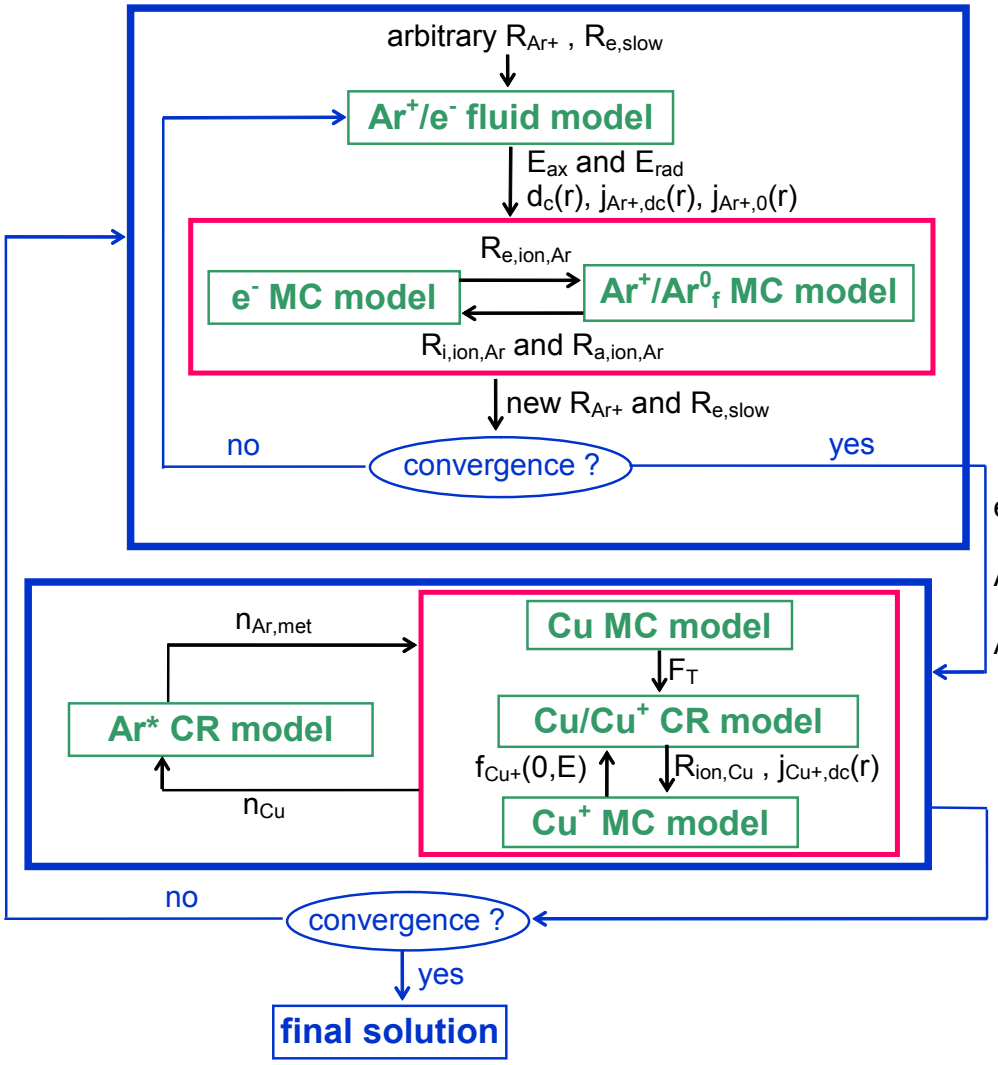




Hybrid model (GD)

Coupling of the models:

"Modeling network"



e^- MC model: - $R_{e,exc,Ar}$, $R_{e,exc,met}$, $R_{e,ion,met}$: for Ar^*_m model
- $R_{e,ion,Cu}$: for Cu model

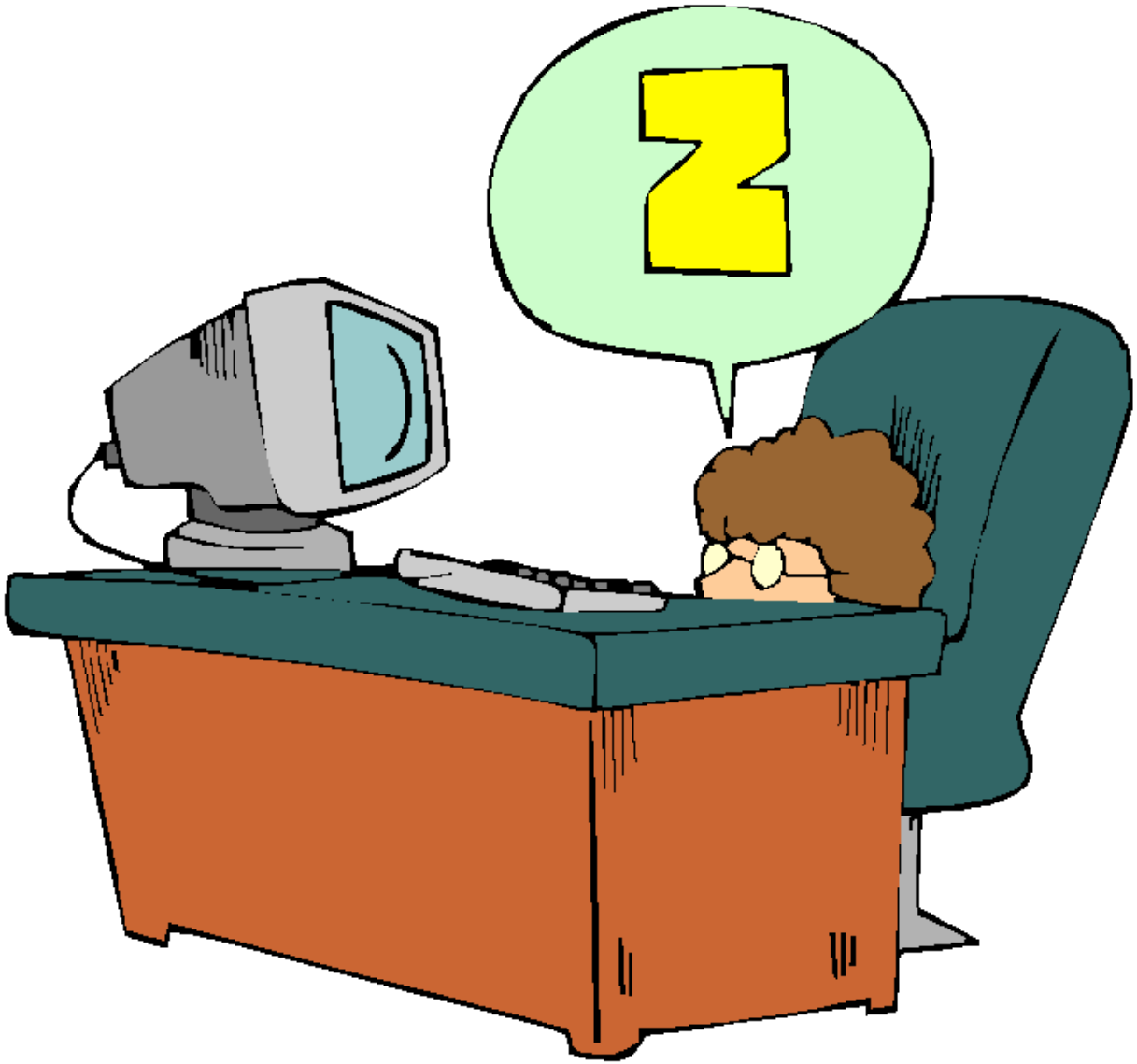
Ar^+/Ar^0_f MC model: - $R_{i,exc,Ar}$, $R_{a,exc,Ar}$: for Ar^*_m model
- $f_{Ar+}(0,E)$, $f_{Ar}(0,E)$: for Cu model

Ar^+/e^- fluid model: - n_{Ar+} , $n_{e,slow}$: for Ar^*_m model
- n_{Ar+} , V : for Cu model

Ar^*_m model: - $n_{Ar,met}$: for $R_{e,exc,met}$ and $R_{e,ion,met}$
- prod, loss: for n_{Ar+} , $n_{e,slow}$

Cu model: - n_{Cu} : for $R_{e,ion,Cu}$
- n_{Cu+} : for E, V
- asymm. CT : for n_{Ar+}
- ioniz.terms: for $n_{e,slow}$

Hybrid model (GD)



Hybrid model (GD)

Input data for the modeling network

- **Electrical data:**

  Voltage, pressure, (gas temperature)

  → Electrical current = calculated self-consistently

- **Reactor geometry:**

  (e.g., cylinder: length, diameter)

- **Gas (mixture)**

- **Cross sections, rate coefficients,**

  transport coefficients,…

All other quantities: calculated self-consistently

Typical calculation results

General calculation results:

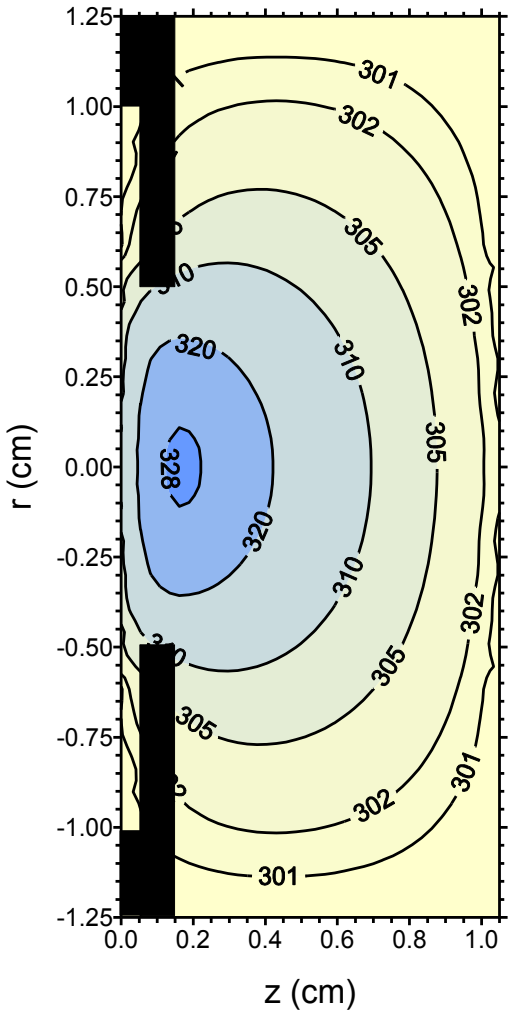
* Electrical characteristics (current, voltage, pressure)
* Electric field and potential distribution
* Densities, fluxes, energies of the plasma species
* Information about collisions in the plasma

