

Technical Plasma: Theoretical side

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- Introduction (some devices and applications)
- Challenges of plasma simulation
- Kinetic Simulation
- Fluid Simulation
- Global models and hybrid models
- Examples & Conclusion





Introduction



Analytical Solution (exact solutuion)

$$\sin(x) = 0.5 \qquad x^2 = 9$$

Numerical solution (approximate solution)

$$\sin(x) + \cos(x) = 0.5$$

Round off errors & Truncation error

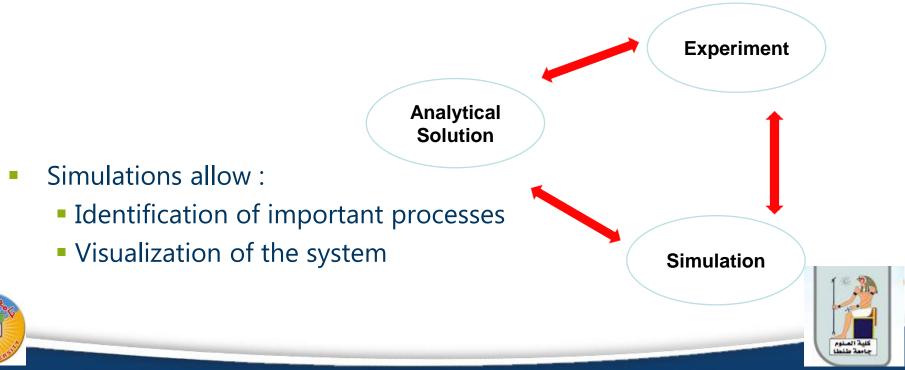
$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!}\dots$$

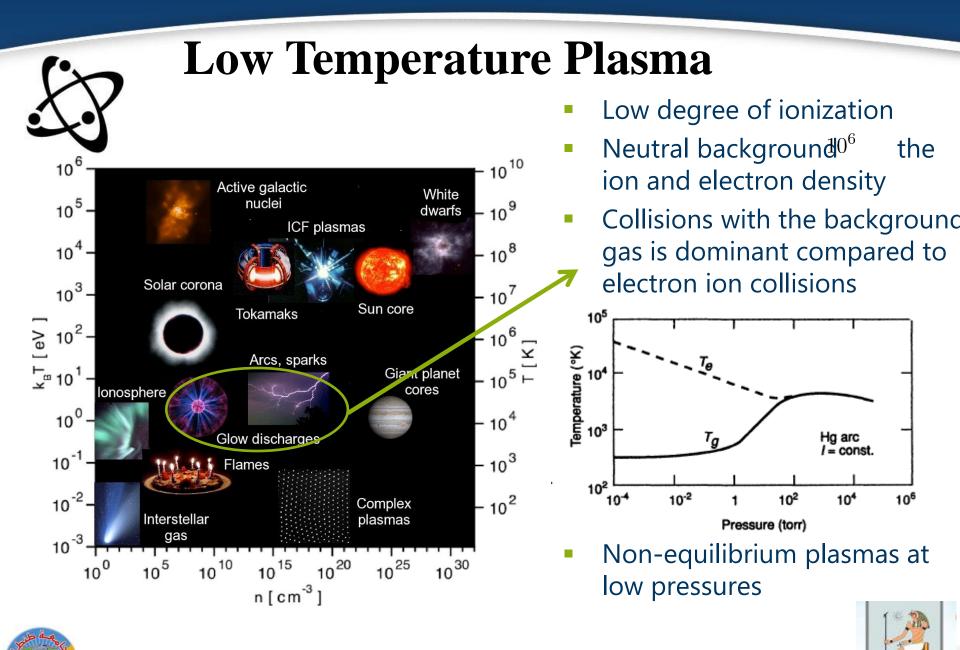


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Do we need simulation?

- Simulations are useful
 - For checking theoretical results
 - For cases wher no theoretical results are available
 - For understanding experimental observations

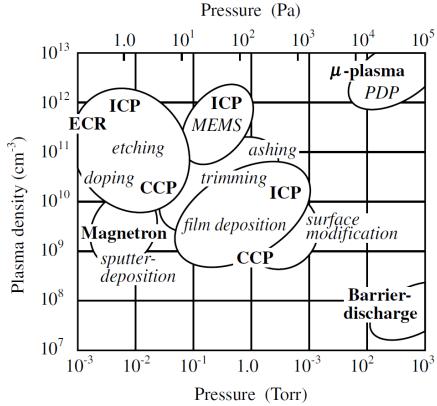




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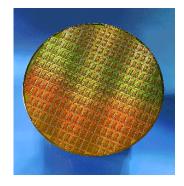
Devices and applications

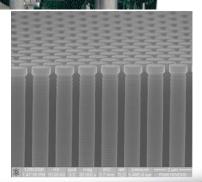


Plasma electronics, Applications in Microelectronic Device Fabrication

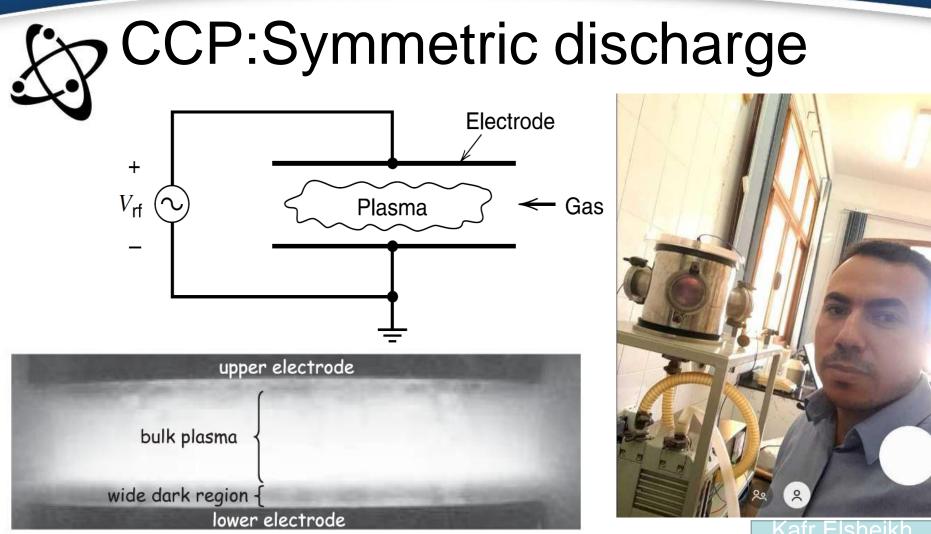
- Capacitive coupled plasma are used in plasma etching and deposition process for production of:
 - Integrated circuits







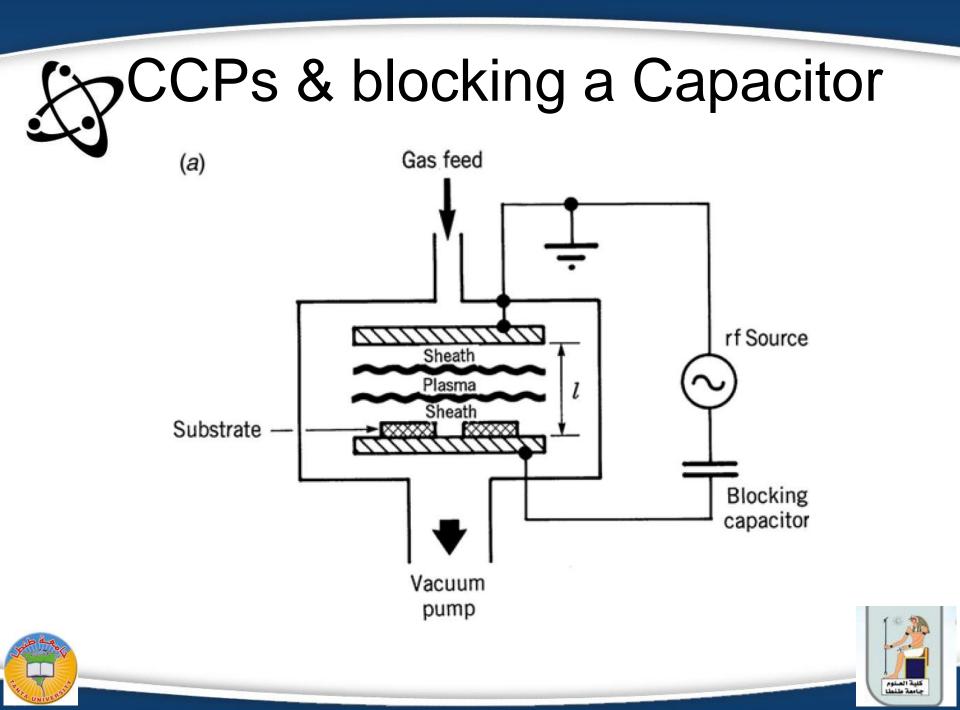






 The ion flux increases and the ion energies decreases by increasing the driving frequency.





Geometrically Asymmetric

- The RF current is constant.
- But the ground electroge
 Area is greater than the powered electrode area.

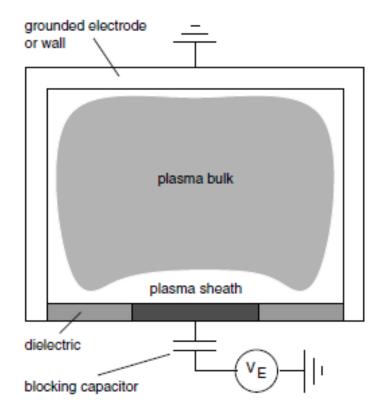
$$J_{\rm g} = I_{\rm rf}/A_g$$

 $J_{\rm p} = I_{\rm rf}/A_p$

$$J_{\rm p} \gg J_{\rm g}$$

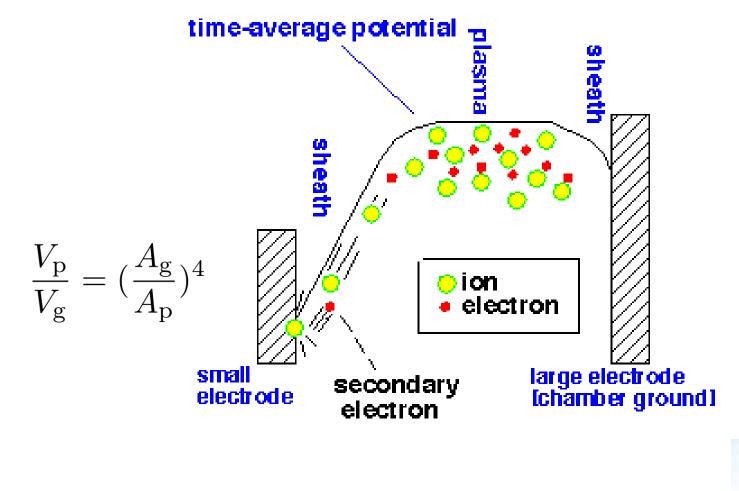
 The blocking capacitor blocks DC currents:

