RUHR-UNIVERSITÄT BOCHUM

EM PIC modeling of CCP discharges

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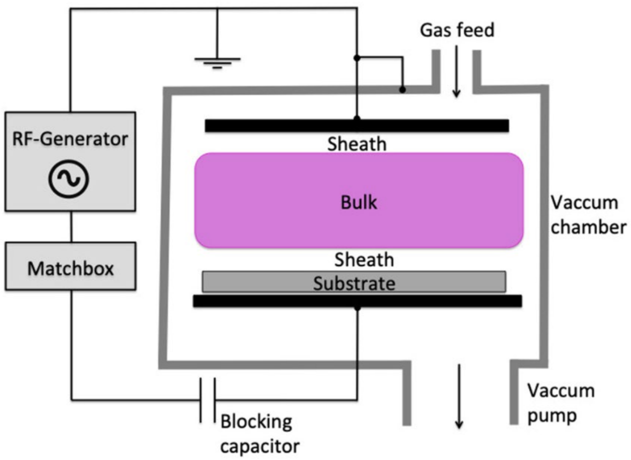
Motivation

CCP reactor



[S. Wilczek et al., J. Appl. Phys. 127 (2020)] 181101]

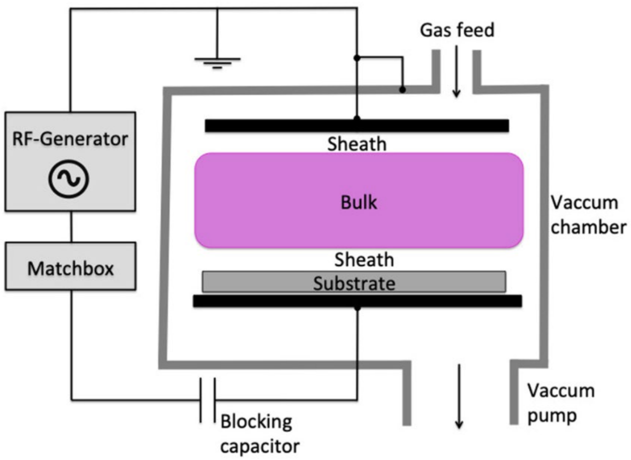
- Higher driving frequency leads to higher ion flux

- Larger wafer size increases throughput

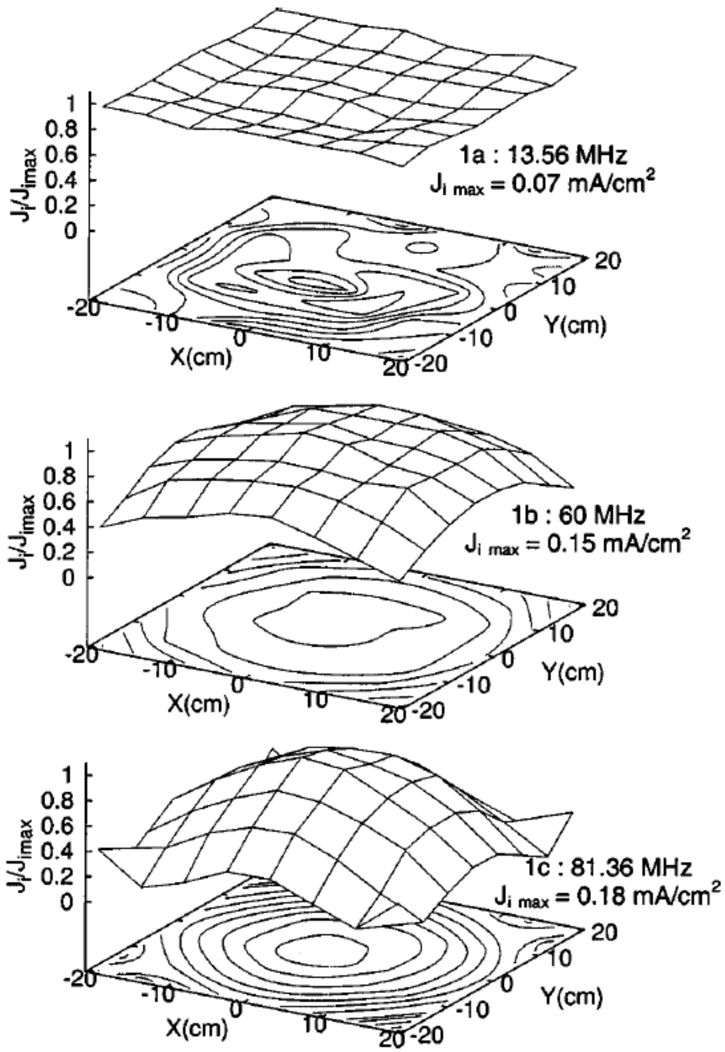
- Plasma (ion flux and energy) uniformity issues

Motivation

CCP reactor



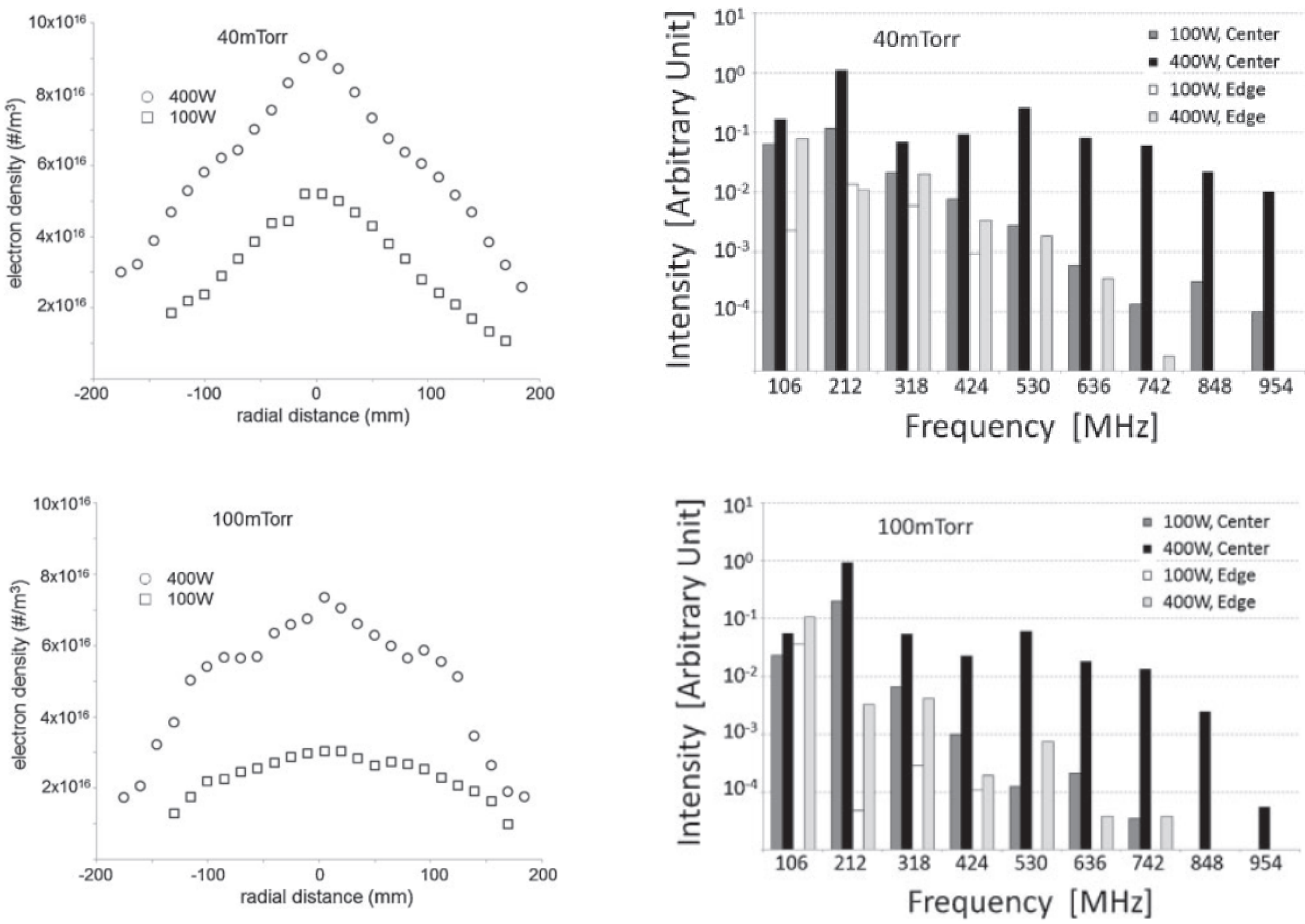
[S. Wilczek et al., J. Appl. Phys. 127 (2020)] 181101]



- Higher driving frequency leads to higher ion flux
- Larger wafer size increases throughput
- Plasma (ion flux and energy) uniformity issues

[A. Perret et al., Appl. Phys. Lett. 83 (2003) 243]

Tokyo Electron Measurements: Test-bench B

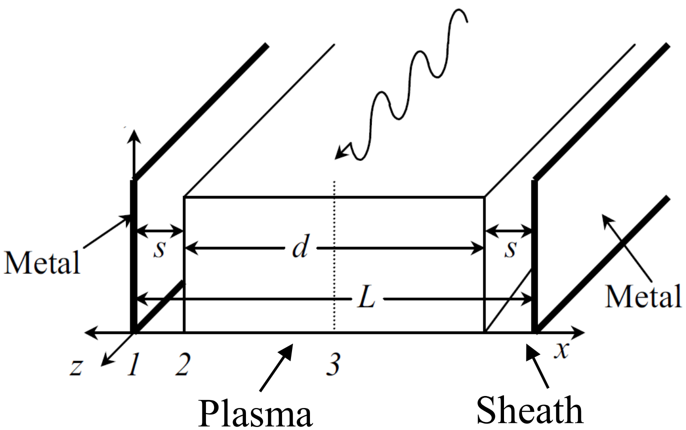


[I. Sawada et al, Jpn. J. Appl. Phys. 53 (2014) 03DB01]

Theory: Normal Modes in a CCP Discharge

Surface Waves in a Cartesian Slab CCP

[K. Bowers, PhD. Thesis, UC Berkeley, 2001,
"High Frequency Electron Resonances and Surface Waves in Unmagnetized Bounded Plasmas"]



$\epsilon_r = 1 - \omega_{pe}^2/\omega^2$ $\qquad \epsilon_r = 1$

$$\begin{cases} \dfrac{d\tilde{E}_z}{dx} = i\left(\omega\tilde{B}_y - k\tilde{E}_x\right) \\ \tilde{B}_y = \dfrac{\omega\epsilon_r}{kc^2}\tilde{E}_x \\ \dfrac{d\tilde{B}_y}{dx} = \dfrac{i\omega\epsilon_r}{c^2}\tilde{E}_z \end{cases}$$

$$\Rightarrow \quad \frac{d^2\tilde{E}_z}{dx^2} - \left(k^2 - \frac{\omega^2\epsilon_r}{c^2}\right)\tilde{E}_z = 0$$

Solution: $\tilde{E}_z = Ae^{\alpha x} + Be^{-\alpha x}$ with $\alpha^2 = k^2 - \omega^2\epsilon_r/c^2$

Boundary & matching conditions at $x = 0, L$ and $x = s, L/2 - s$

and symmetry condition $\tilde{E}_z(x = L/2) = 0$ (anti-symmetric)

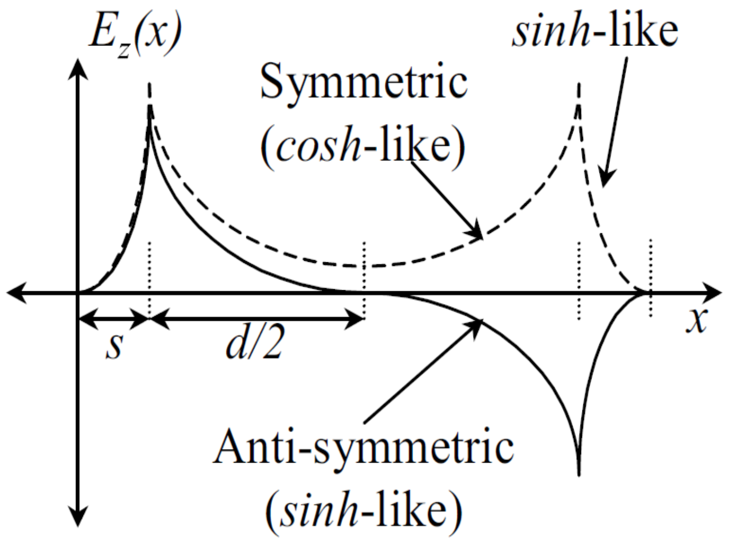
$\tilde{E}_z(x = s) = \tilde{E}_z(x = L/2 - s)$ (symmetric)

