Experimental and simulation study of a capacitively coupled oxygen discharge driven by tailored voltage waveforms

A. Derzsi, I. Korolov, Z. Donkó

Wigner Research Centre for Physics, Hungarian Academy of Sciences, Budapest, Hungary

T. Lafleur, B. Bruneau, E. Johnson, J.P. Booth

LPP-CNRS, LPICM-CNRS, Ecole Politechnique, Palaiseau, France

A.R. Gibson, D. O'Connell, T. Gans

York Plasma Institute, Department of Physics, University of York, UK

Contents

- PIC/MCC model for O_2 discharges
- Multifrequency excitation of capacitive O_2 discharges

  Comparison of simulation and experimental results (dc self-bias, discharge power, ion flux, flux energy distribution of ions, spatiotemporal distribution of the excitation rate)

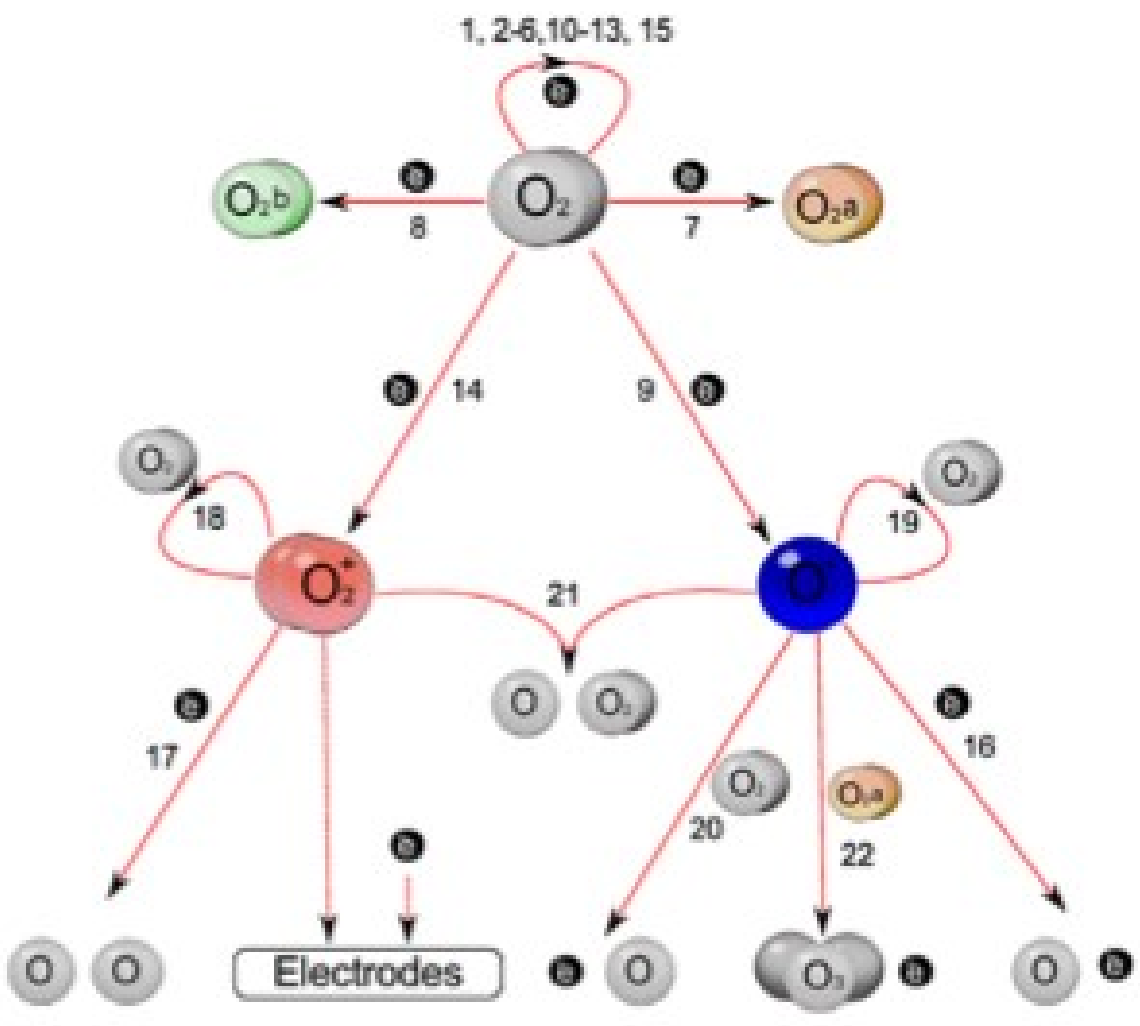
  - peaks / valleys waveforms

  - saw-tooth waveforms

PIC/MCC model for O_2 discharges: particles and processes

- traced particles: e^-, O_2^+, O^-

Elementary processes



	Reaction	Process	C.S.
1	$e^- + O_2 \longrightarrow O_2 + e^-$	Elastic scattering	1
2	$e^- + O_2(r=0) \longrightarrow e^- + O_2(r>0)$	Rotational excitation	2
3	$e^- + O_2(v=0) \longrightarrow e^- + O_2(v=1)$	Vibrational excitation	2
4	$e^- + O_2(v=0) \longrightarrow e^- + O_2(v=2)$	Vibrational excitation	2
5	$e^- + O_2(v=0) \longrightarrow e^- + O_2(v=3)$	Vibrational excitation	2
6	$e^- + O_2(v=0) \longrightarrow e^- + O_2(v=4)$	Vibrational excitation	2
7	$e^- + O_2 \longrightarrow e^- + O_2(a^1\Delta_g)$	Metastable excitation (0.98 eV)	2
8	$e^- + O_2 \longrightarrow e^- + O_2(b^1\Sigma_g)$	Metastable excitation (1.63 eV)	2
9	$e^- + O_2 \longrightarrow O + O^-$	Dissociative attachment	2
10	$e^- + O_2 \longrightarrow e^- + O_2$	Excitation (4.5 eV)	2
11	$e^- + O_2 \longrightarrow O(^3P) + O(^3P) + e^-$	Dissociation (6.0 eV)	2
12	$e^- + O_2 \longrightarrow O(^3P) + O(^1D) + e^-$	Dissociation (8.4 eV)	2
13	$e^- + O_2 \longrightarrow O(^1D) + O(^1D) + e^-$	Dissociation (9.97 eV)	2
14	$e^- + O_2 \longrightarrow O_2^+ + e^- + e^-$	Ionization	3
15	$e^- + O_2 \longrightarrow e^- + O + O(3p^3P)$	Dissociative excitation (14.7 eV)	2
16	$e^- + O^- \longrightarrow e^- + e^- + O$	Electron impact detachment	2
17	$e^- + O_2^+ \longrightarrow O(^3P) + O(^1D)$	Dissociative recombination	2
18	$O_2^+ + O_2 \longrightarrow O_2 + O_2^+$	Elastic scattering[b]	3
19	$O^- + O_2 \longrightarrow O^- + O_2$	Elastic scattering	3
20	$O^- + O_2 \longrightarrow O + O_2 + e^-$	Detachment	3
21	$O^- + O_2^+ \longrightarrow O + O_2$	Mutual neutralization	3
22	$O^- + O_2(a^1\Delta_g) \longrightarrow O_3 + e^-$	Associative detachment	4

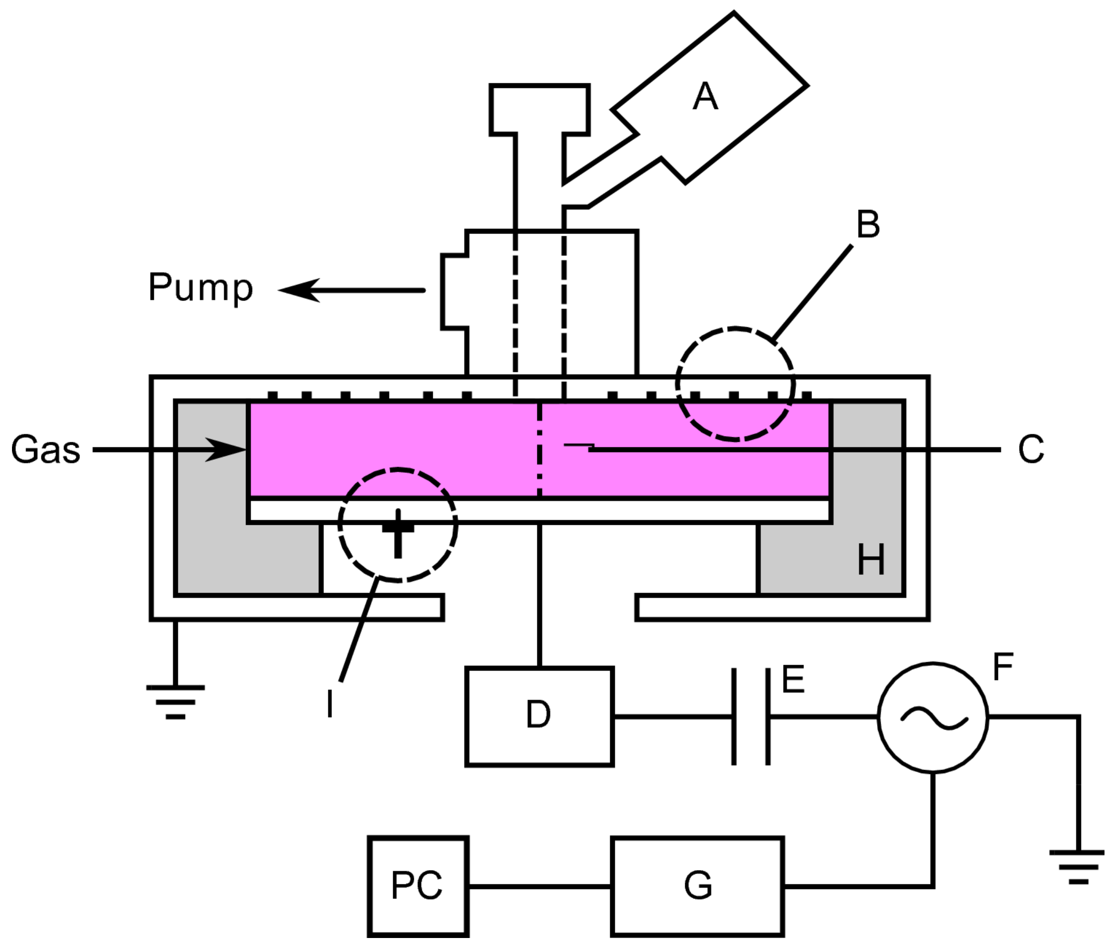
Cross Sections

[1] Biagi-v8.9 database, www.lxcat.net
[2] V. Vahedi, M. Surendra, *Computer Phys. Commun*. **87** 179 (1995) – xpdp1
[3] J.T. Gudmundsson, E. Kawamura, M.A. Lieberman, *Plasma Sources Sci. Technol*. **22** 035011 (2013)
[4] F. X. Bronold, K. Matyash, D. Tskhakaya, R. Schneider and H Fehske, *J. Phys. D: Appl. Phys*. **40** 6583 (2007)