$$\frac{V_{\rm p}}{V_{\rm g}} = (\frac{A_{\rm g}}{A_{\rm p}})^4$$







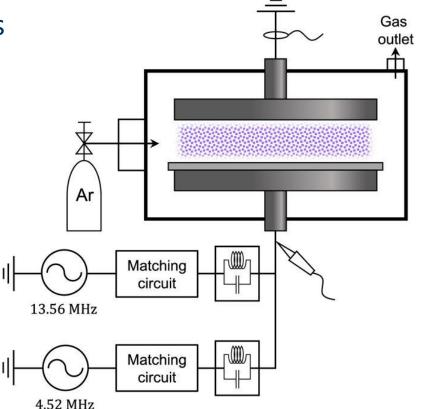






Electrically Asymmetric

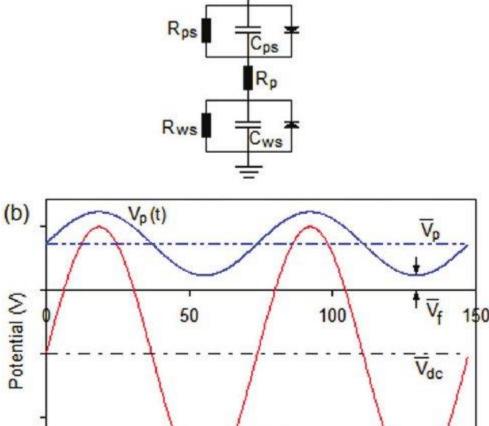
- The high frequency controls the ion plasma bulk (ion flux).
- The lower frequency controls the plasma sheath voltage.
- The phase shift between the two sources controls also the sheath potential.



 The independent control is not always perfect.



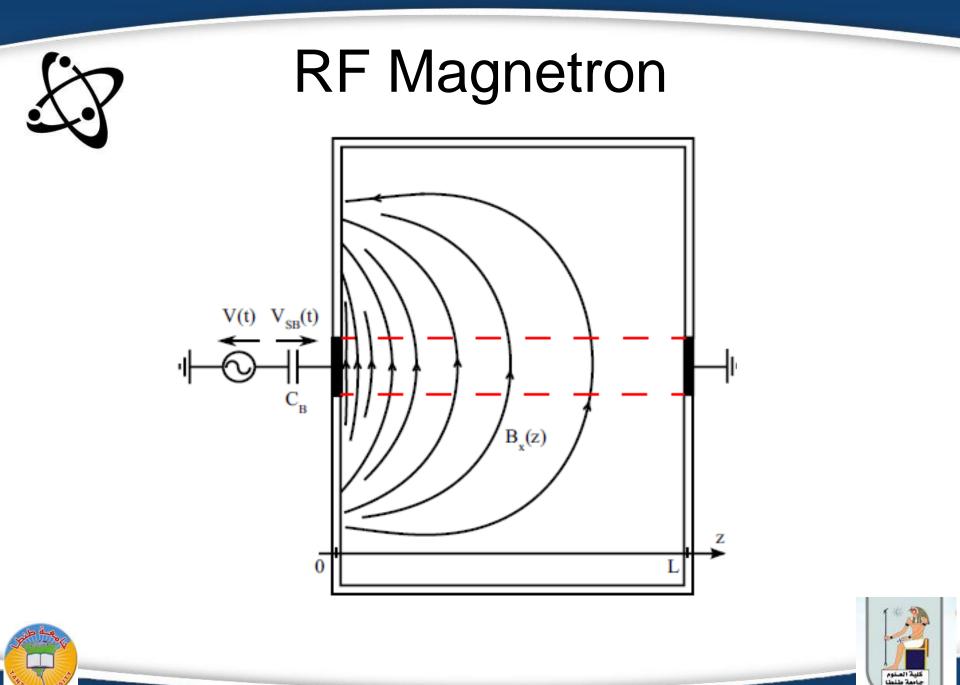
Electrically asymmetric CCP discharges

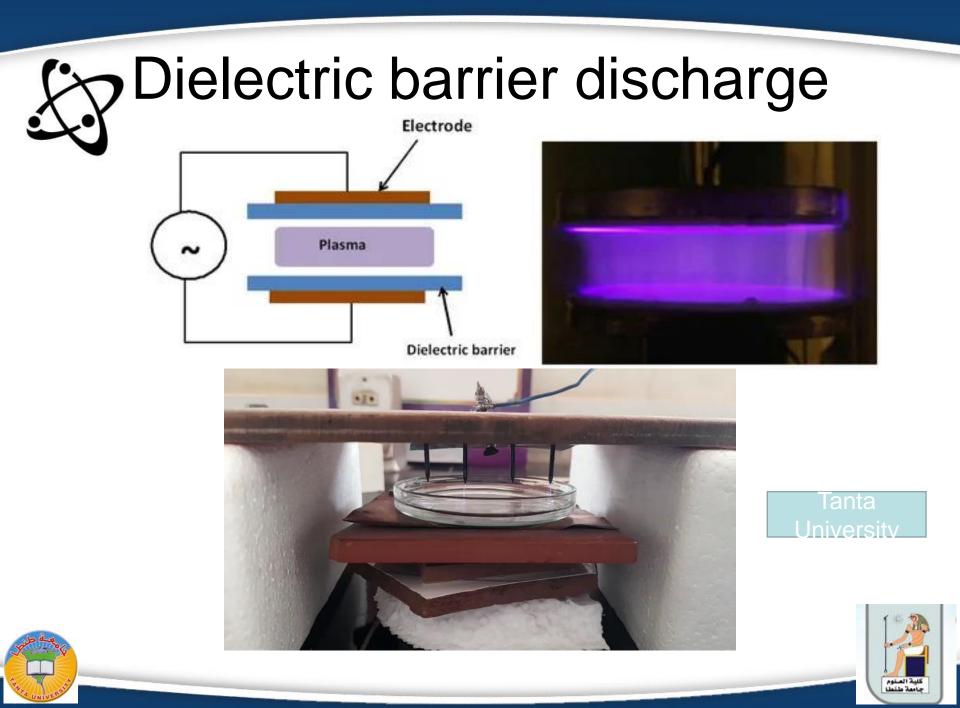


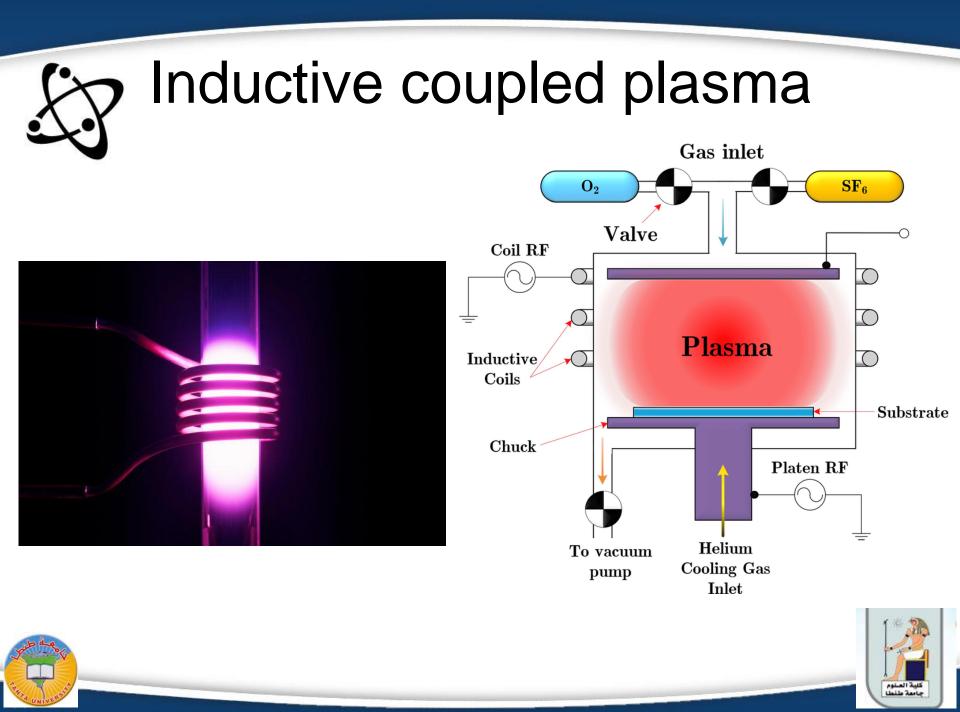
J. Schulze et al, Ruhr University Bochum

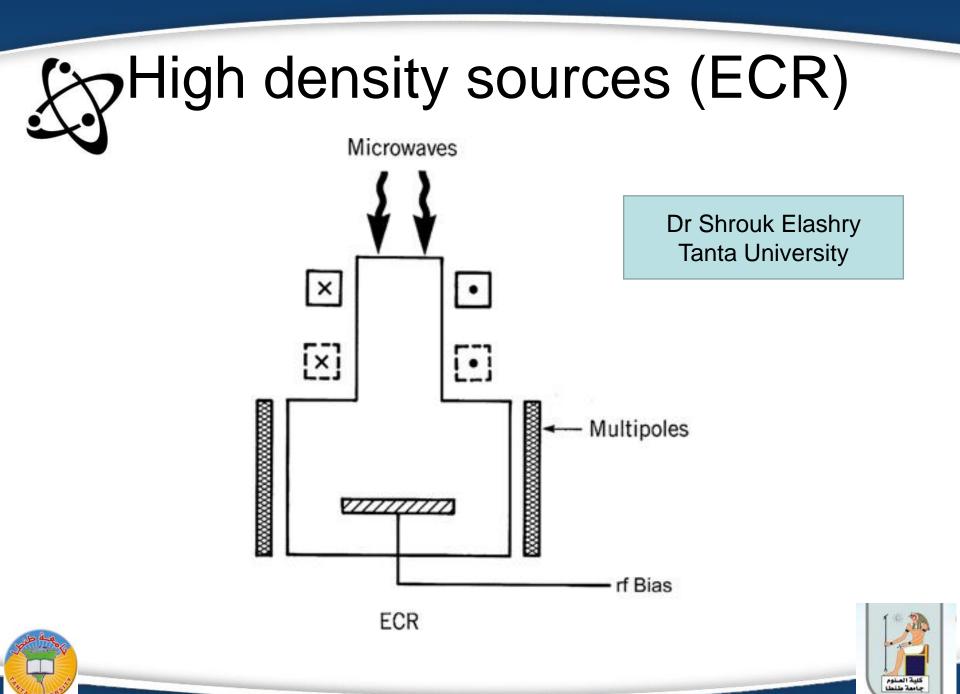
Vrf (t)















