# Basic Research of Electron Dynamics in Low Pressure Capacitively Coupled Plasmas


**S. Wilczek[1], J. Trieschmann[2], J. Schulze[1,3], R. P. Brinkmann[1], Z. Donkó[4], and T. Mussenbrock[2]**

[1]Ruhr-University Bochum, Germany
[2]Brandenburg University of Technology, Cottbus-Senftenberg, Germany
[3]Dalian University of Technology, Dalian, China
[4]Wigner Research Centre for Physics, Budapest, Hungary

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# Electron dynamics in low pressure capacitively coupled radio frequency discharges F

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S. Wilczek, J. Schulze, R. P. Brinkmann, Z. Donkó, J. Trieschmann, and T. Mussenbrock

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**This presentation is based on the tutorial „Electron dynamics in low pressure capacitively coupled radio frequency discharges“, which has already been published as a featured article in Journal of Applied Physics**

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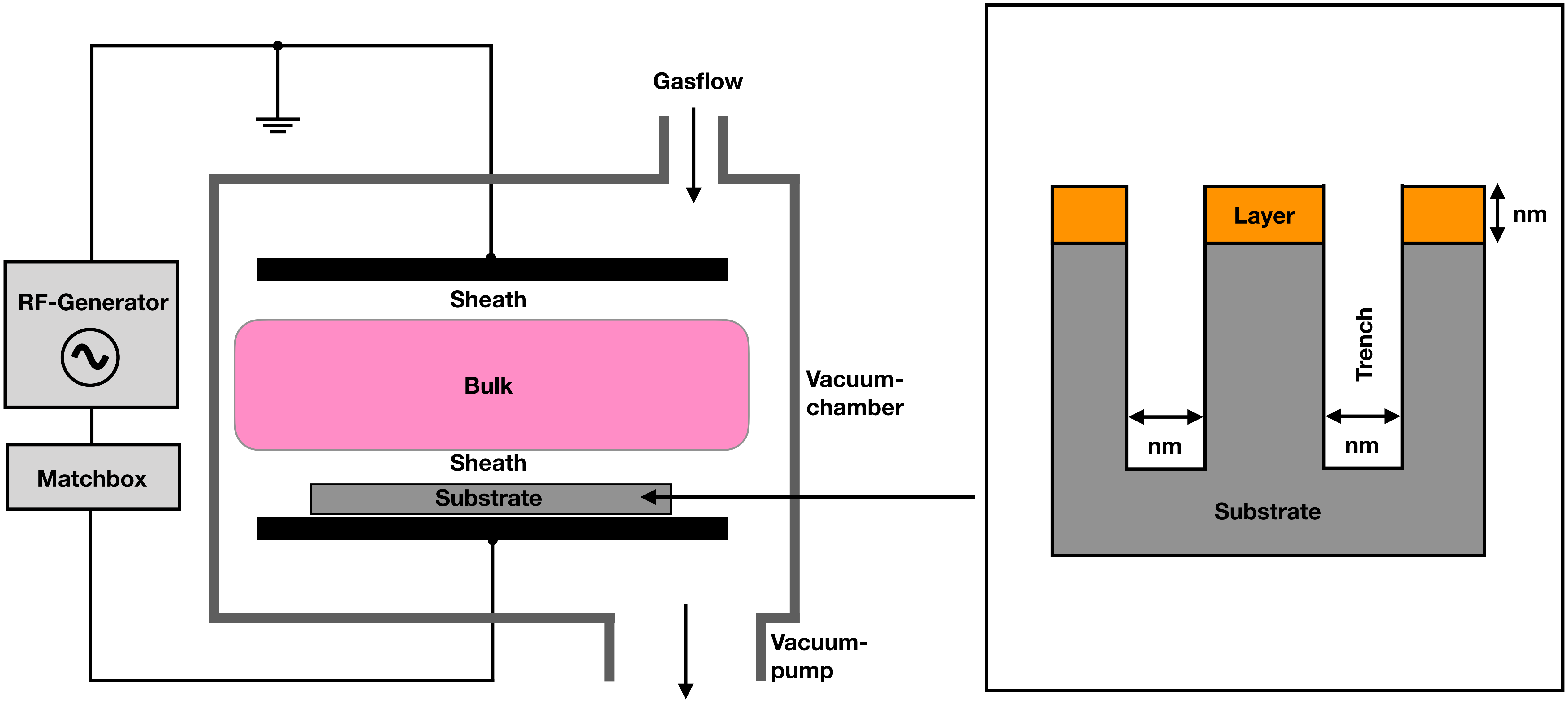
# Motivation: CCRF Discharge




- classical CCRF discharges for etching and deposition processes
- both processes reach the precision of single atomic layers
- requires a fundamental understanding of the particle dynamics in order to obtain a much better process control