Results of importance for applications (sputtering, GD-OES,…):

* Crater profiles, erosion rates at the cathode
* Optical emission intensities
* Effect of cell geometry, operating conditions

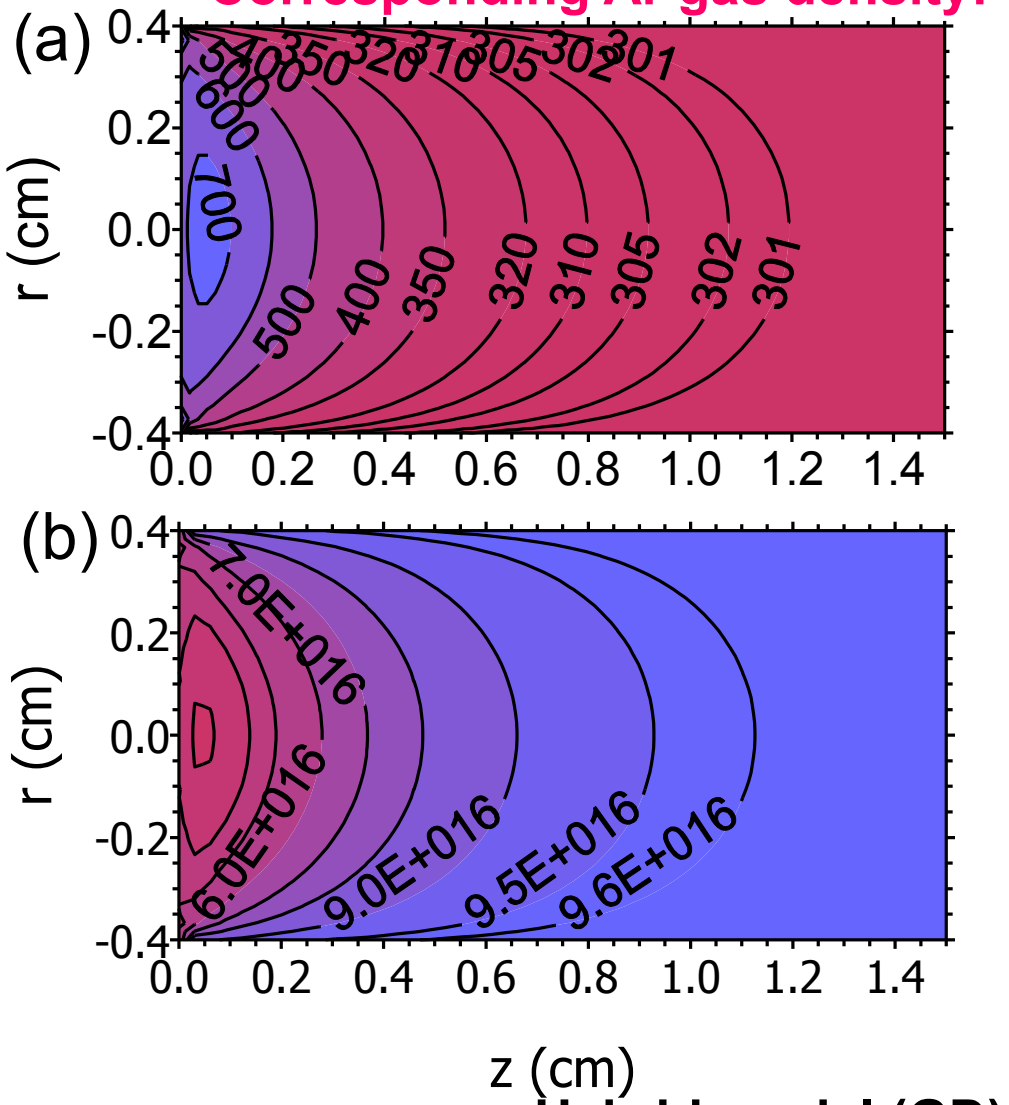
Calculated gas temperature:

VG9000 cell
(1000 V, 3 mA, 75 Pa):



Grimm-type cell
(800 V, 50 mA, 400 Pa)

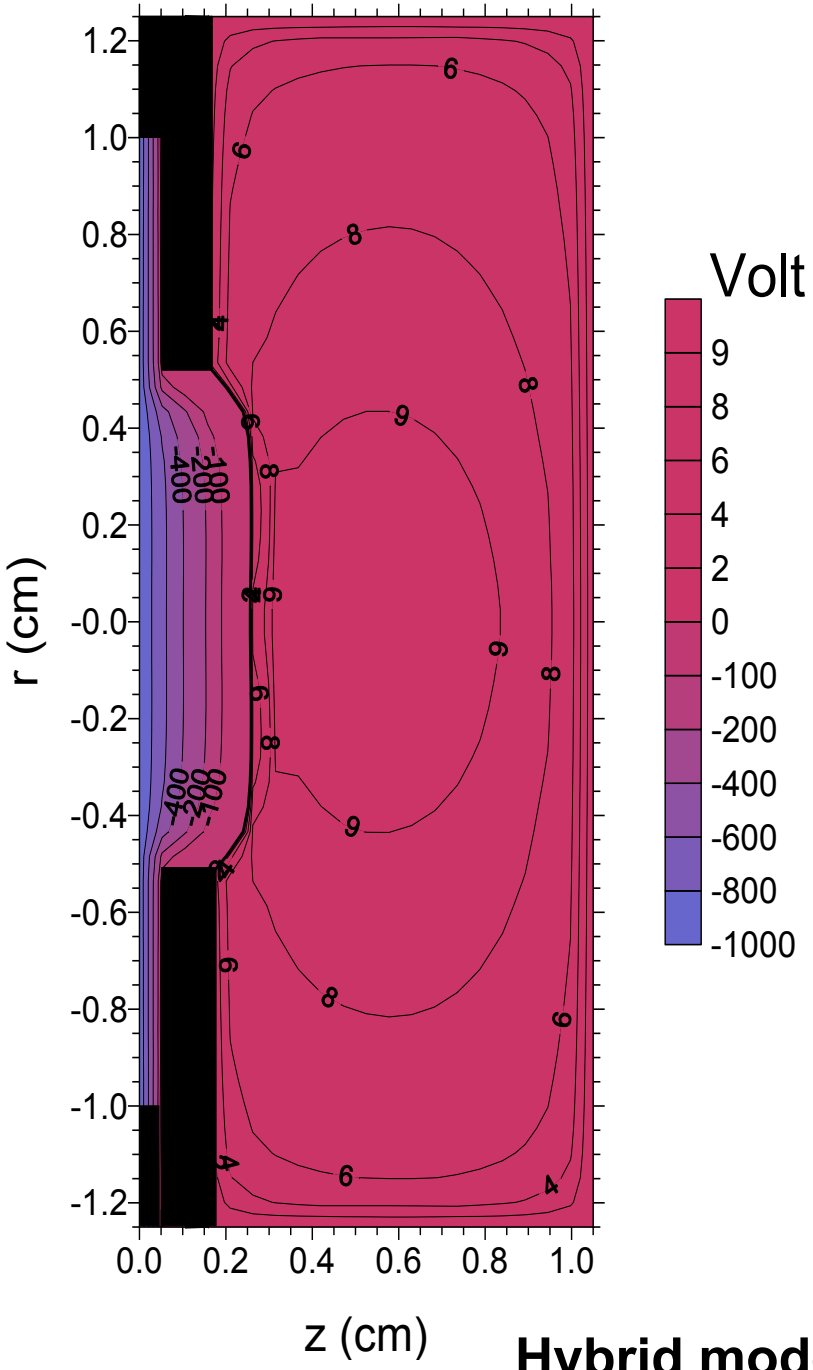
+ Corresponding Ar gas density:



Hybrid model (GD)

Potential distribution:
(VG9000 cell
1000 V, 75 Pa, 3 mA)