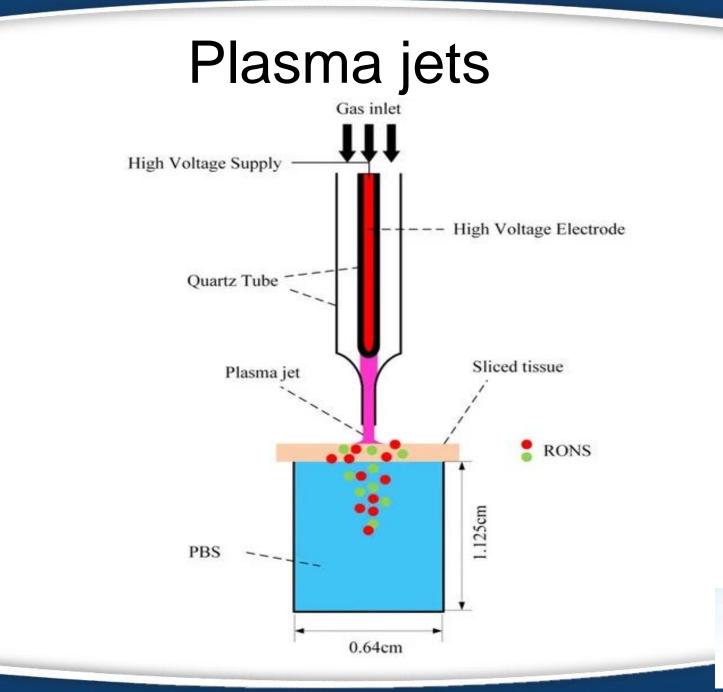
Plasma jets





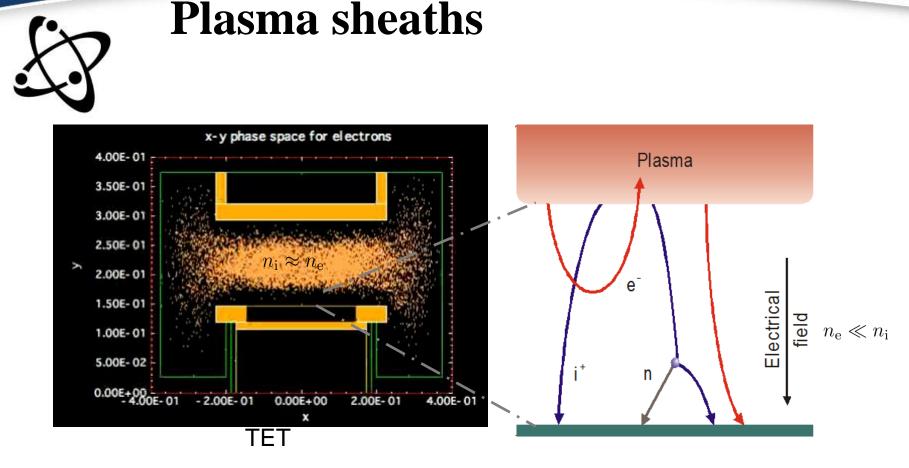


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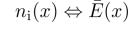




- RF sheaths:
 - High frequency regime
 - Intermediate frequency regime $^{\omega_{\mathrm{RF}}pprox\omega_{\mathrm{pi}}}$
 - Low frequency regime

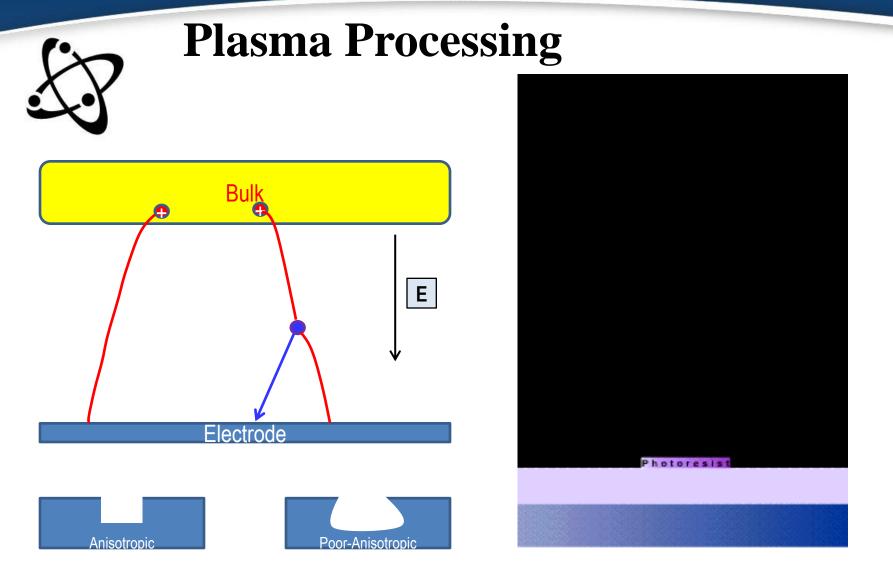
 $\omega_{
m RF}\ll\omega_{
m pi}$

 $\omega_{
m RF}\gg\omega_{
m pi}$



 $n_{\rm i}(x,t) \Leftrightarrow E(x,t)$











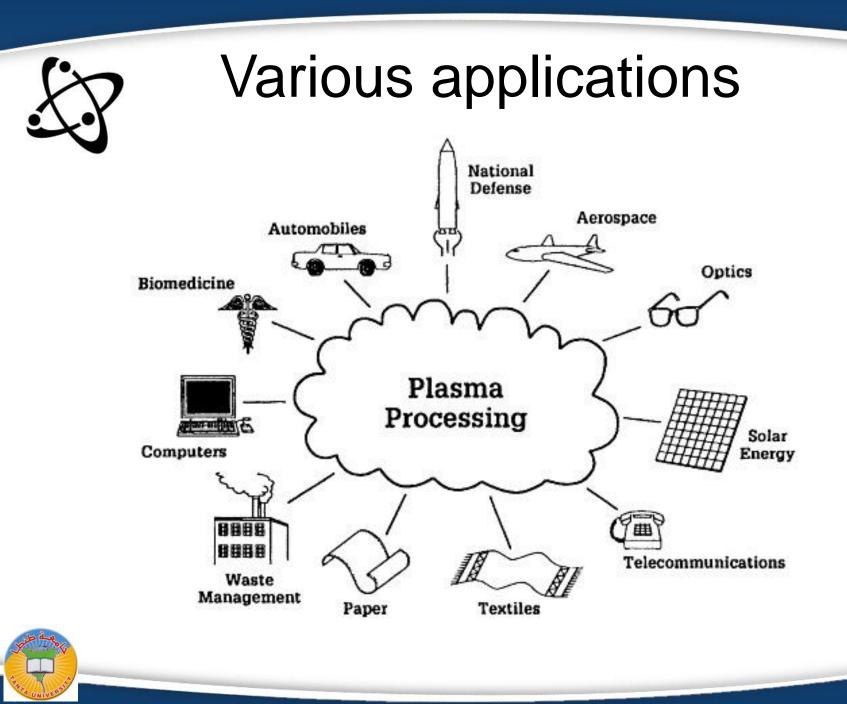
Plasma Chemistry

Dissociation of feedstock gas into active neutral free radicals: $e^- + CF_4 \rightarrow CF_3 + F + e^-$

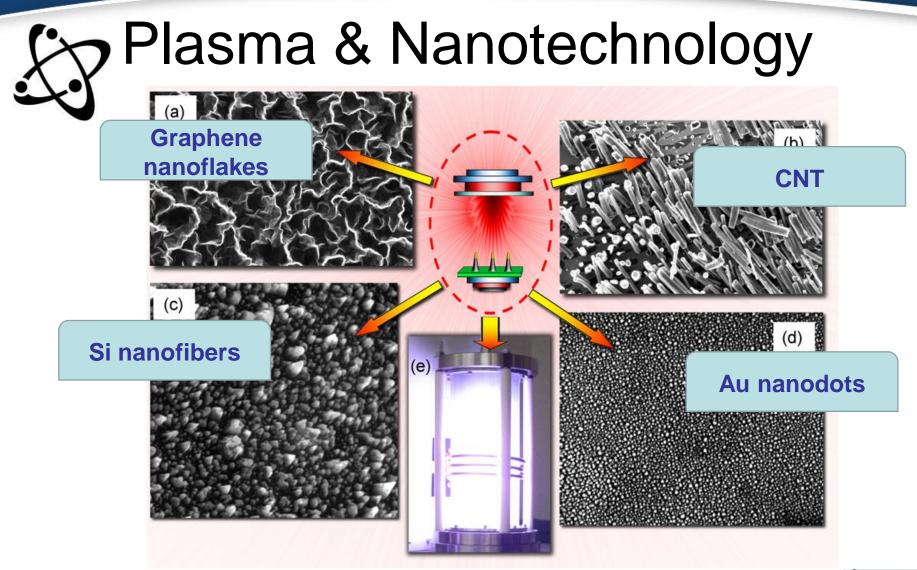
> $e^- + CF_4 \rightarrow CF_2 + 2F + e^$ $e^- + CF_4 \rightarrow CF + F_2 + F + e^-$

• Dissociation of the free radicals $e^- + CF_3 \rightarrow CF_2 + F + e^$ $e^- + CF_2 \rightarrow CF + F + e^-$



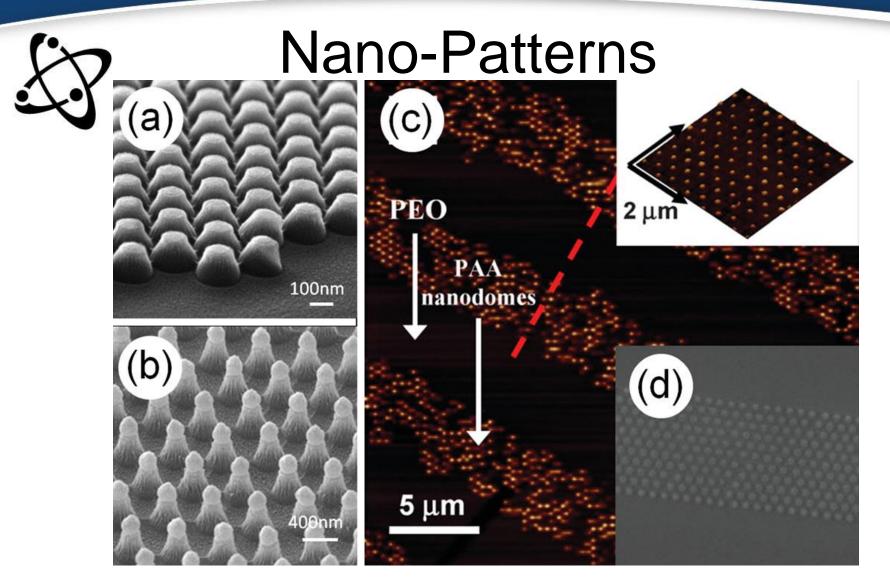


















Challenges of plasma simulation

The most accurate method is to solve the equation of motion of each particle in the plasma.

$$m\frac{d\vec{v}_k}{dt} = e\vec{E}_k + e\vec{v}_k \times \vec{B}_k$$

- No. of particles is very very large $n = 10^9 10^{13} \mathrm{cm}^{-3}$
- Maxwell equations
 $\vec{\nabla} \cdot \vec{D} = \rho_v$ $\vec{\nabla} \cdot \vec{B} = 0$ $\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$ $\vec{\nabla} \cdot \vec{B} = 0$ $\vec{\nabla} \times \vec{H} = \vec{J} + \epsilon \frac{\partial \vec{E}}{\partial t}$
- The collective behaviour and the huge number of particles make the solution impossible in such way.





