# بسم الله الرحمن الرحيم

# Transition from non-neutral regime to neutral regime for capacitively coupled plasma reactors

***By***

**Aya Reda Elsayed Mohamed Elbadawy**

# Outlines

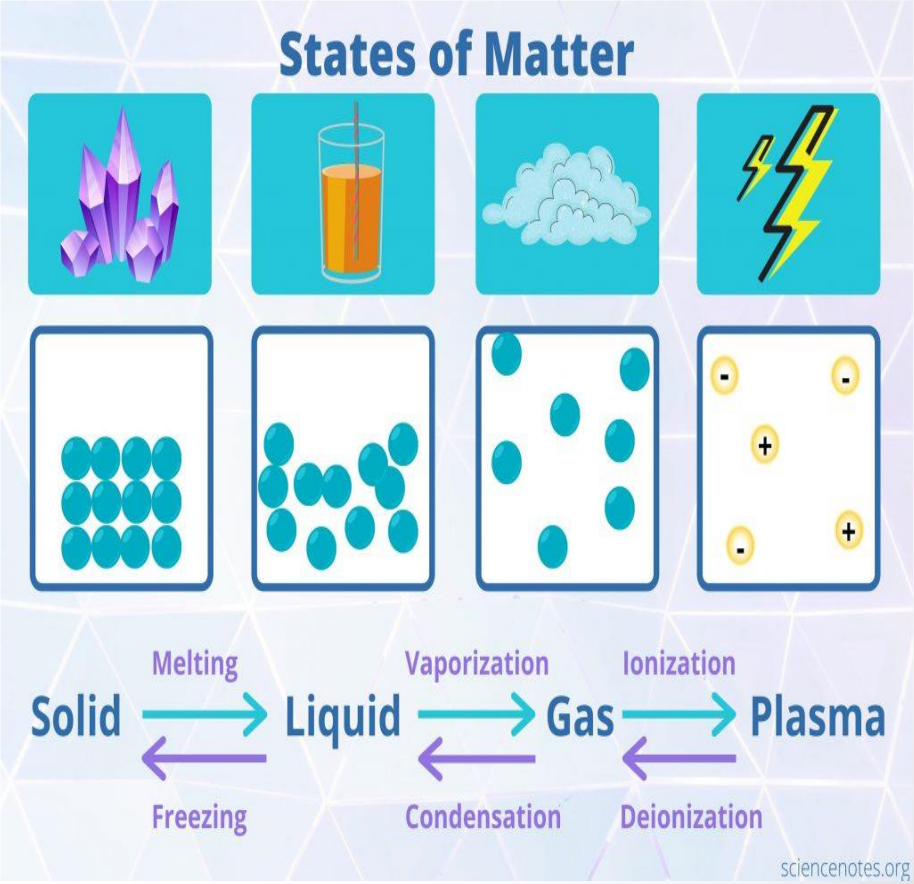
- Introduction to low temperature plasma
- Gas Discharge
- Plasma applications
- Capacitive coupled plasma
- PIC simulation
- PIC simulation parameters for He RF-CCP
- PIC simulation parameters for Ar RF-CCP
- Ion Acoustic modes and solitons
- Sagdeev's method
- The conditions for the transition from neutral plasma to non-neutral plasma.
- Conclusion

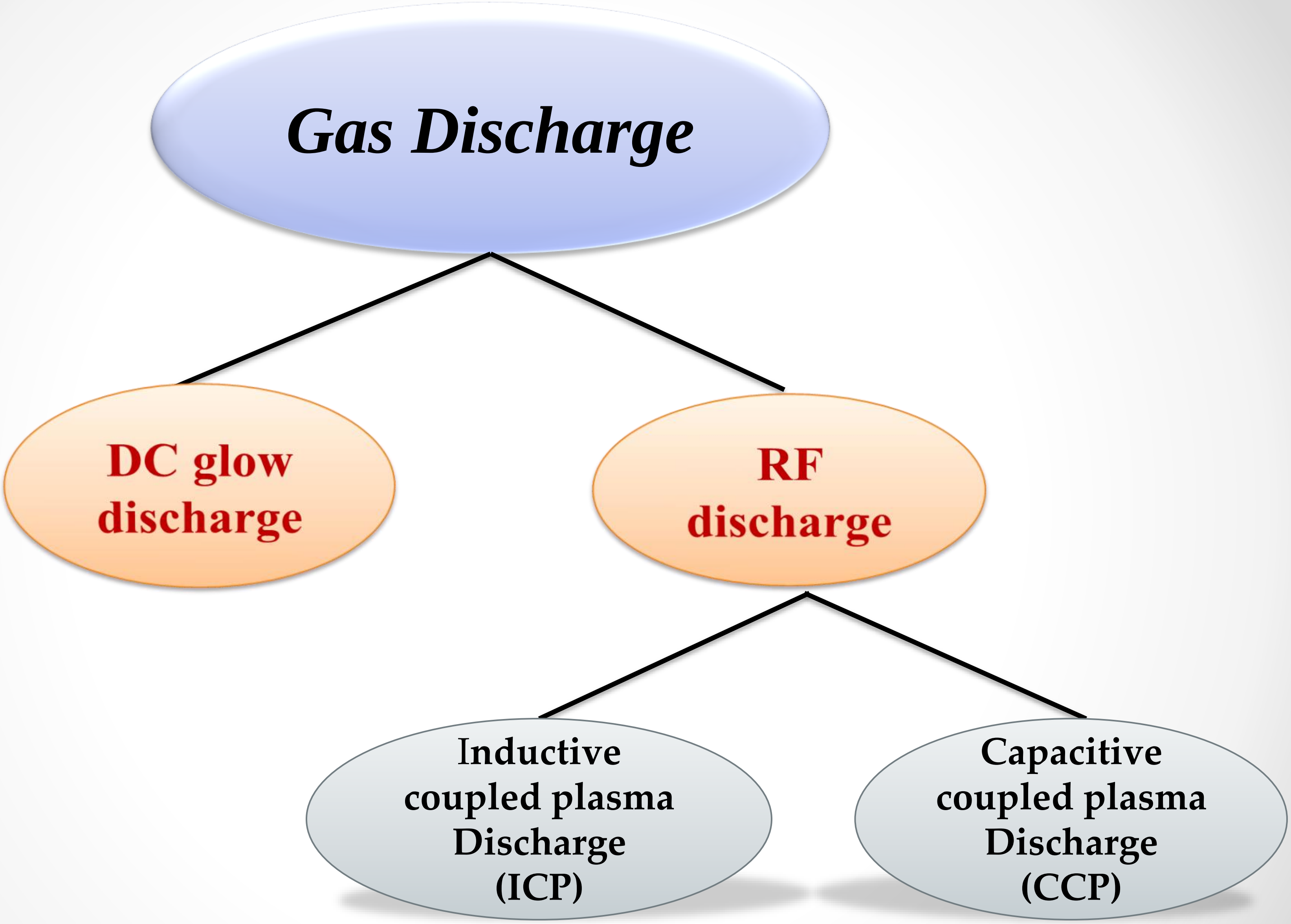
# Motivation

- Studying the effect of pressure, applied voltage, frequency and magnetic field on the properties of the formed plasma.
- Studying the conditions for the transition from neutral plasma to non-neutral plasma.
- Studying the possibility of generating sound waves for ions and generating soliton waves when moving from the neutral plasma to the non-neutral plasma.

# Plasma definition

- Plasma is considered as fourth state of matter and its quasi neutral gas with collective behaviour.




Gas Discharge
DC glow discharge
RF discharge
Inductive coupled plasma Discharge (ICP)
Capacitive coupled plasma Discharge (CCP)

***Medical applications***

- Prostate cancer treatment .
- Living tissues treatment.

***Industrial applications***

- Plasma etching.
- Plasma assisted cutting.
- Processing of semiconductors .
- Manufacture of (IC)

# *Plasma applications*

***Other applications***

- Surface preparation.
- Beam forming plasma antenna .
- Atmospheric pressure plasma jet.

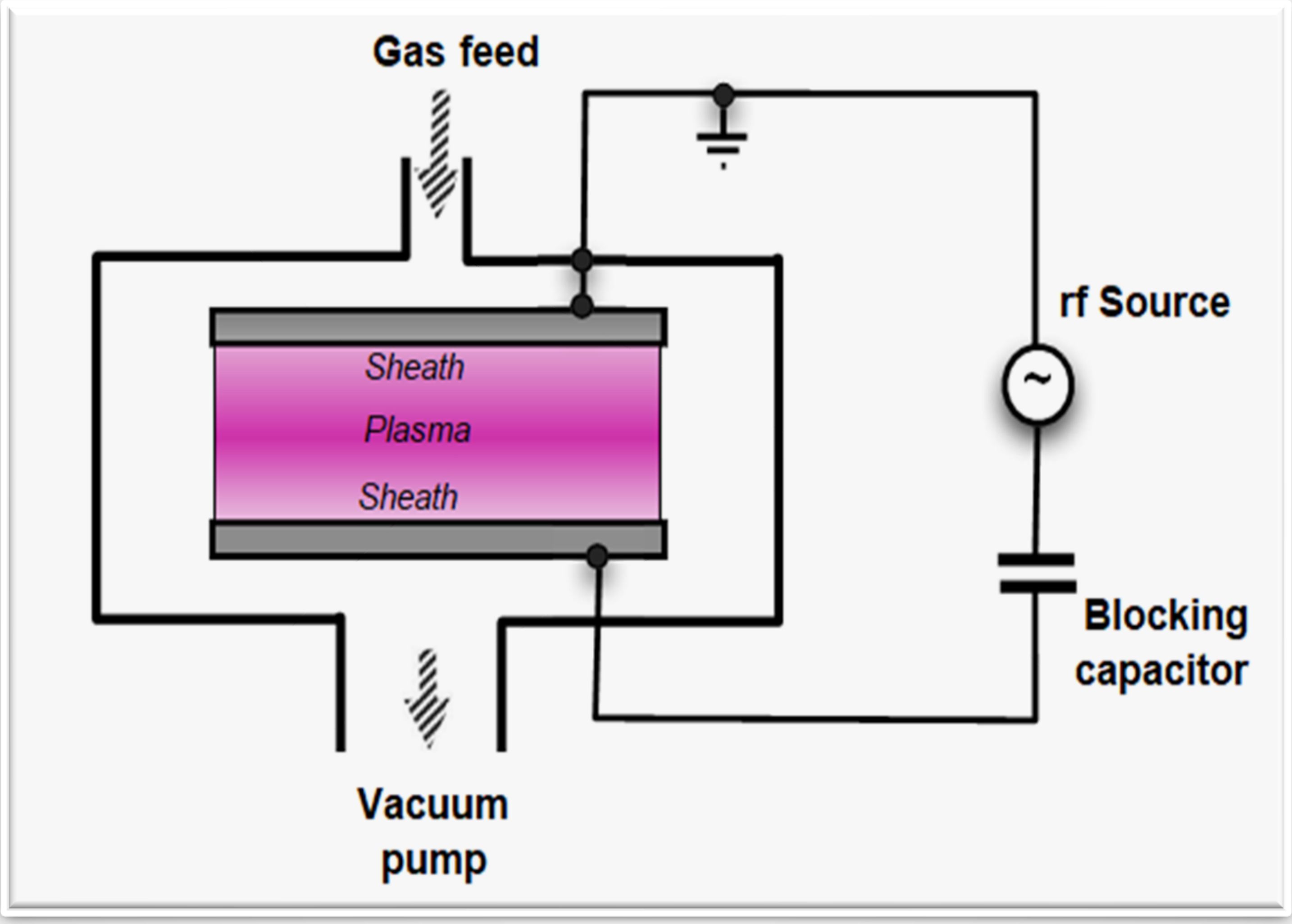
***Capacitive coupled plasma applications***