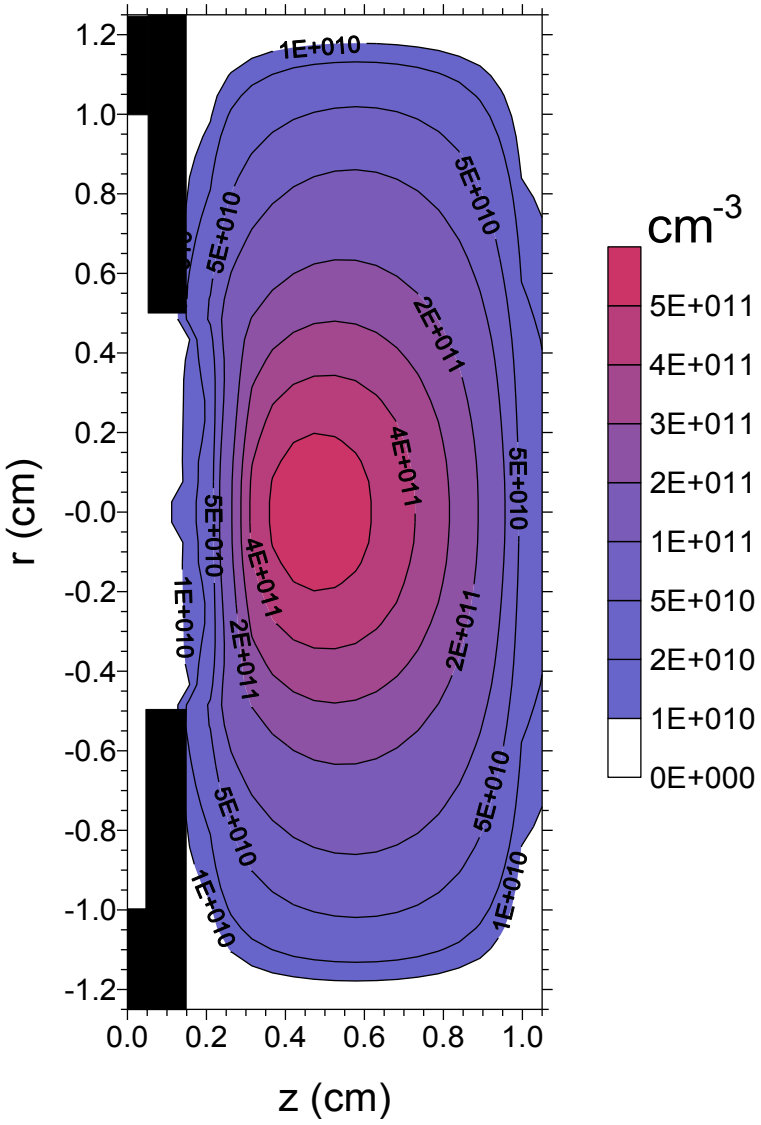
CDS: ca. 2 mm long
NG: major part (9 V)



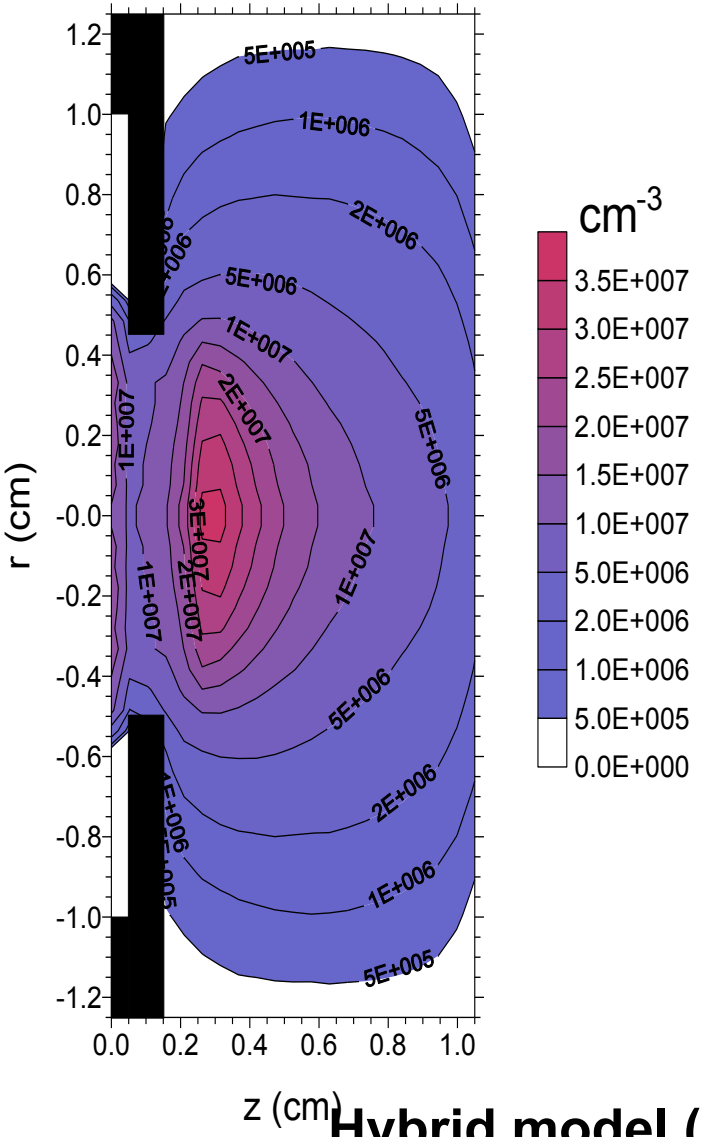
Hybrid model (GD)

Densities: (VG9000: 1000 V, 75 Pa, 3 mA):

Ar^+ ions ~ slow electrons:



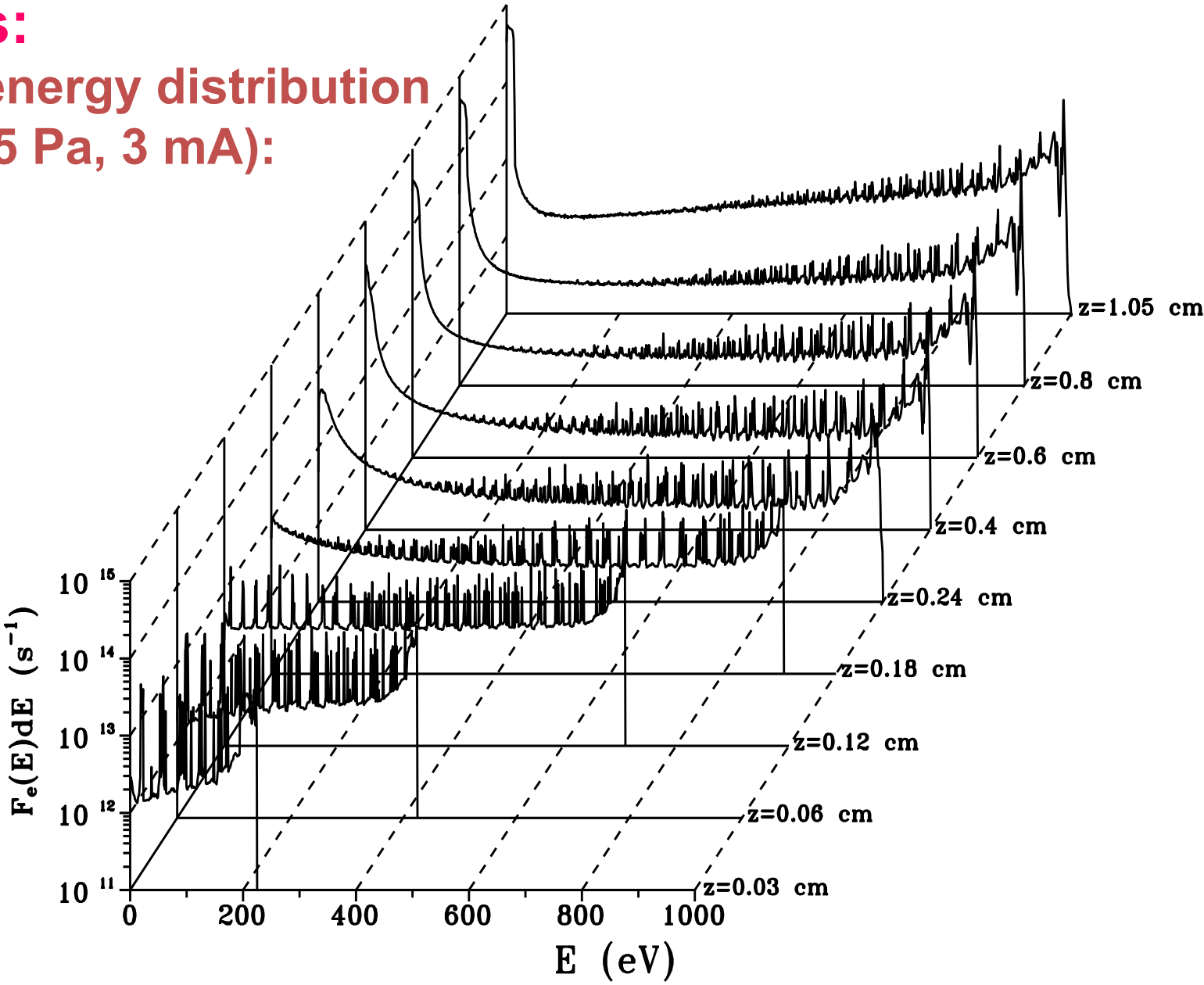
Fast electrons:



Hybrid model (GD)

Energies:

Electron energy distribution (1000 V, 75 Pa, 3 mA):

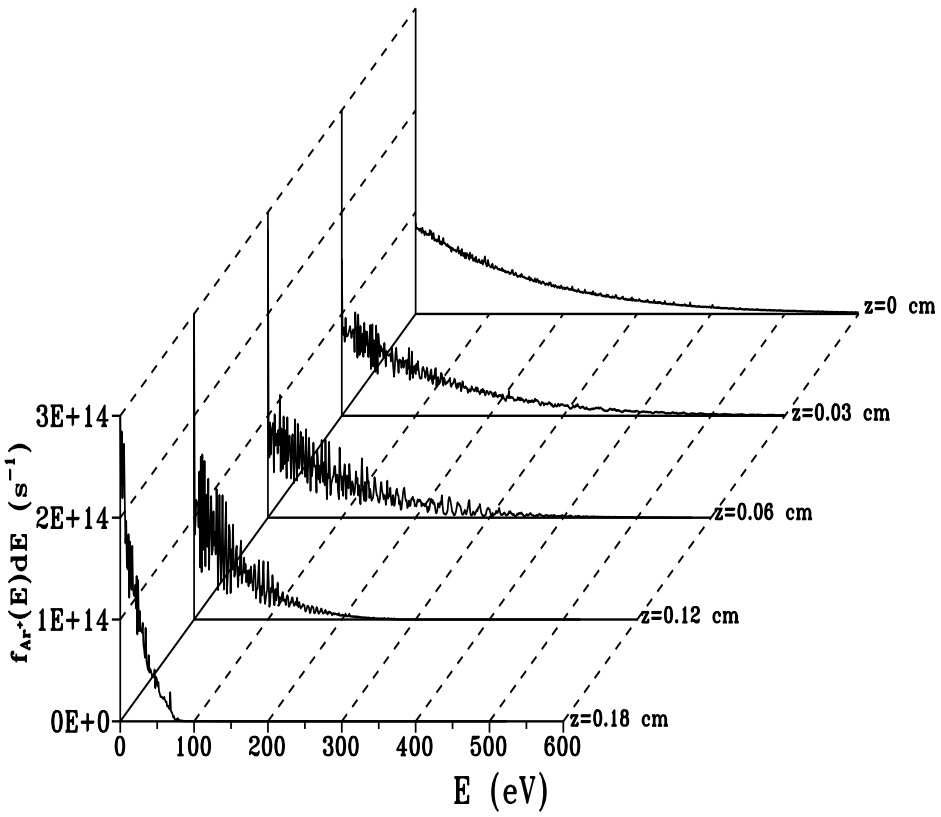


Hybrid model (GD)