# Motivation: Electron Dynamics

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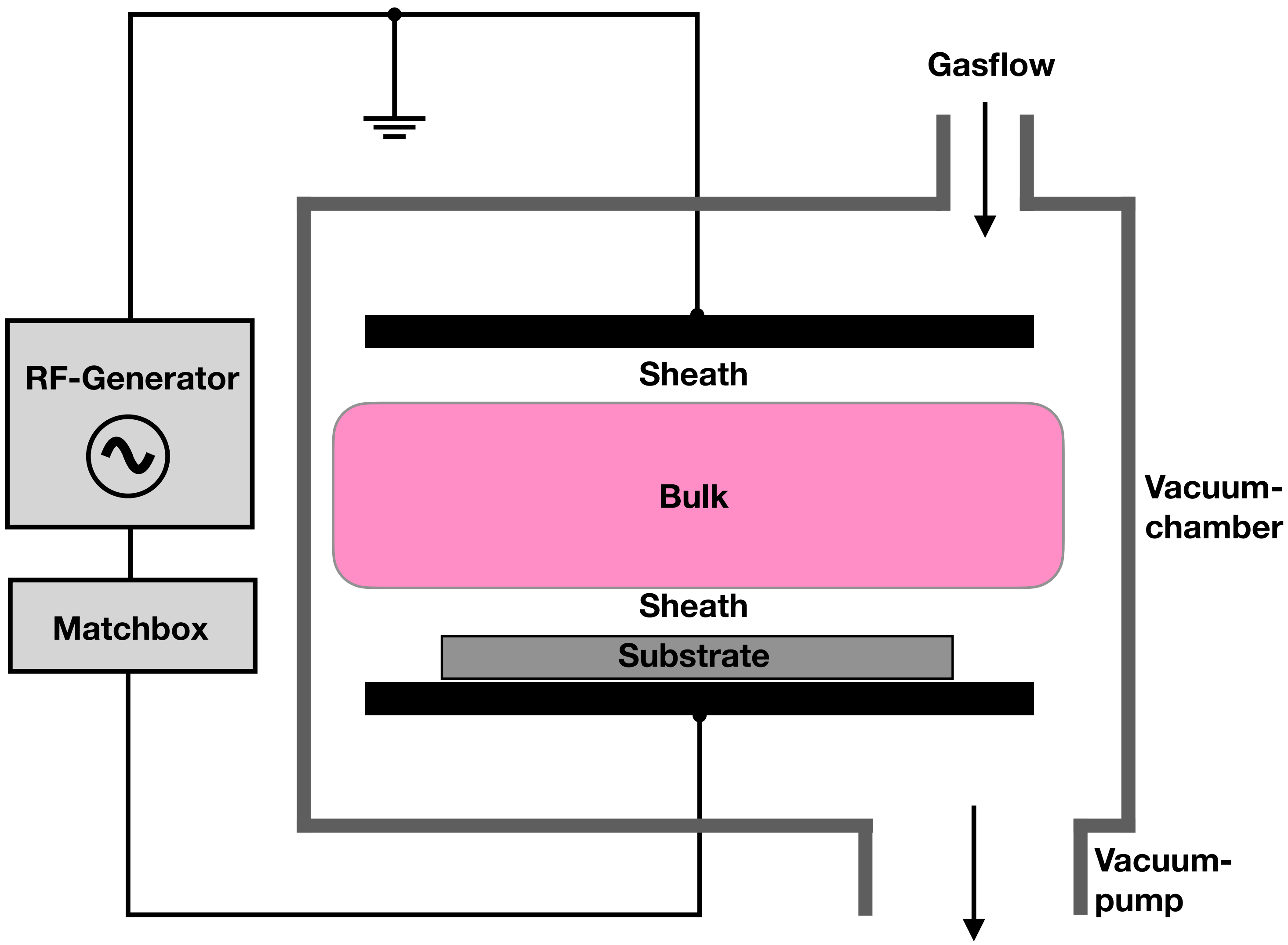
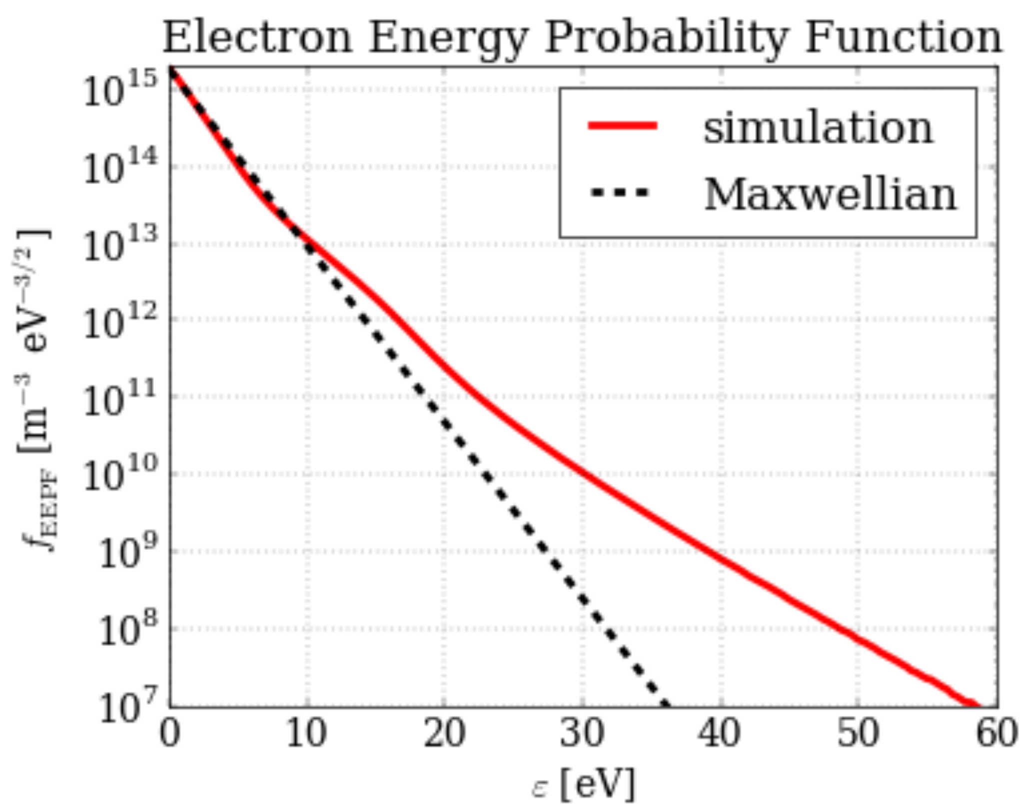