Plasma deposition

Plasma etching

Plasma sputtering

# Capacitive coupled plasma CCP



# Plasma modeling and simulation

- **Equivalent circuit models**
- **Fluid models**
- **Kinetic models**
  - **Monte Carlo Simulation**
  - **PIC Simulation**

# Particle in cell simulation (PIC)

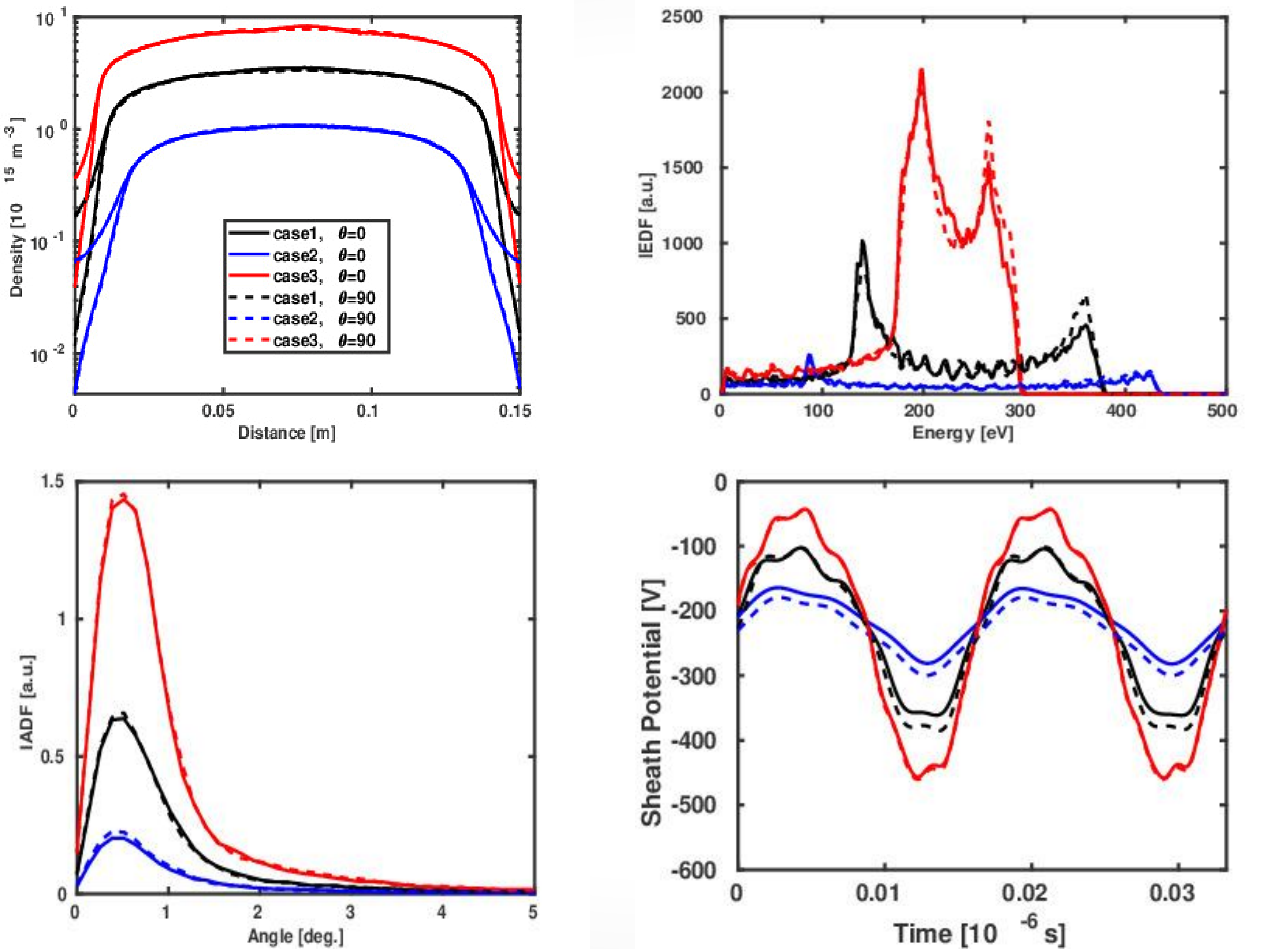
- The code solves the equation of motion of the plasma superparticles in a self-consistent way with Poisson's equations assuming electrostatic approximation; Collisions, e.g., elastic scattering and charge exchange.

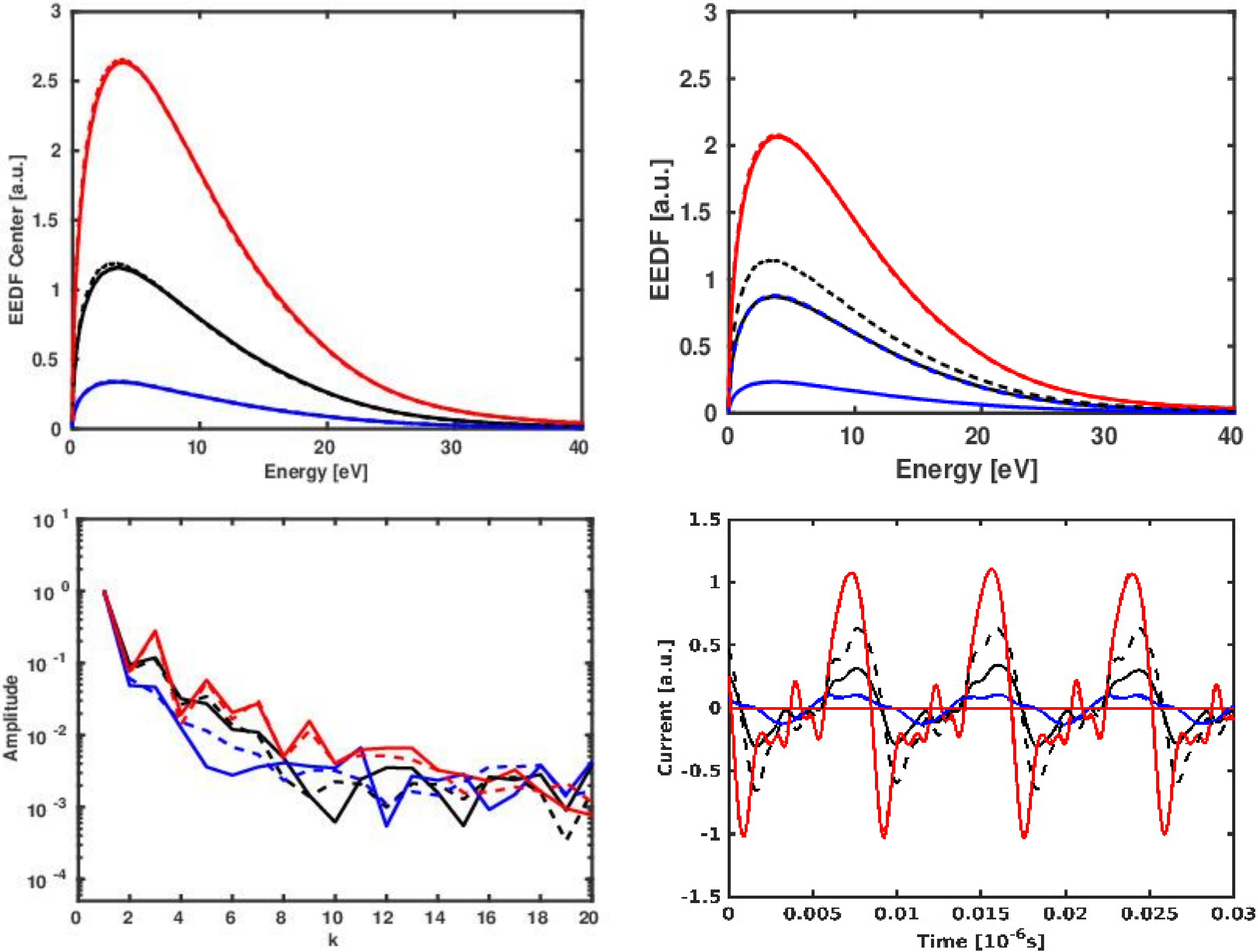
# PIC simulation parameters for He RF-CCP

- The distance between the two planar electrodes is 15 cm and the gap size is discretized into 259 grids.
- The initial ion and electron temperatures are 300 K and 50000 K, respectively.
- The voltages of the frequencies change, where the total is constant, . $V_{60} + V_1 = 500\text{V}$
- The simulation runs for 500 RF periods of the 60 MHZ cycles.
- The simulation stops when there is no variation in the number of superparticles in the entire discharge, i.e., steady state.