The distribution function

The distribution function gives the number of particles per unit volume (particles density) with speed v as a function of time. v_y

$$v_z = \int f(r, v, t) d^3 v$$

• The kinetic equation is an integro- deffrential equations in 7 parameters $\frac{Df}{Dt} = \frac{\partial f}{\partial t} + \vec{v} \cdot \vec{\nabla}_r f + \vec{a} \cdot \vec{\nabla}_v f = \text{collision terms}$

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Macroscopic description

- Instead of known the physical parameters of each particle, one can calculate the average values for the whole plasma system.
- Average plasma density

$$\bar{n} = \int f(r, v, t) d^3 v$$

Average speed

Kinetic energy

$$\bar{v} = \int v f(r, v, t) d^3 v / \bar{n}$$

$$\bar{E}_k = \int \frac{1}{2} m v^2 f(r, v, t) d^3 v / \bar{n}$$

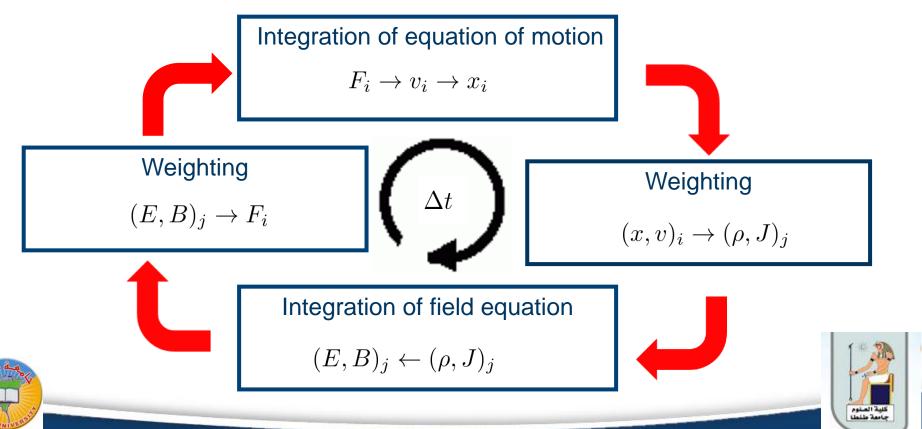
• Avergaes over Boltzman equation

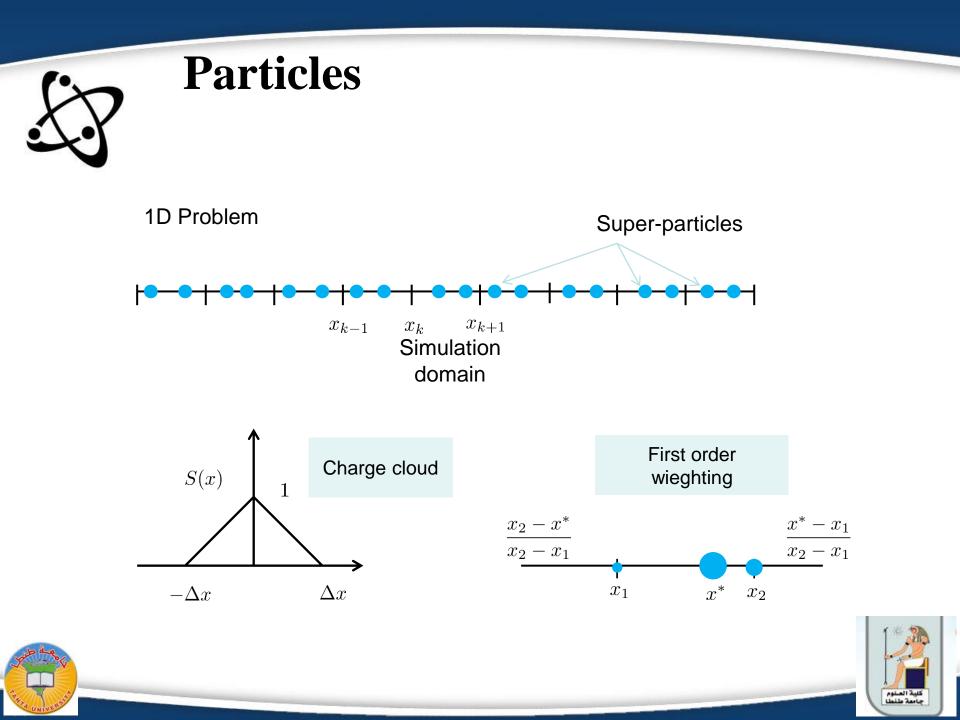
$$mv^{q}\left(\frac{\partial f}{\partial t} + \vec{v} \cdot \vec{\nabla}_{r}f + \vec{a} \cdot \vec{\nabla}_{v}f\right) = \text{collision terms}$$
$$q = 0, 1, 2, 3, \dots$$

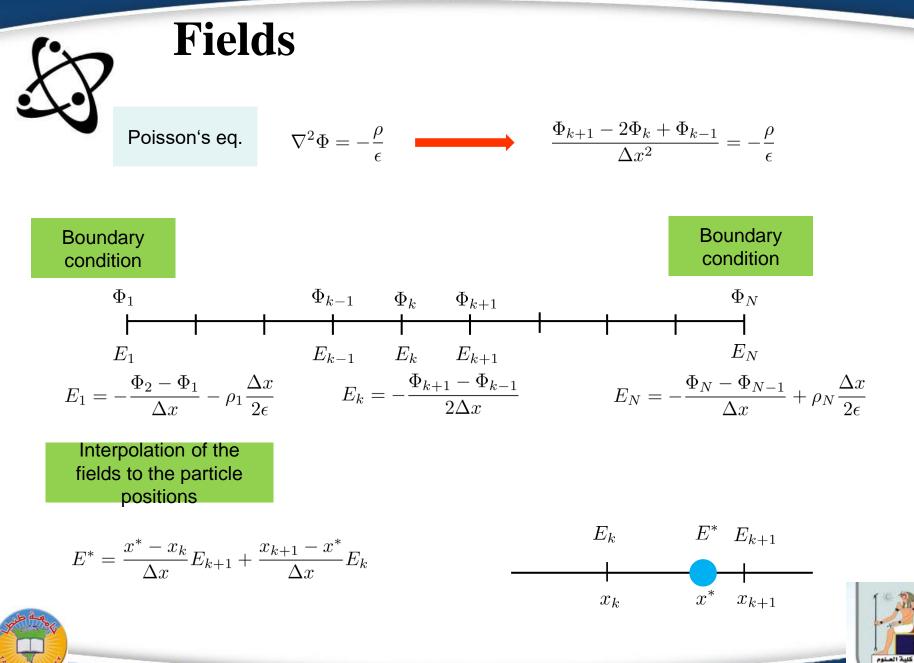


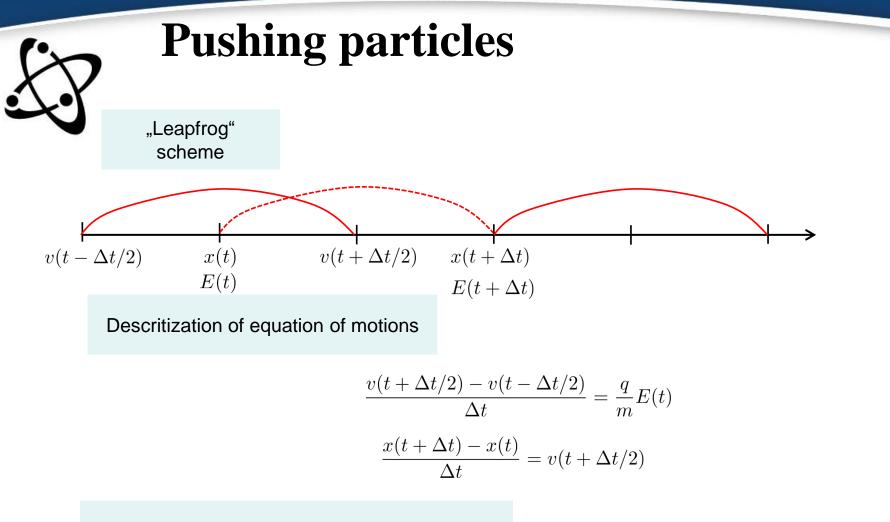
Kinetic Description

- Kinetic means "of or relating to motion".
 - It is impractical to solve the equation of motion of all plasma particles.
 - Boltzman equation is an integro-differential equation.
- Particle-in-Cell : Super particle⁶ 10^9 real particles.









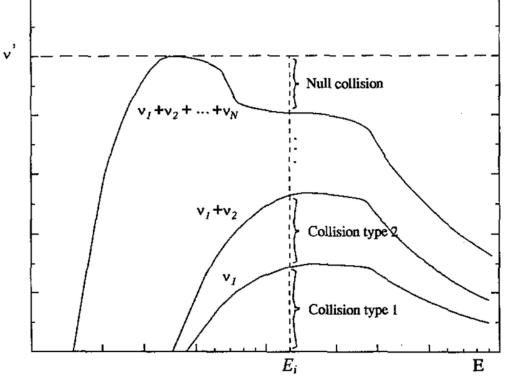
Monte-Carlo Scheme is required for collisions



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Monte Carlo: null collision method

- Many collisions take place: impact ionization, charge exchange hard-shere, ...
- Let the probability of them P1,P2,P3,P4, ...
- Claculate the total probabilities PT
- Calculate relative probabilities
 P1/PT, P2/PT, P3/PT, P4/PT,



- Generate a random number between [0,1]
- if P1/PT = < The randum number < (P1+P2)/PT</p>
- Event 1 takes place
- If not