$p = 3\,\mathrm{Pa}\,(\mathrm{argon})$ $V_0 = 500\,\mathrm{V}$

$f = 13.56\,\mathrm{MHz}$ $L_{\mathrm{gap}} = 50\,\mathrm{mm}$




- optimization of the distribution function is necessary
- however, electrons at low pressures (< 10 Pa) indicate a strong anisotropy
- electron distribution function (red solid line) strongly differs from a Maxwellian distribution (black dashed line)

# Background: Electron Heating

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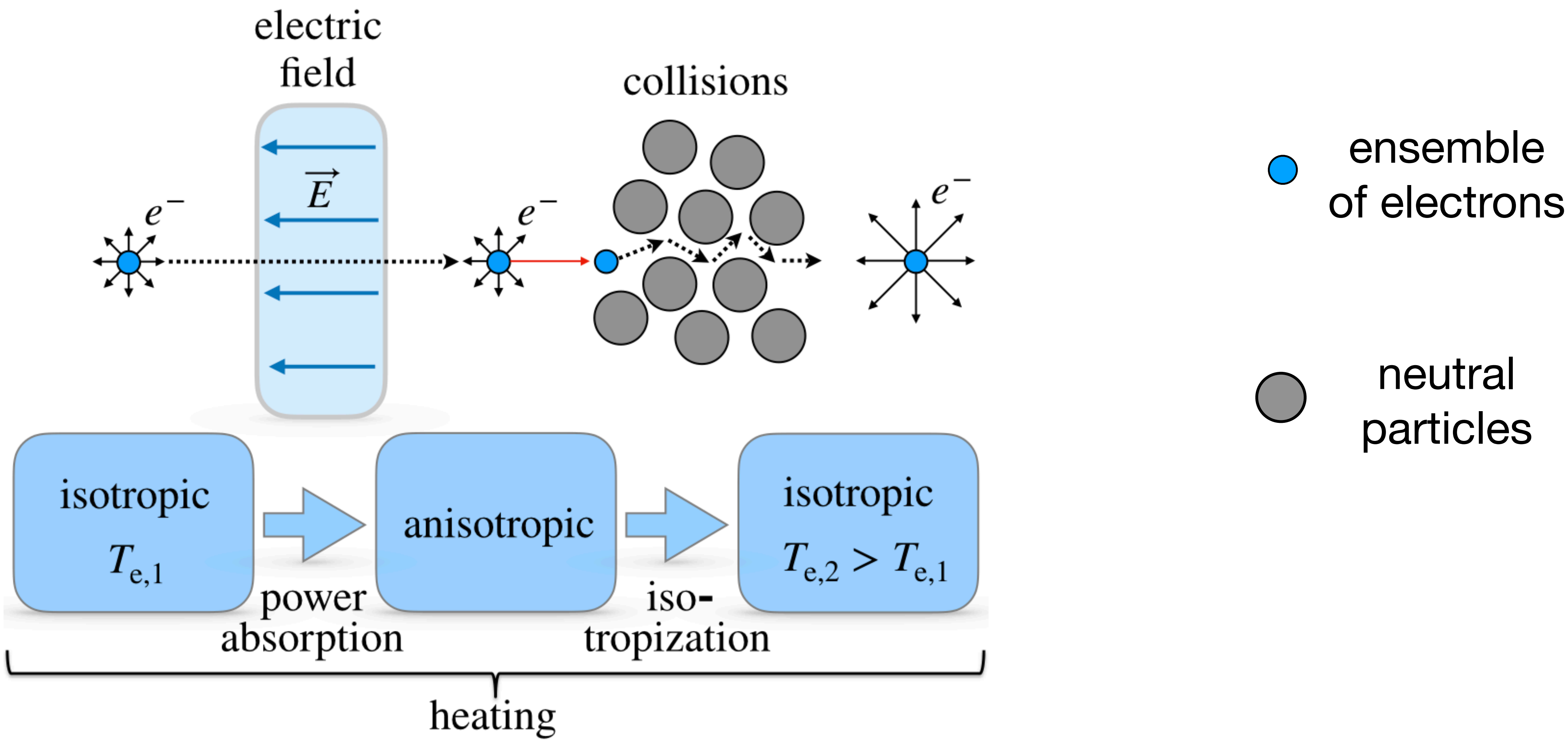
**On of the most fundamental questions:**

**How do the electrons gain and lose their energy?**

- traditionally studied and called as electron heating
- however, heating and power absorption are physically two different mechanisms
- what is the difference between both terminologies?