Measurements in O_2 discharges

DRACULA CCP plasma reactor

LPP-CNRS, Ecole Polytechnique, Palaiseau



A – mass spectrometer

B – ion flux probe array (16)

C – hairpin resonator probe

D – voltage-current probe

E – blocking capacitor (4.5 nF)

F – RF power amplifier

G – arbitrary function generator

H – dielectric spacers between the electrodes

I – high-voltage probe

- dc self-bias voltage
- discharge power
- ion flux
- flux energy distribution of ions

experiment ⟷ simulation

Discharge conditions

Multifrequency tailored voltage waveform

$$\phi(t) = \sum_{k=1}^{N} \phi_k \cos(2\pi k f_1 t + \Theta_k)$$

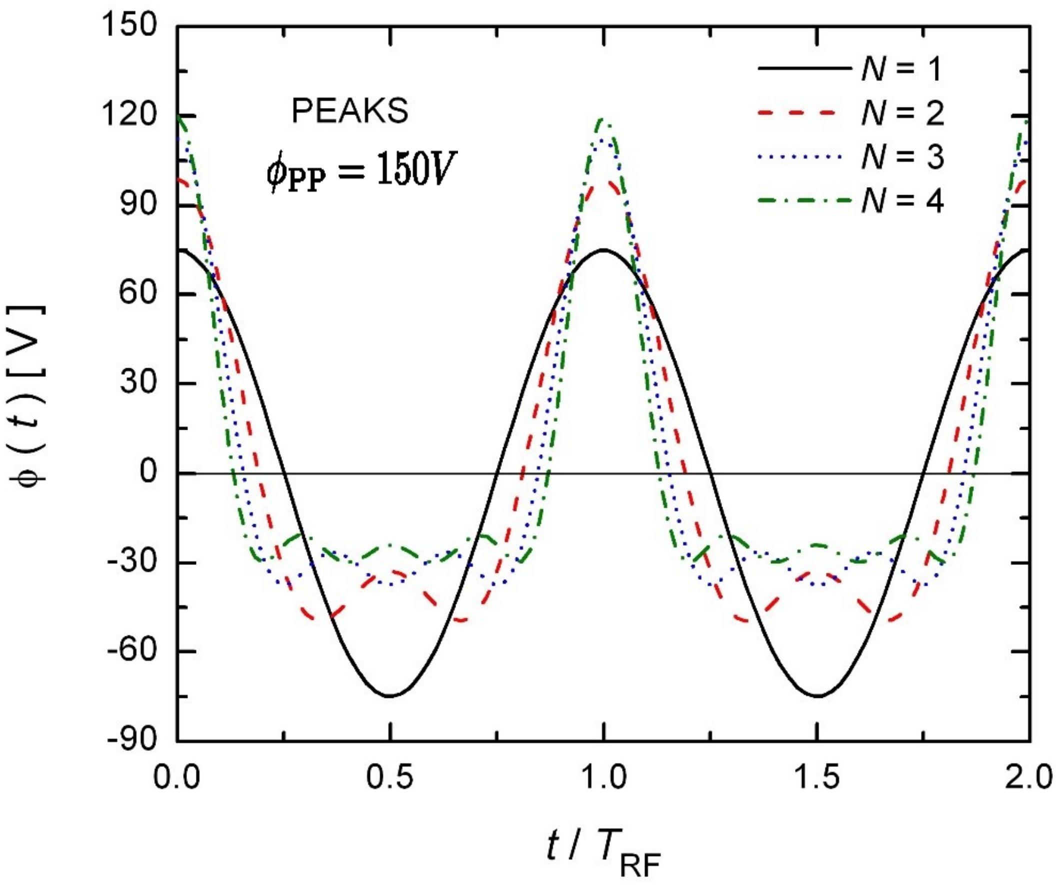
$$\phi_k = \phi_0 \frac{N-k+1}{N} \qquad \phi_0 = \frac{2N}{(N+1)^2}\phi_{PP}$$

- N number of harmonics
- $\Theta_k (k = 1...N)$ phase angles
- ϕ_k amplitude of harmonics
- f_1 fundamental RF frequency

"Peaks" & "Valleys" waveforms

$\Theta_k = 0$ or $\Theta_k = \pi$

- aluminium electrodes: d = 50 cm
- electrode gap: L = 2.5 cm
- gas pressure: 50 mTorr < p < 380 mTorr
- fundamental frequency 13.56 MHz
- number of harmonics $N \leq 4$

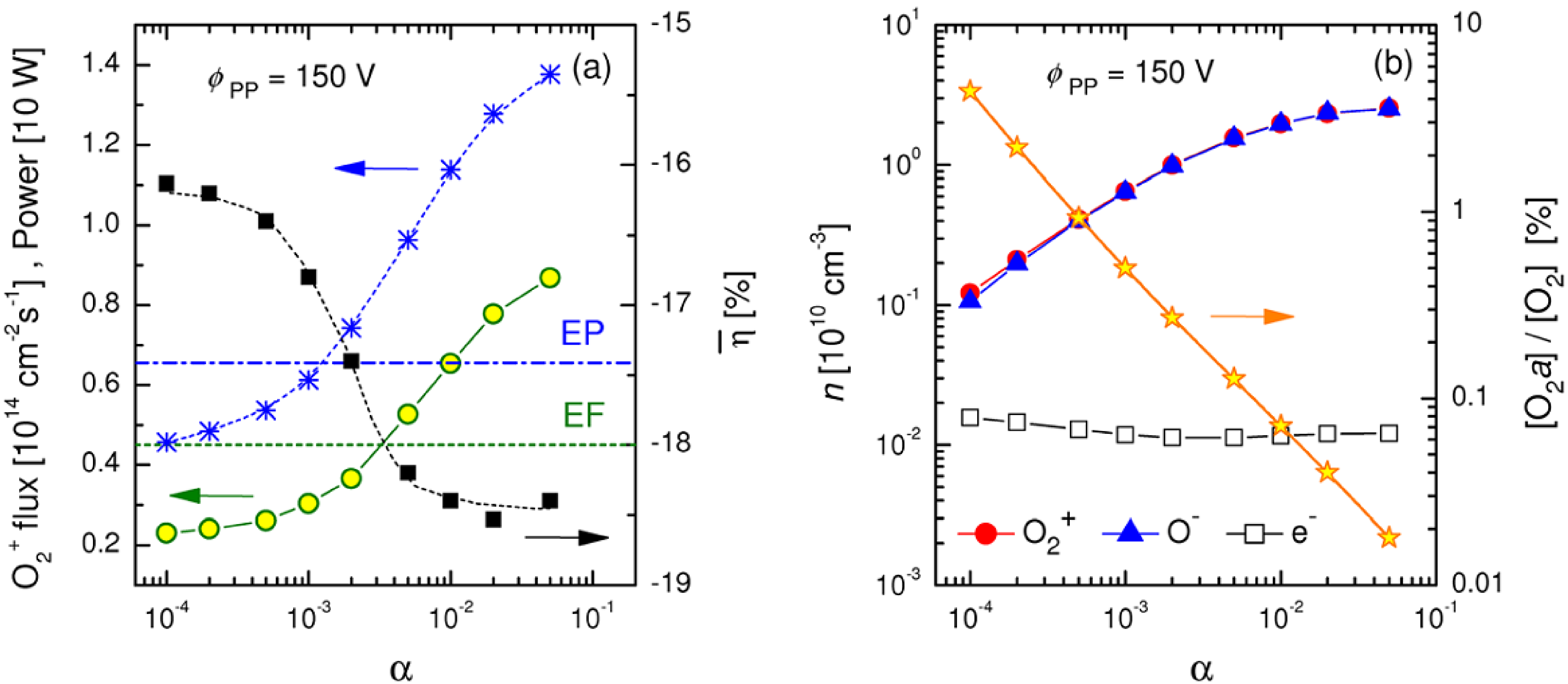


In the simulations

- gas temperature: 300 K
- electron reflection: 0 %
- secondary electron emission: γ = 0

Surface destruction probability of O_2 ($a^1\Delta_g$) molecules (α)

p = 100 mTorr, ϕ_{pp} = 150 V, N = 2



- O_2^+ ion flux at the grounded electrode
- discharge power
- DC self-bias
- EF - measured O_2^+ ion flux
- EP - measured discharge power

- electron density
- O_2^+ ion density
- O^- ion density
- $[O_2\,(a^1\Delta_g)]/[O_2]$ density ratio