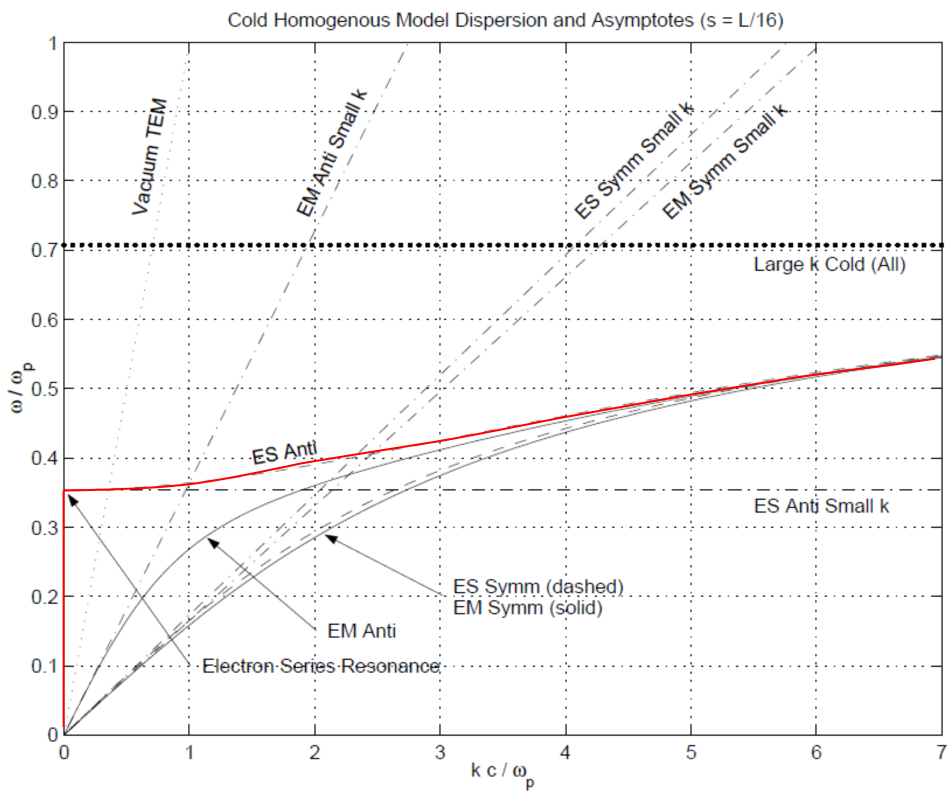
Dispersion Curves of Surface Waves

$$\coth \alpha s = \frac{\alpha}{\beta}\left(\frac{\omega_p^2}{\omega^2} - 1\right)\coth \beta d/2$$ antisymmetric mode

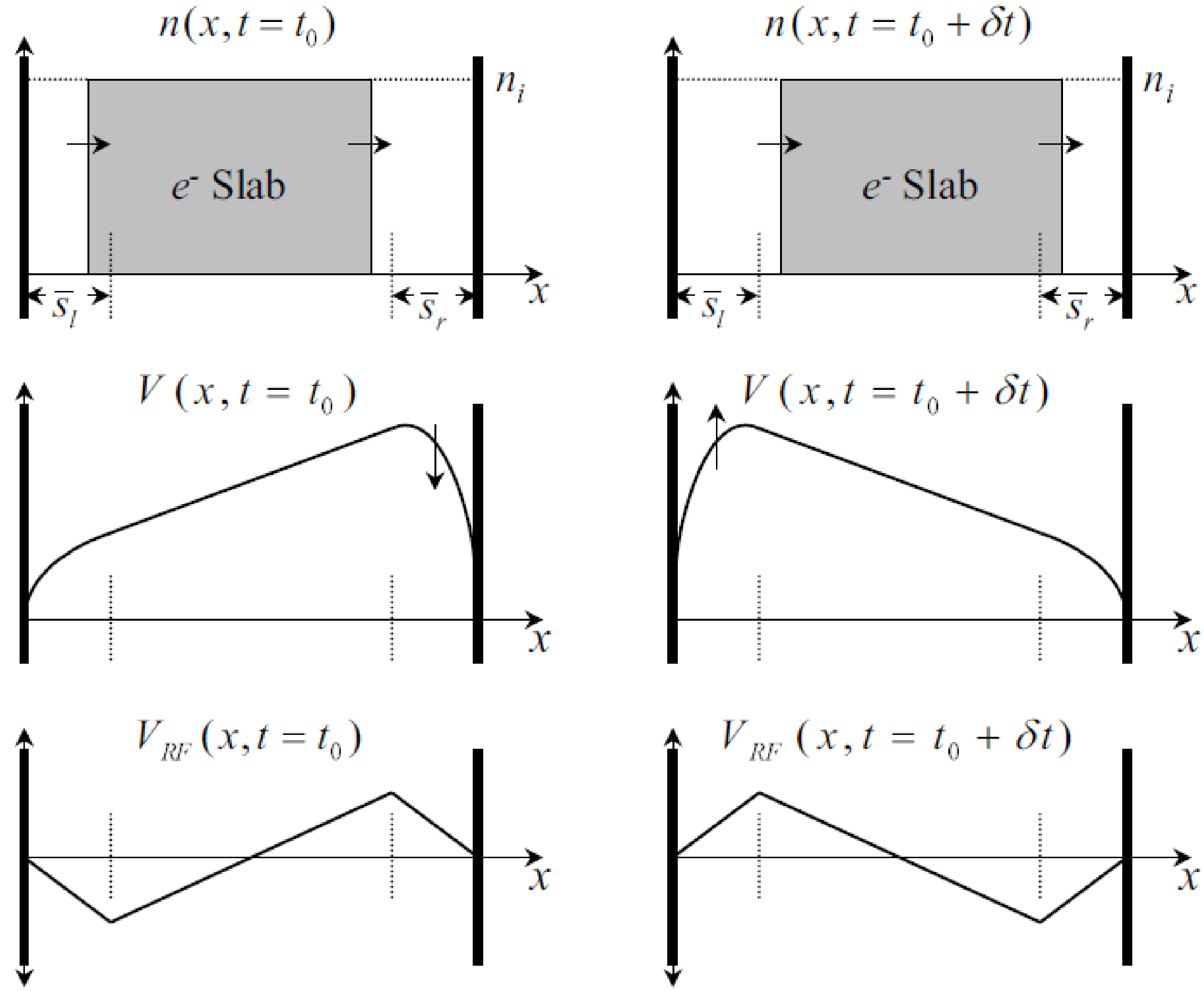
$$\coth \alpha s = \frac{\alpha}{\beta}\left(\frac{\omega_p^2}{\omega^2} - 1\right)\tanh \beta d/2$$ symmetric mode

$$\alpha^2 = k^2 - \omega^2/c^2 \qquad \beta^2 = k^2 - \omega^2/c^2 + \omega_p^2/c^2$$





Moving vs Fixed Slab Model

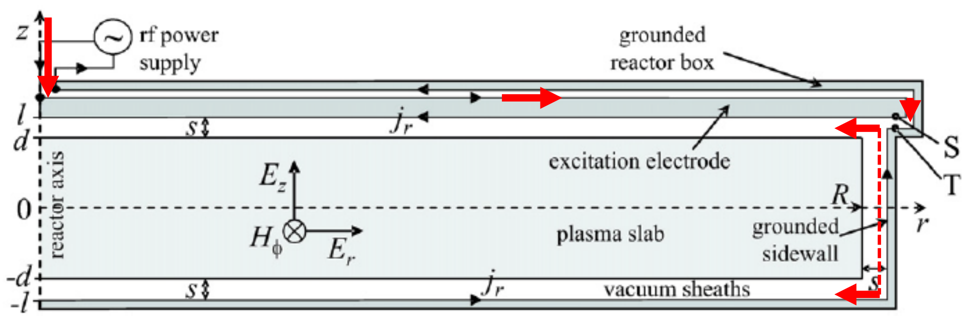


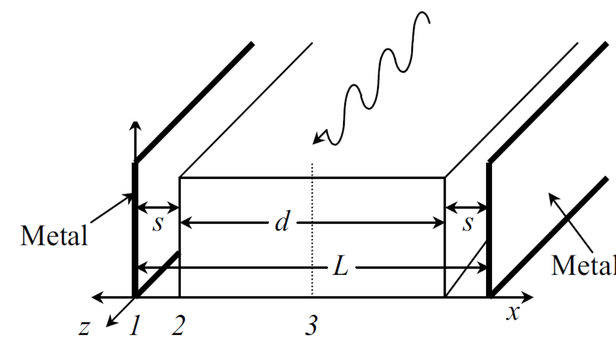
Moving and fixed slab models are equivalent for small amplitudes

Normal modes in a cylindrical CCP

[A.A. Howling et al, Thin Solid Films 515 (2007) 5059]

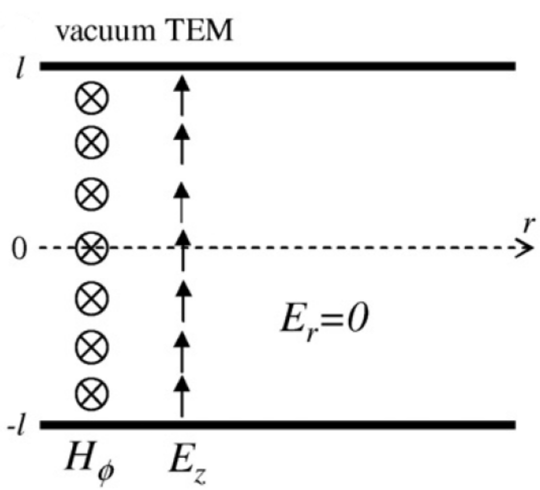
[L. Sansonnens et al, Plasma Sources Sci. Technol. 15 (2006) 302]

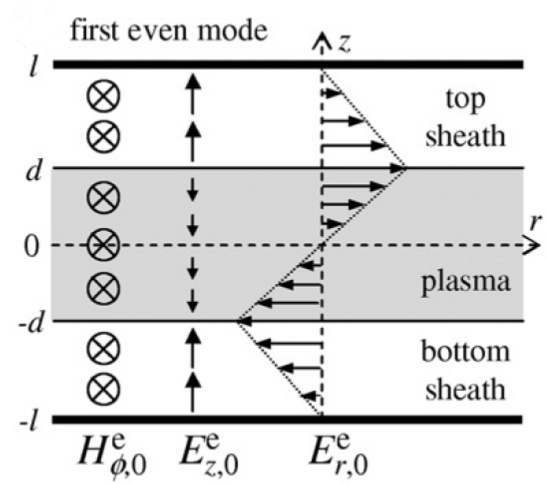


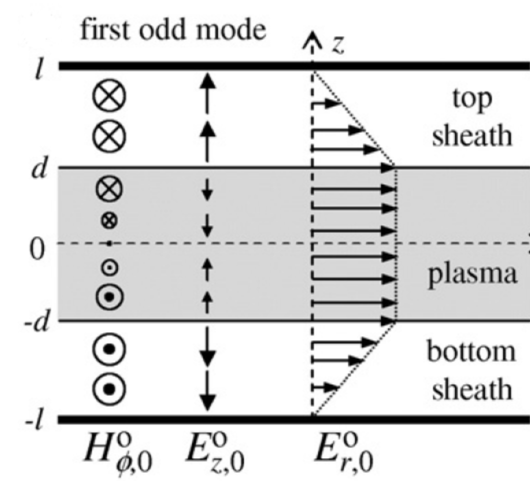


no plasma, TEM mode

with plasma, two quasi-TEM modes

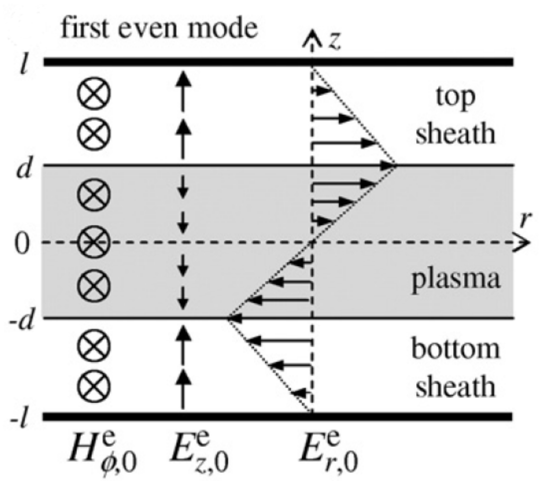


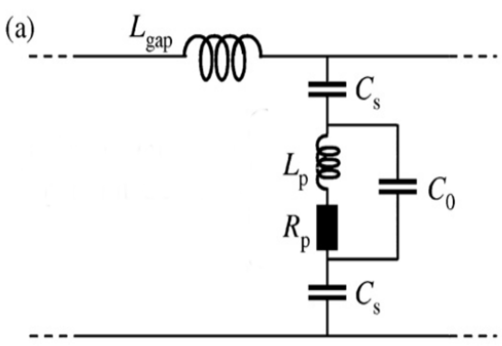




See also [M. Lieberman et al, Phys. Plasmas 23 (2016) 013501]