# What is actually Electron Heating?




1. ensemble of electrons obeys an isotropic velocity distribution with $T_{e,1}$
2. velocity distribution becomes anisotropic due to an acceleration in an electric field along one particular direction (perpendicular to the electrodes)
3. electron energy is redistributed in an isotropic manner by collisions and the ensemble of electrons becomes isotropic but with a higher temperature: $T_{e,2} > T_{e,1}$
4. the combination of power absorption and isotropization is termed heating

# Goal of this Work

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- provide a basic strategy on how to study the electron dynamics at low pressures
- PIC/MCC simulations indicate spatial and temporal results
- animations of fundamental plasma parameters explain the details
- a universal electropositiv (argon, 3 Pa) CCRF discharge scenario is depicted

**The following fundamental questions are addressed:**

- How is the electric field distributed over space and time and how does it influence the electrons
- How is current continuity ensured during the whole rf cycle?
- What is the influence of highly energetic beam electrons?
- How is the electron temperature defined?
- How do the collisional and collisionless electron power absorption really work?

# How to Investigate the Electron Dynamics?

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**PIC/MCC simulations solve the electric field and and the potential based on (electrostatic) Maxwell's (MW) equations. Additionally, every macroscopic quantity (densities, fluxes, temperature, pressure etc.) can be solved in the simulation.**

**(electrostatic) MW equations**

$$-\nabla^2\Phi = \rho/\epsilon_0$$

$$\vec{E} = -\nabla\Phi$$

**Macroscopic (fluid) equations**

$$\frac{\partial}{\partial t}n + \frac{\partial}{\partial x}\Gamma = G - L$$

$$m\frac{\partial}{\partial t}\Gamma + \frac{\partial}{\partial x}P_{\parallel} = qnE - \Pi_{\mathrm{c}}$$

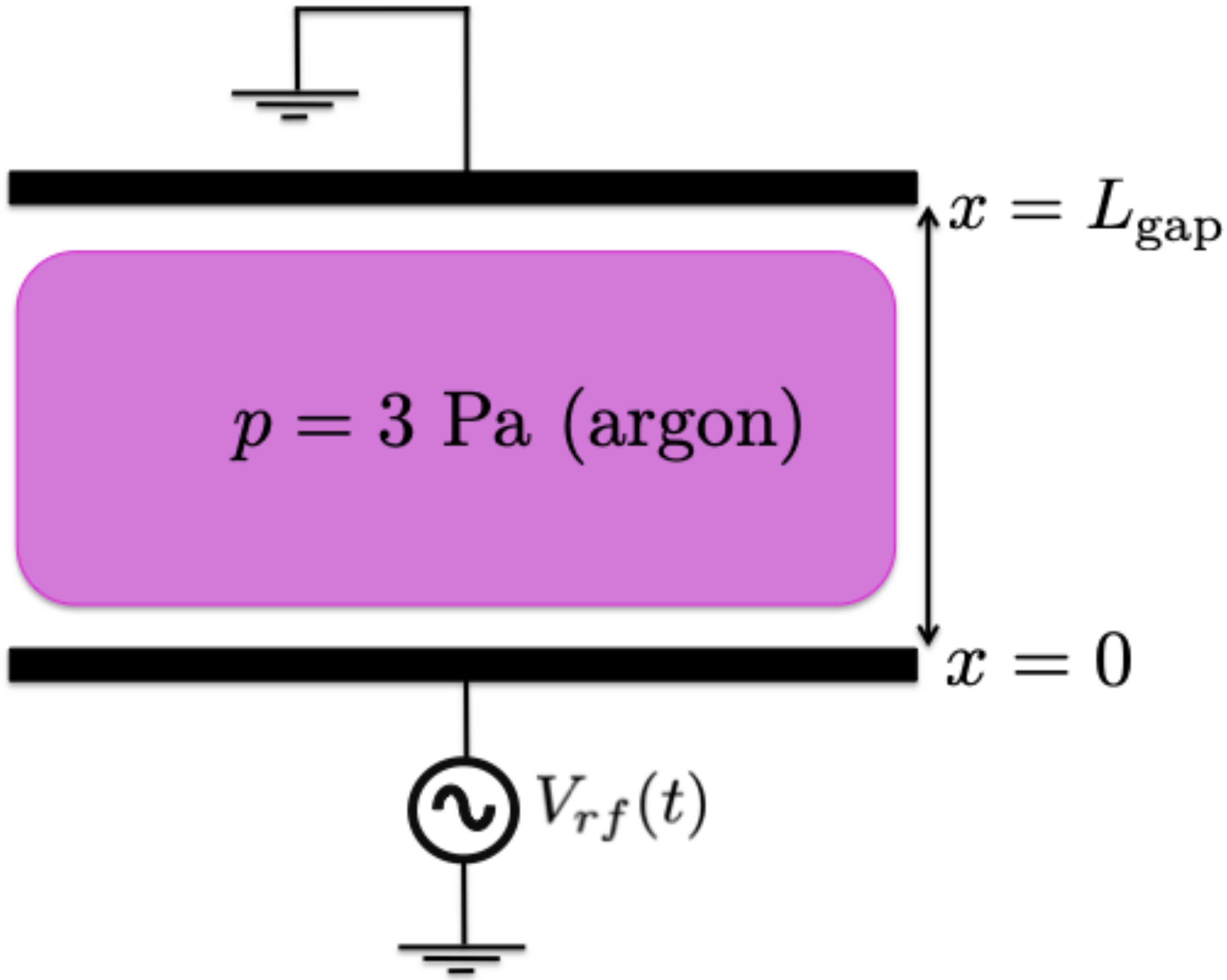
$$\frac{\partial}{\partial t}w + \frac{\partial}{\partial x}Q = q\Gamma E - \varepsilon_c$$