$\alpha = 6 \times 10^{-3}$ - in the simulations

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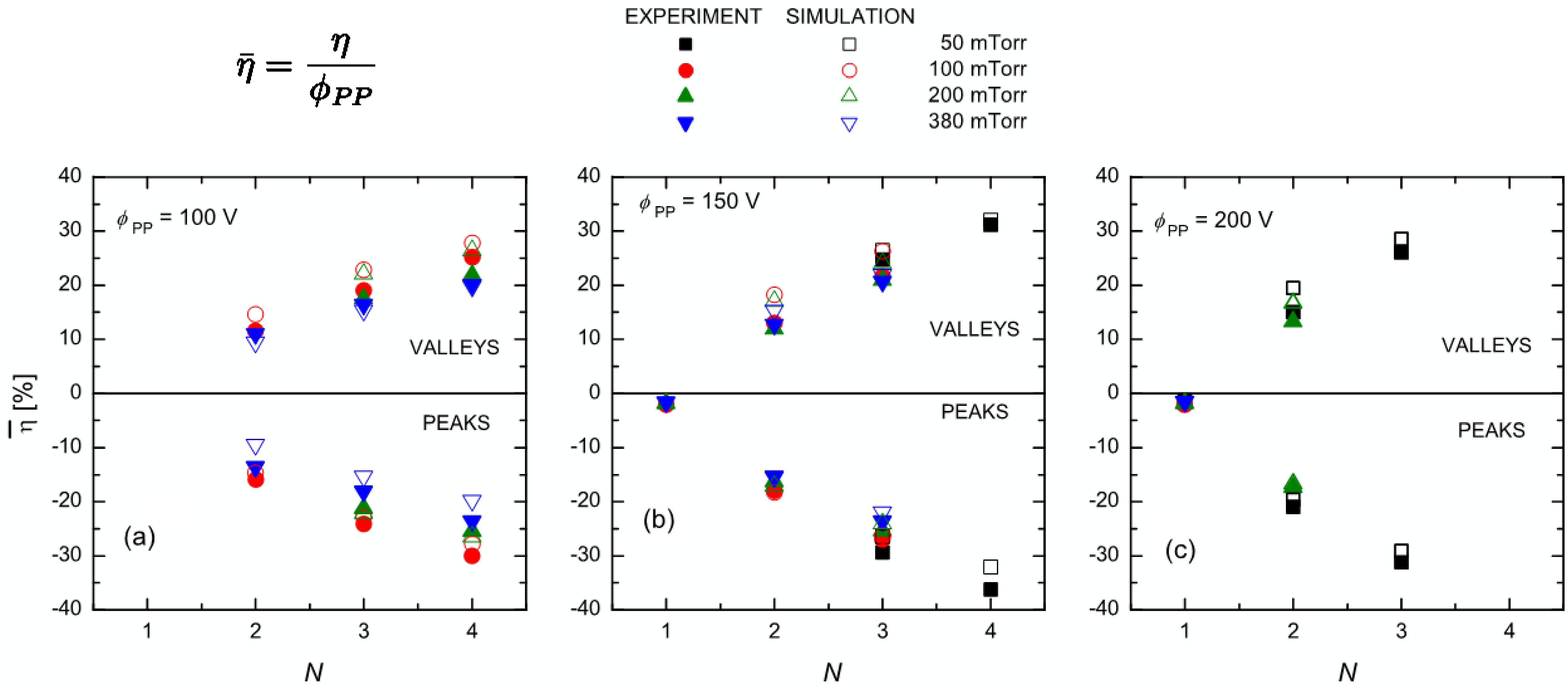
DC self-bias voltage

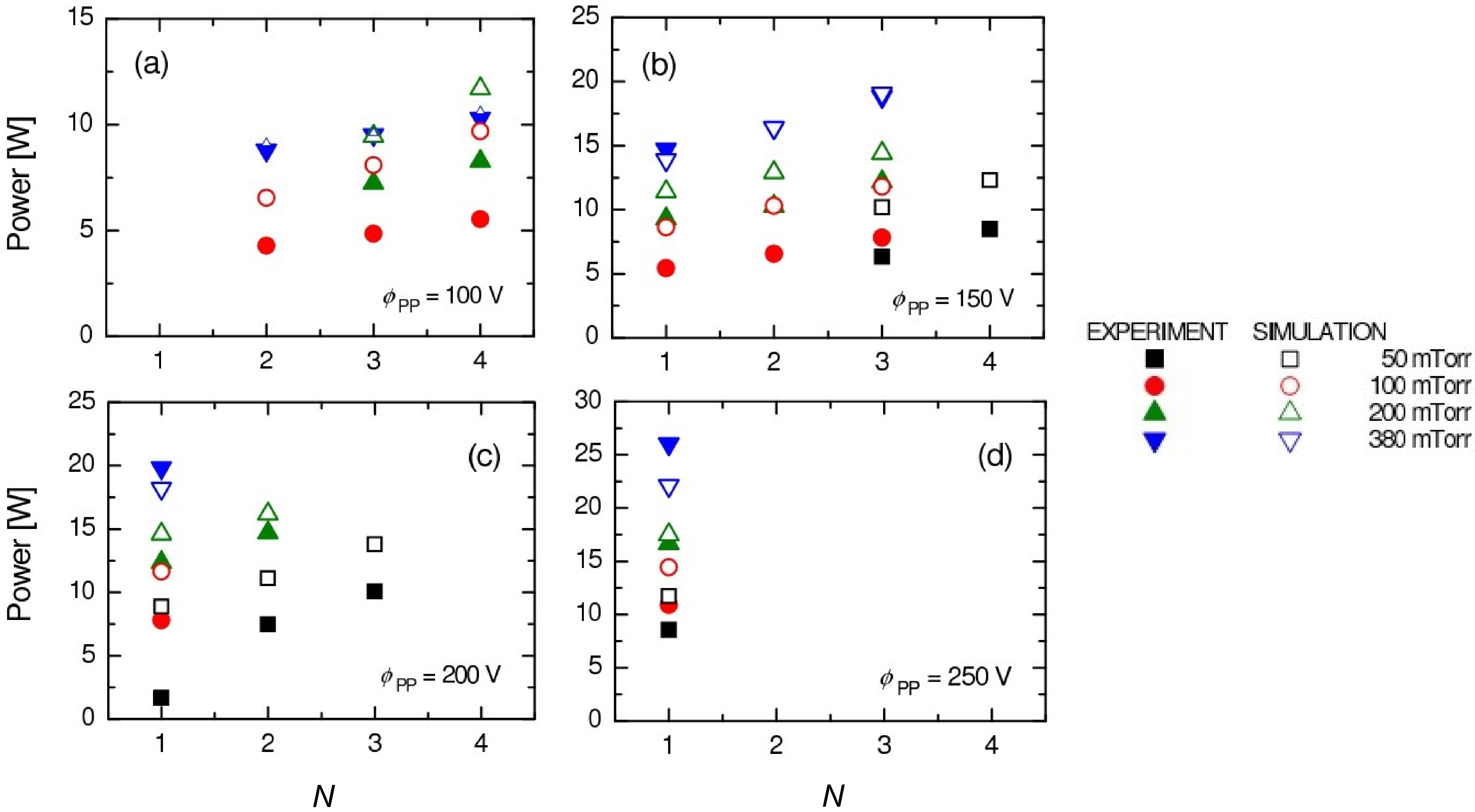
$$\bar{\eta} = \frac{\eta}{\phi_{PP}}$$



Normalized self-bias as a function of the number of driving RF harmonics for different voltage amplitudes, pressures and voltage waveform types.