# At different voltages

| | |
|---|---|
| **source1** | |
| $V_1 = 250$ v | $V_2 = 250$ v |
| $f_1 = 60$ MHz | $f_2 = 1$ MHz |
| Phase shift =0 | Gas pressure =1 pa |
| <u>source2</u> | |
| $V_1 = 100$ v | $V_2 = 400$ v |
| $f_1 = 60$ MHz | $f_2 = 1$ MHz |
| Phase shift =0 | Gas pressure =1 pa |
| <u>source3</u> | |
| $V_1 = 400$ v | $V_2 = 100$ v |
| $f_1 = 60$ MHz | $f_2 = 1$ MHz |
| Phase shift =0 | Gas pressure =1 pa |


Density [10^15 m^-3]
Distance [m]
case1, θ=0
case2, θ=0
case3, θ=0
case1, θ=90
case2, θ=90
case3, θ=90
IEDF [a.u.]
Energy [eV]
IADF [a.u.]
Angle [deg.]
Sheath Potential [V]
Time [10^-6 s]



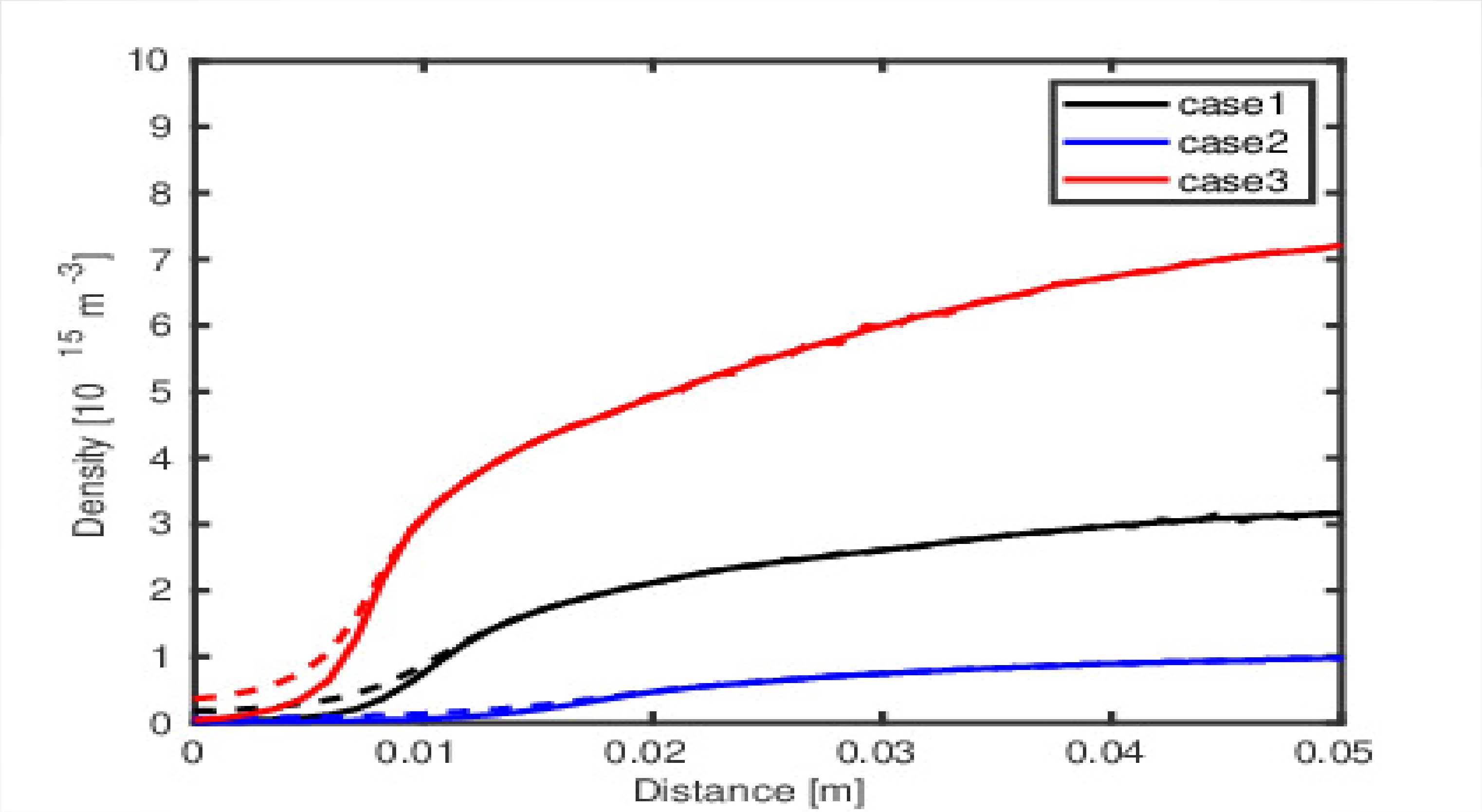
EEDF Center [a.u.]
Energy [eV]
EEDF [a.u.]
Energy [eV]
Amplitude
k
Current [a.u.]
Time [10^-6 s]

# PIC simulation parameters for Ar RF-CCP

- The distance between the two planar electrodes is 5 cm and the gap size is discretized into 129 grids.
- The initial ion and electron temperatures are 300 K and 50000 K, respectively.
- The simulation runs for 5000 RF periods of the 60 MHZ cycles.
- The driven frequencies are 60 MHz and 1 MHz,

$$\boldsymbol{V_{RF} = V_{60}\,\mathbf{sin}(2\pi 60\mathrm{MHz}t) + V_1 \mathbf{sin}(2\pi \mathrm{MHz}t).}$$

- The voltages of the frequencies change, where the total is constant, . $V_{60} + V_1 = 500\mathrm{V}$

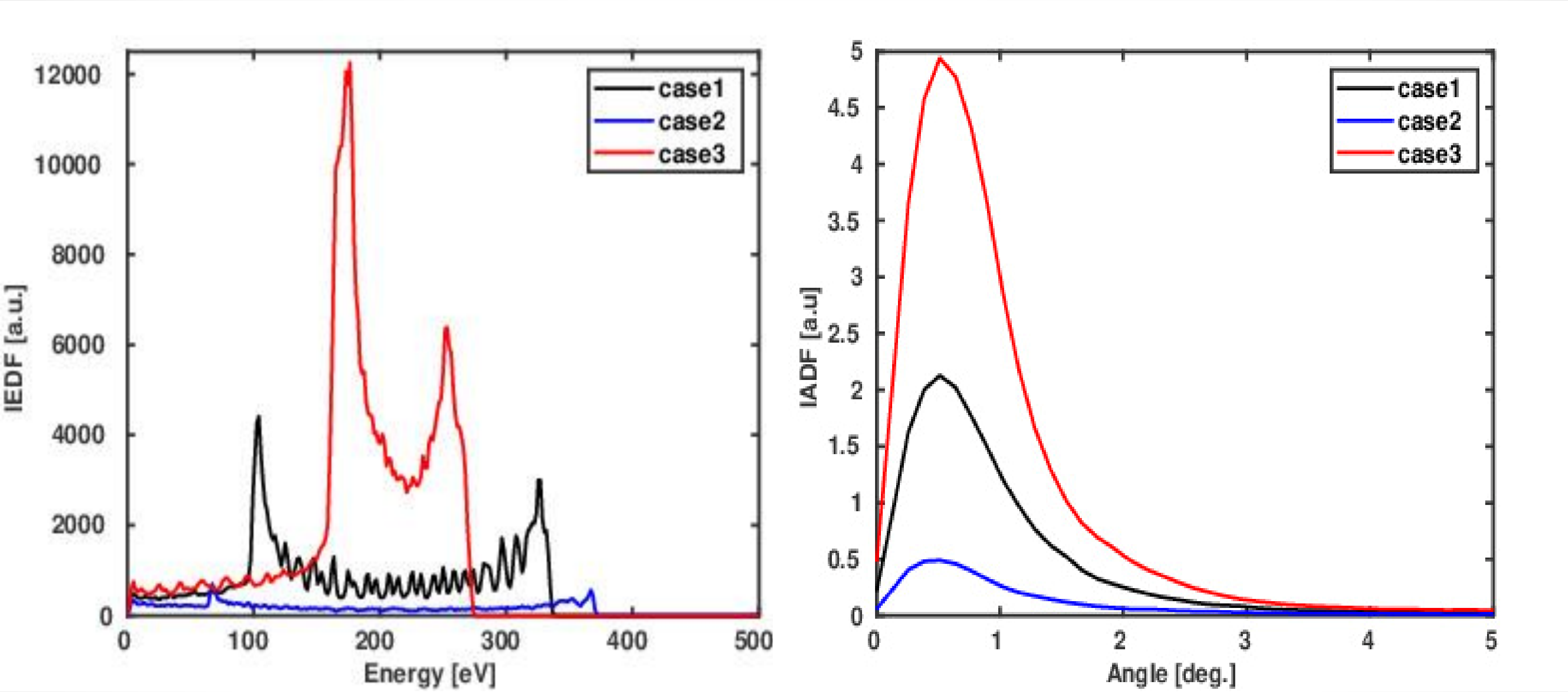



The time average density profile.

In case (1) the voltages are $V_{60}$ = 250V and $V_1$= 250V

In case (2) the voltages are $V_{60}$ = 100V and $V_1$= 400V

In case (3) the voltages are $V_{60}$= 400V and $V_1$ = 100V




- The broadening of the ion energy distribution increases by increasing the amplitude of the 1 MHz signal.
- This allows more processes that would take place at the substrate. In addition, still most of ions hit the target close to normal incidence as in cases (1) and (3).