# Concept of this Investigation

- Chapter 1: Interaction between field and particles
- Chapter 2: Current densities and current conservation
- Chapter 3: Electron beams and inelastic collisions
- Chapter 4: Concept of the kinetic electron temperature
- Chapter 5: Mechanism of electron power absorption

# Simulation Setup

- 1d3v PIC/MCC simulation
- planar, parallel and infinite electrodes
- axial symmetric, translational invariant in y and z
- argon gas pressure: 3 Pa
- gap size: 50 mm
- driving frequency: 13.56 MHz
- voltage amplitude: 500 V
- no surface models



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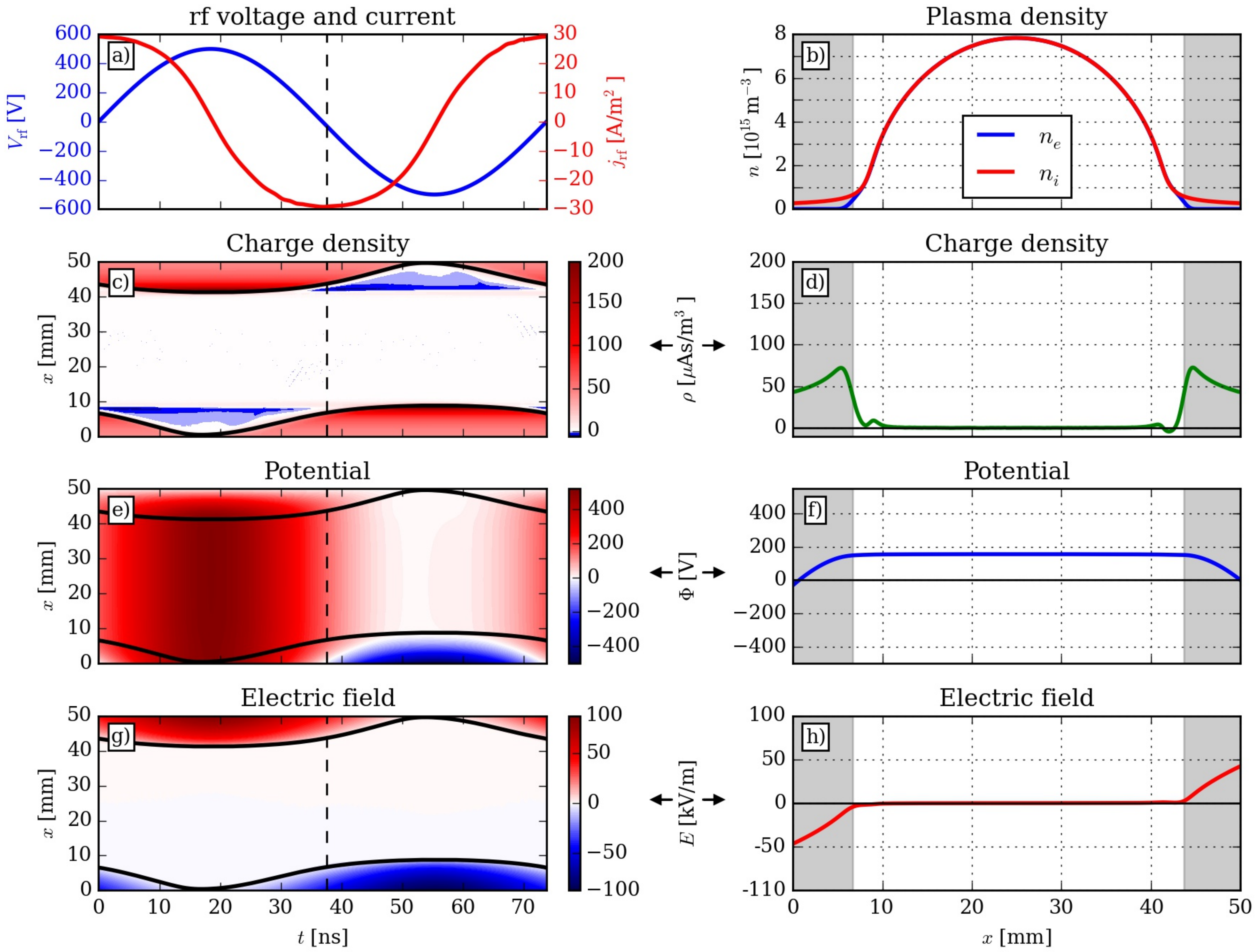
# Interaction between Field and Particles