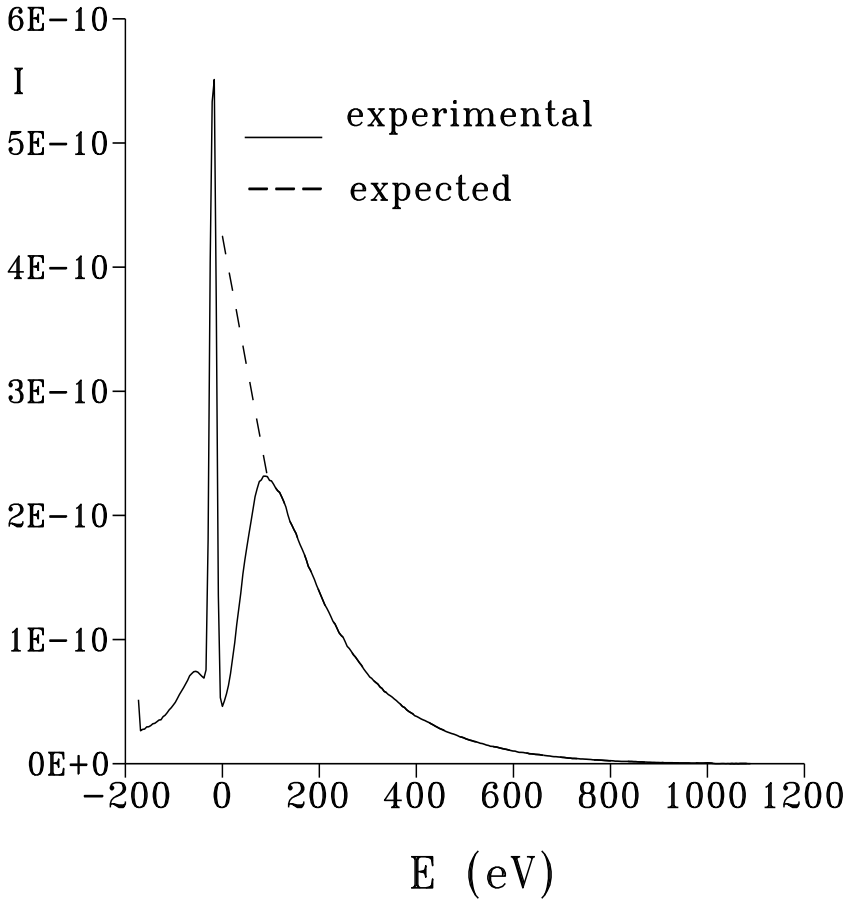
Energies:

Argon ion energy distribution (1000 V, 75 Pa, 3 mA):

Calculated:



Measured (MS):

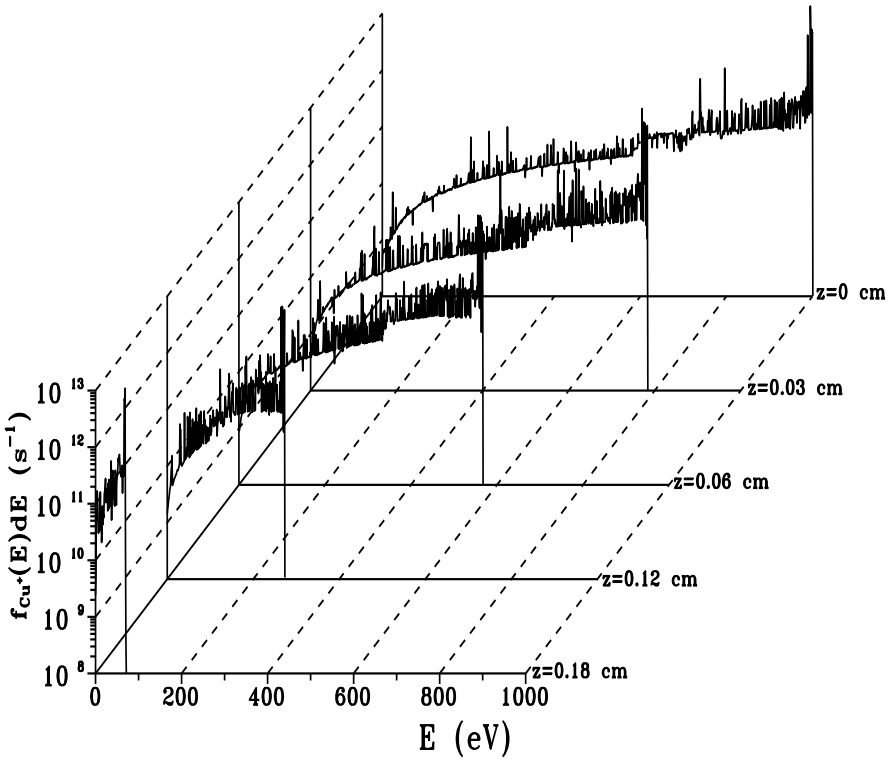


Hybrid model (GD)

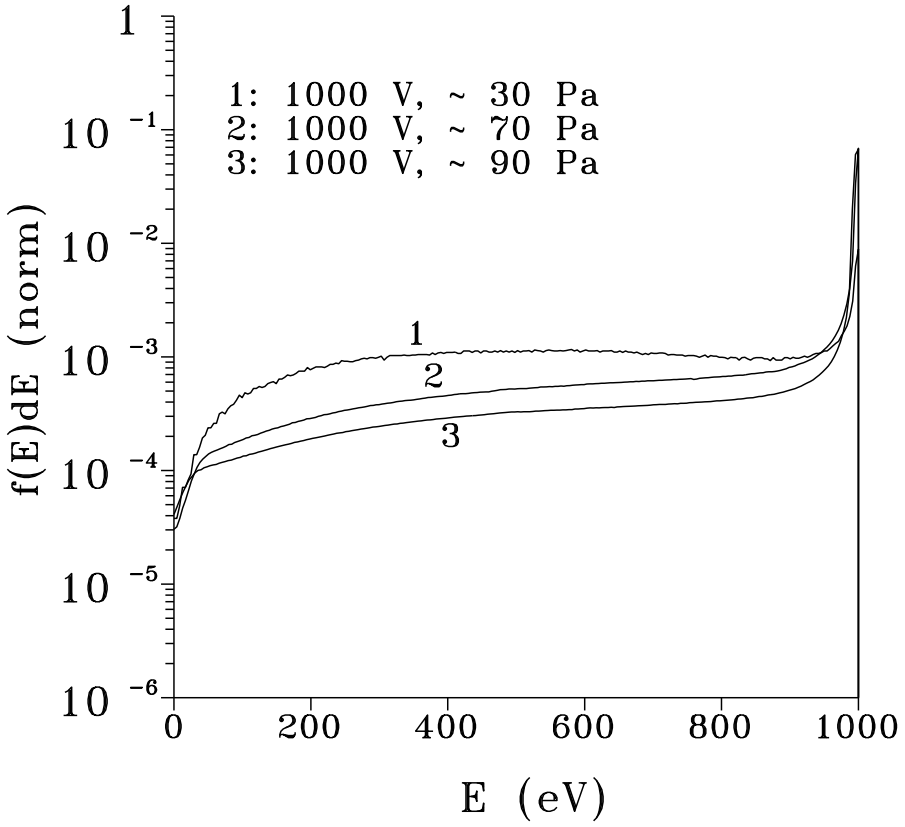
Energies:

Copper ion energy distribution (1000 V, 75 Pa, 3 mA):

Calculated:



Measured (MS):

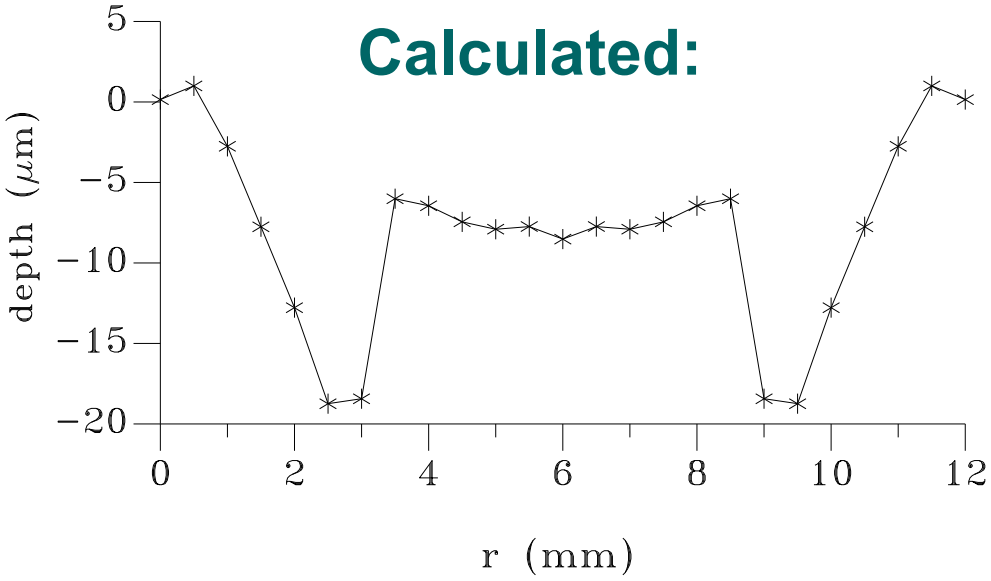


Hybrid model (GD)