A. Derzsi, T. Lafleur, J.-P. Booth, I. Korolov, Z. Donkó, *Plasma Sources Sci. Technol.* **25** 015004 (2016)

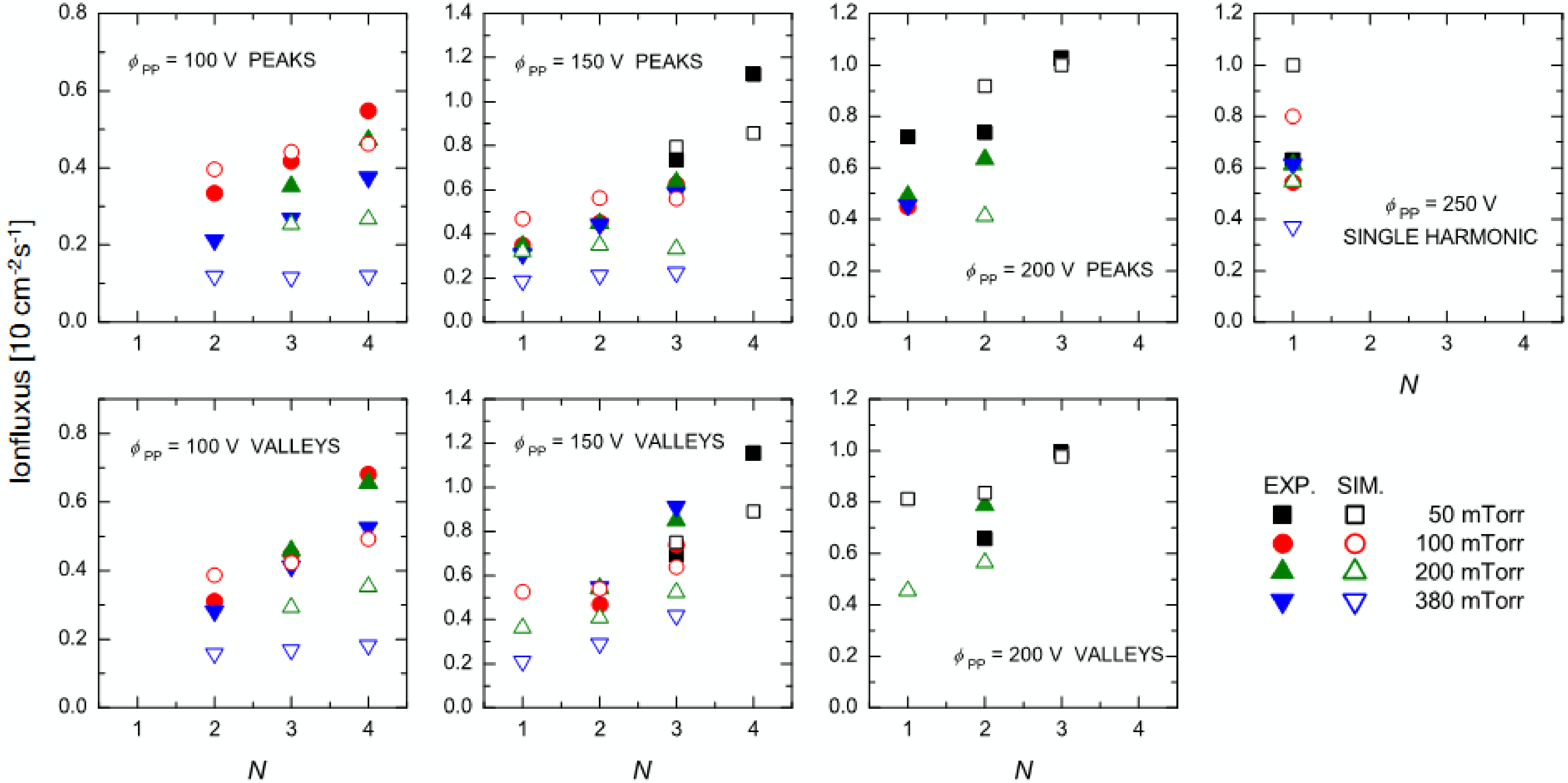
Discharge power



Discharge power as a function of the number of driving RF harmonics for different voltage amplitudes and pressures.

A. Derzsi, T. Lafleur, J.-P. Booth, I. Korolov, Z. Donkó, *Plasma Sources Sci. Technol.* **25** 015004 (2016)

O_2^+ ion flux



O_2^+ ion flux as a function of the number of driving RF harmonics for different voltage amplitudes, pressures and voltage waveform types.

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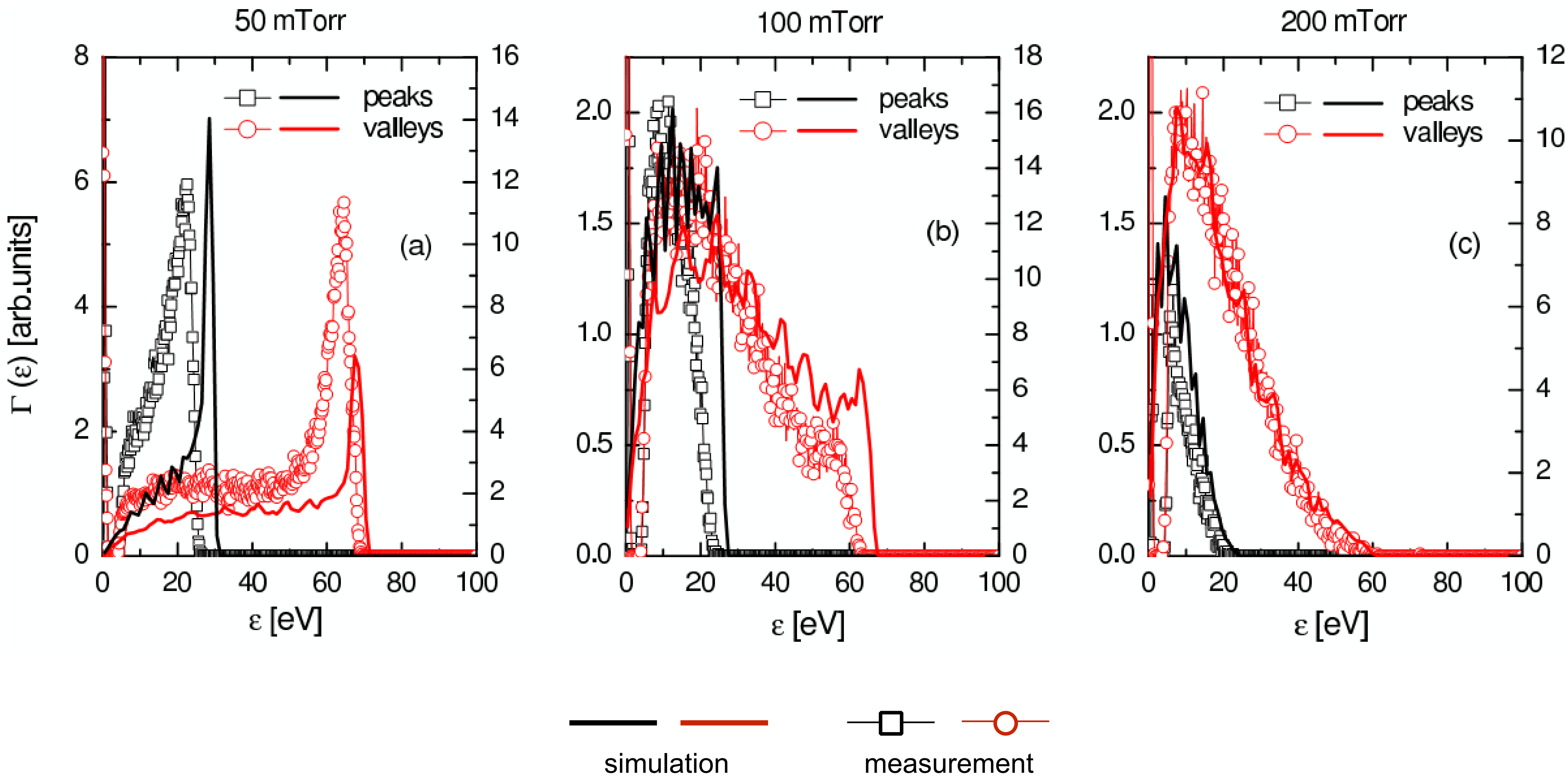
O_2^+ ion flux energy distribution function

N = 3, ϕ_{pp} = 150 V



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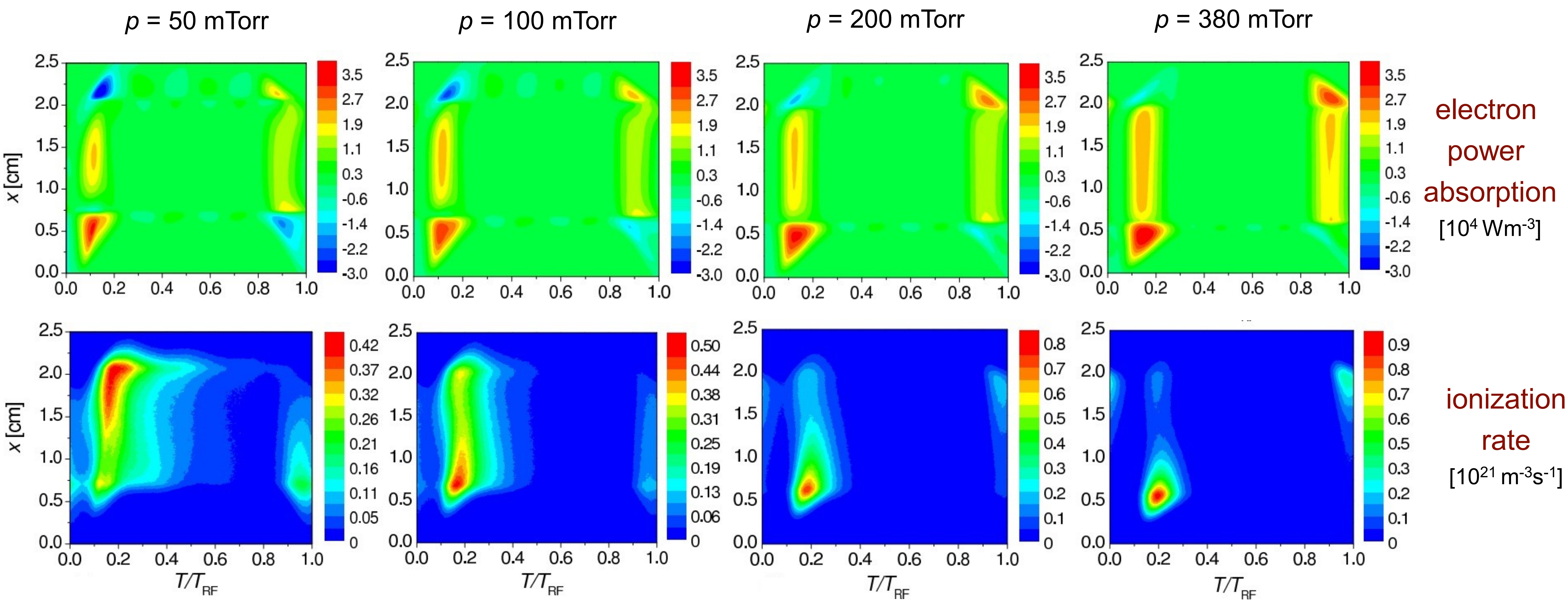
Heating mode transitions - pressure variation

N = 3, ϕ_{PP} = 150 V, “peaks” waveform



PIC/MCC simulation results on the spatio-temporal distribution of the electron power absorption (1st row) and rate of O_2^+ ion production (2nd row) for different pressures.