# Ion Acoustic modes and solitons

- The intermediate radio frequency regime holds the inequality $\omega_{pe} >> \omega_{RF} \approx \omega_{pi}$ .

Where $\omega_{pe}$, $\omega_{RF}$ and $\omega_{pi}$ are the electron plasma frequency, the radio frequency and the ion plasma frequency, respectively.

- In this regime, electrons follow the RF sheath field and the assumption of Boltzmann distribution for electrons is valid.
- Ions cross the sheath with a transit time comparable to the RF period, consequently, their inertia allow them to partially interact with the instantaneous RF sheath field.

- The fluid dynamics of collisionless sheath could be merely summarized with Poisson's equation as follows:

$$\frac{\partial n_{\mathrm{i}}}{\partial t} + \frac{\partial n_{\mathrm{i}} u_{\mathrm{i}}}{\partial x} = 0,$$

$$m_{\mathrm{i}} \frac{\partial u_{\mathrm{i}}}{\partial t} + m_{\mathrm{i}} u_{\mathrm{i}} \frac{\partial u_{\mathrm{i}}}{\partial x} = eE,$$

$$\epsilon_0 \frac{\partial E}{\partial x} = n_{\mathrm{i}} - n_{\mathrm{e0}} \exp(\frac{e\Phi}{T_{\mathrm{e}}}),$$

$$\frac{\partial \Phi}{\partial x} = -E.$$

- By making the normalization by using:

$$x \to x\lambda_{\mathrm{D}},\ t \to t/\omega_{\mathrm{RF}},\ u \to u\sqrt{T_{\mathrm{e}}/m_{\mathrm{i}}},\ n \to n_{\mathrm{i0}}n,$$

$$E \to ET_{\mathrm{e}}/e\lambda_{\mathrm{D}},\ \text{and}\ \Phi \to \Phi T_{\mathrm{e}}/e.\ \ \lambda_{\mathrm{D}} = \sqrt{\frac{\epsilon_0 T_{\mathrm{e}}}{n_{\mathrm{i0}}e^2}}$$

We found :

$$\Omega\frac{\partial n_{\mathrm{i}}}{\partial t} + \frac{\partial n_{\mathrm{i}}u_{\mathrm{i}}}{\partial x} = 0,$$
$$\Omega\frac{\partial u_{\mathrm{i}}}{\partial t} + u_{\mathrm{i}}\frac{\partial u_{\mathrm{i}}}{\partial x} = E,$$

$$\frac{\partial E}{\partial x} = n_{\mathrm{i}} - \mu\exp(\Phi),$$
$$\frac{\partial \Phi}{\partial x} = -E.$$

$\Omega = \omega_{RF}/\omega_{pi}$. $\omega_{RF}$ and $\omega_{pi} = \sqrt{\frac{n_{i0}e^2}{\varepsilon_0 m_i}}$ are RF frequency and the ion plasma frequency, respectively. $\mu = \frac{n_e}{n_i}$ is the ratio of the electron density to the ion density.

- The dispersion relation which is derived when $\mu = 1$ is belong to the plasma bulk. But for the sheath, $\mu < 1$.
- Let expand the dynamical quantities using $A(x,t) = \bar{A}(x) + \delta A(x,t)$, where $\bar{A}(x)$ is the zero-order component and $\delta A(x,t)$ is the first order component. The linearization and assuming $\delta A \sim exp(i\omega t)$ yield:

$$i\Omega\omega\delta n_i + \frac{\partial}{\partial x}(\bar{u}\delta n_i + \bar{n}_i\delta u) = 0,$$

$$i\Omega\omega\delta u_i + \frac{\partial(\bar{u}_i\delta u_i)}{\partial x} = \delta E,$$

$$\frac{\partial\delta E}{\partial x} = \delta n_i - \exp(\bar{\Phi})\delta\Phi,$$

$$\frac{\partial\delta\Phi}{\partial x} = -\delta E.$$

For a plasma with a homogeneous zero order dynamical quantities and holds the quasi-neutrality as in the plasma bulk,

$$\Omega^2\omega^2\bar{n}_\mathrm{i}\delta u_\mathrm{i} - 2i\Omega\omega\bar{n}_\mathrm{i}\bar{u}_\mathrm{i}\frac{\partial\delta u_\mathrm{i}}{\partial x} +$$

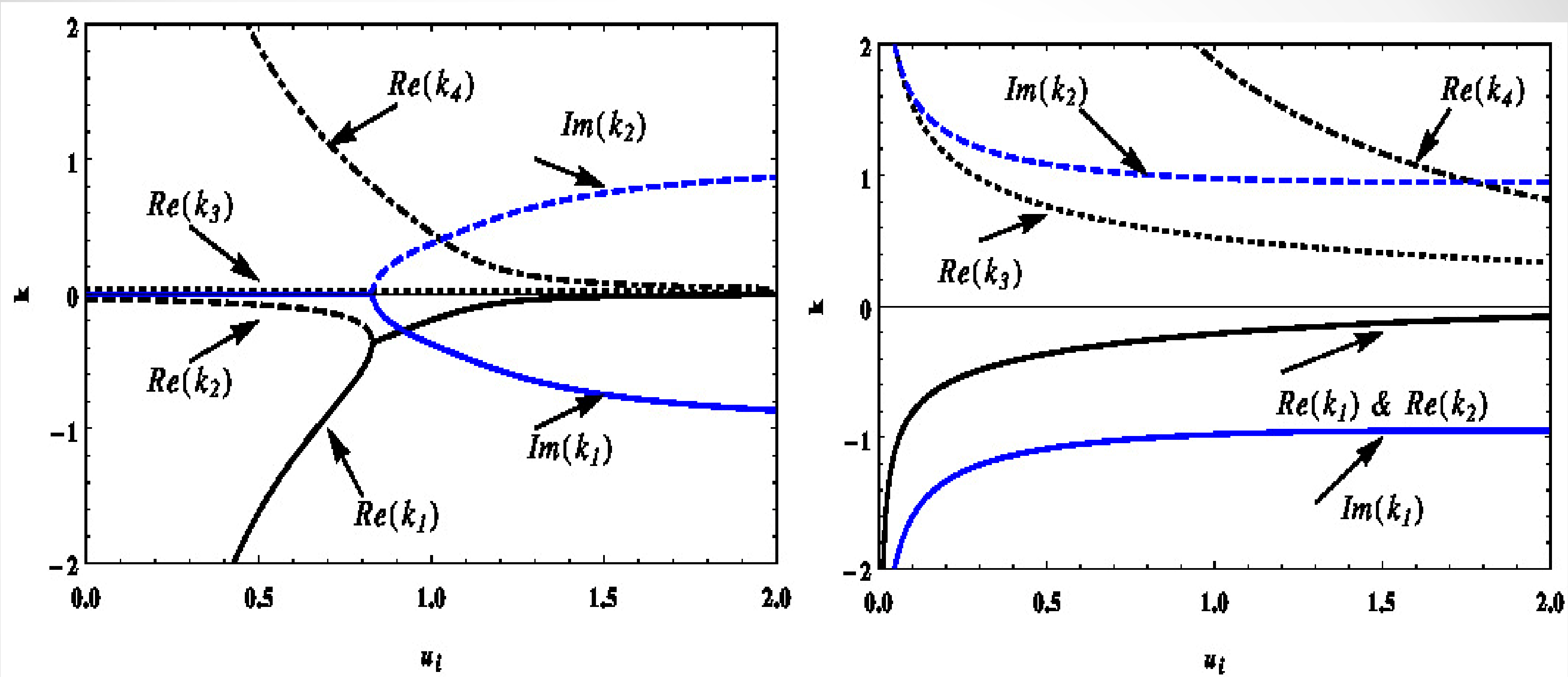
$$(\bar{n}_\mathrm{i} - \bar{n}_\mathrm{i}\bar{u}_\mathrm{i}^2 - \Omega^2\omega^2)\frac{\partial^2\delta u_\mathrm{i}}{\partial x^2} + 2i\Omega\omega\bar{u}_\mathrm{i}\frac{\partial^3\delta u_\mathrm{i}}{\partial x^3} + \bar{u}_\mathrm{i}^2\frac{\partial^4\delta u_\mathrm{i}}{\partial x^4} = 0.$$