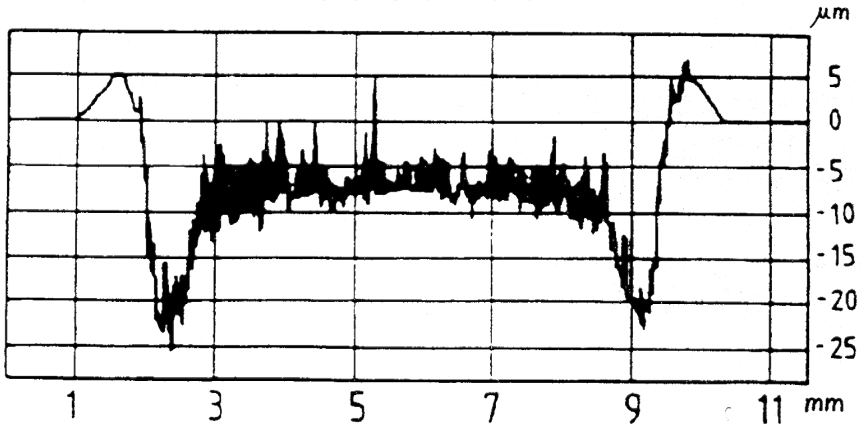
Information about sputtering at the cathode:

Crater profile after 45 min. sputt. (VG9000: 1000 V, 75 Pa, 3 mA):

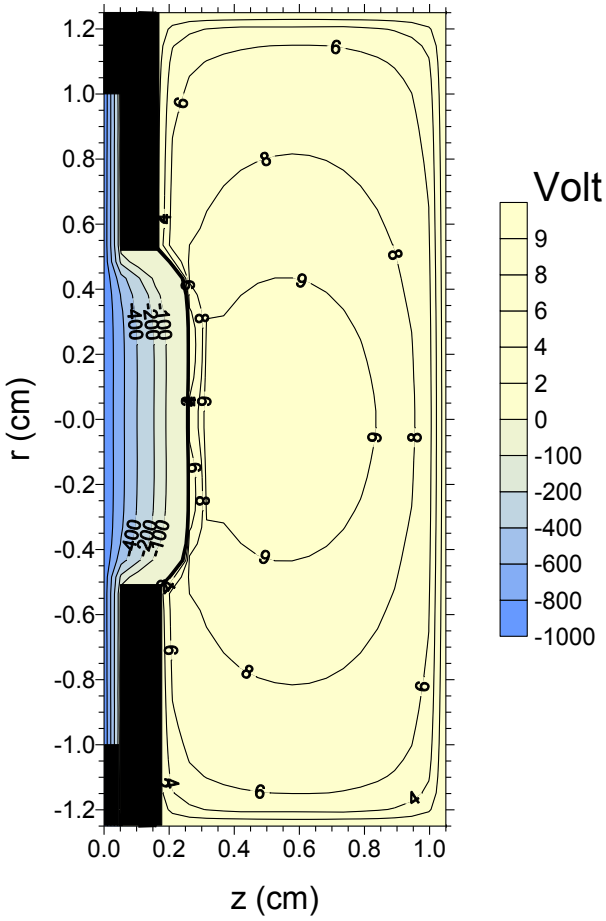
Calculated:



Measured:

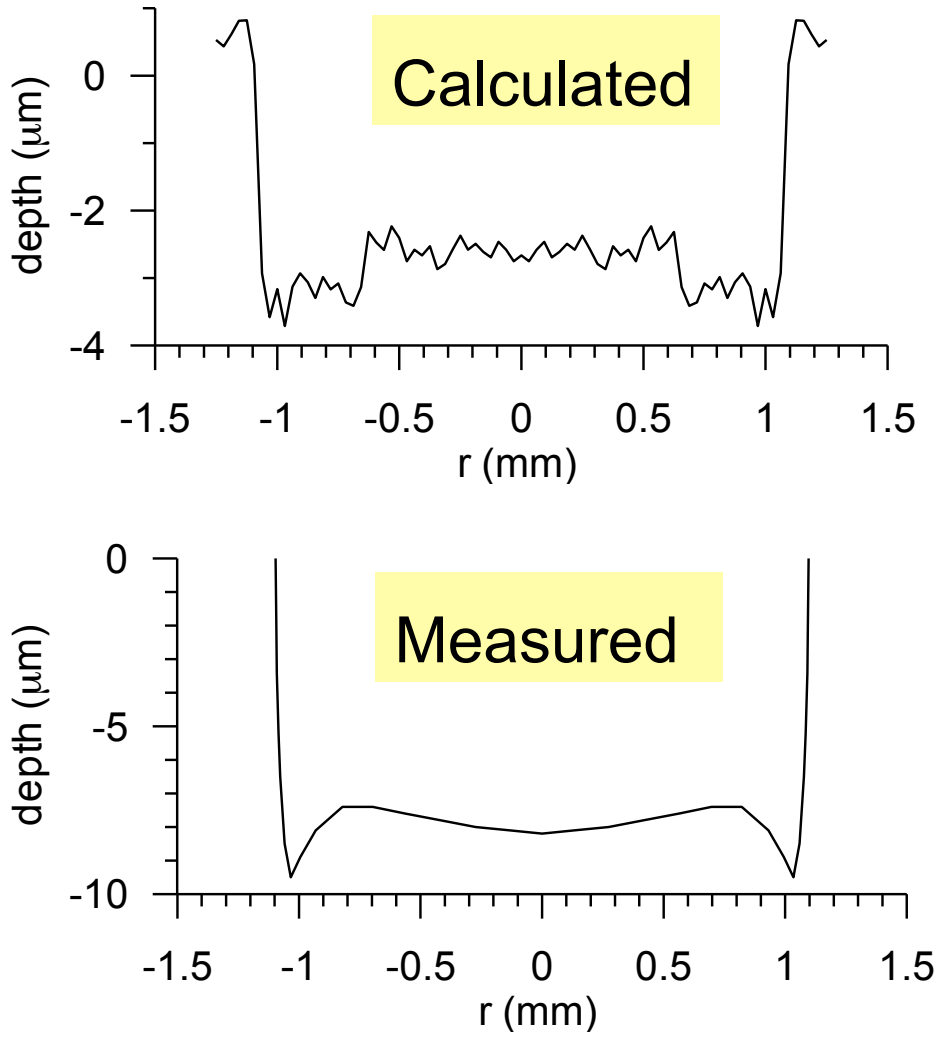


Crater edge effect due to anode front plate:

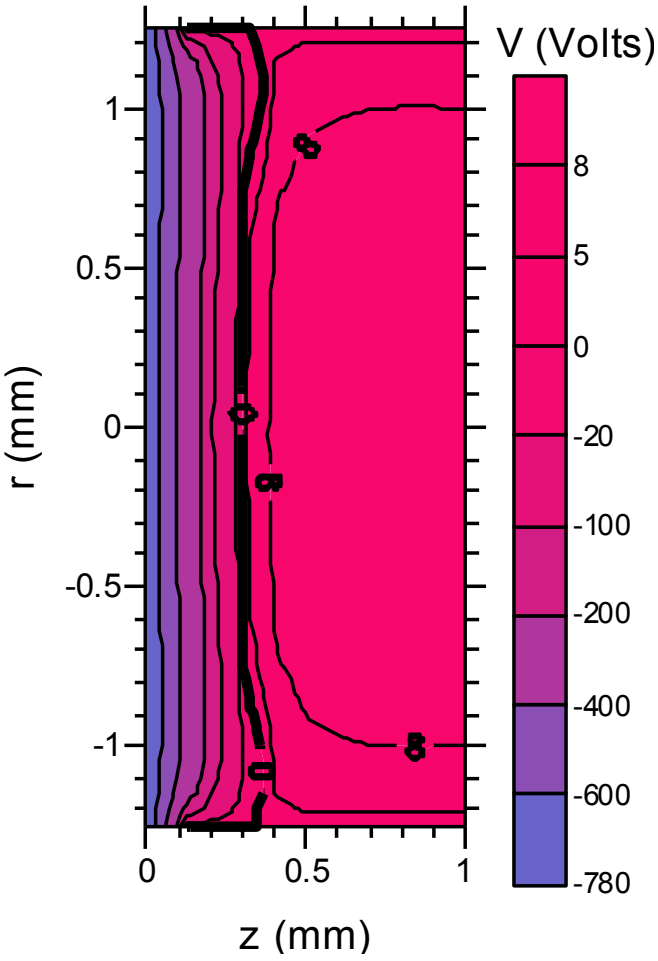


Hybrid model (GD)