(P1+ P2)/PT= < The randum number < (P1+P2+P3)/PT



Challenges of PIC simulation

- Numerical instabilities:
 - Accuracy criterion $\omega_p \Delta t \leq 0.2$
 - Courant criterion $v_{\max}\Delta t \leq \Delta x$
 - The computational grid has to resolve the Debye lenge $\lambda x \leq \lambda_D$
- In order to have a good statistics, a resonable high number of particles per Debye lenght must be used $\underline{1}$
- Keep the probability for collisions small

$$P_{\rm coll} = 1 - e^{-\nu t} \le 0.1$$

- Alternatives:
 - Implicit schems
 - Parrallilization





Fluid Models

 Continuity, momentum, and energy equations are closed with Poisson's equation



$$\begin{aligned} \frac{\partial n_{\rm e,i,m}}{\partial t} + \vec{\nabla} \cdot \vec{\Gamma}_{\rm e,i,m} &= G_{\rm e,i,m} - L_{\rm e,i,m}, \\ \vec{\Gamma}_{\rm e,i,m} &= \operatorname{sign}(q_{\rm e,i,m}) \ n_{\rm e,i,m} \ \mu_{\rm e,i,m} \ \vec{E} - D_{\rm e,i,m} \vec{\nabla} n_{\rm e,i,m}, \\ \frac{\partial n_{\rm e} T_{\rm e}}{\partial t} &= -\vec{\nabla} \cdot \left(\frac{5}{3} T_{\rm e} \vec{\Gamma}_{\rm e} - \frac{5}{3} n_{\rm e} D_{\rm e} \vec{\nabla} T_{\rm e}\right) - e \vec{\Gamma}_{\rm e} \cdot \vec{E} - n_{\rm e} n_{\rm G} k_{\rm loss}, \end{aligned}$$

and

$$T_{\rm i} = T_{\rm m} = 0.026 \ eV.$$





Fluid Models

Ar atomic processes considered in the

simulation		
Equation of	Rate of Reaction Coefficient	
Reaction		
e + Ar → Ar+ + 2e	impact- ionization	K _{ei} = 1.253 × 10 ⁻⁷ exp(-18.618/T _e) cm³/s
$e + Ar \rightarrow Ar^* + e$	collisional- excitation	Kex = 3.712 × 10 ⁻⁸ exp(-15.06/T _e) cm ³ /s
$e + Ar^* \rightarrow Ar^+ + 2e$	impact- ionization	K _{mi} = 2.05 × 10 ⁻⁷ exp(-4.95/T _e) cm³/s
e + Ar [*] → Ar + e	collisional- deexcitation	K _{em} = 1.818 × 10 ⁻⁹ exp(-2.14/T _e) cm³/s
e + Ar [*] → Ar ^r + e	radiative- deexcitation	K _r = 2 × 10 ⁻⁷ cm³/s
Ar* + Ar* → Ar+ + Ar + e	collisional- ionization	$K_{mm} = 6.2 \times 10^{-10} \text{ cm}^3/\text{s}$
Ar* + Ar → 2Ar	collisional- deexcitation	K _{2q} = 3.0 × 10 ⁻¹⁵ cm ³ /s
$Ar^* + 2Ar \rightarrow Ar + Ar_2$	attachment	K _{3q} = 1.1 × 10 ⁻³¹ cm ⁶ /s



Main reactions and the corresponding rate coefficients in the Ar/CF₄ discharge plasma.

м.,	Reaction equation	Reaction rate coefficient
	$CF_3^- + Ar^+ \rightarrow CF_3 + Ar$	$1 \times 10^{-7} \text{ cm}^3 \text{ s}^{-1}$
	$F^- + Ar^+ \rightarrow F + Ar$ $CF_4 + Ar^+ \rightarrow CF_3^+ + F + Ar$	$1 \times 10^{-7} \text{ cm}^3 \text{ s}^{-1}$ 9.58 × 10 ⁻¹⁰ cm ³ s ⁻¹
	$\operatorname{Ar} + \operatorname{CF}_3^+ \to \operatorname{CF}_3^+ \operatorname{Ar}^+$	$1 \times 10^{-9} \mathrm{cm^3 s^{-1}}$

Chengjie Bai et al 2018 J. Phys. D: Appl. Phys. 51 255201

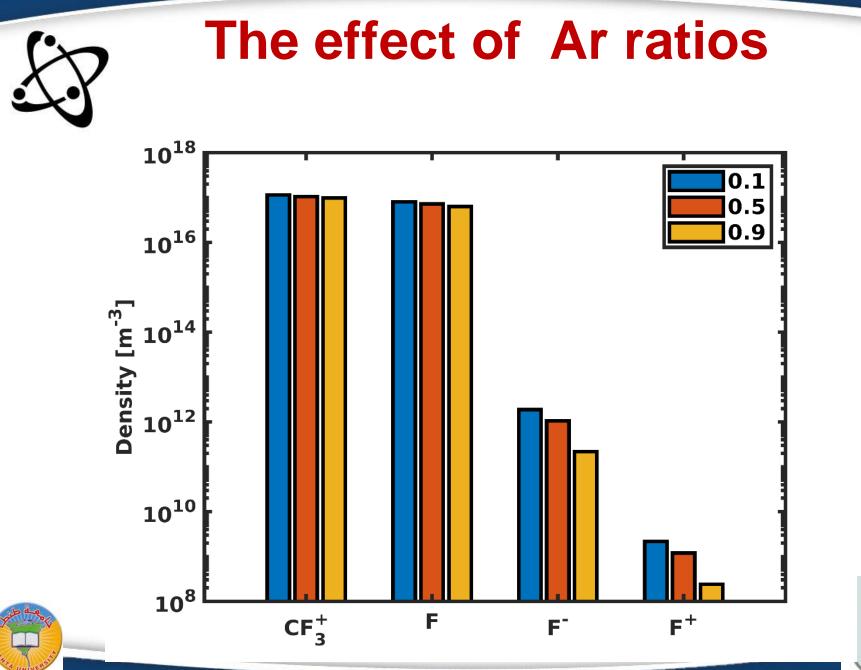


Main reactions and the corresponding reaction rate coefficients in the CF₄ discharge plasma.

	Reaction equation
	$CF_4 + e \rightarrow CF_4^+ + 2e$
[•.	$CF_3 + e \rightarrow CF_3^+ + 2e$
	$F + e \rightarrow F^+ + 2e$
X V	$CF_4 + e \rightarrow CF_4^*(12.5 eV)$
· \ .•Y	$CF_4 + e \rightarrow CF_4^*(8 eV) +$
	$CF_4 + e \rightarrow CF_4(V13) +$
	$CF_4 + e \rightarrow CF_4(V24) +$
	$CF_4 + e \rightarrow CF_3^+ + F +$
	$CF_4 + e \rightarrow CF_2^+ + F_2 +$
	$CF_4 + e \rightarrow CF^+ + F_2 +$
	$CF_4 + e \rightarrow CF_3 + F^+ +$
	$CF_4 + e \rightarrow CF_3 + F + e$
	$CF_4 + e \rightarrow CF_2 + 2F +$
	$CF_3 + F^- \rightarrow CF_4 + e$
	$CF_2 + F^- \rightarrow CF_3 + e$
	$CF + F^- \rightarrow CF_2 + e$
	$CF_3 + F \rightarrow CF_4$
	$CF_2 + F \rightarrow CF_3$
	$CF+F \rightarrow CF_2$
	$CF_3^- + CF_3^+ \rightarrow 2CF_3$
	$F^- + CF_3^+ \rightarrow F + CF_3$
	$F^- + CF_2^+ \rightarrow F + CF_2$

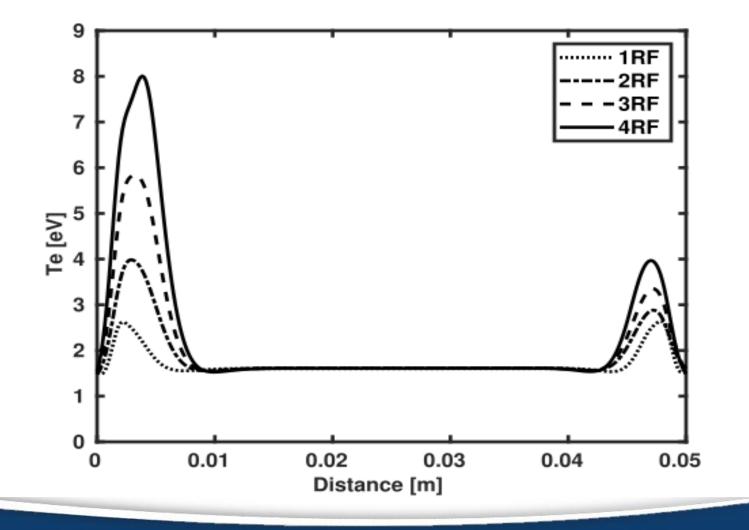
Reaction equation	Reaction rate coefficient	
$CF_4 + e \rightarrow CF_4^+ + 2e$	Calculated by BOLSIG+	
$CF_3 + e \rightarrow CF_3^+ + 2e$	$1.4 \times 10^{-11} (11605 \times T_e)^{0.6481} \exp(-9.8/T_e) \text{ cm}^3 \text{ s}^{-1}$	
$F + e \rightarrow F^+ + 2e$	$7.489 \times 10^{-13} (11605 \times T_e)^{0.8595} \exp(-17.6/T_e) \text{ cm}^3 \text{ s}^{-1}$	
$CF_4 + e \rightarrow CF_4^*(12.5 \text{ eV}) + e$	Calculated by BOLSIG+	
$CF_4 + e \rightarrow CF_4^*(8 eV) + e$	Calculated by BOLSIG+	
$CF_4 + e \rightarrow CF_4(V13) + e$	Calculated by BOLSIG+	
$CF_4 + e \rightarrow CF_4(V24) + e$	Calculated by BOLSIG+	
$CF_4 + e \rightarrow CF_3^+ + F + 2e$	$1.159 \times 10^{-11} (11605 \times T_e)^{0.7645} \exp(-17.2/T_e) \text{ cm}^3 \text{ s}^{-1}$	
$CF_4 + e \rightarrow CF_2^+ + F_2 + 2e$	$2.886 \times 10^{-11} (11605 \times T_e)^{0.5108} \exp(-22.8/T_e) \text{ cm}^3 \text{ s}^{-1}$	
$CF_4 + e \rightarrow CF^+ + F_2 + F + 2e$	$2.296 \times 10^{-14} (11605 \times T_e)^{1.09} \exp(-27.0/T_e) \text{ cm}^3 \text{ s}^{-1}$	
$CF_4 + e \rightarrow CF_3 + F^+ + 2e$	$1.482 \times 10^{-13} (11605 \times T_e)^{0.9375} \exp(-34.7/T_e) \text{ cm}^3 \text{ s}^{-1}$	
$CF_4 + e \rightarrow CF_3 + F + e$	$2 \times 10^{-9} \exp(-13/T_e) \text{ cm}^3 \text{ s}^{-1}$	
$CF_4 + e \rightarrow CF_2 + 2F + e$	$5 \times 10^{-9} \exp(-13/T_e) \text{ cm}^3 \text{ s}^{-1}$	
$CF_3 + F^- \rightarrow CF_4 + e$	$5 \times 10^{-10} \mathrm{cm^3 s^{-1}}$	
$CF_2 + F^- \rightarrow CF_3 + e$	$5 \times 10^{-10} \mathrm{cm^3 s^{-1}}$	
$CF + F^- \rightarrow CF_2 + e$	$5 \times 10^{-10} \mathrm{cm^3 s^{-1}}$	
$CF_3 + F \rightarrow CF_4$	$2 \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$	
$CF_2 + F \rightarrow CF_3$	$1.3 \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$	
$CF + F \rightarrow CF_2$	$5.2 \times 10^{-15} \mathrm{cm^3 s^{-1}}$	
$CF_3^- + CF_3^+ \rightarrow 2CF_3$	$4 \times 10^{-7} \mathrm{cm^3 s^{-1}}$	
$F^- + CF_3^+ \rightarrow F + CF_3$	$4 \times 10^{-7} \mathrm{cm}^3 \mathrm{s}^{-1}$	
$F^- + CF_2^+ \rightarrow F + CF_2$	$1 \times 10^{-7} T_g^{-0.5} \text{ cm}^3 \text{ s}^{-1}$	
$F^- + CF^+ \rightarrow F + CF$	$1 \times 10^{-7} T_g^{-0.5} \text{ cm}^3 \text{ s}^{-1}$	
$F^- + F^+ \rightarrow F_2$	$4 \times 10^{-7} T_{\rm g}^{-0.5} {\rm cm}^3 {\rm s}^{-1}$	
$CF_2^+ + e \rightarrow CF + F$	$4 \times 10^{-8} \text{ cm}^3 \text{ s}^{-1}$	
$CF^{+} + e \rightarrow C + F$	$4 \times 10^{-8} \mathrm{cm}^3 \mathrm{s}^{-1}$	
$CF_3^+ + e \rightarrow CF_3$	$9.6 \times 10^{-7} \mathrm{cm^3 s^{-1}}$	
$F^+ + e \rightarrow F$	$4 \times 10^{-8} \text{ cm}^3 \text{ s}^{-1}$	
$CF_4^+ \rightarrow CF_3^+ + F$	$3.3 \times 10^5 \mathrm{s}^{-1}$	
$CF_4 + e \rightarrow CF_3 + F^-$	$4.8 \times 10^{-12} \text{ cm}^3 \text{ s}^{-1}$	
$CF_4 + e \rightarrow CF_3^- + F$	$3.28 \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$	
$CF_2 + F_2 \rightarrow CF_3 + F$	$4.56 \times 10^{-13} \text{ cm}^3 \text{ s}^{-1}$	
$CF_3 + F_2 \rightarrow CF_4 + F$	$1.88 \times 10^{-14} \text{ cm}^3 \text{ s}^{-1}$	
$CF_3^- + F \rightarrow CF_3 + F^-$	$5 \times 10^{-8} \text{ cm}^3 \text{ s}^{-1}$	1 1 🖓 🎆
$2CF_4^*(12.5 \text{ eV}) \rightarrow 2CF_4$	$4.9 \times 10^{-4} \mathrm{cm^3 s^{-1}}$	and a second
$2CF_4^*(8 \text{ eV}) \rightarrow 2CF_4$	$4.9 \times 10^{-4} \mathrm{cm^3 s^{-1}}$	
$2CF_4(V13) \rightarrow 2CF_4$	$4.9 \times 10^{-4} \mathrm{cm^3 s^{-1}}$	All Sull
$2CF_4(V24) \rightarrow 2CF_4$	$4.9 \times 10^{-4} \mathrm{cm^3 s^{-1}}$	كلية العنوم