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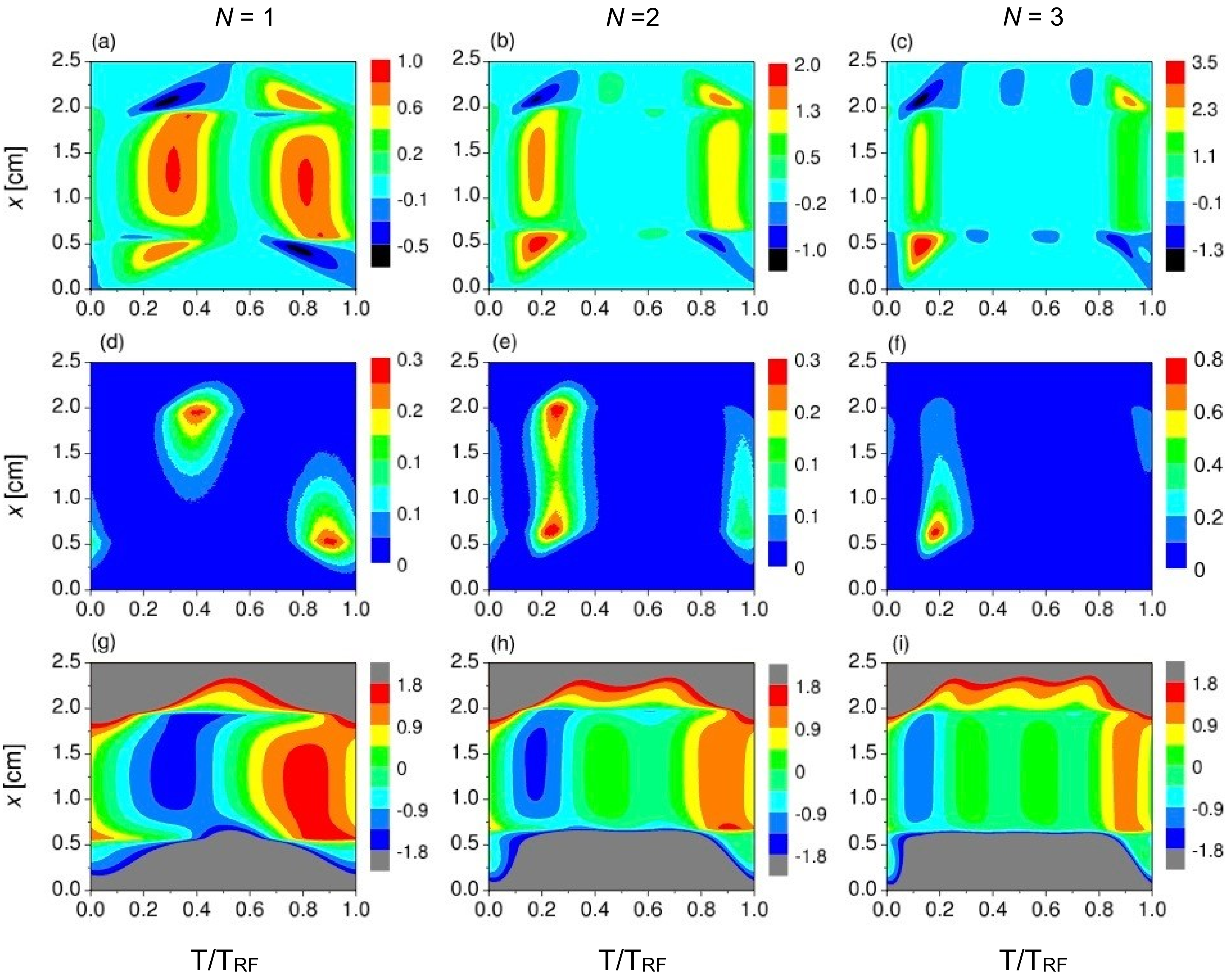
Heating mode transitions – variation of *N*



p = 200 mTorr
ϕ_{pp} = 150 V
"peaks" waveform

electron power absorption
[10^4 Wm^{-3}]

ionization rate
[10^{21} m^{-3}s^{-1}]

electric field
[10^3 Vm^{-1}]

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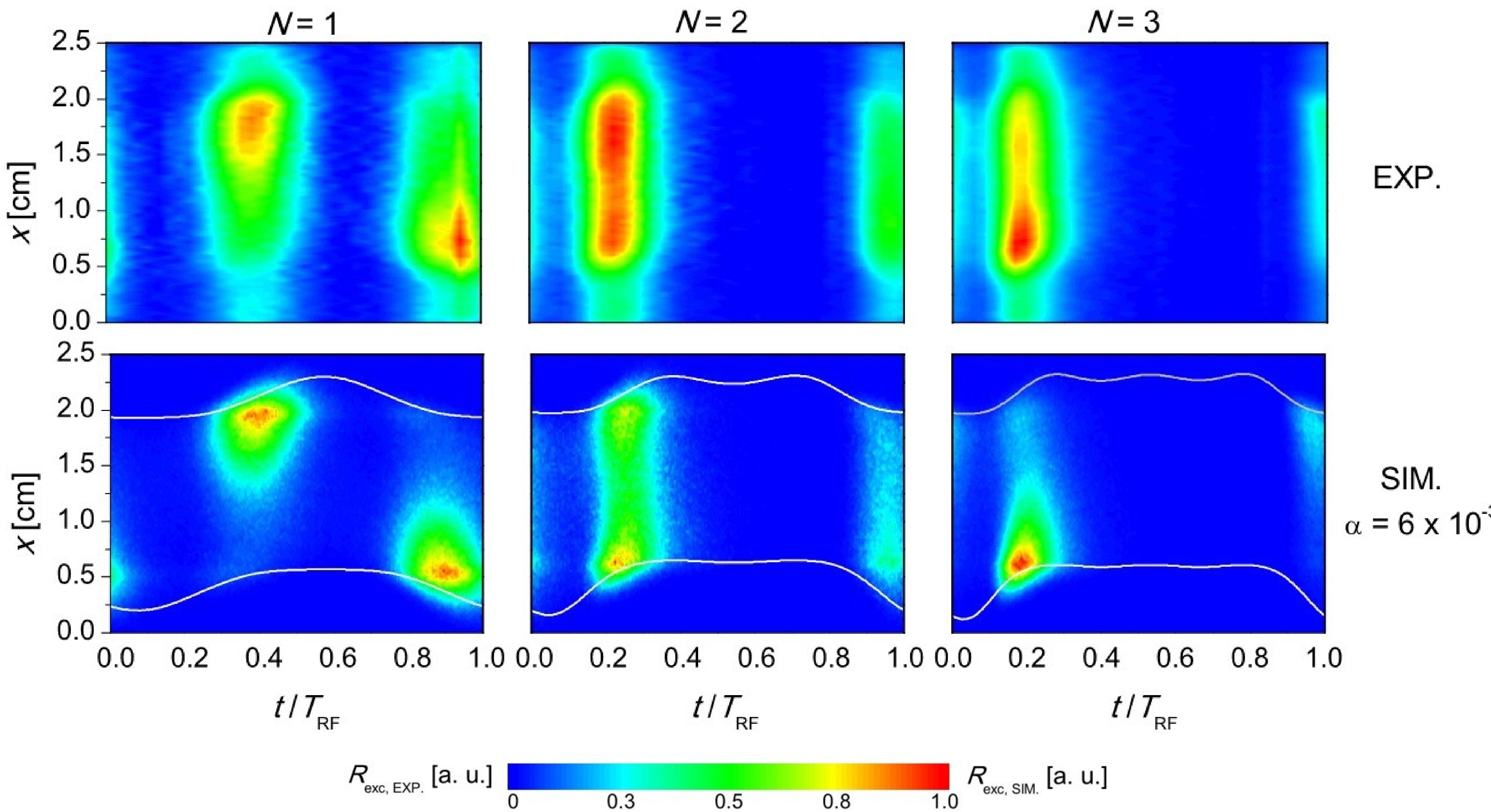
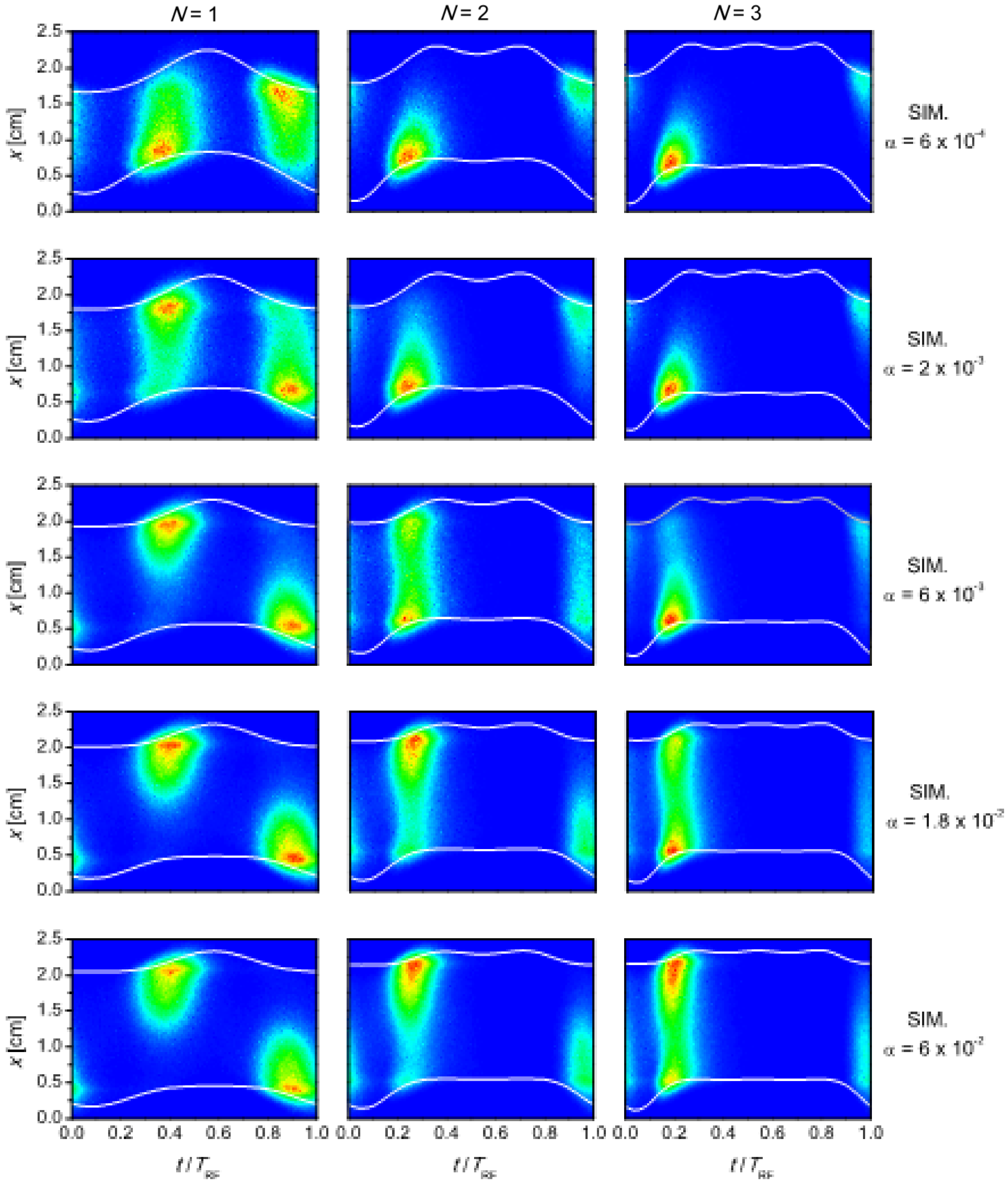
Heating mode transitions: experiment, simulation