Grimm cell



Craters more flat
Because equipot.lines // cathode

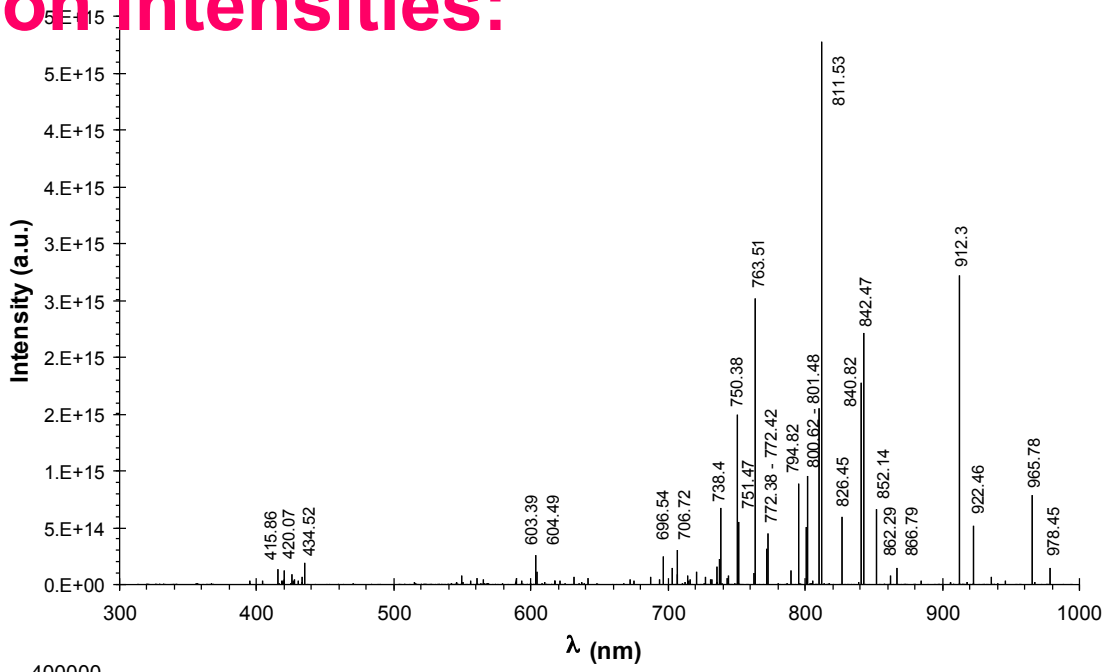


Hybrid model (GD)

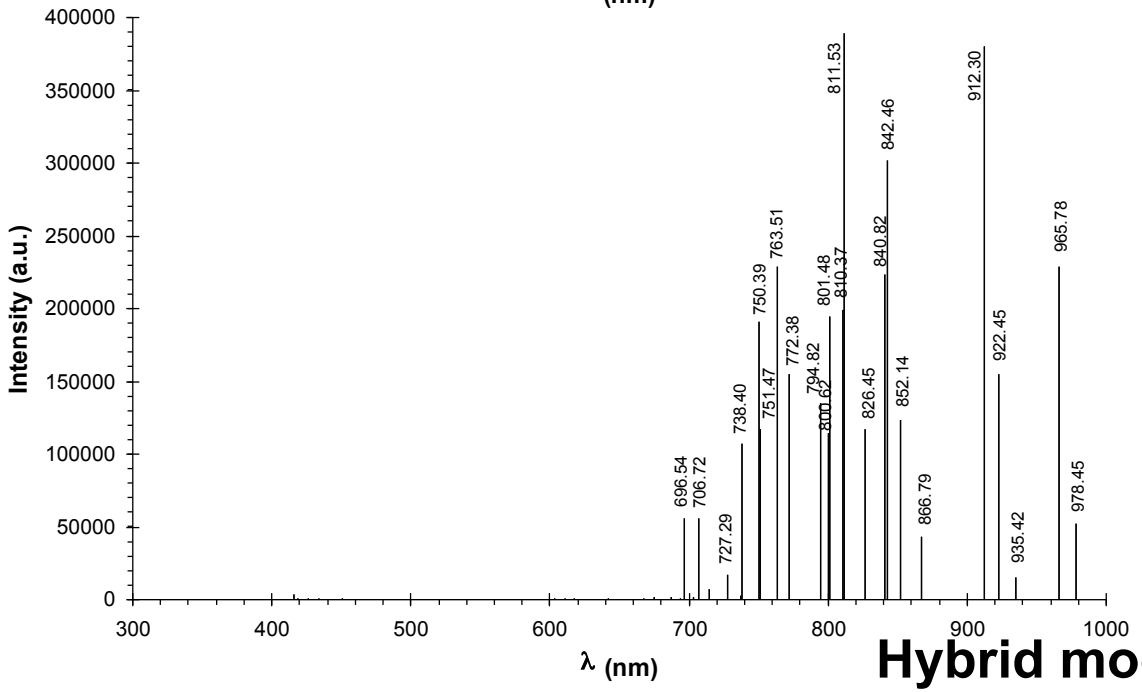
Optical emission intensities:

Ar(I) spectrum

Calculated:



Measured:



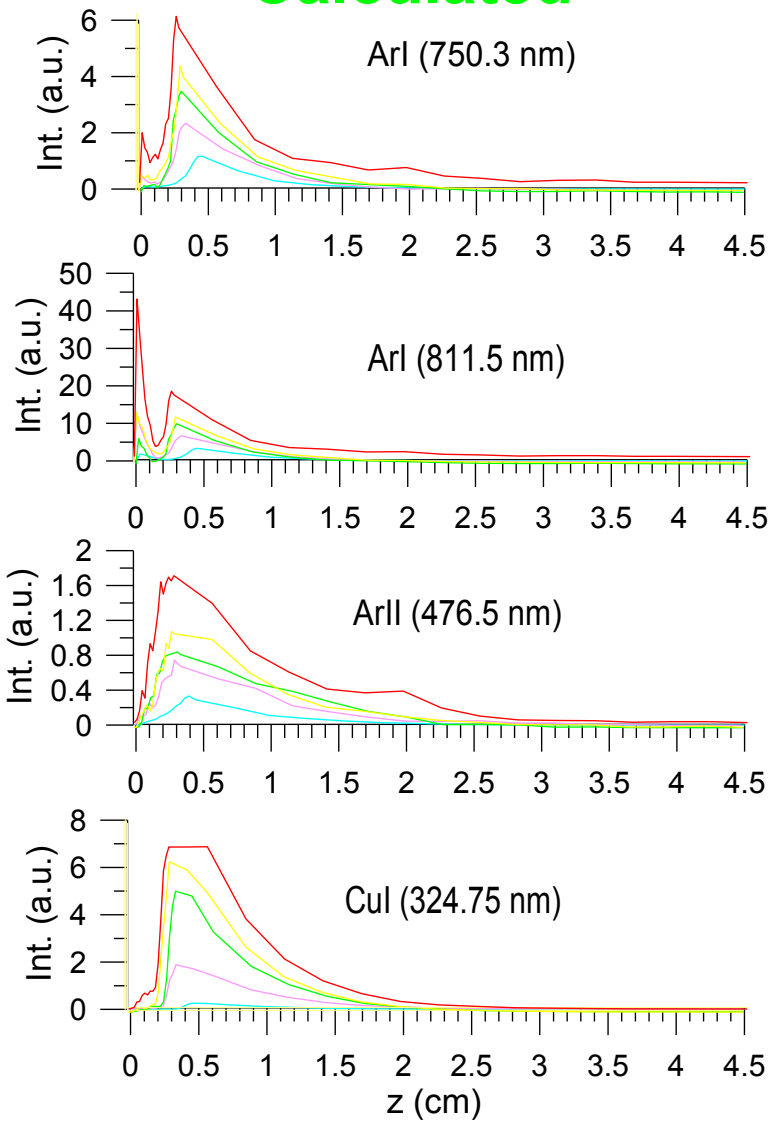
Hybrid model (GD)