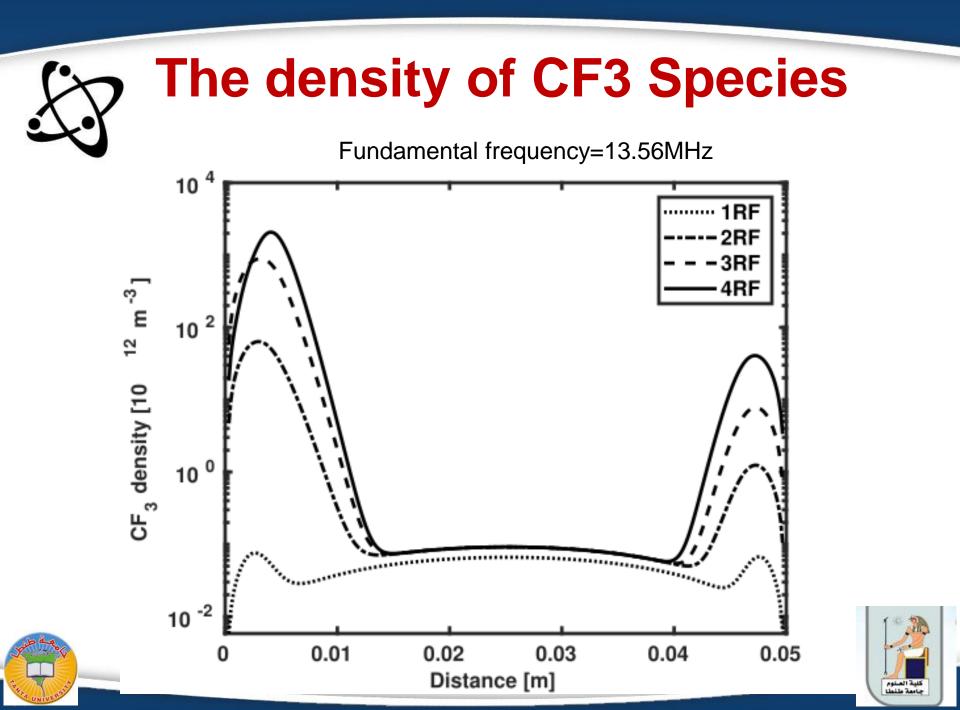




The electron temperature Fundamental frequency=13.56MHz



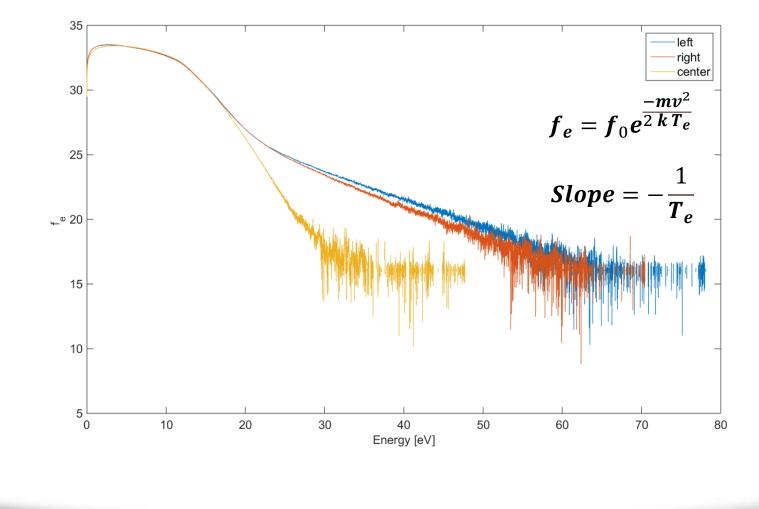
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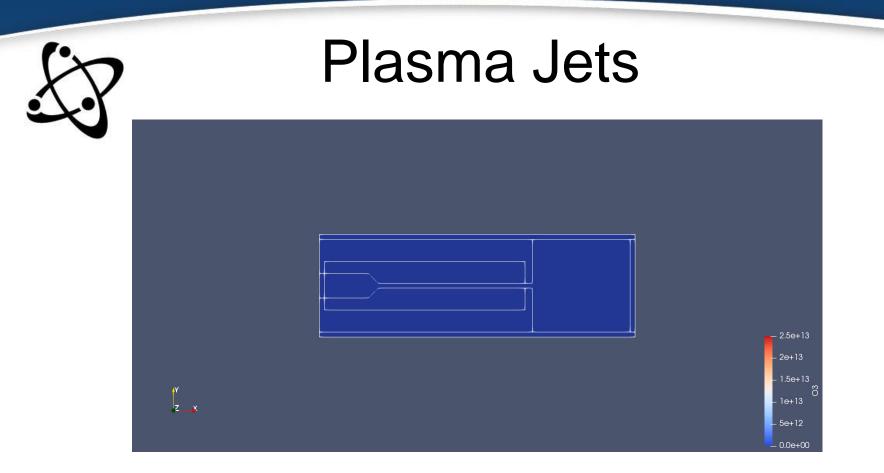
Kinetic Confirmation-Symmetric discharge 35 left right 30 center 25 $f_e = f_0 e^{\frac{-mv^2}{2 k T_e}}$ ൗ 20 $Slope = -\frac{1}{T_e}$ 15 10 10 20 40 0 30 50 Energy [eV]

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Kinetic Confirmation-Asymmetric discharge



کلیڈ انسان کا ا



Ruhr-Universität Bochum Fakultät für Elektrotechnik und Informationstechnik Lehrstuhl für Angewandte Elektrodynamik und Plasmatechnik (AEPT)





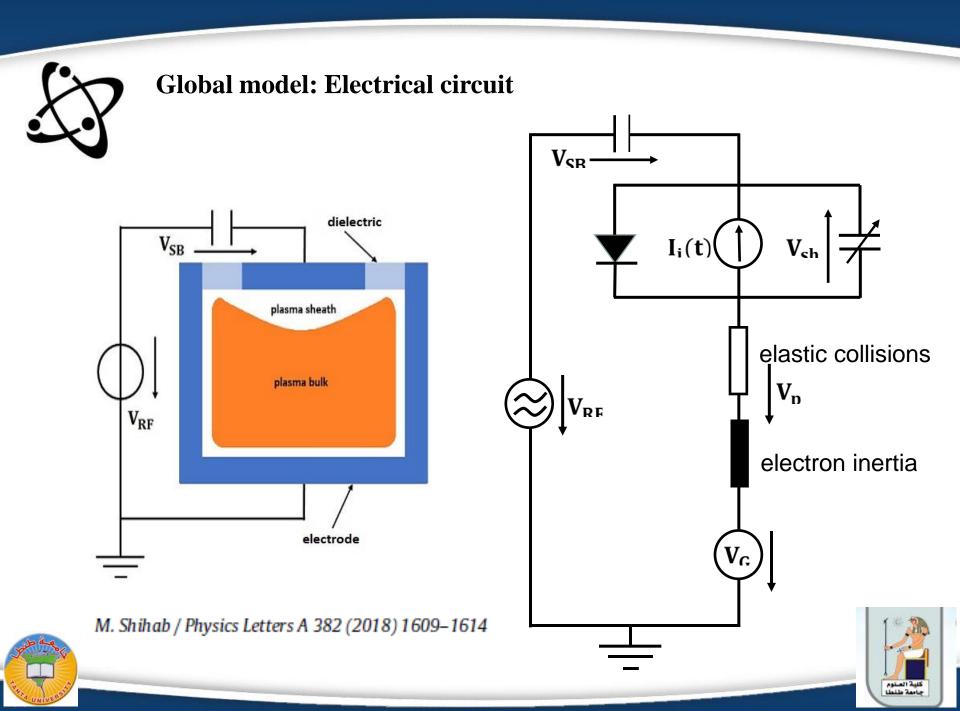
Global model: Zero dimensional model

$$\frac{\partial n_e}{\partial t} = n_e n_s k_i - n_e n_s k_r - \text{loss term}$$

Note

- If right hand side always positive = Simulation diverge with time
- If right hand side always negative = the plasma density vanishes with time
- We are looking for balance situation. Comparison with experiments is highely required.