Even (Symmetric) Mode: Always Around





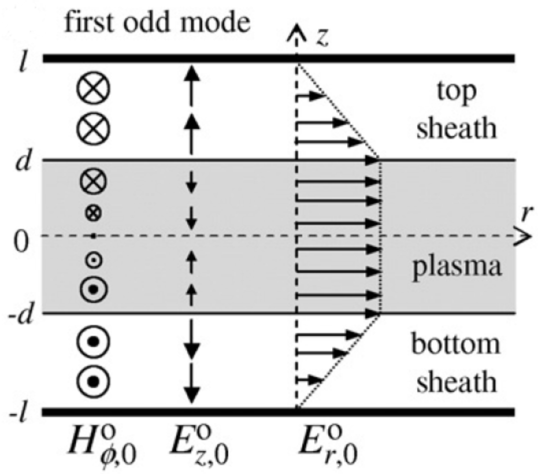
Compared to the vacuum case, effective relative permittivity is

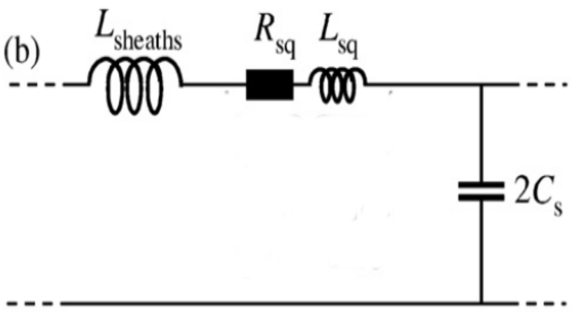
$$\varepsilon_{\rm eff} = \frac{s+d}{s}$$

Therefore, the effective EM velocity is

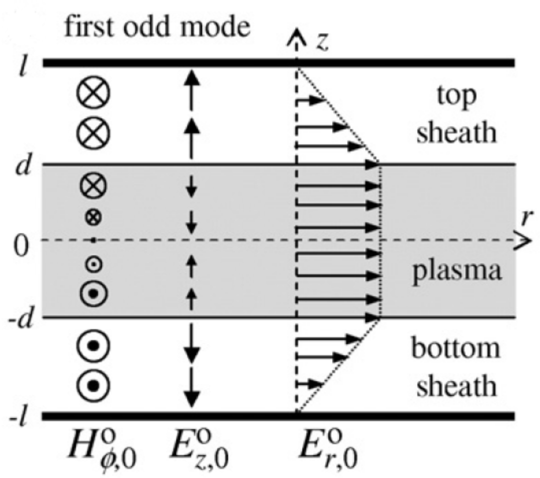
$$c_{\rm eff} = c/\sqrt{\varepsilon_{\rm eff}} = c/\sqrt{1+d/s} \ll c$$

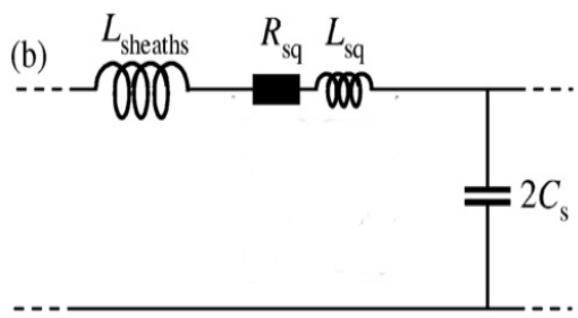
Physical Nature of the Odd (Antisymmetric) Mode

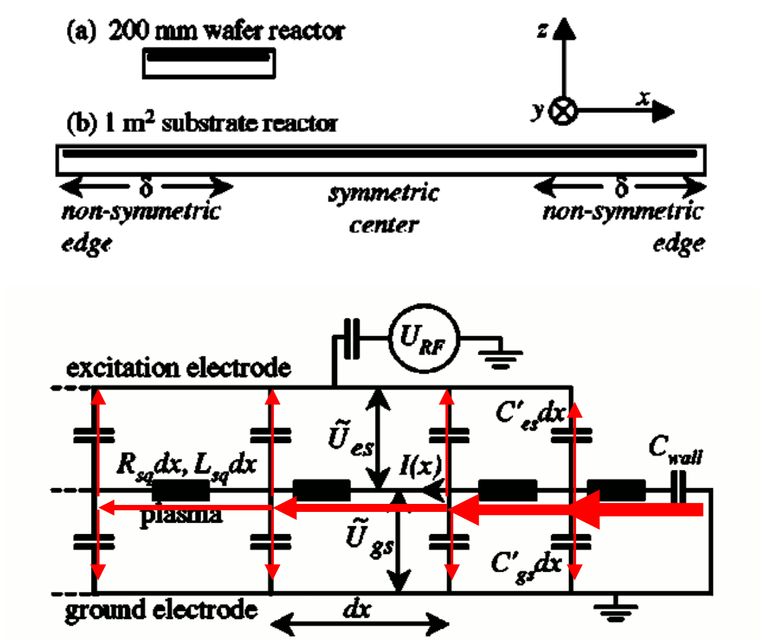




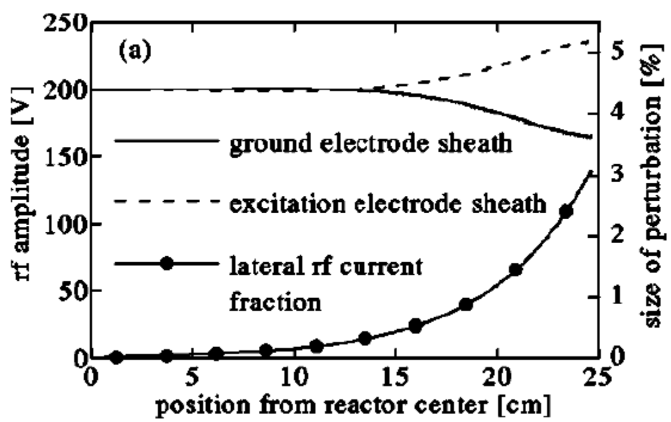
Physical Nature of the Odd (Antisymmetric) Mode





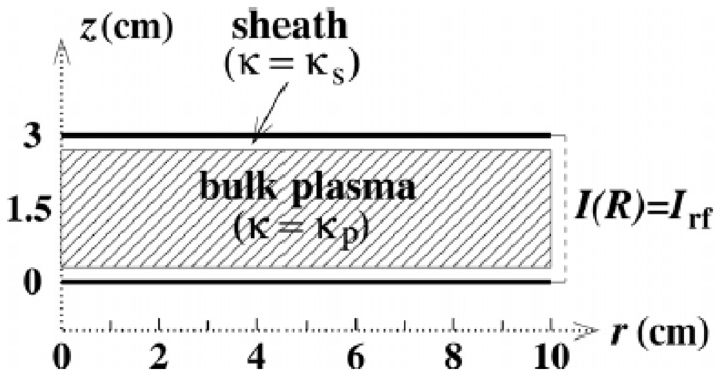


Radially nonuniform rf plasma potential!

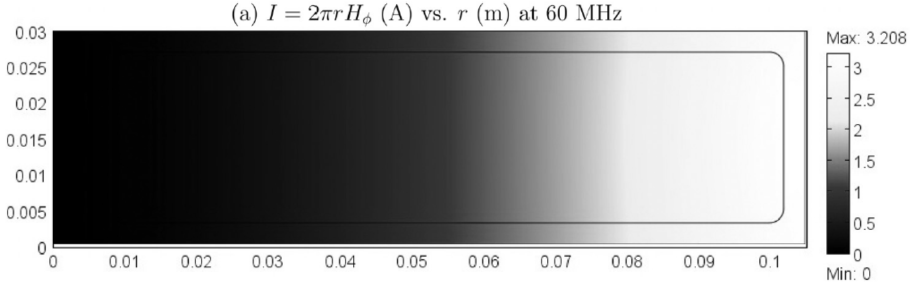


[A.A. Howling et al., J. Appl. Phys., 96, 5429 (2004)]

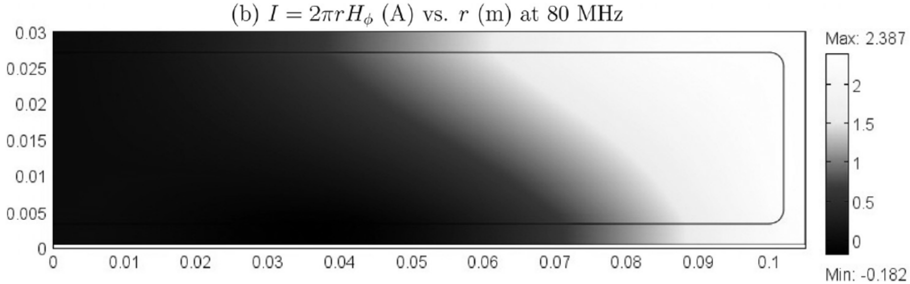
Excitation of the Odd Mode and Symmetry Breaking



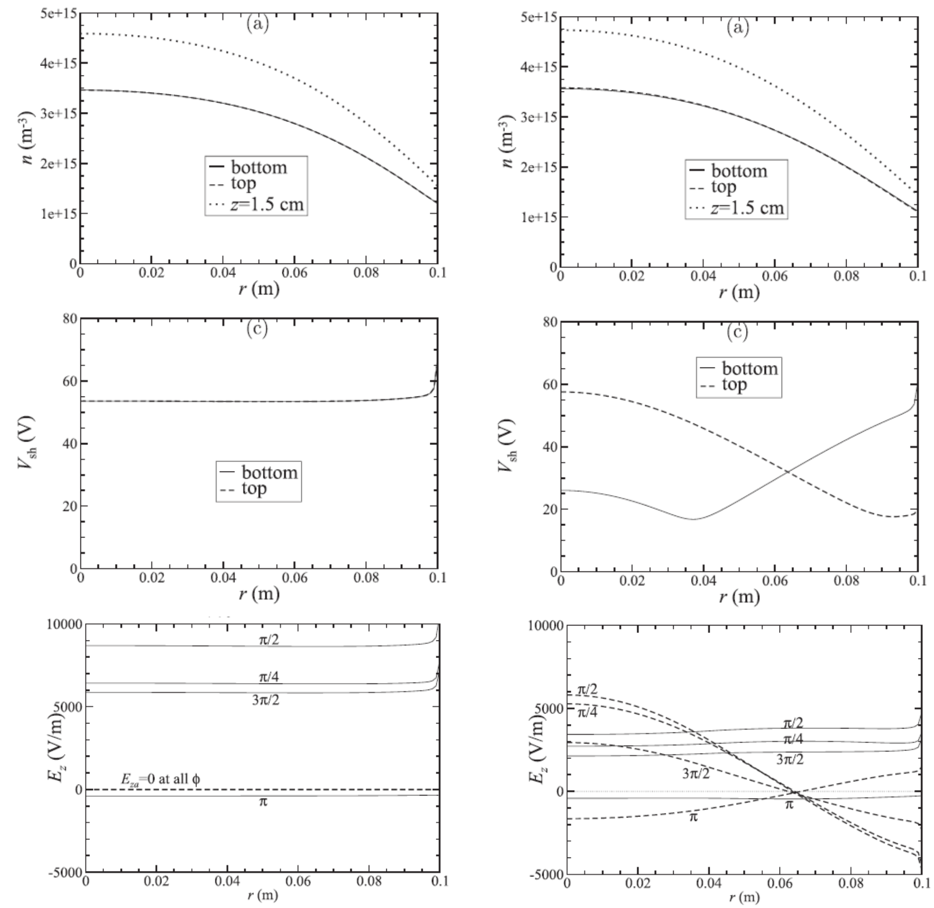
(a) $I = 2\pi r H_\phi$ (A) vs. r (m) at 60 MHz