Optical emission intensities

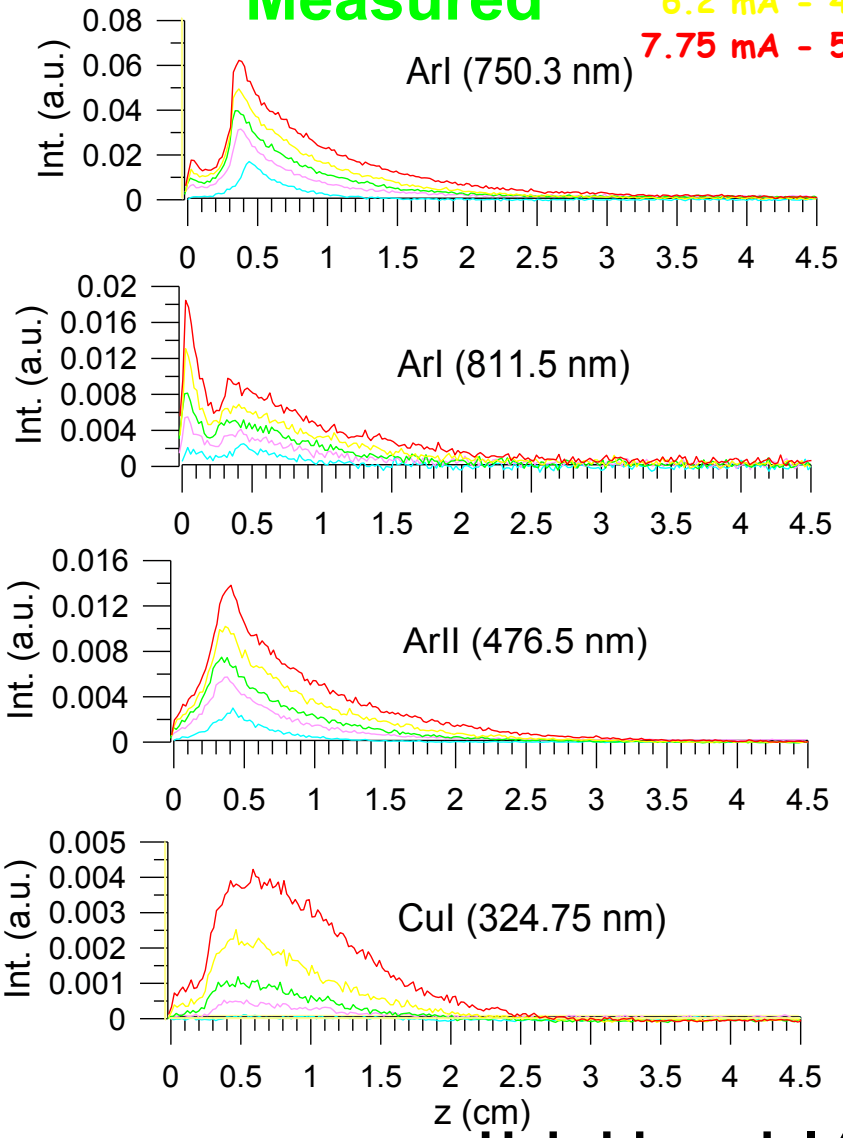
DC: 0.6 Torr

1.55 mA - 417 V
3.1 mA - 455 V
4.65 mA - 480 V
6.2 mA - 495 V
7.75 mA - 505 V

Calculated



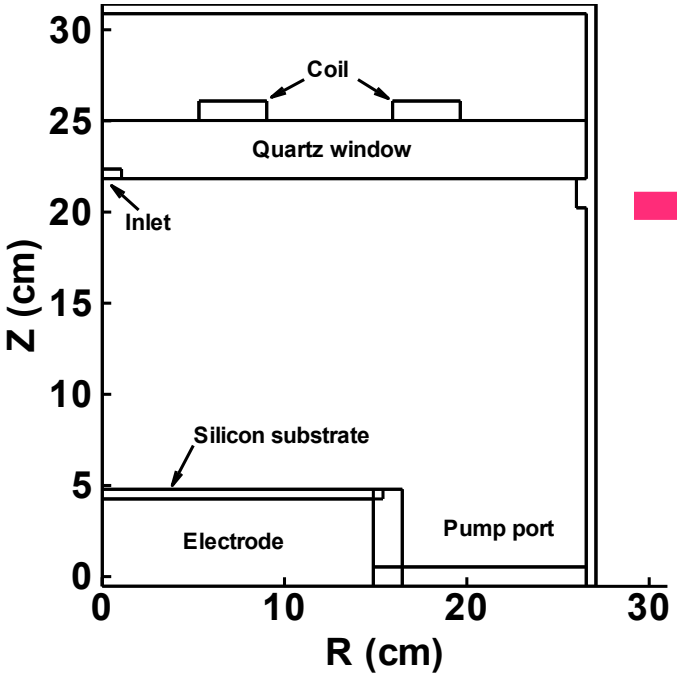
Measured



Hybrid model (GD)

E. Hybrid model for ICP etch reactor

HPEM (M.Kushner, University of Michigan)



Maxwell equations
E, B fields

Monte Carlo
(electrons)
n_e, T_e, *EEDF*, *reaction rates*

Fluid
(heavy particles)
n_i, Γ_i, E_s

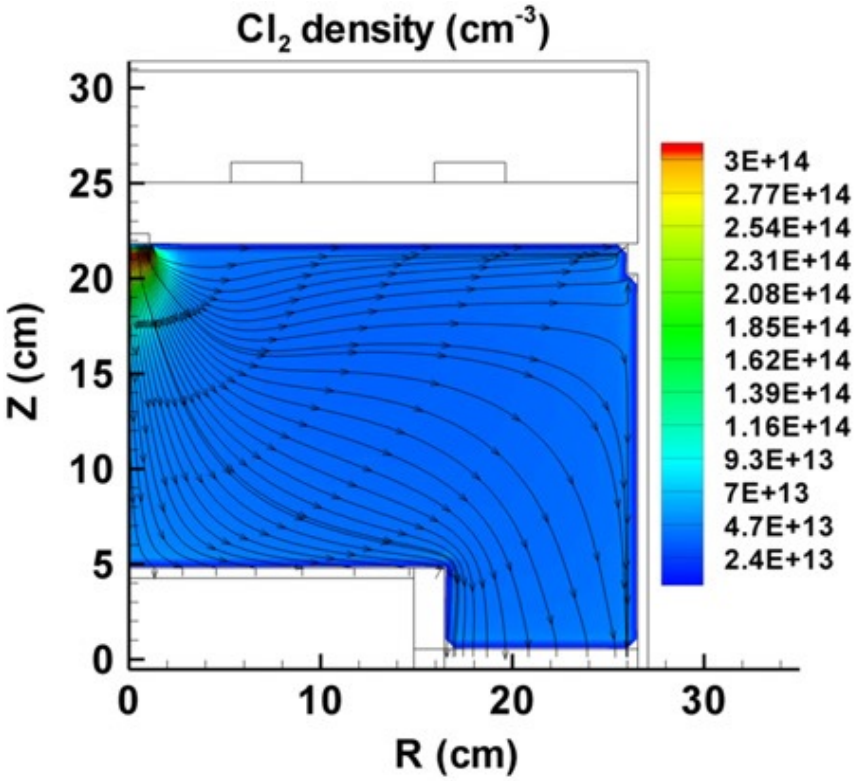
Monte Carlo
(heavy particles)
IEDF, IADF

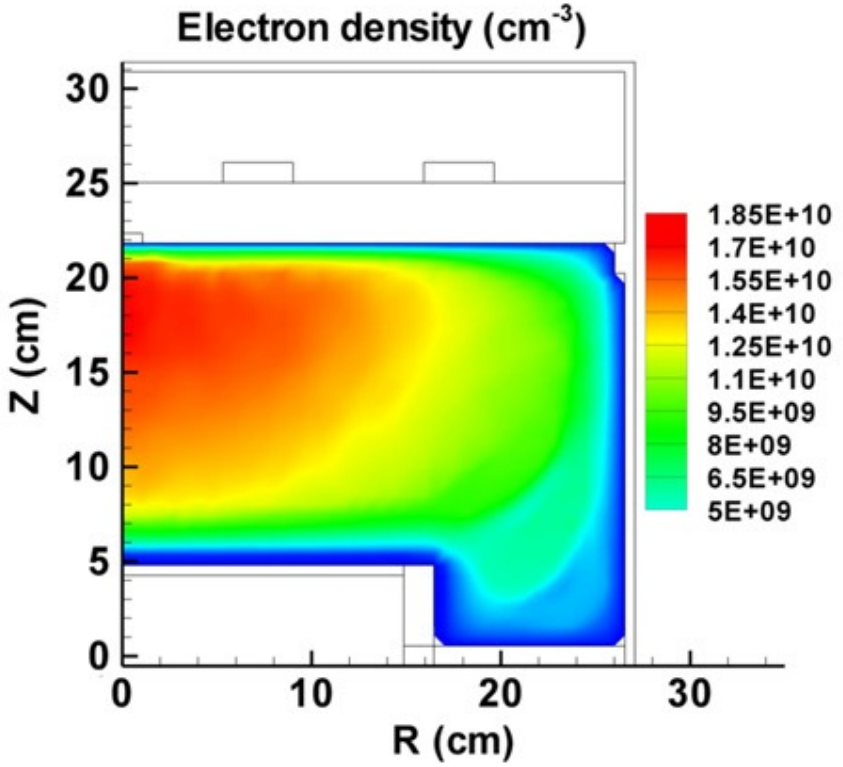
Surface modeling
surface reactions, Γ_{Ri}

Monte Carlo
(heavy particles)
etch profile evolution

Hybrid model (ICP etch reactor)

Calculated species densities (Cl_2, e^-)



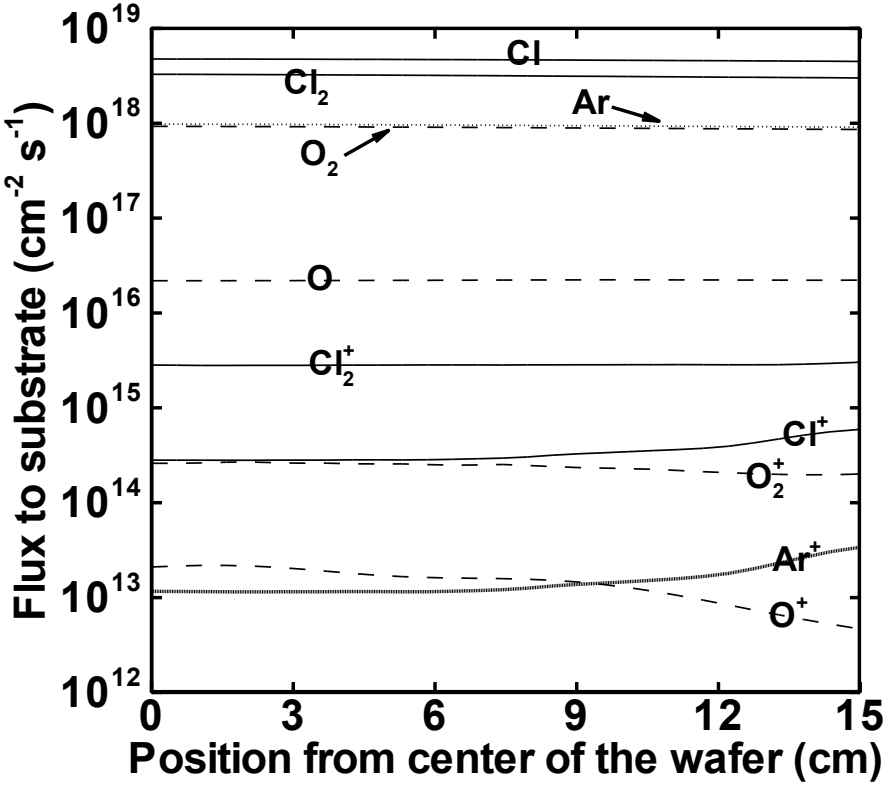


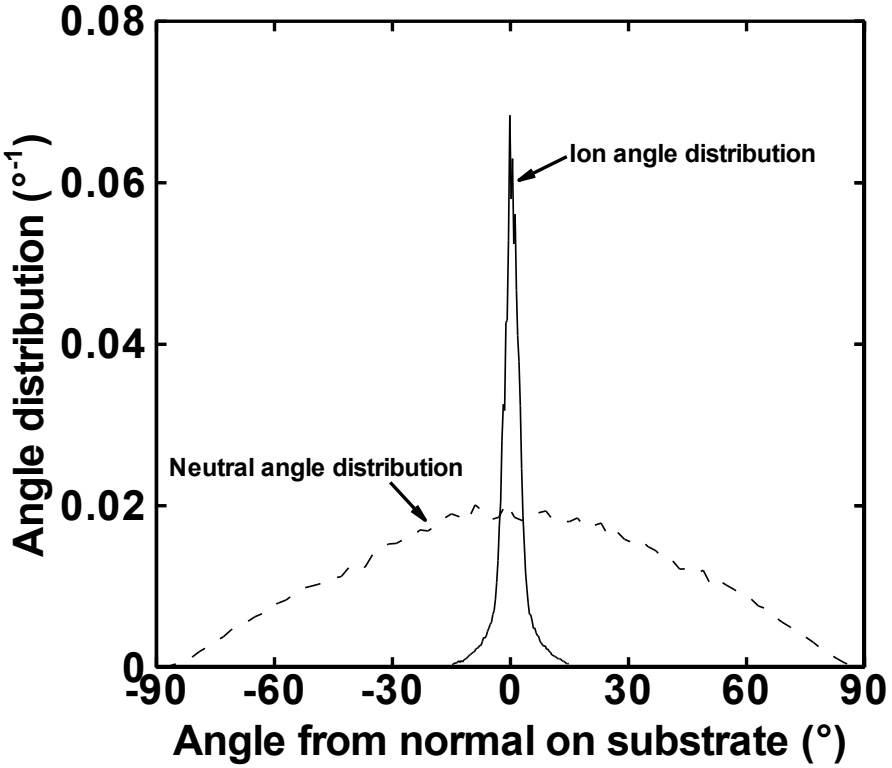
- Cl_2: Maximum near inlet, then depletion (chemical reactions)