Model equations

$$\frac{dQ(t)}{dt} = -I - en_{s}(t)A_{s}u_{s}(t) + en_{B}\sqrt{(T_{e}/2\pi m_{e})}A_{s}\exp(-eV_{s}(t)/T_{e})$$

$$V_{s}(t) = \frac{Q^{2}(t)}{2\epsilon_{0}en_{s}(t)A_{s}^{2}}$$

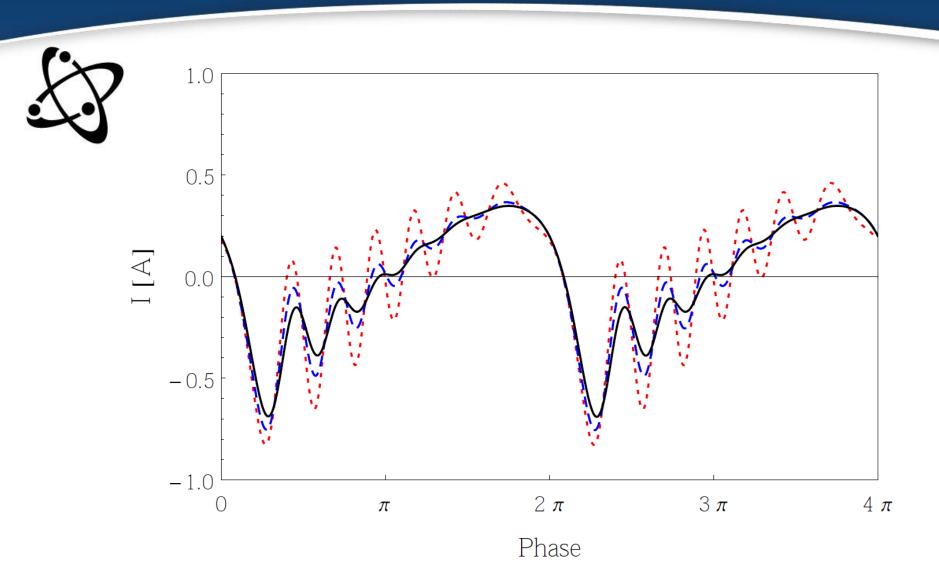
$$\frac{m_{e}L_{B}}{e^{2}n_{B}A_{B}}\left(\frac{dI(t)}{dt} + \nu_{eff}I(t)\right) = V_{s}(t) - V_{G} - V_{SB}(t) + V_{RF}(t)$$

$$V_{G} = \frac{T_{e}}{2e}\ln(\frac{m_{i}}{2\pi m_{e}})$$

$$C\frac{dV_{SB}(t)}{dt} = I(t)$$

$$P(t) = \frac{m_{e}L_{B}}{e^{2}n_{B}A_{B}}\nu_{eff}I^{2}(t) \qquad \bar{P}(t) = \frac{m_{e}L_{B}}{e^{2}n_{B}A_{B}\tau}\int_{0}^{t}\nu_{eff}I^{2}(t)dt$$





50 mTorr Black, 30 mTorr Blue, 10

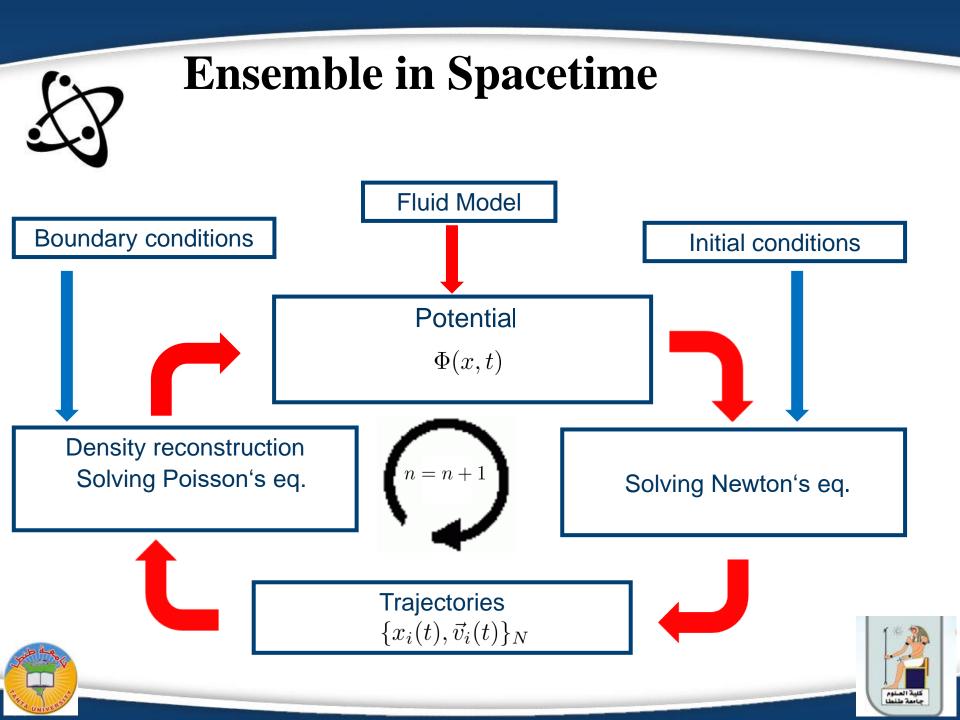




Ensemble-in-Spacetime Kinetic Sheath model

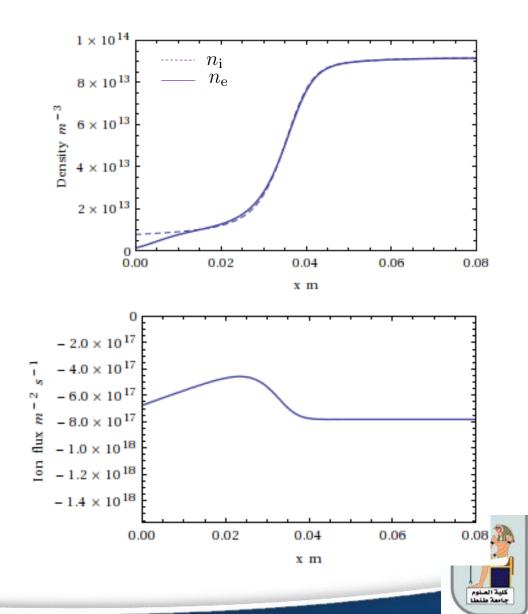








Ion dynamics



The intermediate regime

 $\omega_{\rm RF} \approx \omega_{\rm pi}$



IEDFs

HF regime **IMF** regime LF regime $\omega_{\rm RF} \approx \omega_{\rm pi}$ $\omega_{\rm RF} \ll \omega_{\rm pi}$ $\omega_{\rm RF} \gg \omega_{\rm pi}$ 0.2 MHz 2 MHz 100 50 150 10 MHz IED 0.5 r 50 150 100 20 MHz 0.4 100 0.3 100 80 MHz 0.2 0.1 0.0 Ľ 0 Ion energy 200 50 100 150

Argon plasma $n_i = 10^{10} \text{cm}^{-3}$

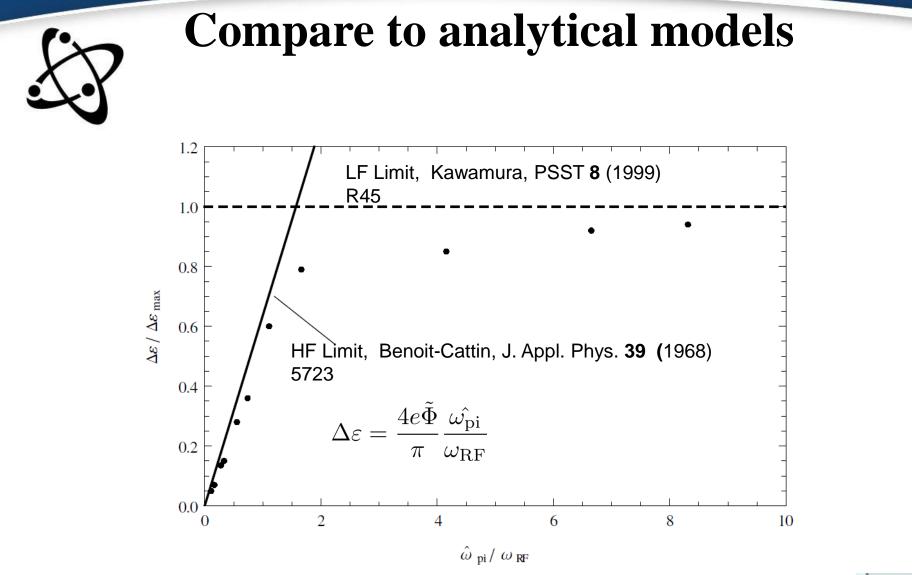




Verification of the EST Model



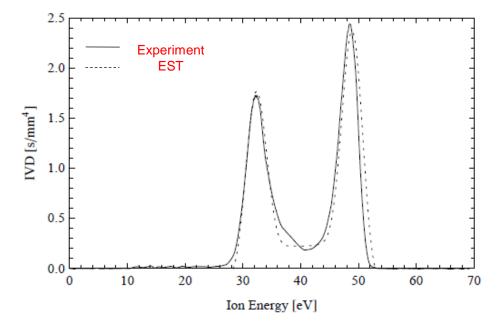




M. Shihab et al, J. Phys.D: Appl. Phys.45 (2012) 185202



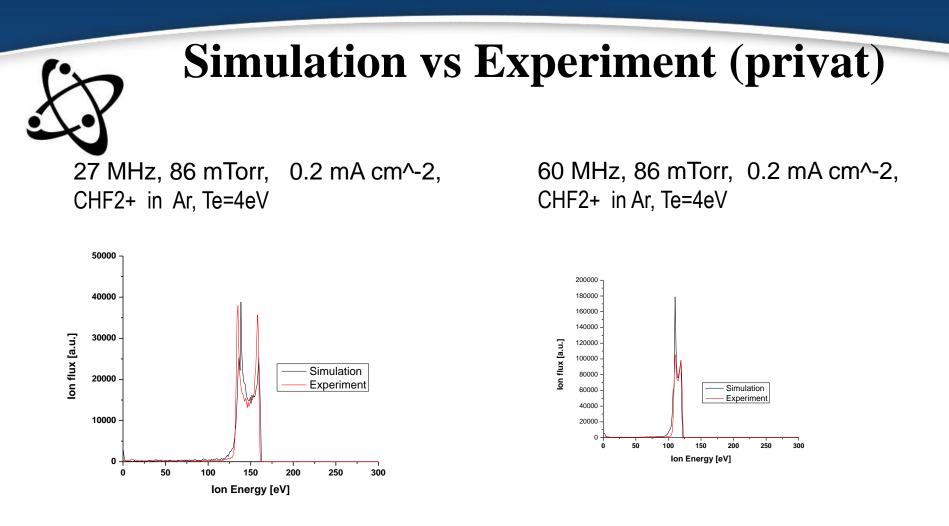




T. Baloniak et al J. Phys. D: Appl. Phys. **43** 335201 2010

M. Shihab et al. 30th ICPIG, Belfast, UK, 2011





- **The same species under the same conditions except the driven RF frequency.**
- Decreasing the driven RF frequencies leads to shorter ion transit times with respect to the driven RF period and consequently a wider IED.