(b) $I = 2\pi r H_\phi$ (A) vs. r (m) at 80 MHz

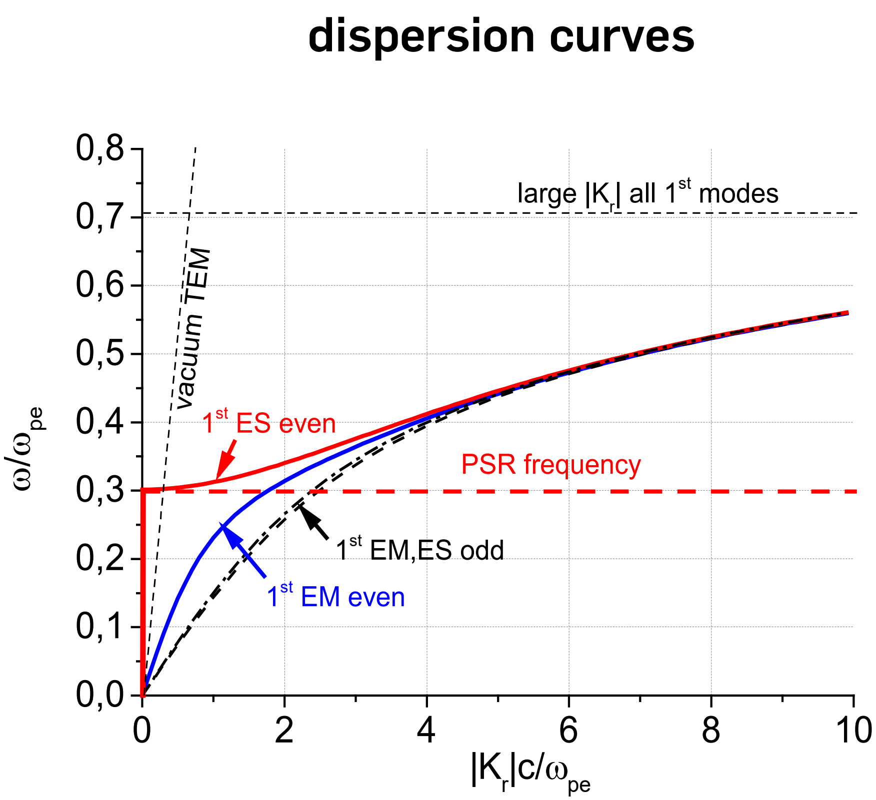


60 MHz 80 MHz



[E. Kawamura et al., Phys. Plasmas, 25, 093517 (2018)]

Dispersion Curves



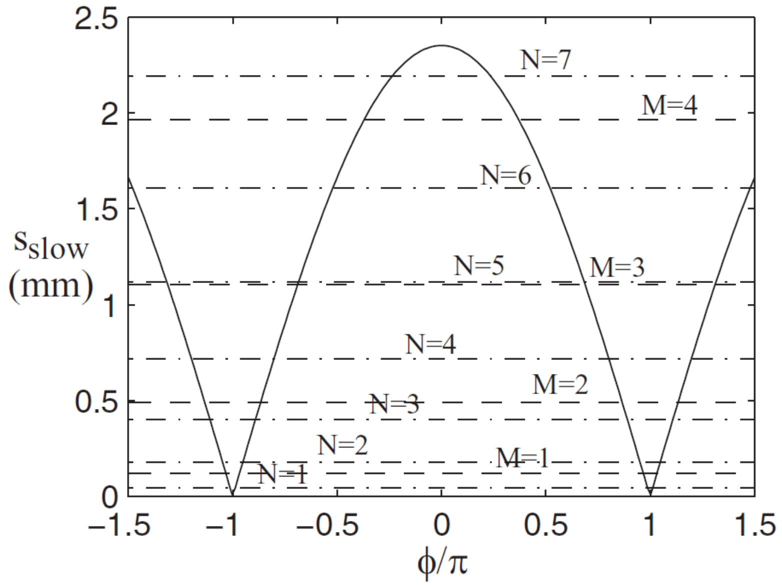
Electron drift diffusion-based fluid models are not sufficient:
[D. Eremin, IEEE Trans. Plasma Sci. 45(4) (2017) 527]

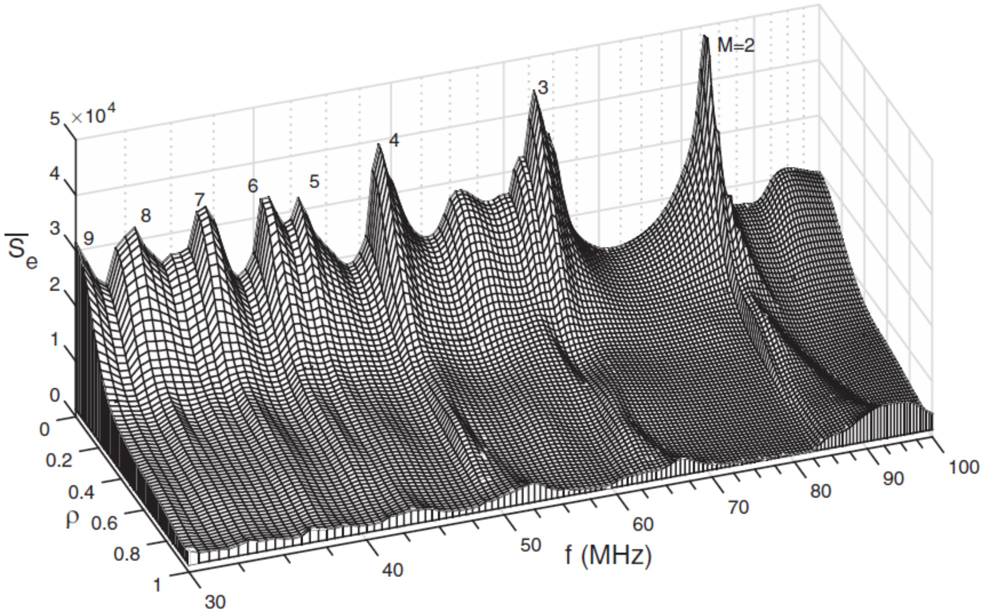
Spatial Mode Resonances

[M.A. Lieberman et al., Plasma Sources Sci. Technol. 24, 055011, (2015)]

PSR resonance: $N\omega = \omega_{PSR} = \omega_{pe}\sqrt{\frac{s}{l}}$

Spatial resonance: $k \approx \frac{\omega_{SW}}{c}\sqrt{\frac{l}{s}} = \frac{\chi_{0m}}{R}$ $\Rightarrow$ $\omega_{SW} = M\omega = \frac{c\chi_{0m}}{R}\sqrt{\frac{s}{l}}$





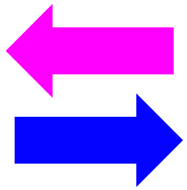
PIC Simulations of Normal Mode Excitation in CCPs

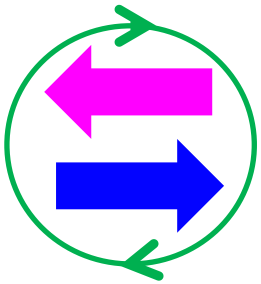
Particle-in-Cell (PIC) Algorithm

(Super)particles

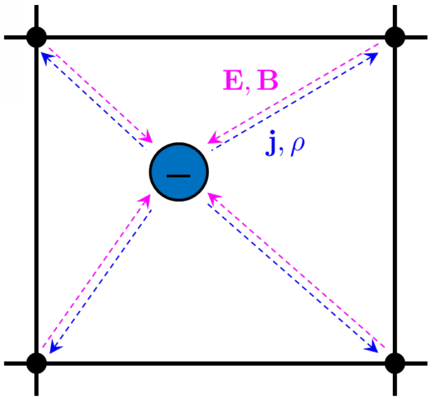
$$\frac{d}{dt}\mathbf{v} = \frac{q}{m}\left(\mathbf{E} + \mathbf{v}\times\mathbf{B}\right)$$
$$\frac{d}{dt}\mathbf{x} = \mathbf{v}$$

decoupled over Δt
(explicit)





coupled over Δt
(implicit)



Grid

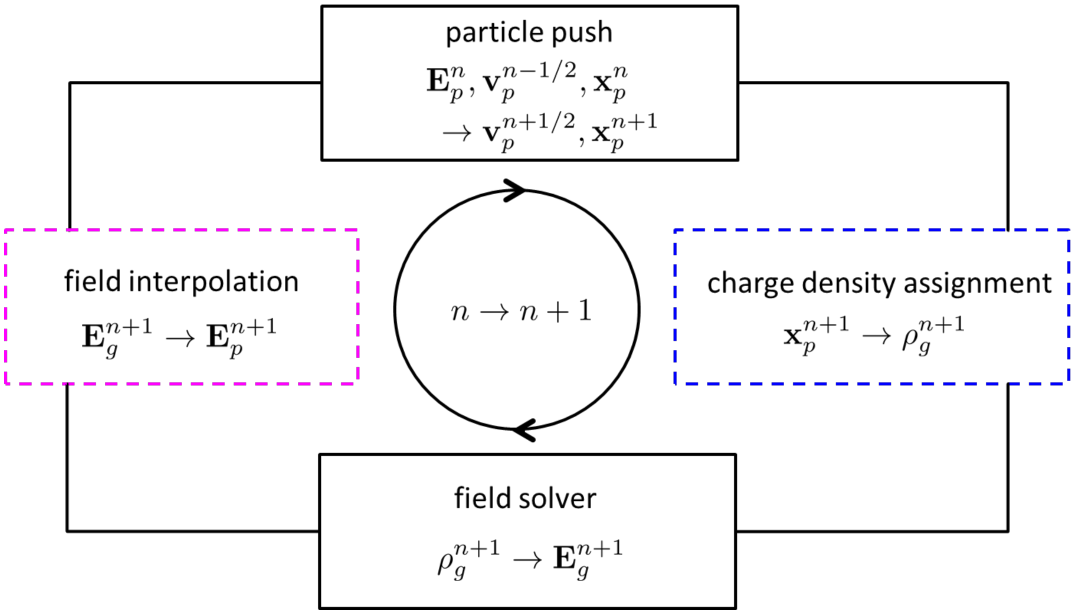
electromagnetic field model

$$\frac{\partial}{\partial t}\mathbf{E} = c^2\nabla\times\mathbf{B} - \frac{\mathbf{j}}{\epsilon_0}$$
$$\frac{\partial}{\partial t}\mathbf{B} = -\nabla\times\mathbf{E}$$
$$\nabla\cdot\mathbf{E} = \frac{\rho}{\epsilon_0}$$
$$\nabla\cdot\mathbf{B} = 0$$

electrostatic field model

$$\nabla\cdot\mathbf{E} = \frac{\rho}{\epsilon_0}$$
$$\left(\nabla^2\phi = -\frac{\rho}{\epsilon_0}\right)$$

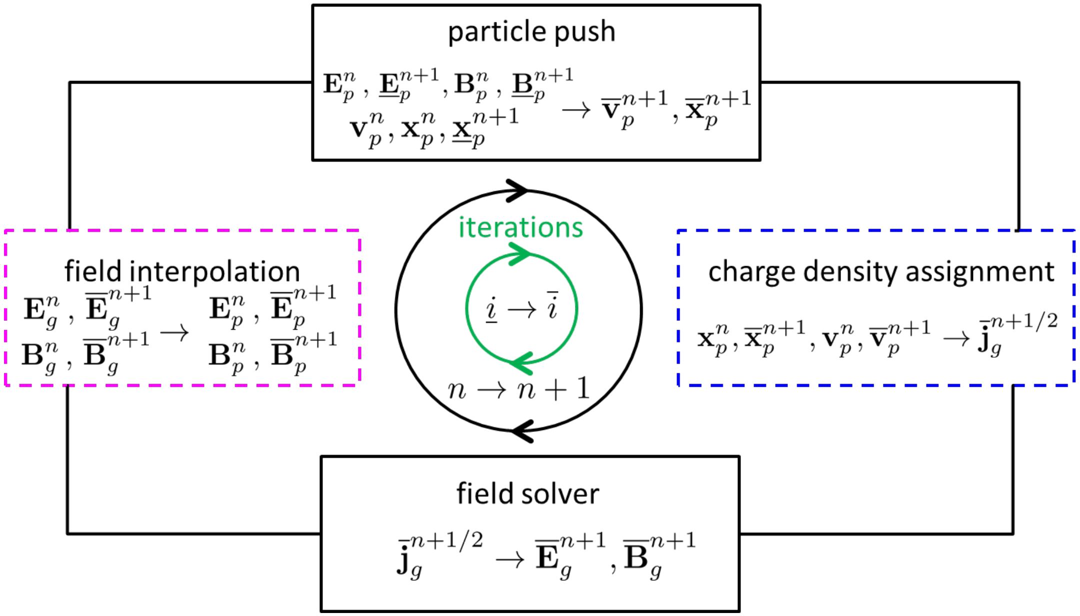
Explicit Electrostatic PIC



Simple algorithm:

- Detached evolution of fields and particles during a time step
- Exact momentum conservation, but numerical heating
- Restrictive stability conditions $\Delta x < \lambda_{De}\,,\ \Delta t < \omega_{pe}^{-1}$

Energy-conserving implicit electromagnetic PIC

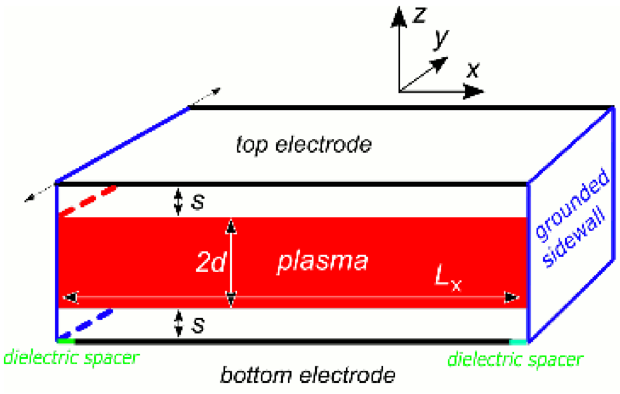


Advanced algorithm:

- Consistent evolution of fields and particles during a time step
- Exact energy conservation, thus no numerical heating
- High numerical stability independent of the plasma density
- Formulation for non-uniform grids to resolve, e.g., sheaths

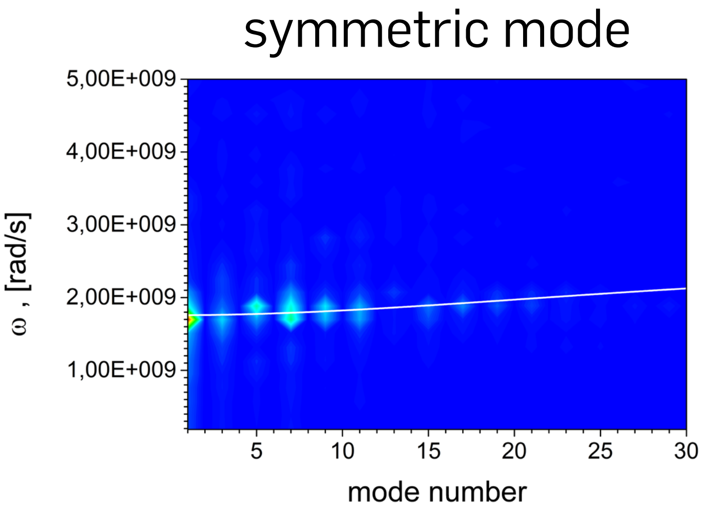
[S. Markidis and G. Lapenta, J. Comput. Phys. 230 (2011) 7037]
[G. Chen and L. Chacon, D.C. Barnes, J. Comput. Phys. 230 (2011) 7018]
[D. Eremin, J. Comput. Phys. 452 (2022) 110934]
[D. Eremin et al., Plasma Sources Sci. Technol. 32 (2023) 044007]

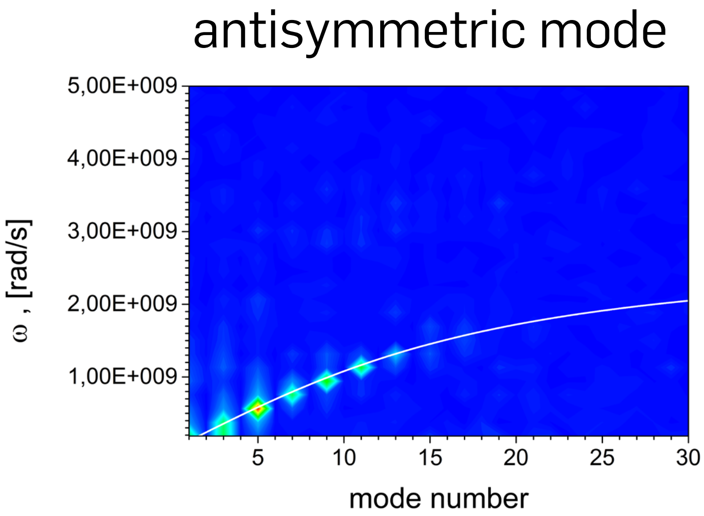
2D ES PIC Simulations in Cartesian Geometry



[D. Eremin et al. Plasma Process Polym. 14 (2017) 1600164]

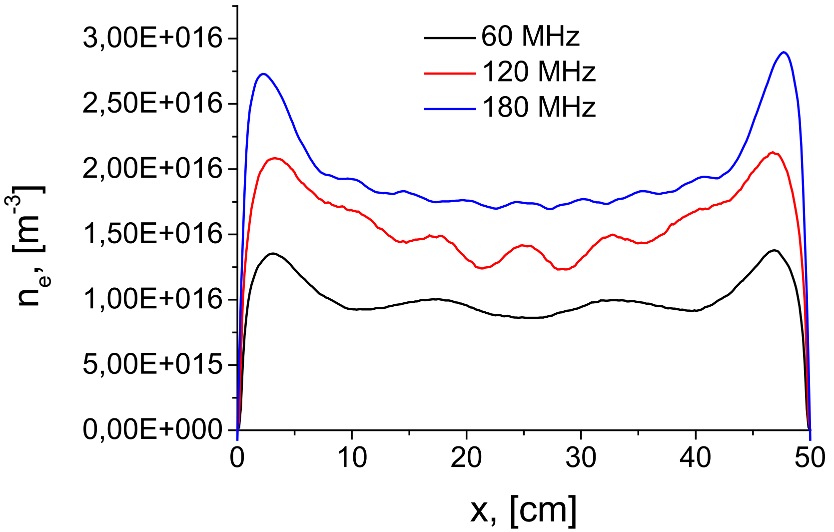
[D. Eremin IEEE Trans. Plasma Sci. 45 (2017) 527]

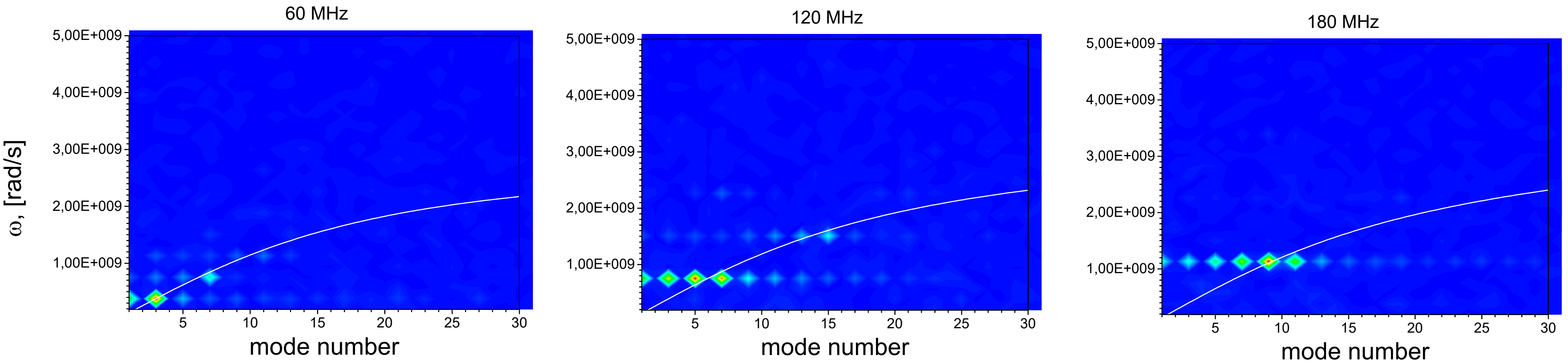




$$E_z \sim \sin\left(\frac{\pi(2n-1)x}{L_x}\right)$$

Forced Excitation of the Antisymmetric Mode





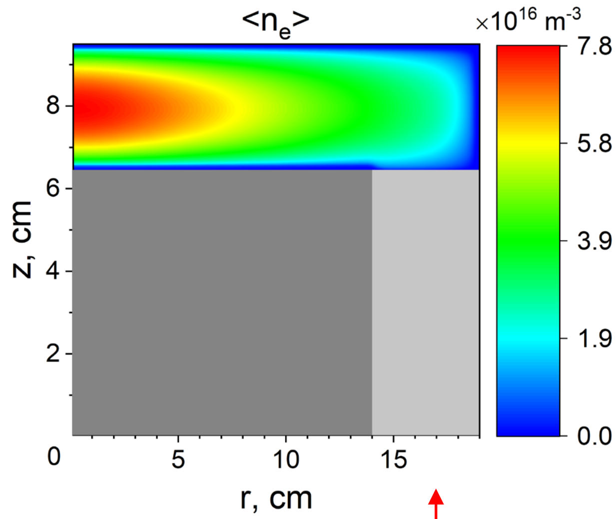
$$\omega/k \approx \omega_{pe}\sqrt{sd} \qquad k \to 0$$

2D EM PIC Simulations in Cylindrical Geometry

[D. Eremin et al., Plasma Sources Sci. Technol. 32 (2023) 044007]

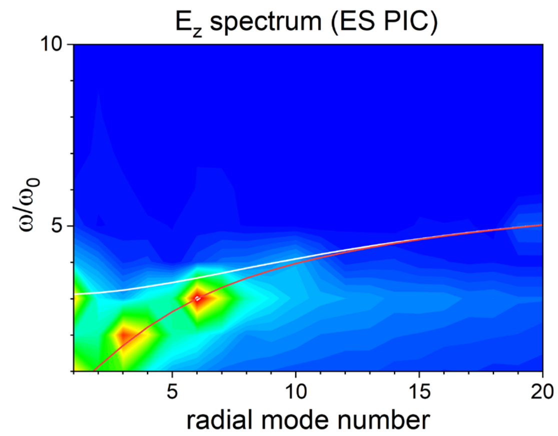
ECCOPIC2M code:

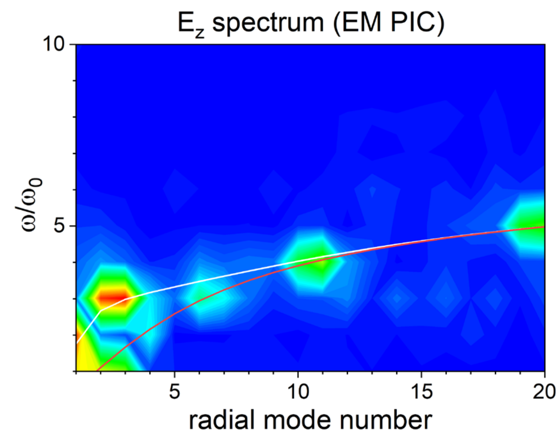
model geometry



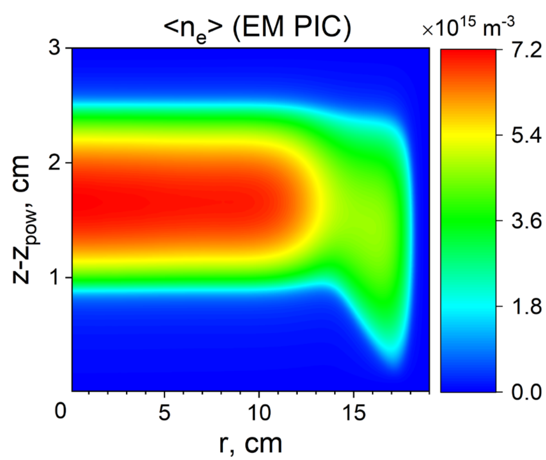
incoming TEM wave

Test 1: dispersion curves: PIC vs analytical prediction

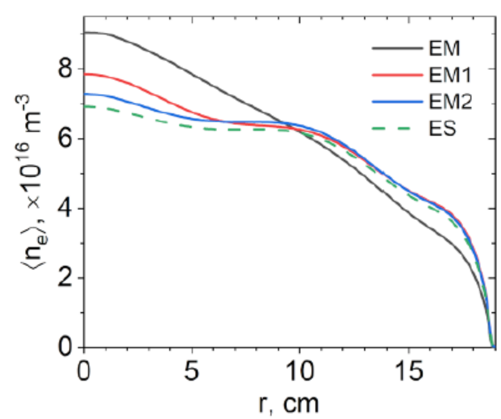




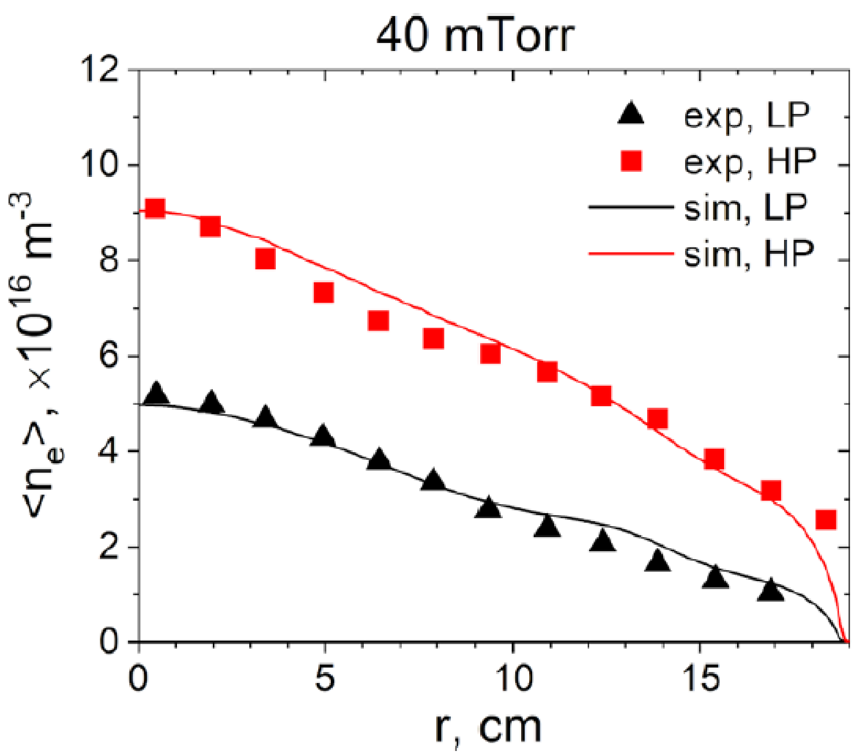
Test 2: 13.56 MHz case

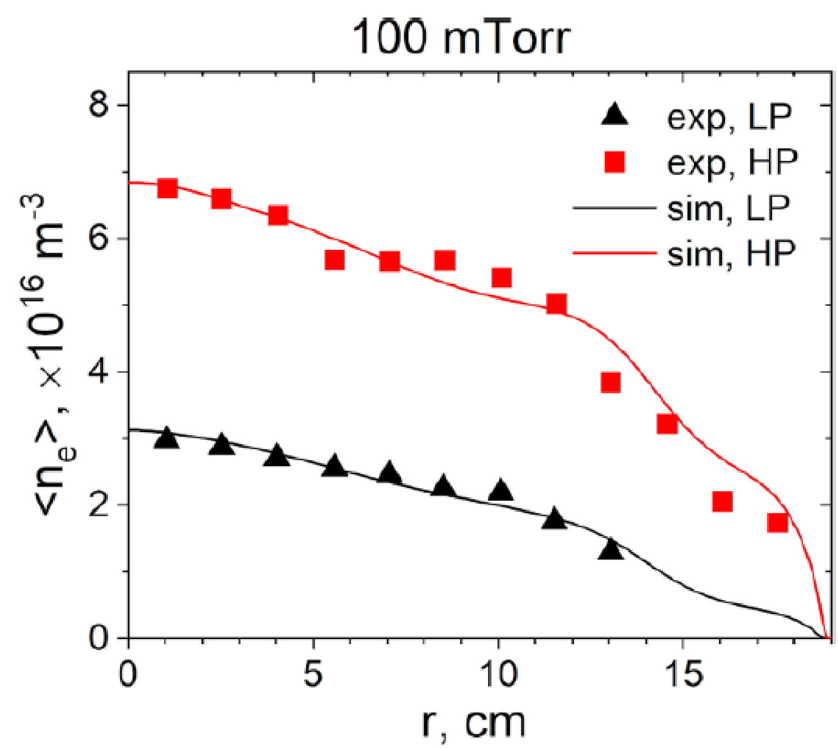


Test 3: EM to ES, 106 MHz



Validation of ECCOPIC2M





electron density comparison:

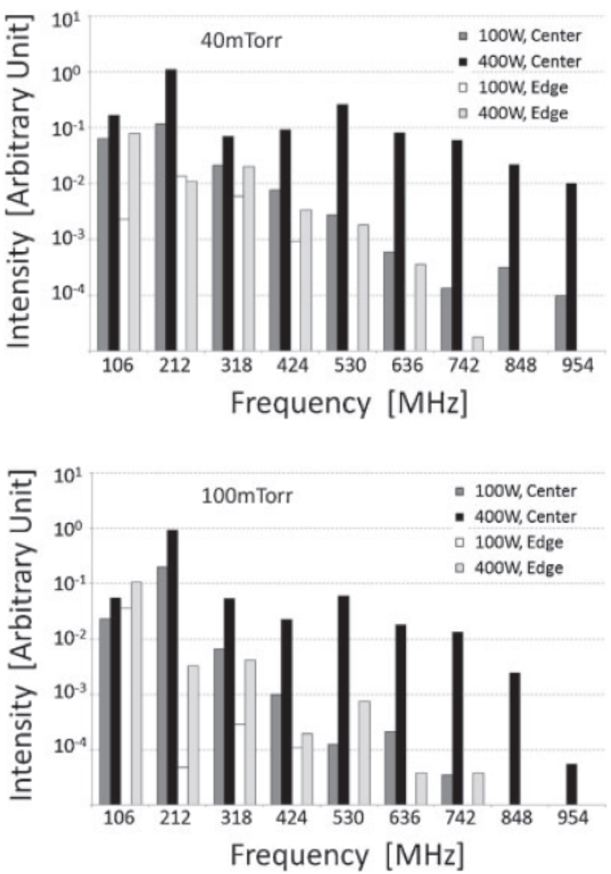
experiment [I. Sawada et al, Jpn. J. Appl. Phys. 53 (2014) 03DB01]

vs

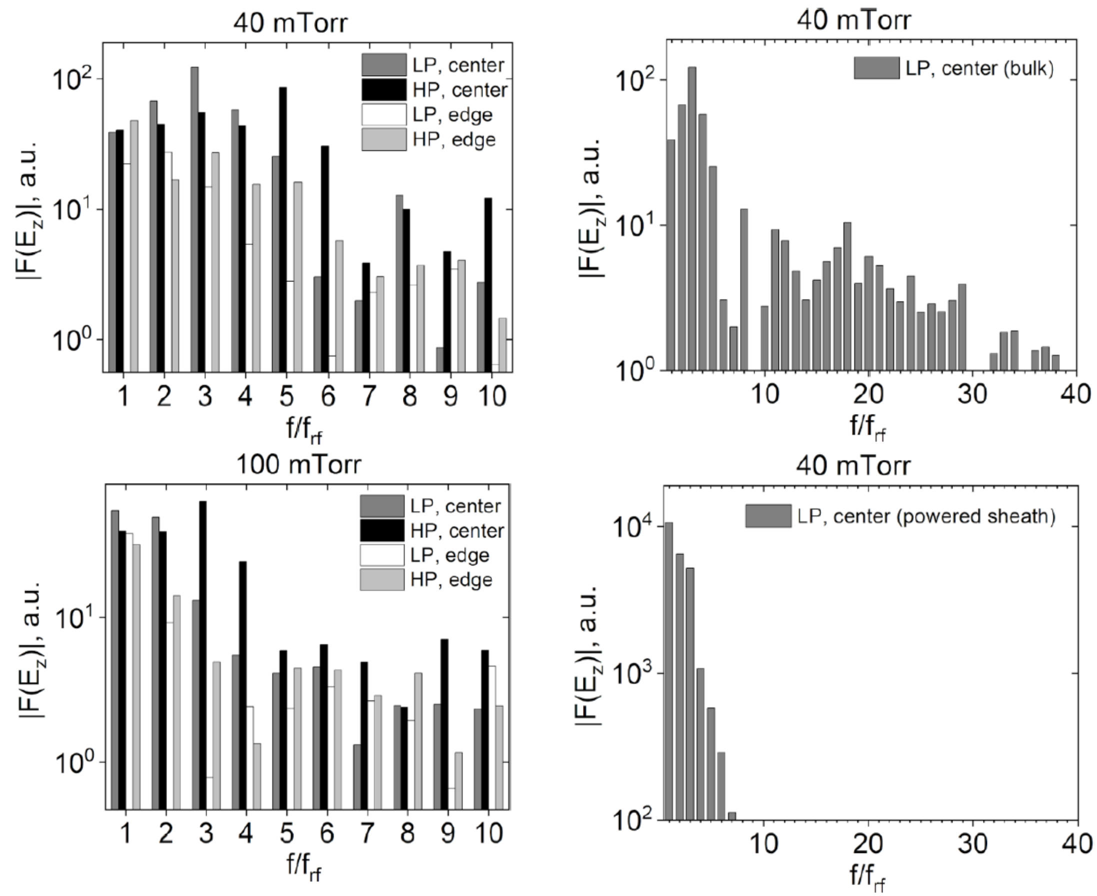
EM PIC/MCC simulations (ECCOPIC2M)

Harmonic content: experiment vs ECCOPIC2M

experiment:

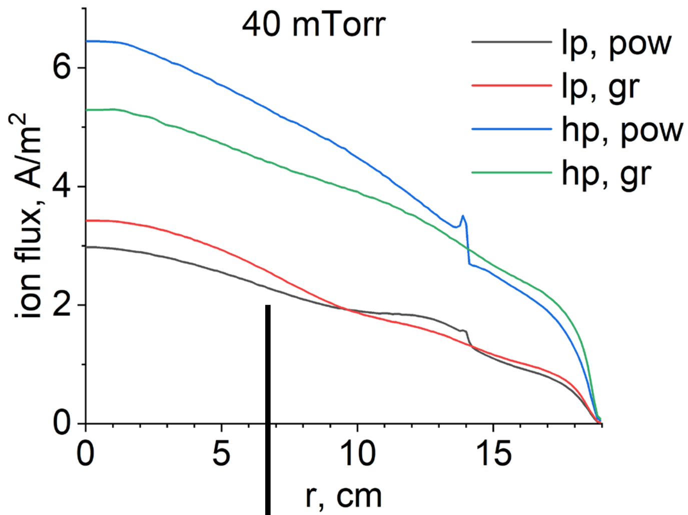


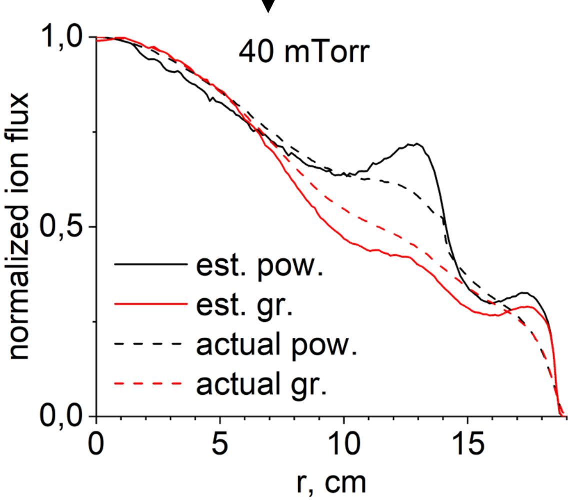
PIC/MCC simulations:



Radial Uniformity of Ion Flux and Energy

Ion flux



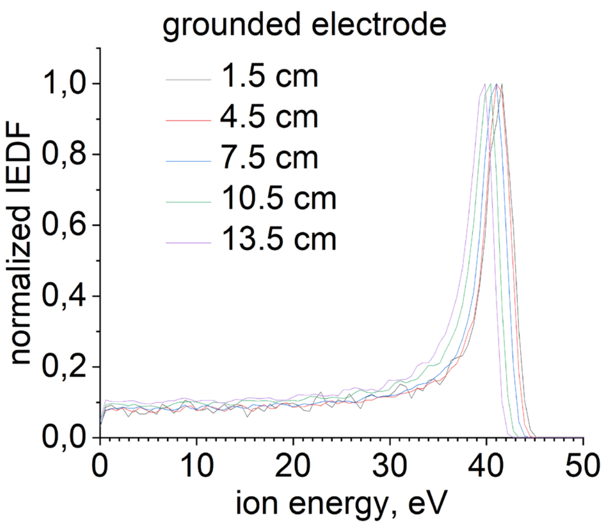


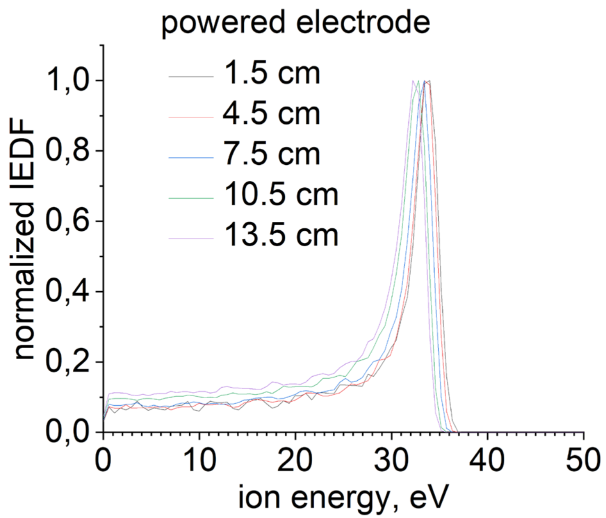
estimate from

the ionization source:

$$\Gamma(r) = -\int_0^{z_*} dz S(r,z)$$

IEDF, EM PIC/MCC

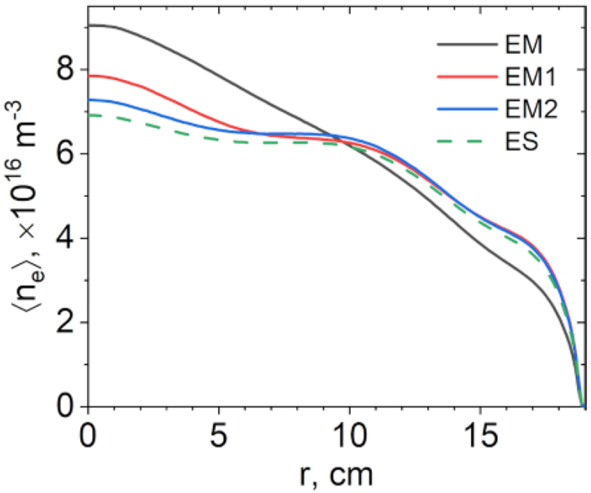




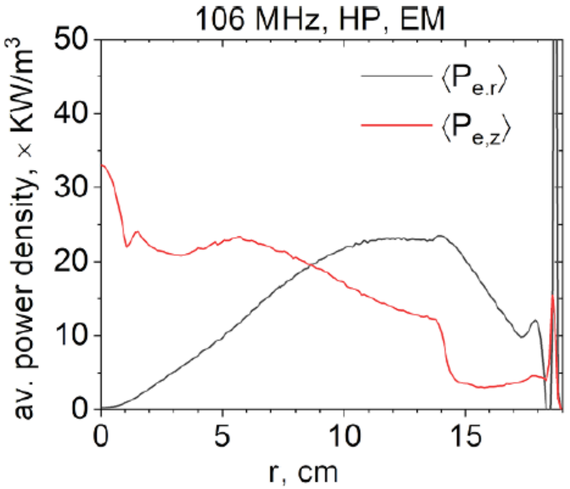
Power absorption by electrons: EM vs ES

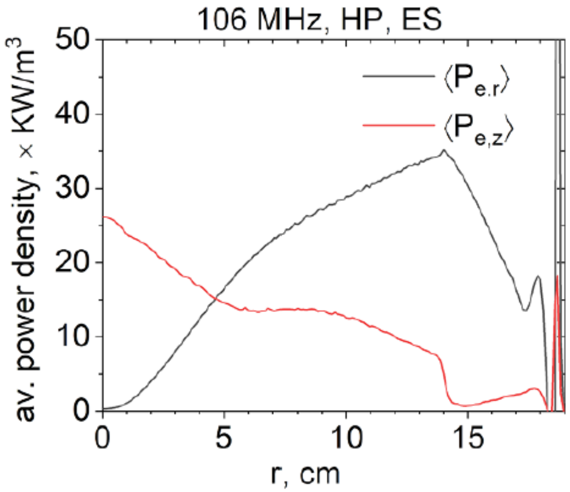
electron density

profile transition from ES to EM case



average absorbed power profiles

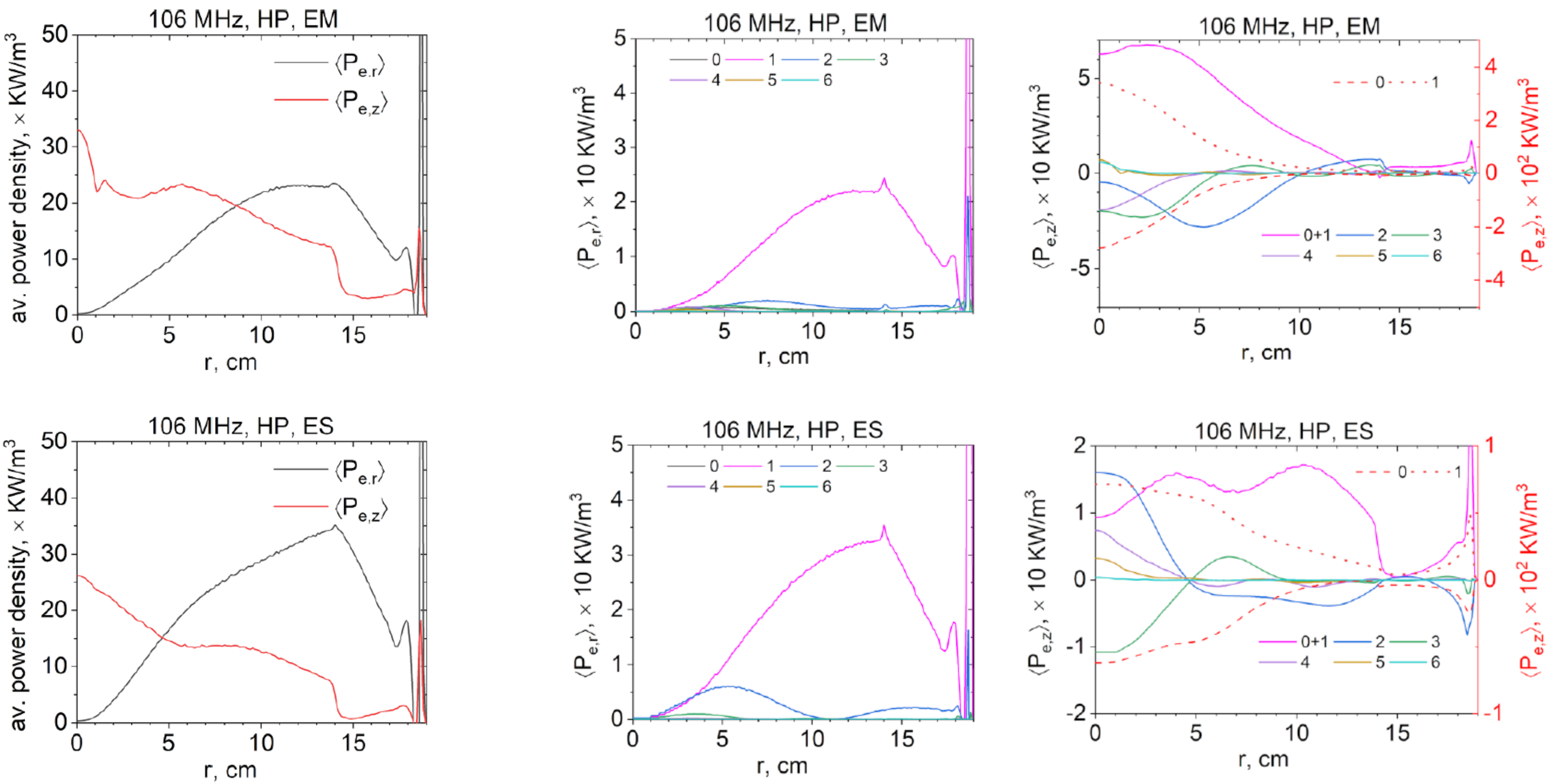




Radial power absorption is not due to the inductive heating, but due to the antisymmetric mode!