- fundamental parameters are shown in the movie on the next slide (please use the link on the next slide in order to open the movie)
- rf voltage at the driven electrode (blue line in a) is the input of the PIC/MCC simulation as well as the boundary value for Maxwell's equations
- the rf current density at the electrode (red line in a) is the output of the system
- ion density (red line in b) is not time modulated and the electron density (blue line in b) follows the rf frequency: $\omega_{\mathrm{pi}} \ll \omega_{\mathrm{rf}} \ll \omega_{\mathrm{pe}}$
- resulting charge density (c and d) indicates the space charge in the sheath region
- potential (e and f) shows a self-adjusted bulk potential during the rf cycle, which must be higher than the potential at the electrodes (to confine the electrons)
- electric field (g and h) indicates the strong amplitude in the sheath and increases during sheath expansion and decreases during the collapsing sheath phase

# Interaction between Field and Particles




**Link to Movie 1**

# Interaction between Field and Particles

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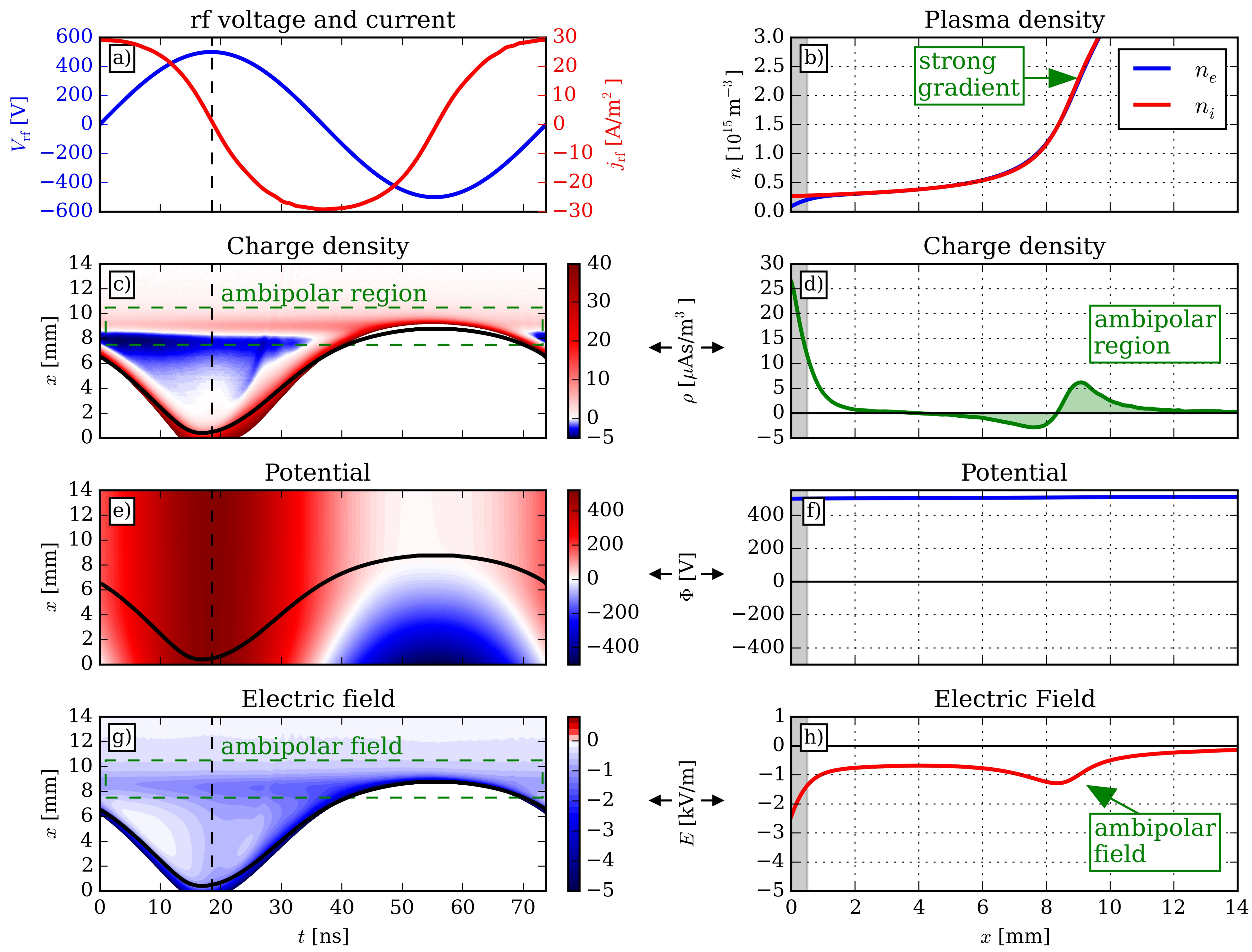
- frequently, the features of the ambipolar electric field are hidden, since the amplitude of the ambipolar electric field in front of the plasma sheath edge (black solid lines) is weak, but many electrons can traverse through this field
- therefore, it is useful to zoom into the plasma sheath region (0 mm - 14 mm) and adjust the color scale in order to highlight the importance of the ambipolar field (movie on the next slide)
- a double layer of positive and negative charges exists in the amipolar region, since electrons move away from the ions in a region of strong density gradients
- consequently, the ambipolar field arises (highlighted by the green markers) and electrons gain energy in this field