Letting $\delta u_\mathrm{i} \sim \exp(-ikx)$, we obtain the dispersion relation

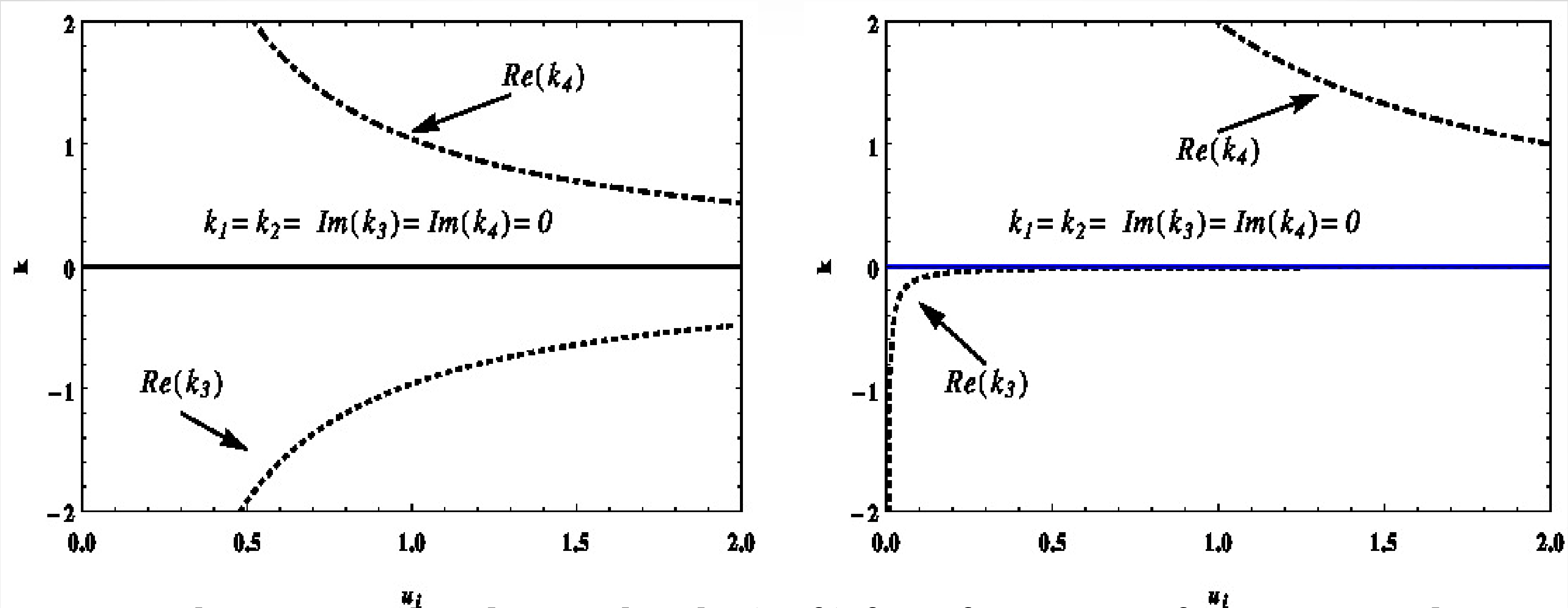
$$-k^2 + k^2\bar{u}_\mathrm{i}^2 + \frac{k^4\bar{u}_\mathrm{i}^2}{\bar{n}_\mathrm{i}} - 2k\bar{u}_\mathrm{i}\Omega\omega - \frac{2k^3\bar{u}_\mathrm{i}\Omega\omega}{\bar{n}_\mathrm{i}} + \Omega^2\omega^2 + \frac{k^2\Omega^2\omega^2}{\bar{n}_\mathrm{i}} = 0$$

This is the dispersion relation , By making analysis to the last equation
We can solve it by K or ω but K has 4 roots and ω has 2 roots , so we will continue with ω

$$\omega_{1,2} = \frac{k^3\bar{u}_\mathrm{i} + k\bar{n}_\mathrm{i}\bar{u}_\mathrm{i} \pm \bar{n}_\mathrm{i}k\sqrt{1 + k^2/\bar{n}_\mathrm{i}}}{\Omega(k^2 + \bar{n}_\mathrm{i})}$$




- The roots in the plasma bulk: (Left) for a frequency of $0.04\ \omega_{pi}$ and (Right) for a frequency of $0.99\ \omega_{pi}$.
- In the left panel, Re($k_2$) and Re($k_1$) are congruent for speeds greater than $\sim 0.85$.




The roots in the plasma sheath: (Left) for a frequency of 0.04 $\omega_{pi}$ and (Right) for a frequency of 0.99 $\omega_{pi}$.

- In the plasma Bulk we assumed that K ranged between 0.04 $\omega_{pi}$ to 0.99 $\omega_{pi}$ .
- Noticed that K has to parts ( real and imaginary ) and inside the sheath imaginary part = 0
- In ω analysis it is a real value because it is a stable system.

- This is the dispersion relation , By making analysis to the last equation

$$\omega_{1,2} = \frac{k^3\bar{u}_i + k\bar{n}_i\bar{u}_i \pm \bar{n}_i k\sqrt{1 + k^2/\bar{n}_i}}{\Omega(k^2 + \bar{n}_i)}$$

- It is clear that no complex $\omega$ is obtained for real k so that all modes described by the dispersion relation are stable.

We can solve it by K or ω but K has 4 roots and ω has 2 roots , so we will continue with ω .

- In the normalized frame, if the ion density $\overline{n}_i(x) = 1$ and $\overline{u}_i = -1$, $\Omega = 1$, then the dispersion relation can be approximately simplified into:

$$\omega_{1,2} \approx -(k \pm 1).$$

# Is there a soliton?

- By solving the equations by the sagdeev's method.

$\xi = x - Mt$, where M is (Mach number). $\varphi = 0$ , $u_i = -1$ , $n_i = 1$ and multiply it by $\frac{d\varphi}{d\xi}$ then integral over

$$\frac{1}{2}\left(\frac{d\varphi}{d\xi}\right)^2 + V(\varphi) = 0$$

where the first term plays the role of kinetic energy, while the second term represents the potential energy which known as Sagdeev potential and is given by

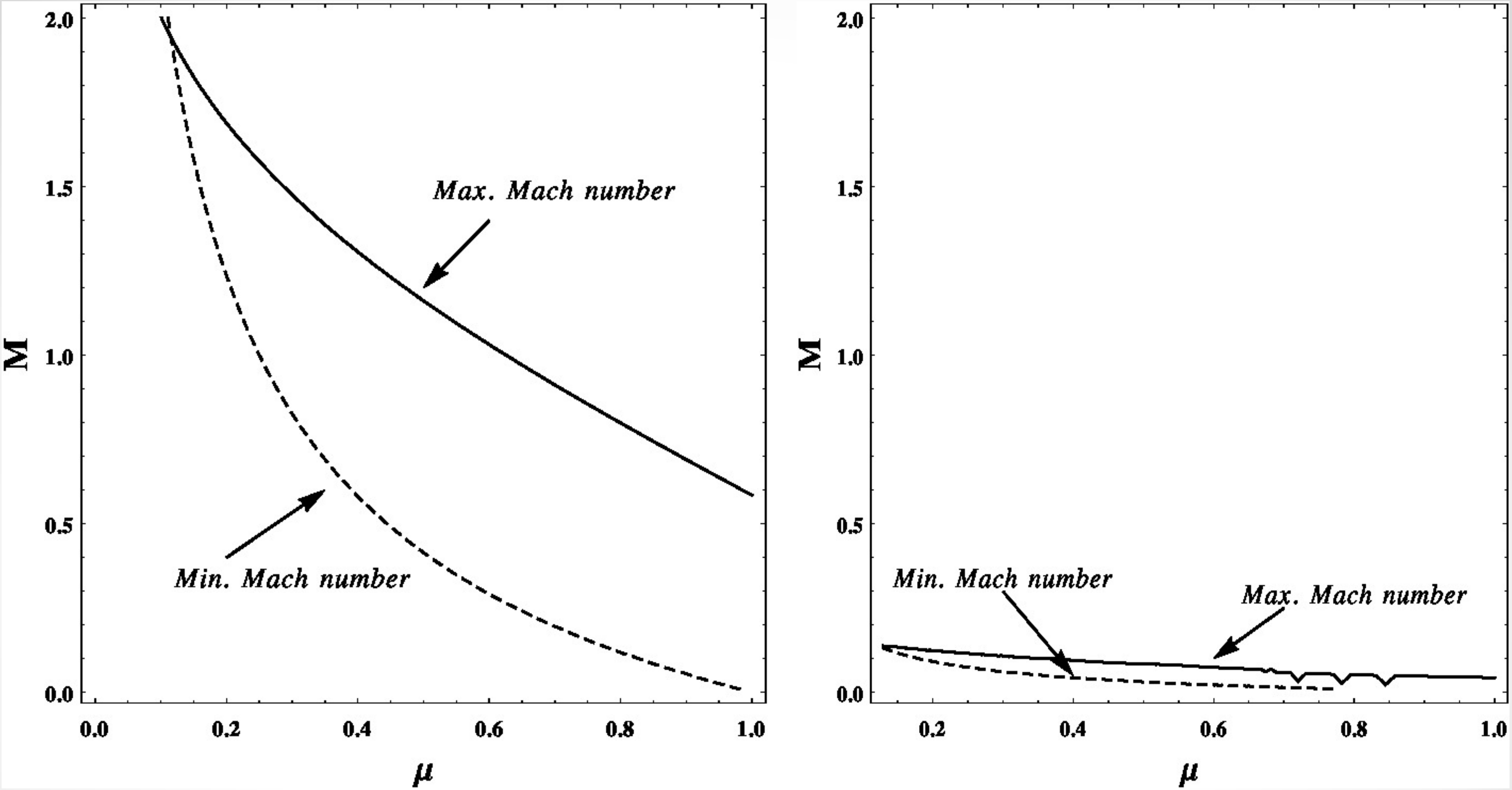
$$V(\varphi) = (M\Omega + 1)^2 \left(1 - \sqrt{1 - \frac{2\varphi}{(M\Omega + 1)^2}}\right) - \mu\,(e^{\varphi} - 1)$$

The conditions for the existance of soliton waves are (i) The potential $V(\varphi)$ has the maximum value if $\frac{d^2V(\varphi)}{d\xi^2} < 0$ at$\varphi = 0$. This condition yields the inequality

$$\frac{1}{(M\Omega+1)^2} - \mu \leq 0$$

(ii) The existance of soliton waves requires also $V(\varphi_{\text{max}}) \geq 0$, where the maximum potential $\varphi_{\text{max}}$ is determined by $\varphi_{\text{max}} = \frac{1}{2}(M\Omega + 1)^2$. This implies the following inequality

$$(M\Omega+1)^2 - \mu\left(e^{\frac{1}{2}(M\Omega+1)^2} - 1\right) \geq 0$$




Minimum (dashed line) and maximum (solid line) Mach numbers are required for solitons generation.
(Left) when $\Omega = \mathbf{1}$; i.e., the intermediate radiofrequency regime, $\boldsymbol{\omega_{pi} = \omega_{RF}} \sim \mathbf{1}\ \boldsymbol{MHz}$, (Right) when $\Omega = \mathbf{13.56}$.