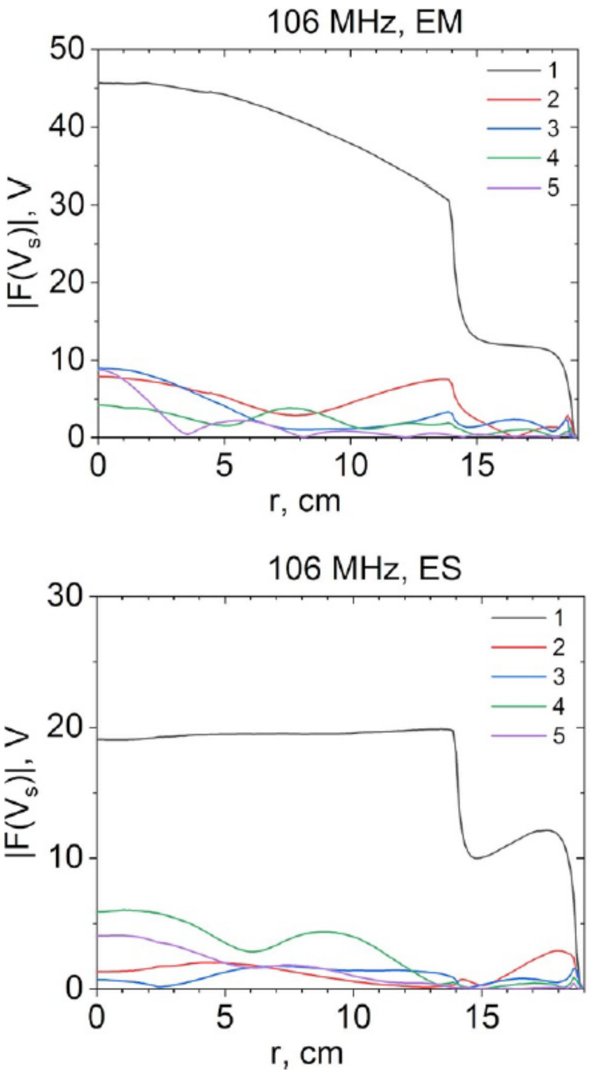
Harmonic analysis

contributions to the average power from separate harmonics

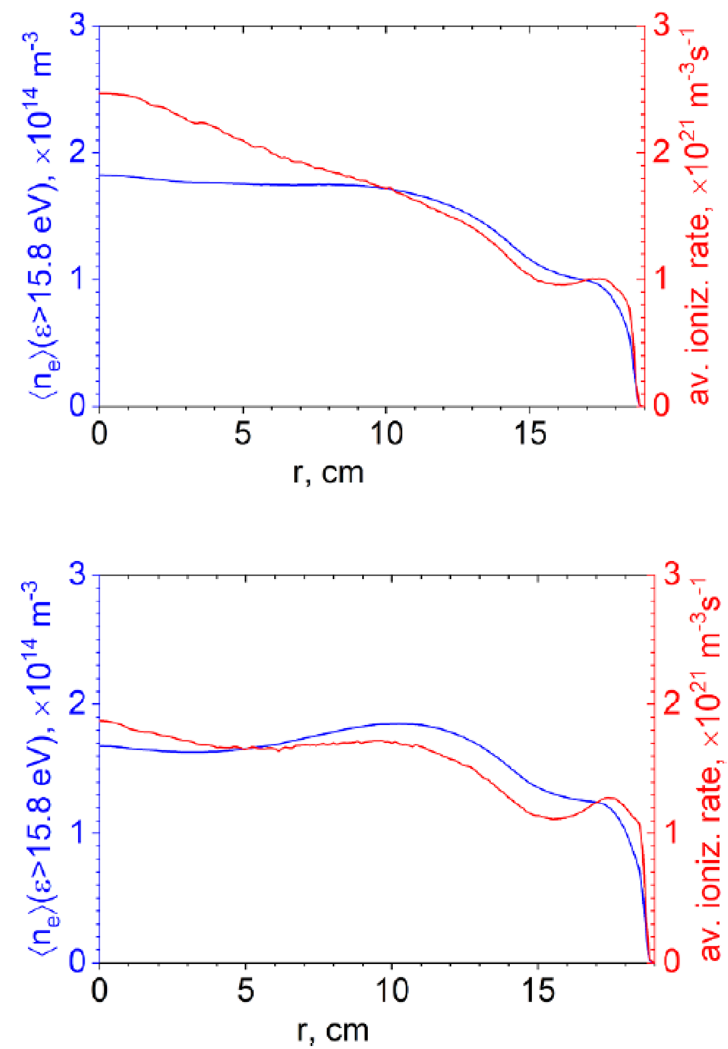


Electron Energization by Different Modes

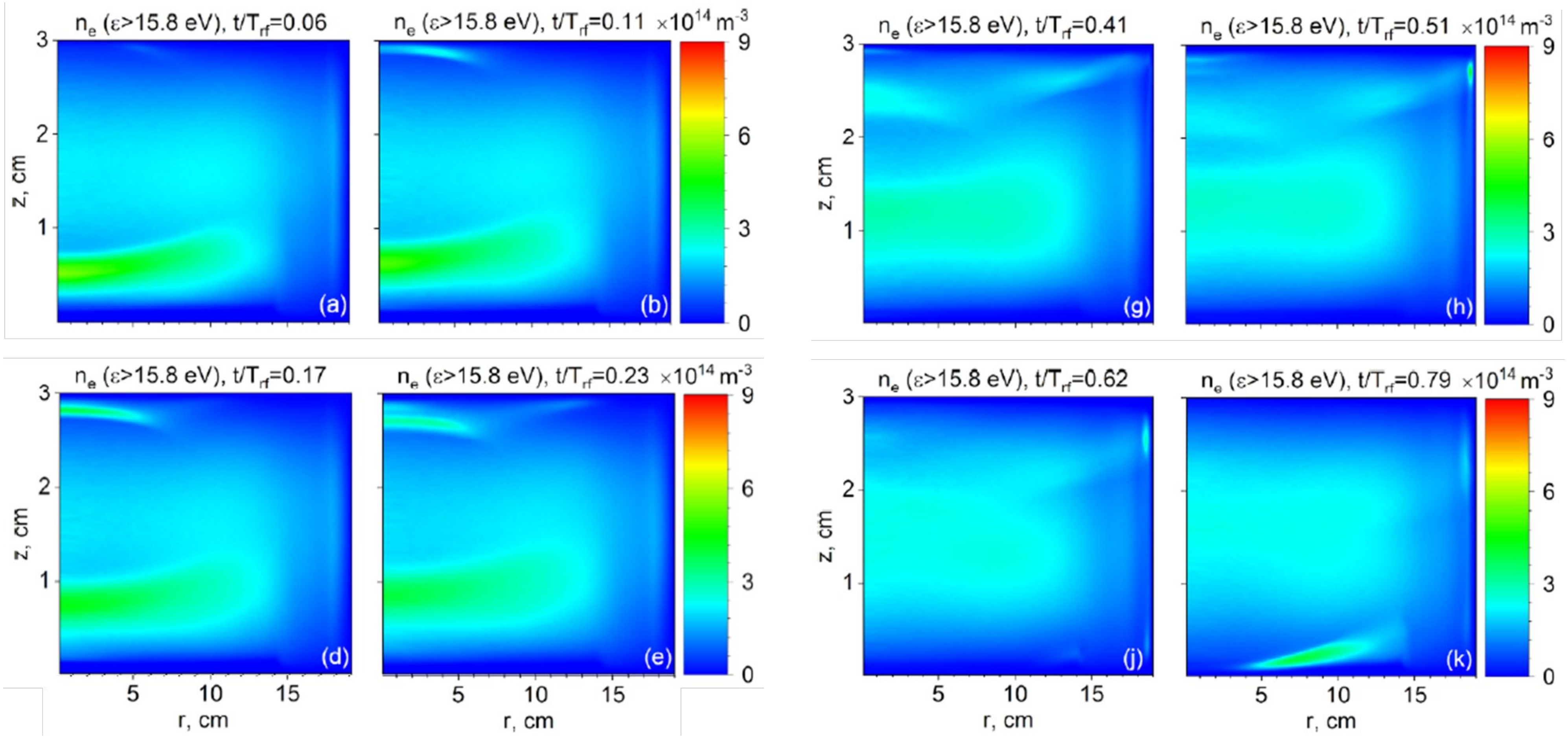
Surface mode harmonic amplitudes



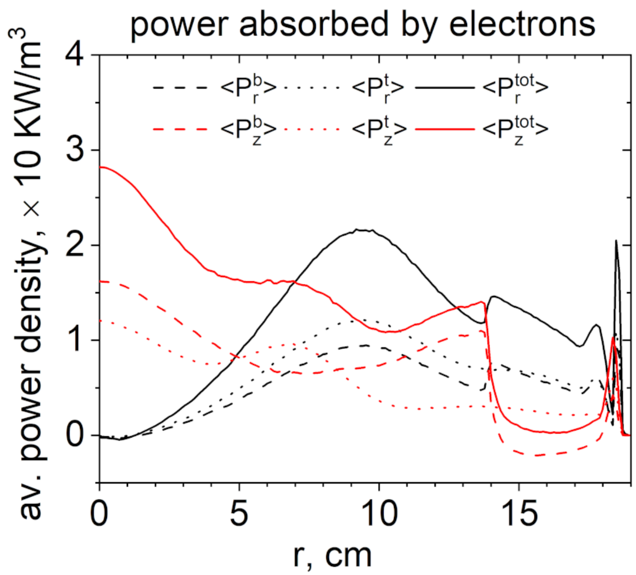
Energetic electron and ionization rate profiles

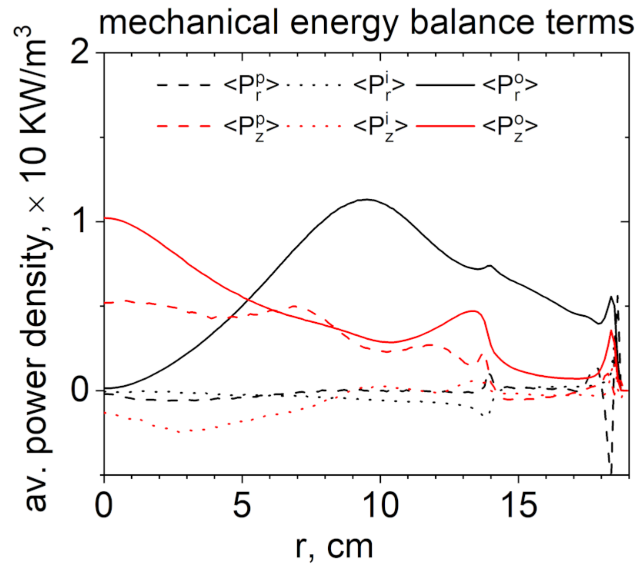


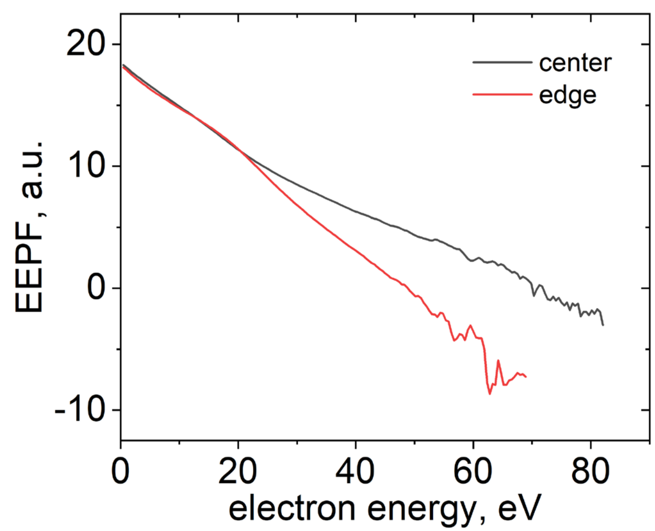
Electron Energization by Different Modes (cont.)



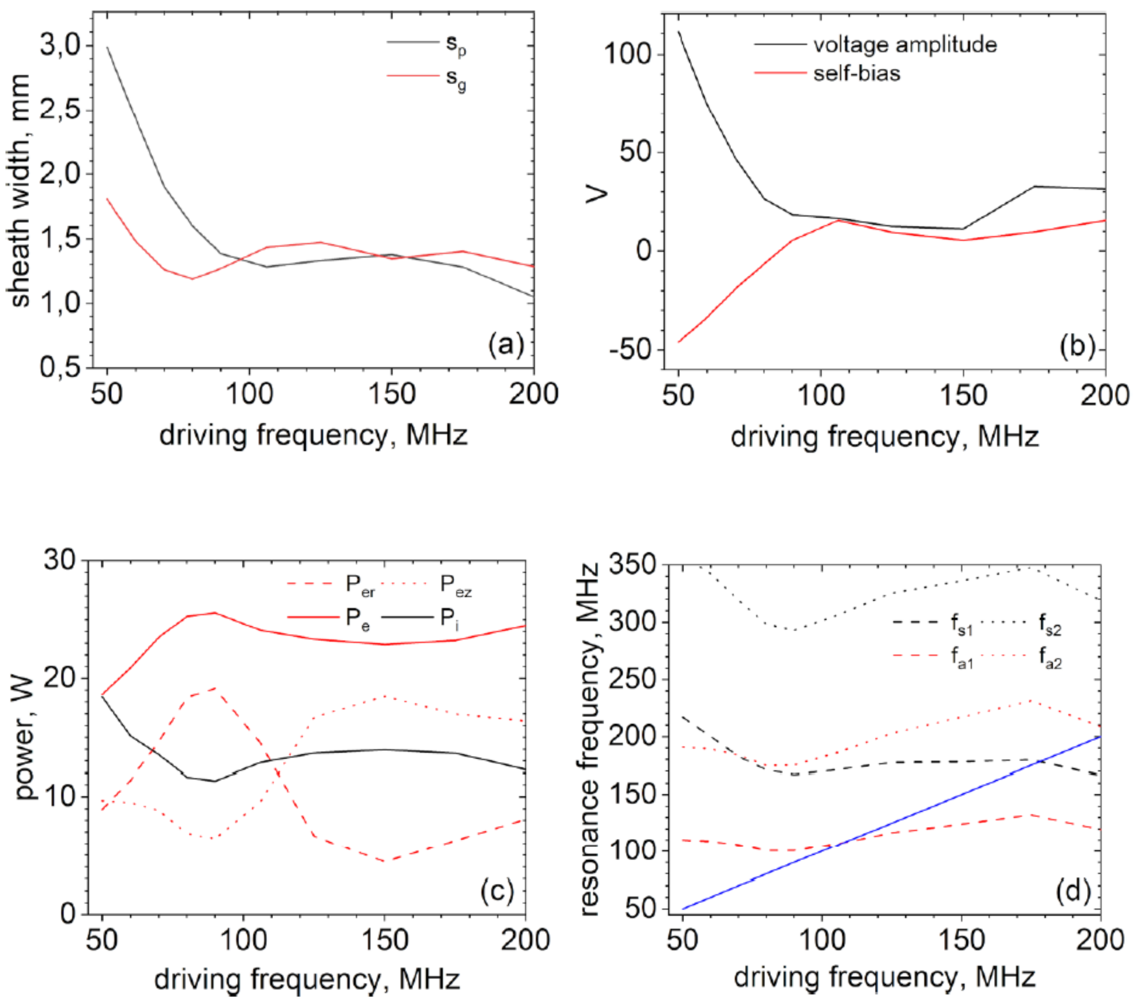
Mechanical Energy Balance Analysis

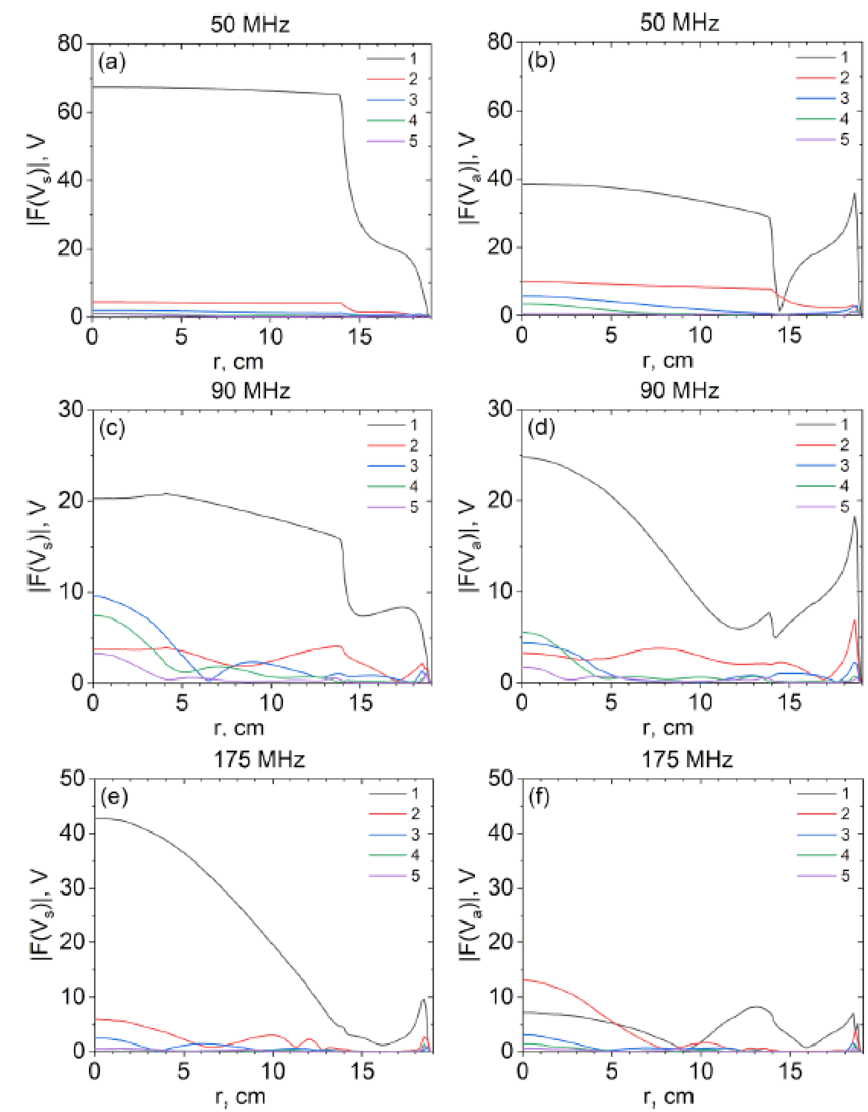






Driving Frequency Scan and Resonant Mode Excitation





Conclusions

- An energy- and charge-conserving implicit electromagnetic particle-in-cell/Monte Carlo code ECCOPIC2M is validated with VHF CCP experimental data for four cases with different gas pressure and absorbed power
- Comparison of the power absorption radial profiles between EM and ES simulations reveals that it alone does not govern the radial plasma density profile nonuniformity
- A more important parameter is the radially resolved EEDF, which reflects amount of energetic electrons above the ionization threshold, since the ionization profile determines the plasma density and ion flux radial profiles. It is shown that electrons are energized primarily due to interaction with (symmetric) surface modes at the sheath. The corresponding interaction is manifested through a significant “pressure heating” contribution in the mechanical energy balance. The antisymmetric modes heat electrons primarily via the inefficient Ohmic heating
- A driving frequency scan demonstrates that various surface mode resonances result in peaks on the total power absorption in the radial (for asymmetric modes) and the axial (for symmetric modes) direction

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