# Interaction between Field and Particles




**Link to Movie 2**

# Concept of this Investigation

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- Chapter 1: Interaction between field and particles
- Chapter 2: Current densities and current conservation
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- Chapter 4: Concept of the kinetic electron temperature
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# Current Densities and Current Conservation

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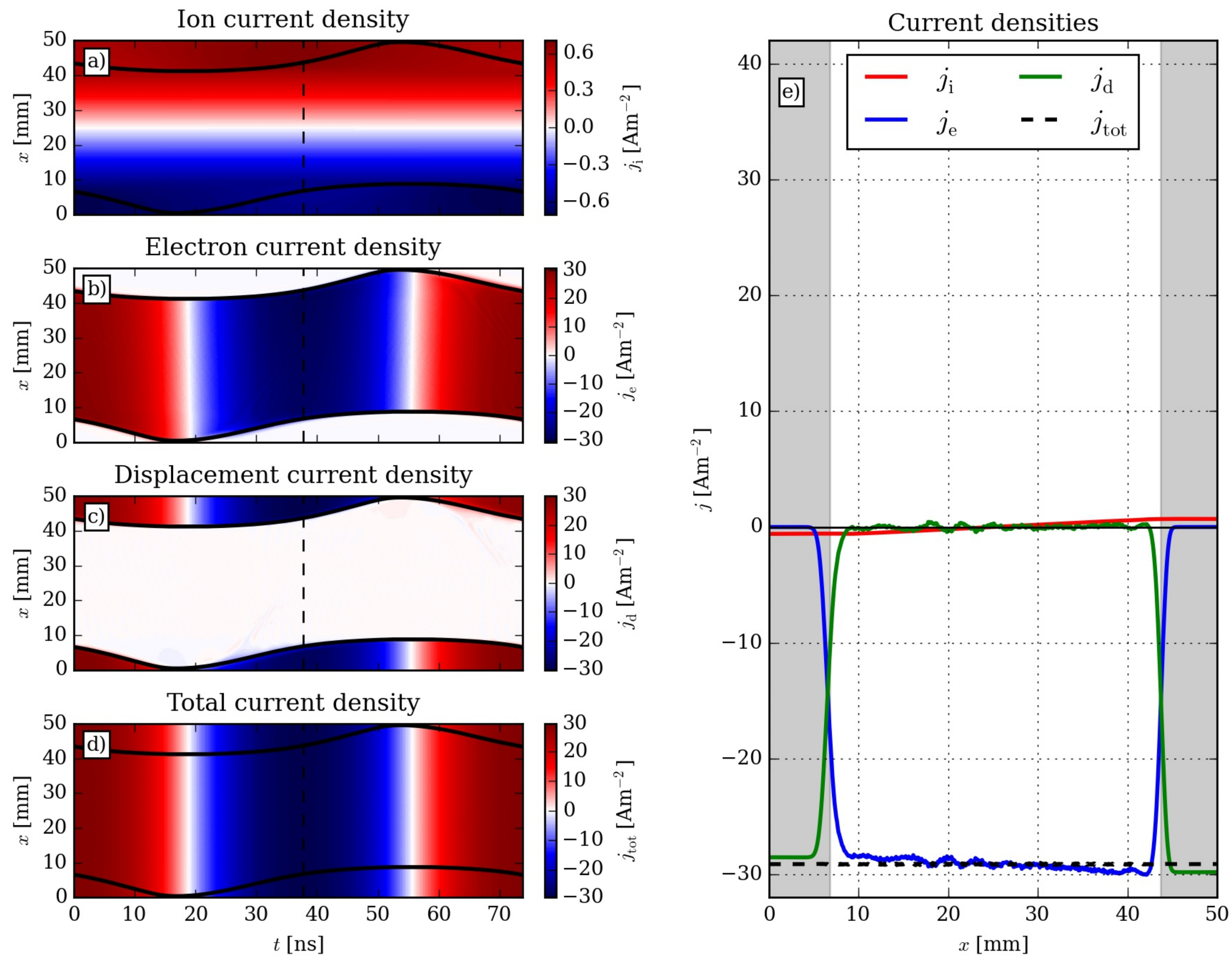
- current densities indicate the collective behavior of the particles (movie on the next slide)
- current conservation for the electron, ion and displacement current density must be ensured all the time
- the ion current density (a and red line in e) contributes weakly to the total current density (d and black dashed line in e) due to the low mean velocity of ions
- the electron current density (b and blue line in e) is dominant in the plasma bulk
- the displacement current density (c and green line in e) is dominant in the sheath region
- the total current density (black dashed line in e) is always a constant due to current conservation