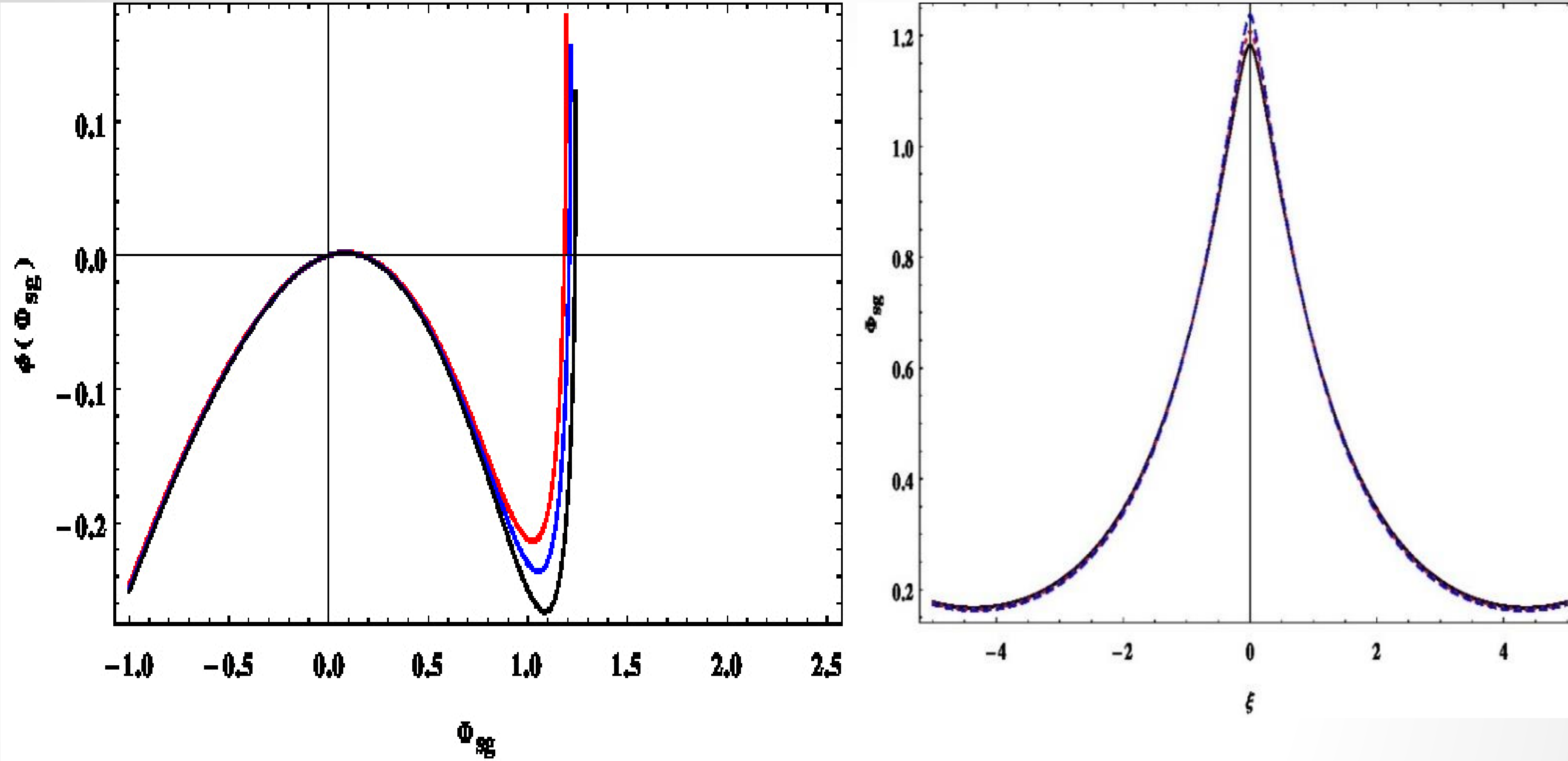
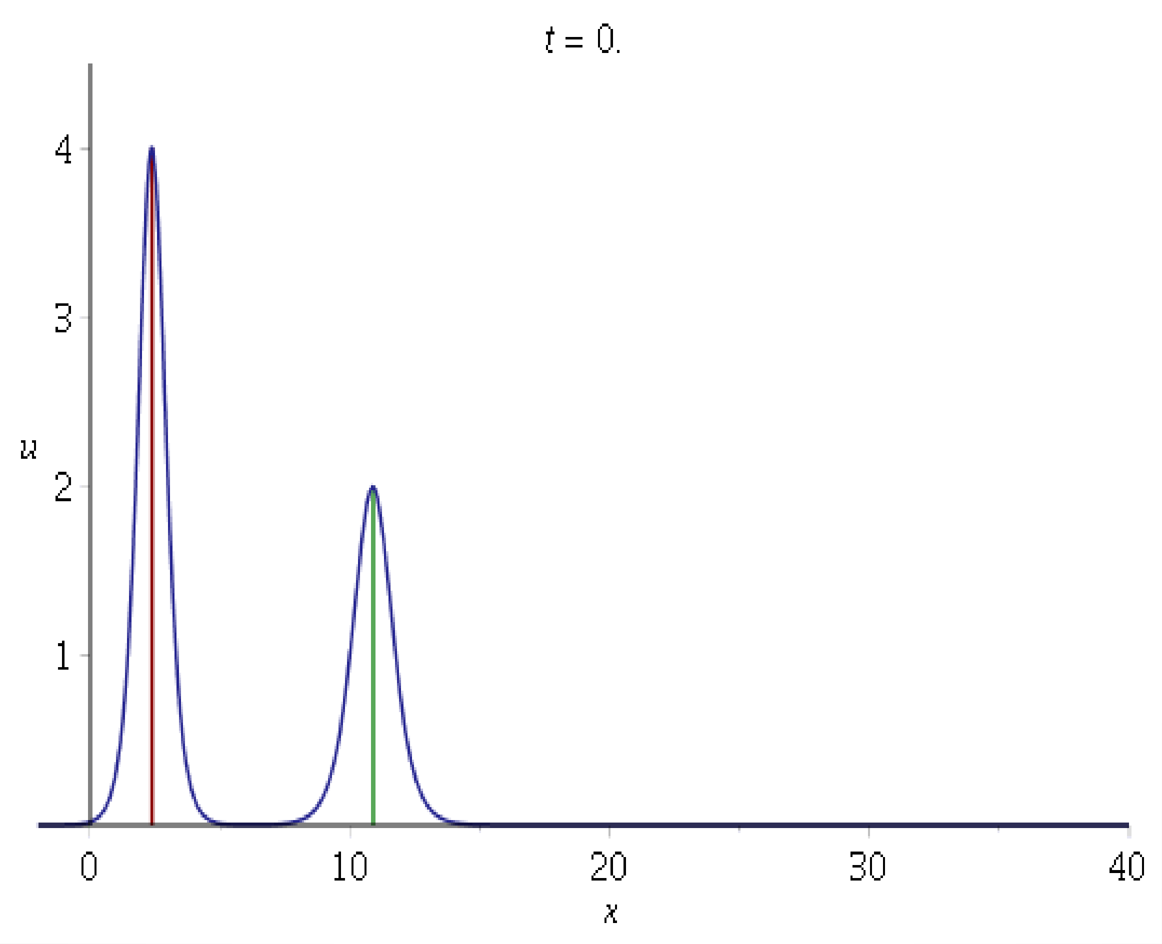


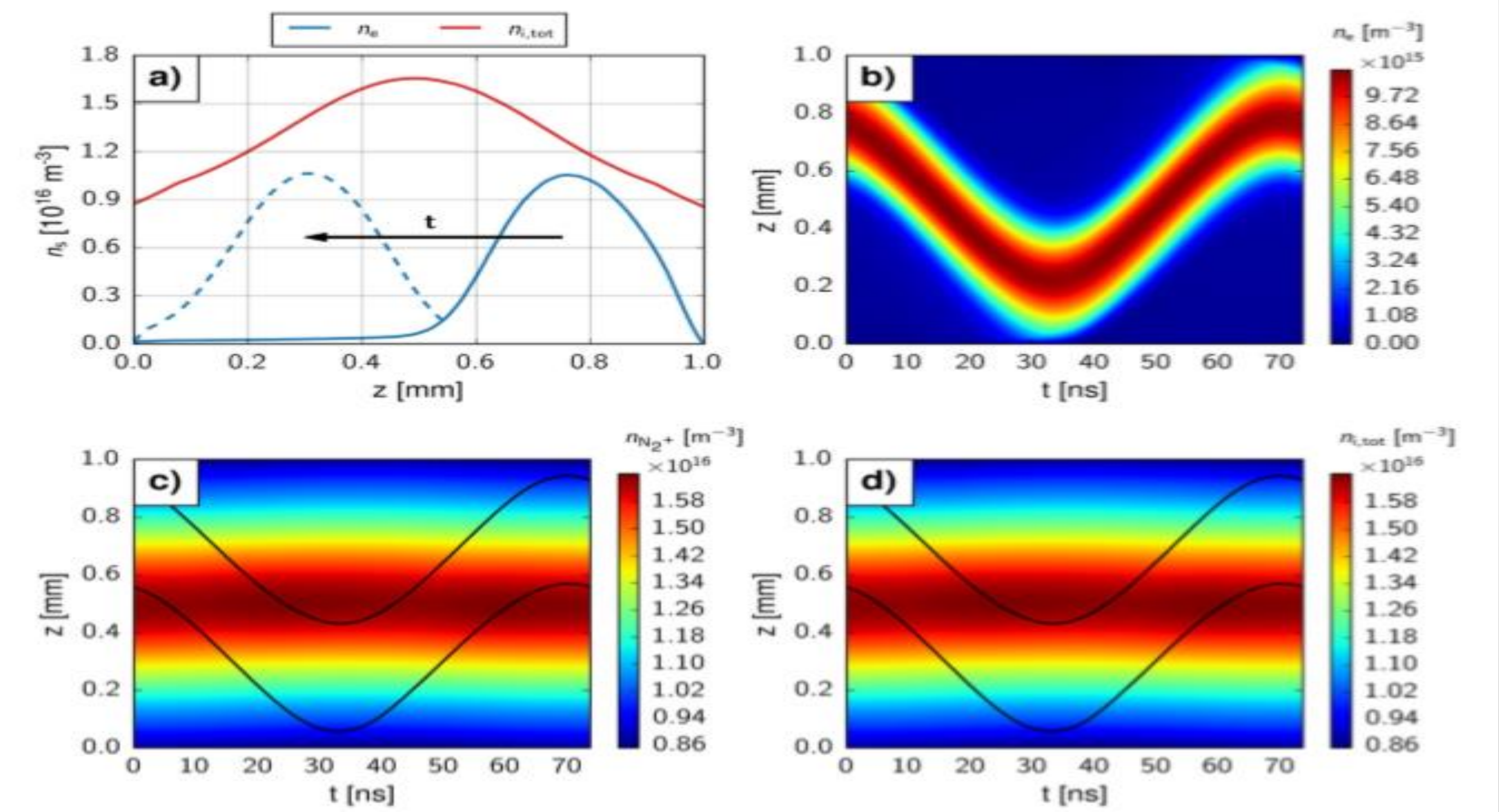

Figure (Left) Variation of Sagdeev potential versus electrostatic potential.