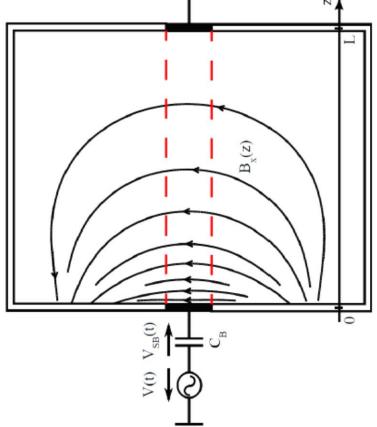


The code may predict an experiment



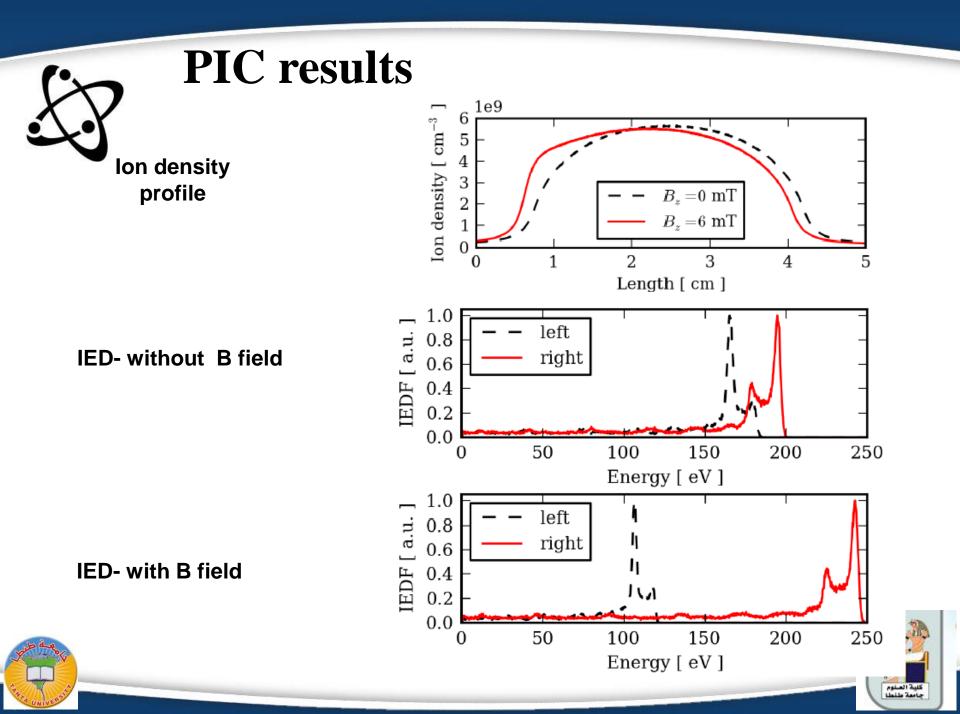






J. Trieschmann, M. Shihab et al J. Phys. D: Appl. Phys. 46 084016 2013



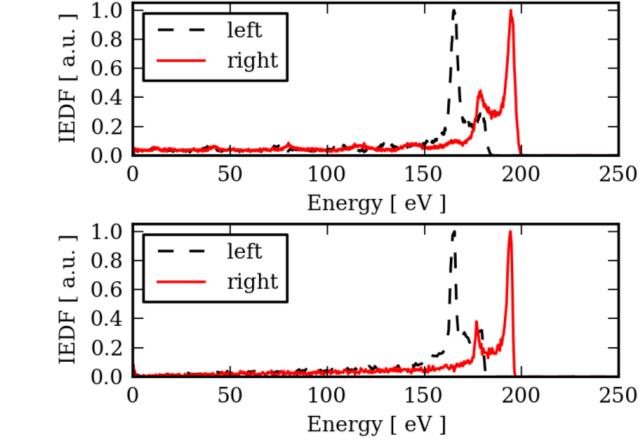




EST vs PIC

PIC





J. Trieschmann, M. Shihab et al J. Phys. D: Appl. Phys. 46 084016 2013

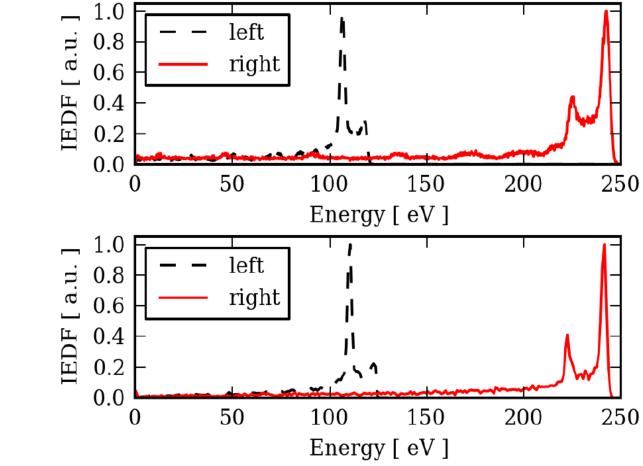




EST vs PIC

PIC





J. Trieschmann, M. Shihab et al J. Phys. D: Appl. Phys. 46 084016 2013



Experimental verif	ication		
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The electrical asymmetry effect allows control of the discharge symmetry, the DC self-bias, and	3. Analytical RF sheath model	cell simulations of	
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The code may be a part in the experiment

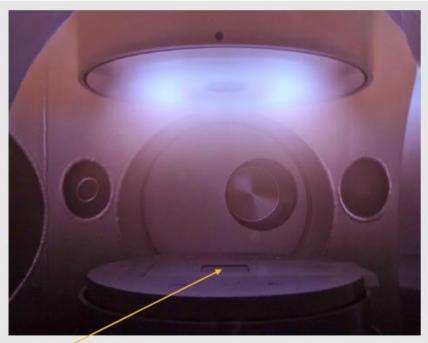




Deposition of Al₂O₃

The film stoichiometry is a function of the energy per deposited ato \bar{a}

- Alumina is widely used:
 - microelectronics
 - hard coating
 - absorbent
 - catalyst
- Alumina is an insulator.
- IED can not be measured, then Simulation.



 $(Al + O_2 + Ar)$ on Si substrate

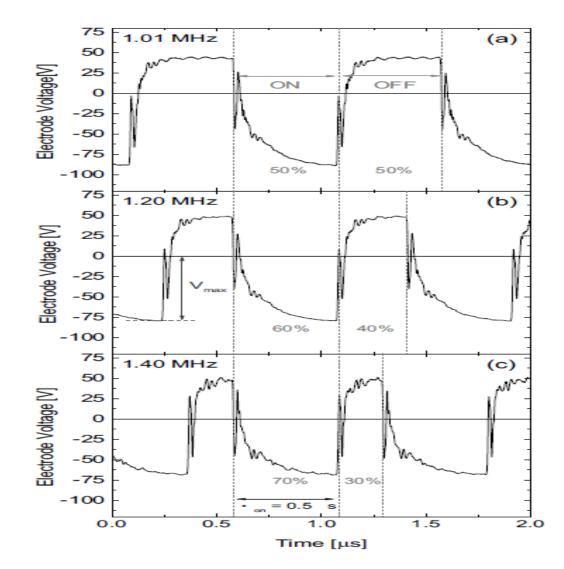
Prenzel, Ruhr University Bochum



M. Prenzel , ... M. Shihab et al J. Phys. D: Appl. Phys. 46 (2013) 084004

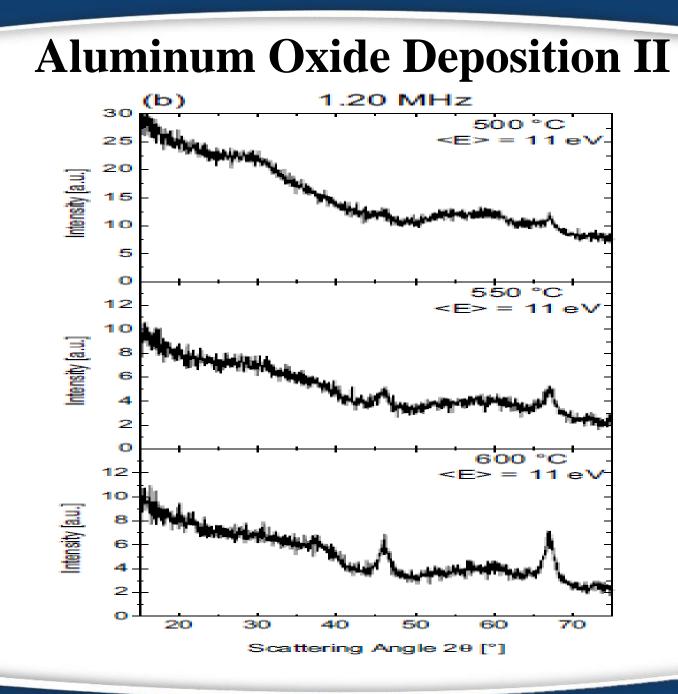


Aluminum Oxide Deposition I













- The simulation gives approximate solution.
- There are different models: Kinetic models as PIC, Fluid models, global models, and hybrid models
- The results must be compared with analytical or exprimental or simulated results.
- We should do calculations to interpret the experiment results, explain phenomena, or even propose an experiment.





Thanks!





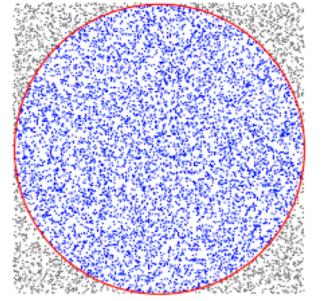


Monte-Carlo Simulation

- Use random numbers to solve problems.
- Are numbers really random?

$$\frac{A_{sq}}{A_{sh}} = \frac{l^2}{\pi r^2}$$

$$\frac{A_{sq}}{A_{sh}} = \frac{4r^2}{\pi r^2} = \frac{N_{sq}}{N_{sp}}$$



$$\pi = 4 * N_{sp} / N_{sq}$$