Phase-resolved excitation rate of the O($^3p^3P$) excited state obtained from PROES (1st row) and PIC/MCC simulation results on the spatio-temporal distribution of the dissociative excitation rate (2nd row) for different numbers of harmonics.

p = 200 mTorr, ϕ_{PP} = 150 V, f_1 = 13.56 MHz, peaks waveform

Heating mode transitions: effect of α



PIC/MCC simulation results on the spatio-temporal distribution of the dissociative excitation rate for different values of α.

p = 200 mTorr,
ϕ_{PP} = 150 V,
f_1 = 13.56 MHz,
peaks waveform

Discharge conditions - amplitude asymmetry & slope asymmetry

"Peaks" & "Valleys" waveforms

$$\phi(t) = \sum_{k=1}^{N} \phi_k \cos(2\pi k f_1 t + \Theta_k)$$

$\Theta_k = 0$ or $\Theta_k = \pi$

N number of harmonics

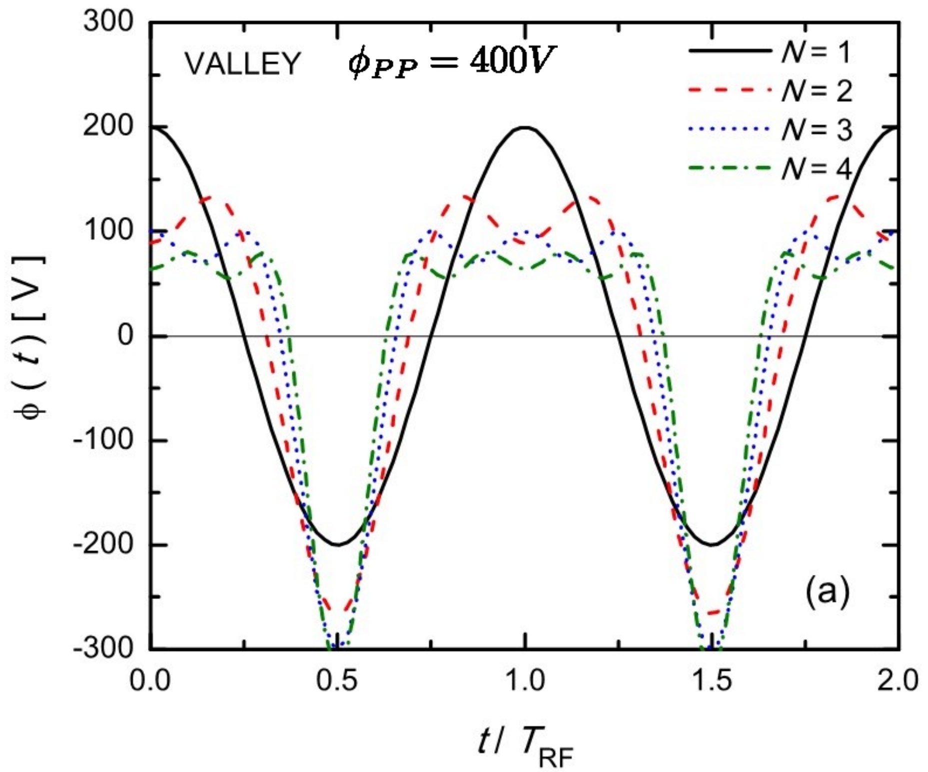
$\Theta_k (k = 1...N)$ phase angles

ϕ_k amplitude of harmonics

f_1 fundamental RF frequency

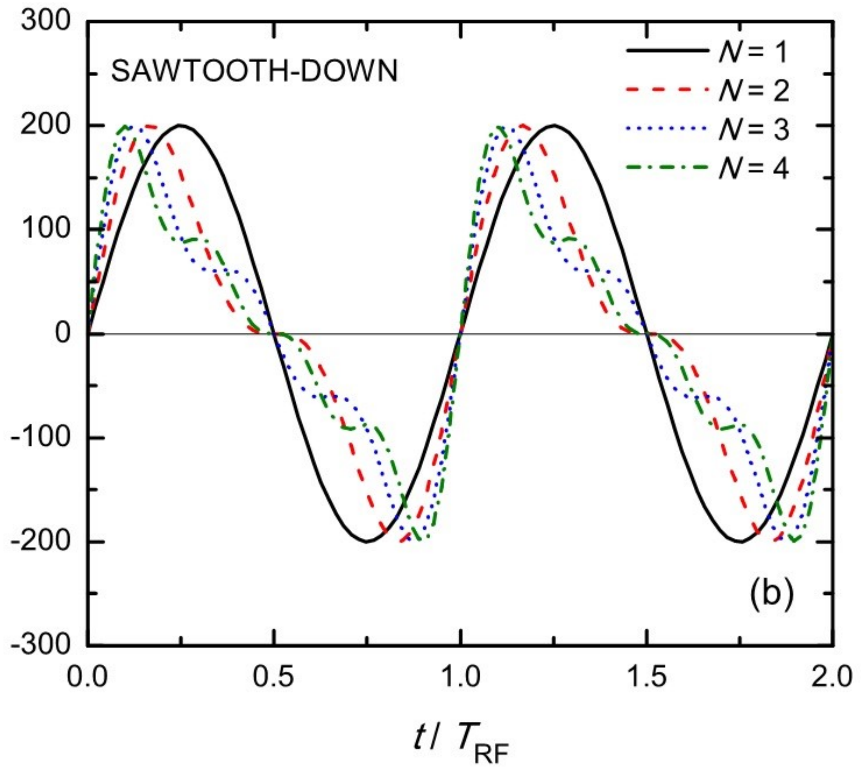