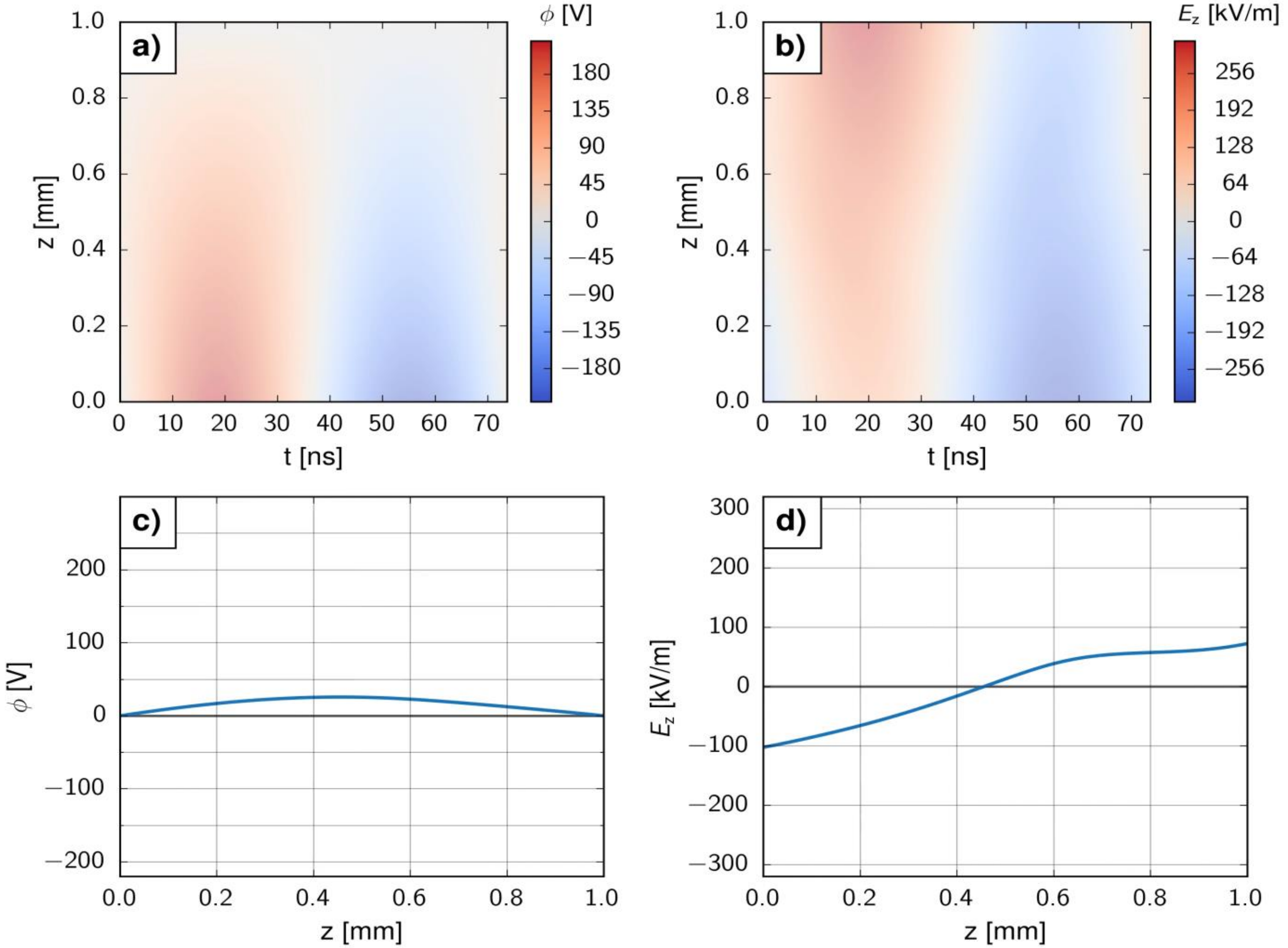
(Right) The profiles for the soliton wave against the normalized spatial coordinate. Here, $\Omega = 1$, $\mu = 0.9533$, and $M = 0.5451$, $M = 0.5588$, and $M = 0.5757$ for red line, blue line, and black line, respectively.