  Fairly uniform density profile
- Electrons: Maximum in center/near coil (ioniz.degree ~ 10^{-4})

Hybrid model (ICP etch reactor)

Calculated fluxes + angul.distrib. to wafer

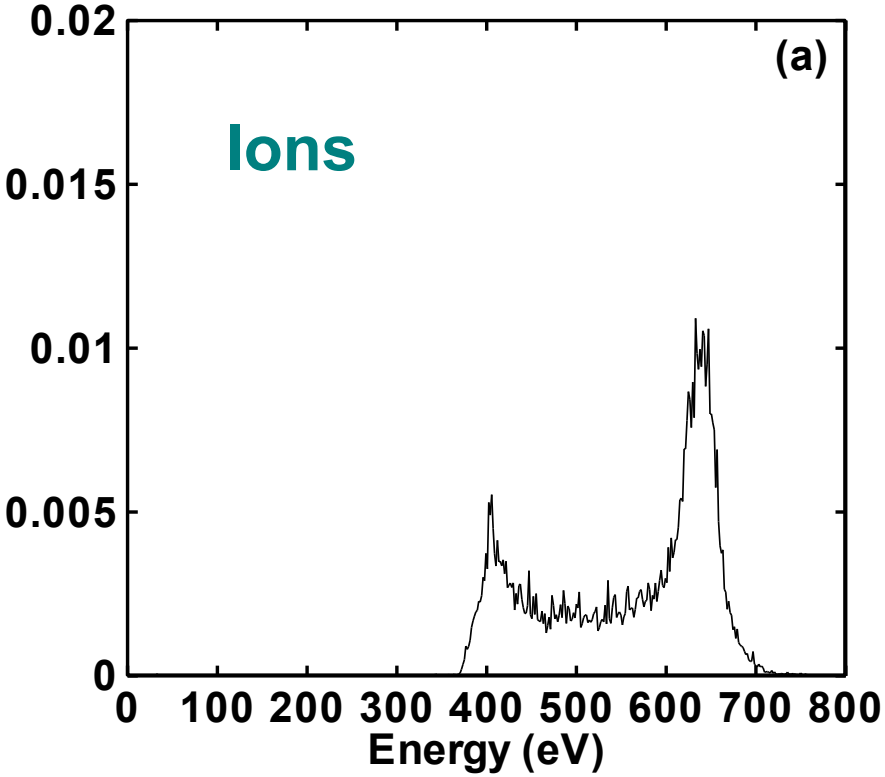


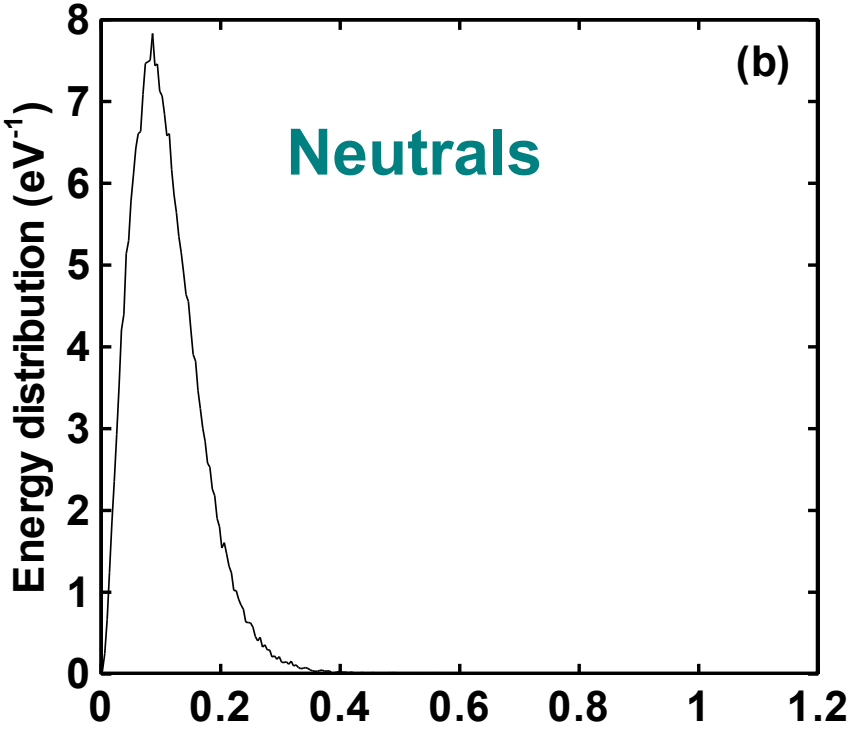


- Ion fluxes ± 1000x lower than neutral fluxes
- Ions: narrow angular distribution (directed by E-field)
- Neutrals: wide angular distribution

Hybrid model (ICP etch reactor)

Calculated energy distributions to wafer





- Ions: bimodal distribution (rf bias at substrate):
  Ions "feel" rf bias amplitude ($time_{sheath}$ < 1 rf cycle)
- Neutrals: Maxwellian distribution at low E

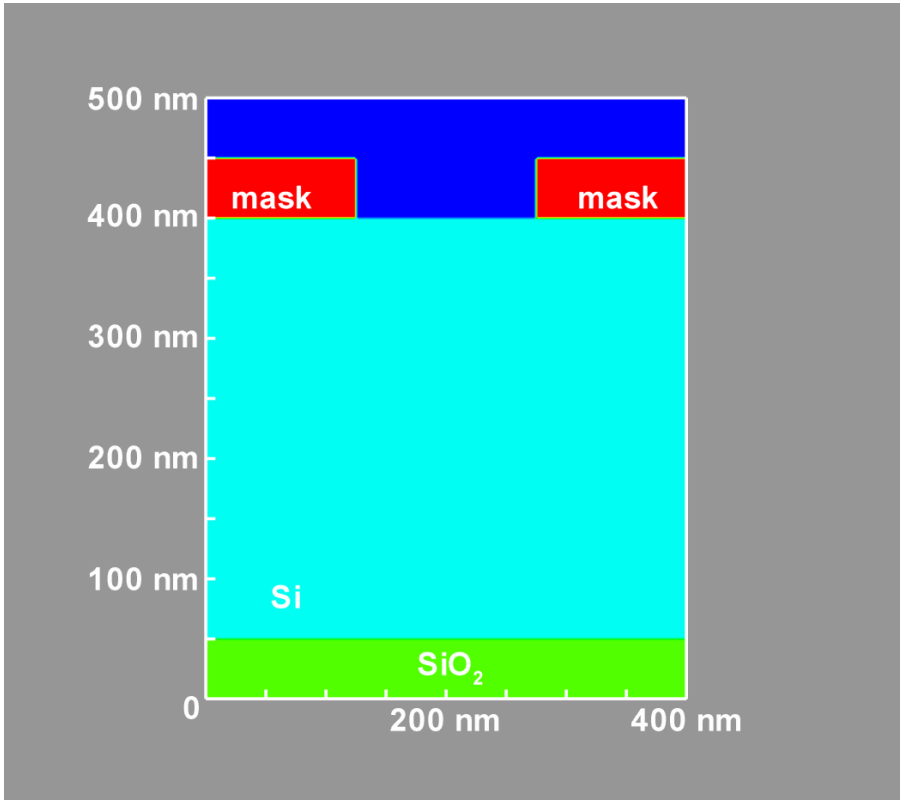
Hybrid model (ICP etch reactor)

Etch profile calculations

Input:

- Fluxes, energy and angular distributions of bombarding species (from plasma model)

- Surface reaction probabilities (etch, oxid, sputt, redepos) of the various species ($Cl^{(+)}$, $Cl_2^{(+)}$, $O^{(+)}$, $O_2^{(+)}$, Ar^+) on the various surface sites (Si, SiCl,$SiCl_2$, $SiCl_3$, SiO, SiO_2)



Hybrid model (ICP etch reactor)

Summary

Plasma modeling :

Most appropriate model depends on application:

- **Fluid (1D or 2D) or (0D) chemical kinetics modeling:**
  - * **Detailed information on plasma chemistry**
  - * **± fast**
- **Particle-in-cell – Monte Carlo simulations:**
  - * **Microscopic – non-equilibrium behavior**
- **Monte Carlo modeling:**
  - * **Faster, but not self-consistent**
- **Hybrid Monte Carlo - fluid simulations:**
  - * **Combination: combines the advantages + eliminates the drawbacks of individual models**
  - * **Extra information (etch profiles, OES,...)**
- **Molecular dynamics simulations: Surface modeling**

End of Presentation

ISPC 2015

22nd International Symposium on Plasma Chemistry

- July 5 – 10, 2015
- University of Antwerp, Belgium