$$\phi_k = \phi_0 \frac{N - k + 1}{N}$$

$$\phi_0 = \frac{2N}{(N+1)^2} \phi_{PP}$$



"Sawtooth" waveforms

$$\phi(t) = \pm\phi_0 \sum_{k=1}^{N} \frac{1}{k} sin(2\pi k f_1 t)$$

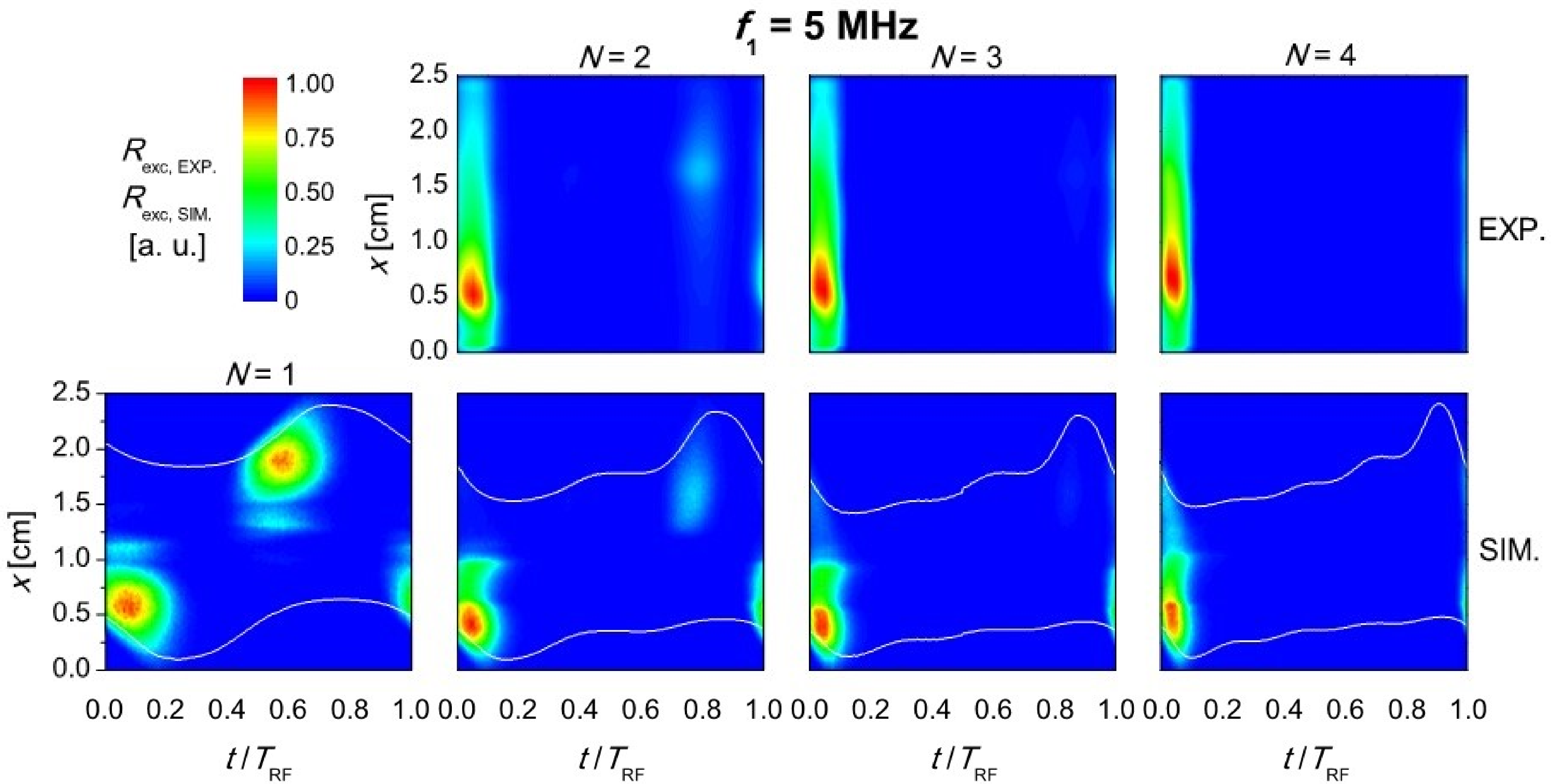


- electrode gap: 2.5 cm
- gas pressure: 50 mTorr - 700 mTorr
- fundamental frequency 5 MHz, 10 MHz, 15 MHz
- number of harmonics $N \leq 4$

- dc self-bias voltage
- excitation rate

experiment ⟷ simulation

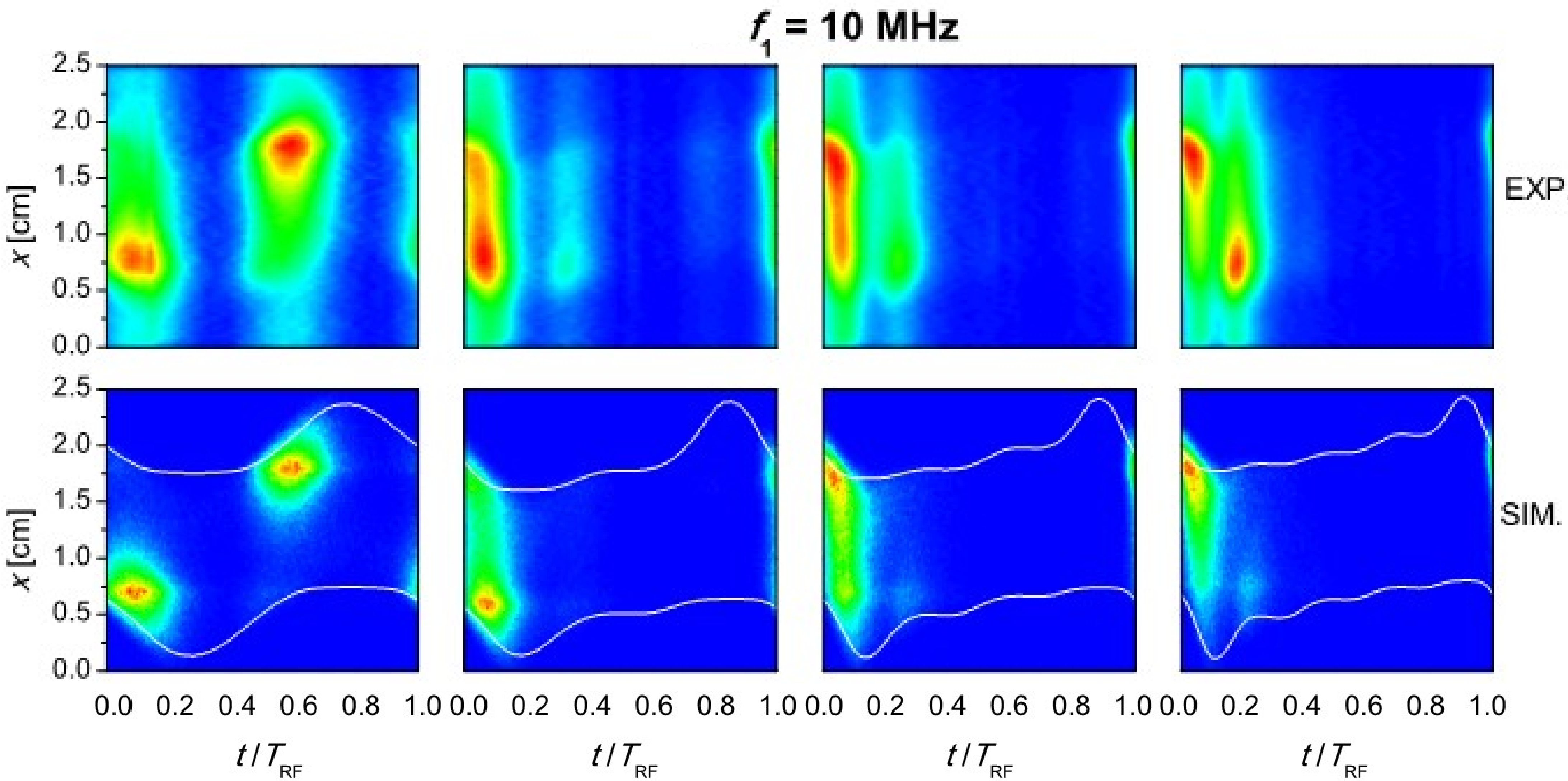
Sawtooth waveforms - Excitation rates, f_1 = 5 MHz



Spatio-temporal maps of the excitation rate obtained for different numbers of harmonics: experimental data derived from PROES (1st row) and PIC/MCC simulation results (2nd row) for different numbers of harmonics.

p = 150 mTorr, ϕ_{PP} = 400 V, f_1 = 5 MHz, sawtooth-down type waveforms

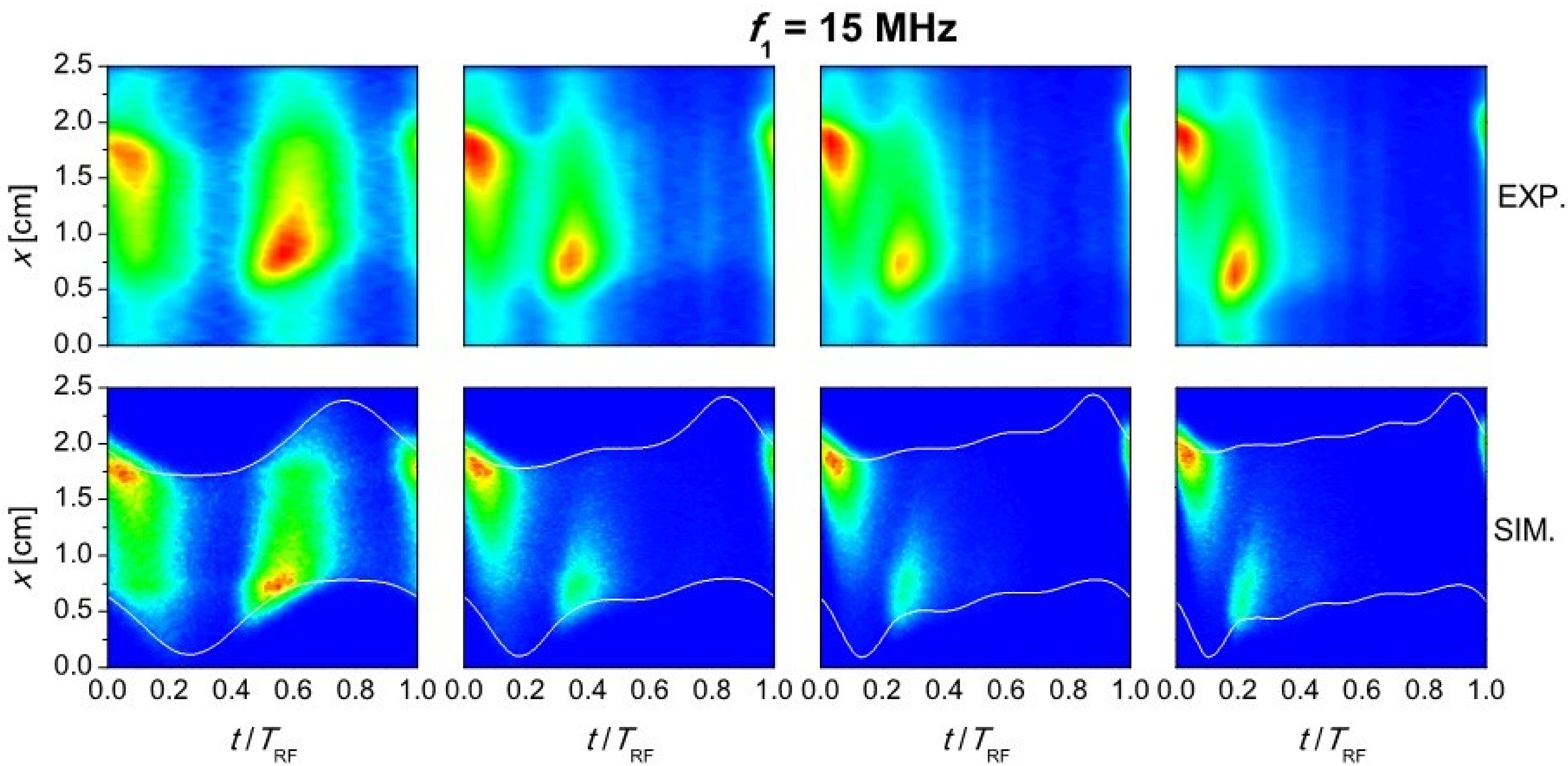
Sawtooth waveforms - Excitation rates, f_1 = 10 MHz