# Soliton waves



# The conditions for the transition from neutral plasma to non-neutral plasma in plasma jet at atmospheric pressure

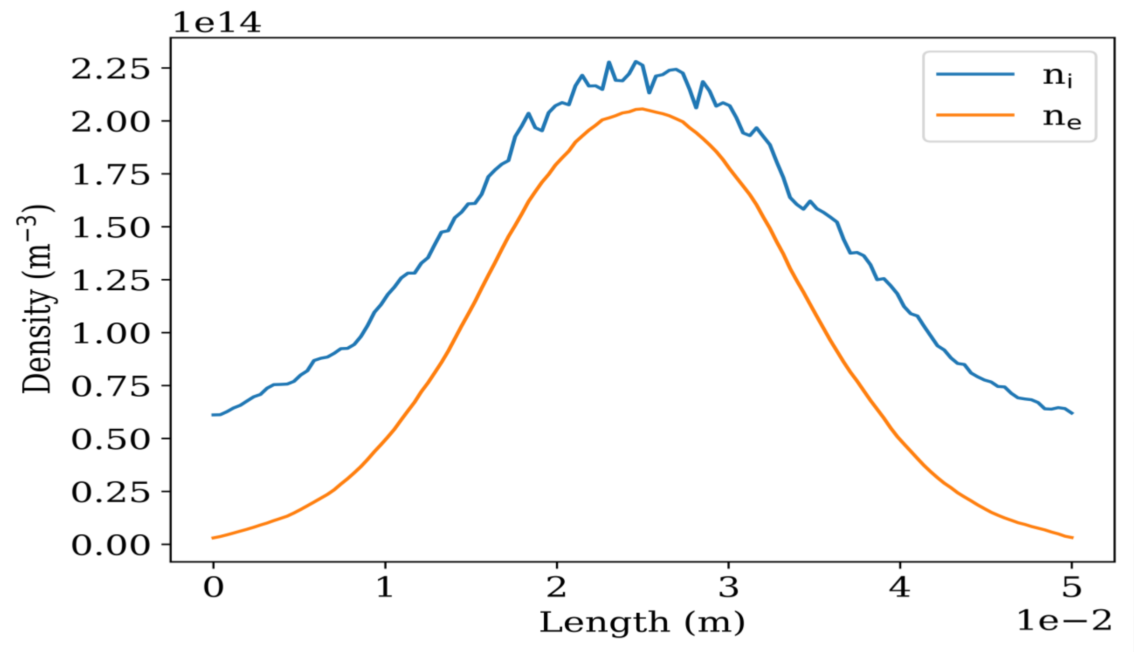


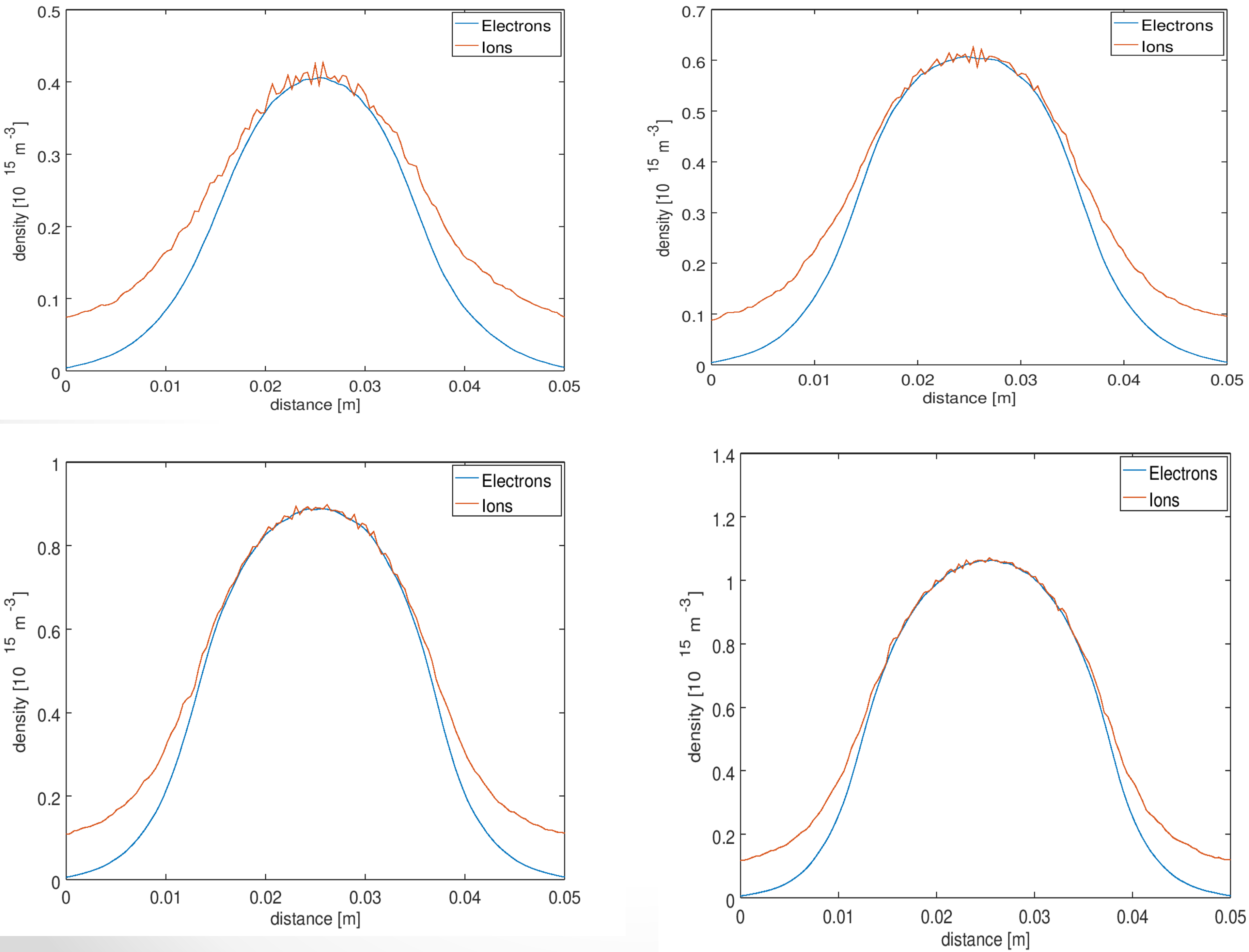


a)
b)
c)
d)
ϕ [V]
$E_z$ [kV/m]
z [mm]
t [ns]
ϕ [V]
$E_z$ [kV/m]
z [mm]

# The conditions for the transition from neutral plasma to non-neutral plasma in CCP

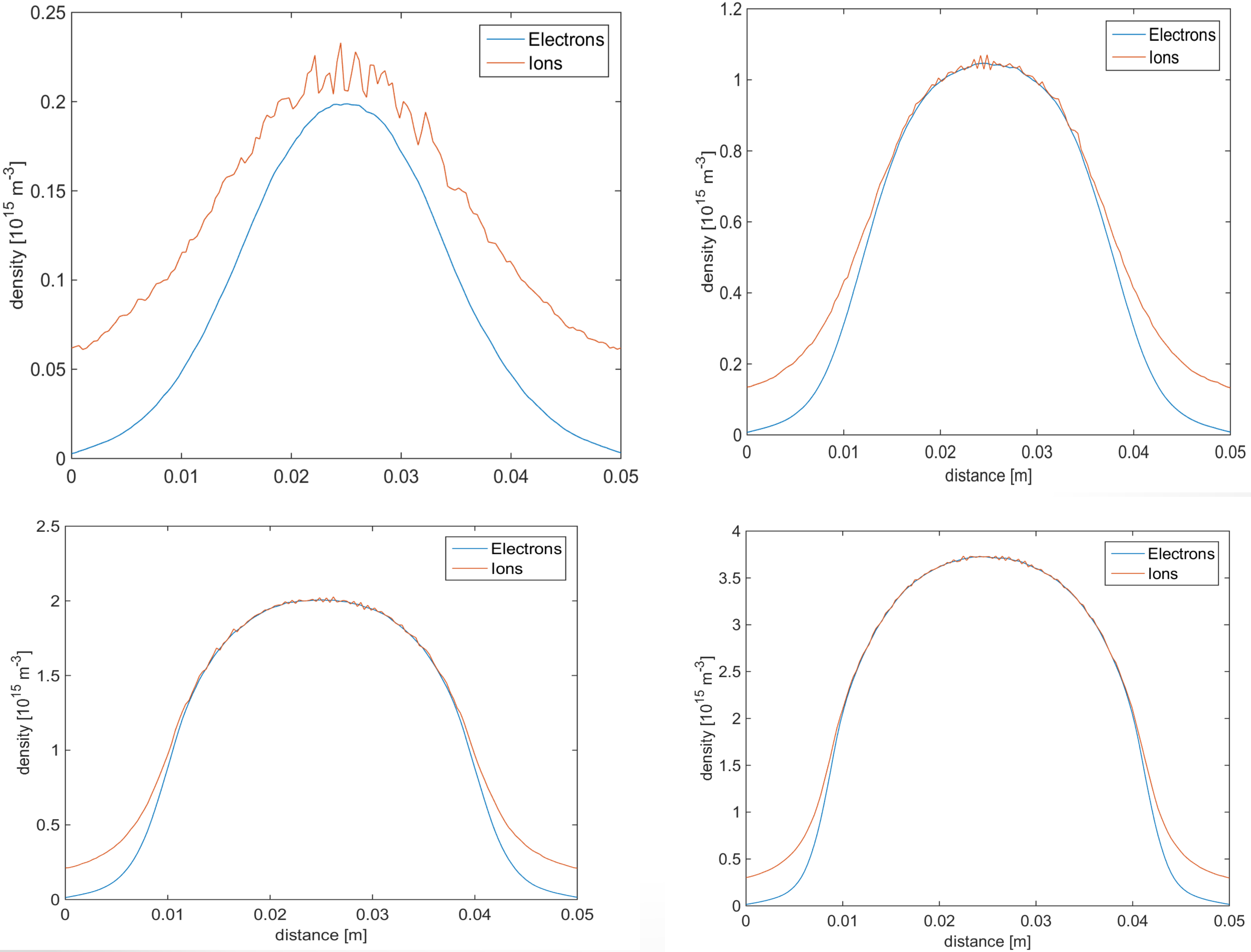
- At different pressure 2 pa, 3 pa,4 pa,5 pa and 6 pa respectively, plasma bulk not excited  at small pressure as shown in the next figures




Electrons
Ions
density [10^15 m^-3]
distance [m]
Electrons
Ions
density [10^15 m^-3]
distance [m]
Electrons
Ions
density [10^15 m^-3]
distance [m]
Electrons
Ions
density [10^15 m^-3]
distance [m]

# At different voltages

| | |
|---|---|
| **source1** | |
| $V_1 = 100$ v | $V_2 = 400$ v |
| $f_1 = 60$ MHz | $f_2 = 1$ MHz |
| Phase shift =0 | Gas pressure =2 pa |
| source2 | |
| $V_1 = 200$ v | $V_2 = 300$ v |
| $f_1 = 60$ MHz | $f_2 = 1$ MHz |
| Phase shift =0 | Gas pressure =2 pa |
| source3 | |
| $V_1 = 400$ v | $V_2 = 100$ v |
| $f_1 = 60$ MHz | $f_2 = 1$ MHz |
| Phase shift =0 | Gas pressure =2 pa |


Electrons
Ions
density [10^15 m^-3]
0.25
0.2
0.15
0.1
0.05
0
0
0.01
0.02
0.03
0.04
0.05
Electrons
Ions
density [10^15 m^-3]
1.2
1
0.8
0.6
0.4
0.2
0
0
0.01
0.02
0.03
0.04
0.05
distance [m]
Electrons
Ions
density [10^15 m^-3]
2.5
2
1.5
1
0.5
0
0
0.01
0.02
0.03
0.04
0.05
distance [m]
Electrons
Ions
density [10^15 m^-3]
4
3.5
3
2.5
2
1.5
1
0.5
0
0
0.01
0.02
0.03
0.04
0.05
distance [m]

# Conclusion

- The broadening of the ion energy distribution at the substrate exist when using intermediate radiofrequencies in the range of 1MHz.
- This help in controlling etching, deposition and sputtering.
- The broadening has been represented in terms of excitation of ion acoustic waves and soliton.
- At small pressure plasma bulk not found.

Plasma Sources Science and Technology

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# The ion transit effects on the sheath dynamics inthe intermediate radiofrequency regime: excitationsof ion-acoustic waves and solitons

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## Abstract

The capacitively coupled plasma is investigated kinetically utilizing the particle- in-cell technique. The Argon (Ar) plasma is generated via two radio-frequencies. The plasma bulk density increases by increasing the voltage amplitude of the high frequency (≥ 13.56 MHz) which is much greater than the ion plasma frequency. The intermediate radio-frequencies ( ≈ 1 MHz) which are comparable to the ion plasma frequency causes a broadening of the ion energy distribution considerably, i.e., ions gain energies above and lower than the time-averaged energy. The good agreement between published experimental results and our theoretical calculations via the Ensemble- in-Spacetime model confirms the modulation of ions around time-averaged values. Intermediate frequencies allow ions to respond partially to the instantaneous electric field. The response of ions to the instantaneous electric field is investigated semi- analytically. The dispersion relation of the plasma sheath and bulk are derived. Stable ion acoustic modes are found. The ion-acoustic modes have two different velocities and carry energy from the sheath edge to the electrode. Also, intermediate frequencies excite solitons in the plasma sheath; the results may help to explain the ion density, flux, and energy modulation, and, consequently, the broadening of the ion energy distribution.

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# Simulation and modeling of radio-frequency atmospheric pressure plasmas in the non-neutral regime

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**Abstract**

Radio-frequency-driven atmospheric pressure plasma jets (RF APPJs) play an essential role in many technological applications. This work studies the characteristics of these discharges in the so-called non-neutral regime where the conventional structure of a quasi-neutral bulk and an electron depleted sheath does not develop, and the electrons are instead organized in a drift-soliton-like structure that never reaches quasi-neutrality. A hybrid particle-in-cell/Monte Carlo collisions (PIC/MCC) simulation is set up, which combines a fully kinetic electron model via the PIC/MCC algorithm with a drift-diffusion model for the ions. In addition, an analytical model for the electron dynamics is formulated. The formation of the soliton-like structure and the connection between the soliton and the electron dynamics are investigated. The location of the electron group follows a drift equation, while the spatial shape can be described by Poisson–Boltzmann equilibrium in a co-moving frame. A stability analysis is conducted using the Lyapunov method and a linear stability analysis. A comparison of the numerical simulation with the analytical models yields a good agreement.

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# Thank you