Spatio-temporal maps of the excitation rate obtained for different numbers of harmonics: experimental data derived from PROES (1st row) and PIC/MCC simulation results (2nd row) for different numbers of harmonics.

p = 150 mTorr, ϕ_{PP} = 400 V, f_1 = 10 MHz, sawtooth-down type waveforms

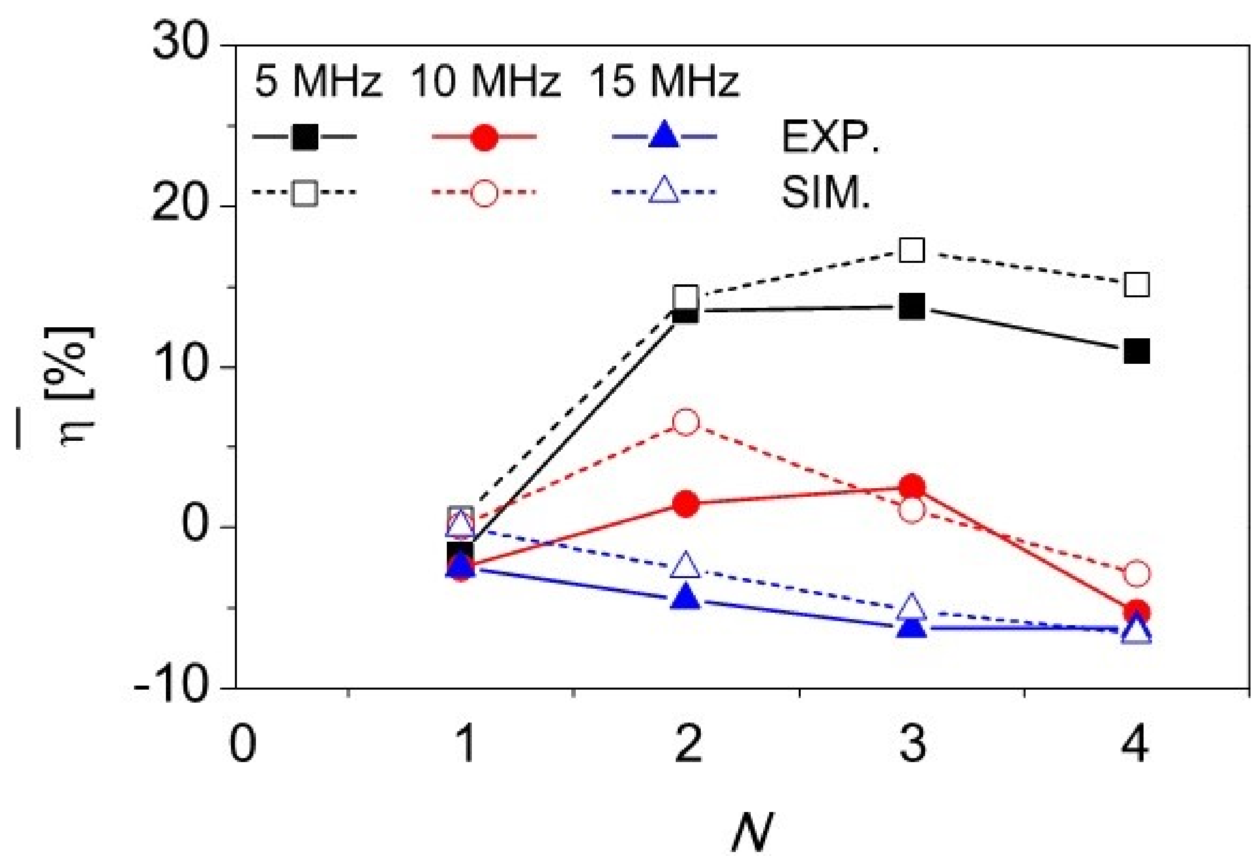
Sawtooth waveforms - Excitation rates, f_1 = 15 MHz



Spatio-temporal maps of the excitation rate obtained for different numbers of harmonics: experimental data derived from PROES (1st row) and PIC/MCC simulation results (2nd row) for different numbers of harmonics.

p = 150 mTorr, ϕ_{PP} = 400 V, f_1 = 15 MHz, sawtooth-down type waveforms

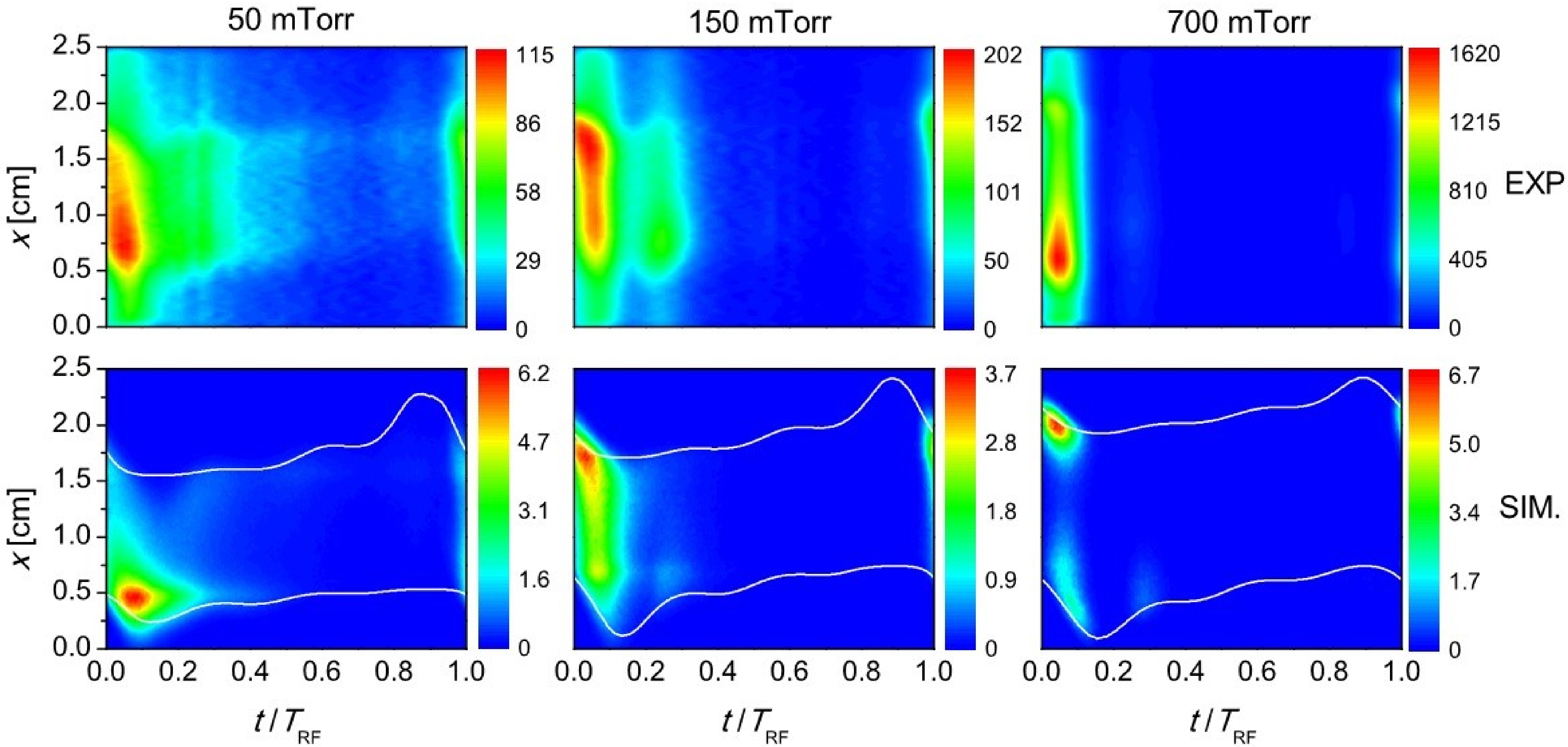
Sawtooth waveforms - DC self-bias



Normalized dc self-bias as a function of the number of driving harmonics, obtained experimentally and from PIC/MCC simulations

p = 150 mTorr, ϕ_{PP} = 400 V, f_1 = 5 MHz, sawtooth-down type waveforms

Sawtooth waveforms - Excitation rates, f_1 =10 MHz, pressure variation



Spatio-temporal maps of the excitation rate obtained from PROES measurements (1st row) and PIC/MCC simulations (2nd row) for different pressures.

N = 3 ϕ_{PP} = 400 V, f_1 = 10 MHz, sawtooth-down type waveforms

Summary

- We have developed a PIC/MCC model for capacitive O_2 discharges
- Several discharge characteristics have been determined both experimentally and via PIC/MCC simulations - test of the collision-reaction model
- Study of capacitive O_2 discharges driven by tailored voltage waveforms

➞ Including new species and processes in the model

➞ Realistic description of surface processes

➞ Benchmarks against simulations and experiments

Experimental and simulation study of a capacitively coupled oxygen discharge driven by tailored voltage waveforms

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