**Current Conservation:**

$$\frac{\partial j_{\mathrm{tot}}}{\partial x} = \frac{\partial}{\partial x}(\underbrace{j_{\mathrm{i}} + j_{\mathrm{e}}}_{j_{\mathrm{c}}} + j_{\mathrm{d}}) = 0$$

# Current Densities and Current Conservation




**Link to Movie 3**

# Current Densities and Current Conservation

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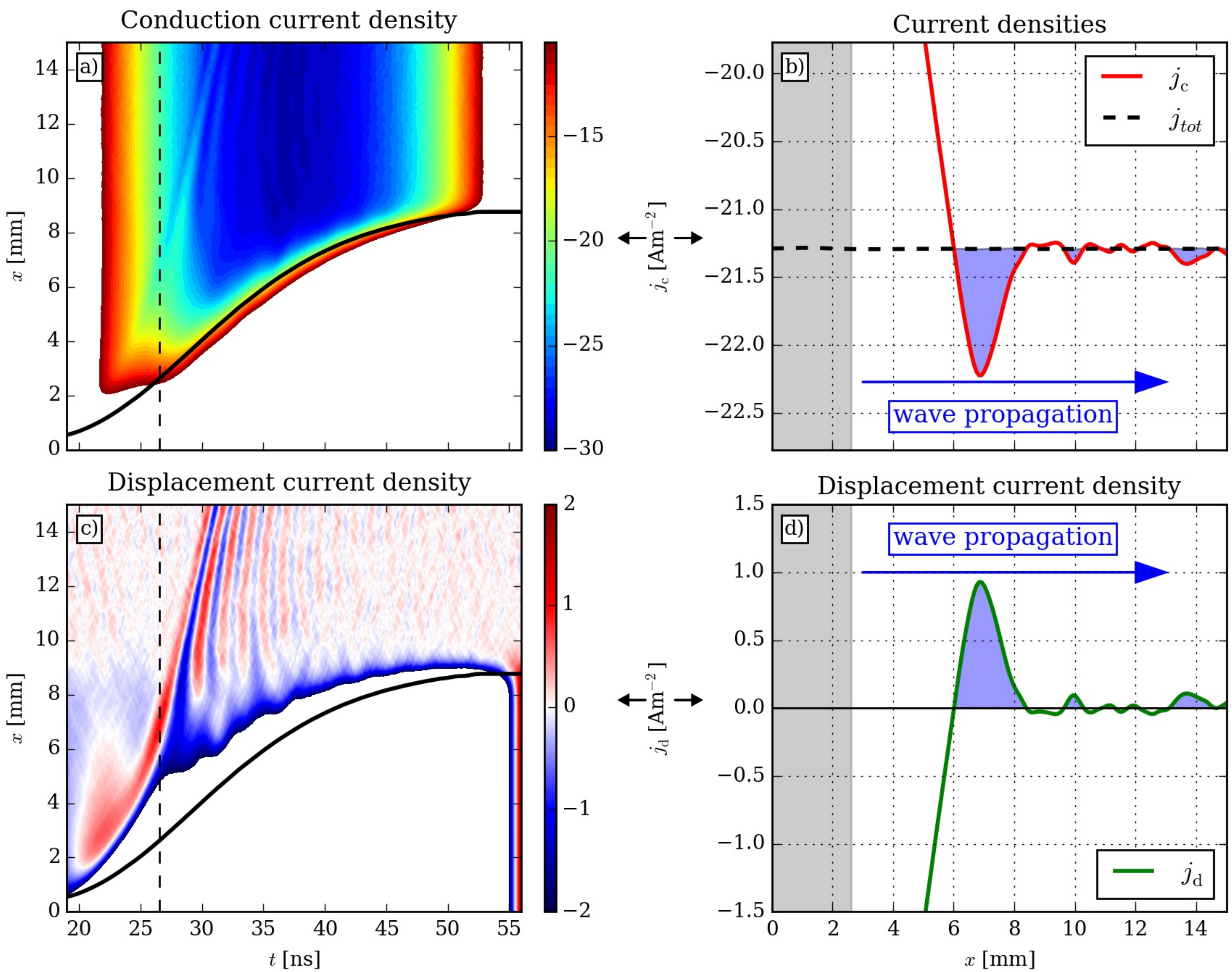
- in order to highlight the relatively weak wave dynamics in this scenario, the current densities are highlighted and adjusted during sheath expansion at the driven electrode (0 mm - 14 mm), the movie shows the propagation of electrostatic waves
- during sheath expansion the anisotropic acceleration of electrons leads to a strong increase of the conduction current density (a and red line in b) which exceeds the total current density
- due to current conservation the displacement current density (c and d) must compensate this effect
- this leads to the generation of electrostatic waves which propagate through the discharge
- these wave dynamics are more pronounced in asymmetric discharges (excitation of the plasma series resonance) and in discharges with high number of secondary electrons

# Current Densities and Current Conservation




**Link to Movie 4**

# Concept of this Investigation

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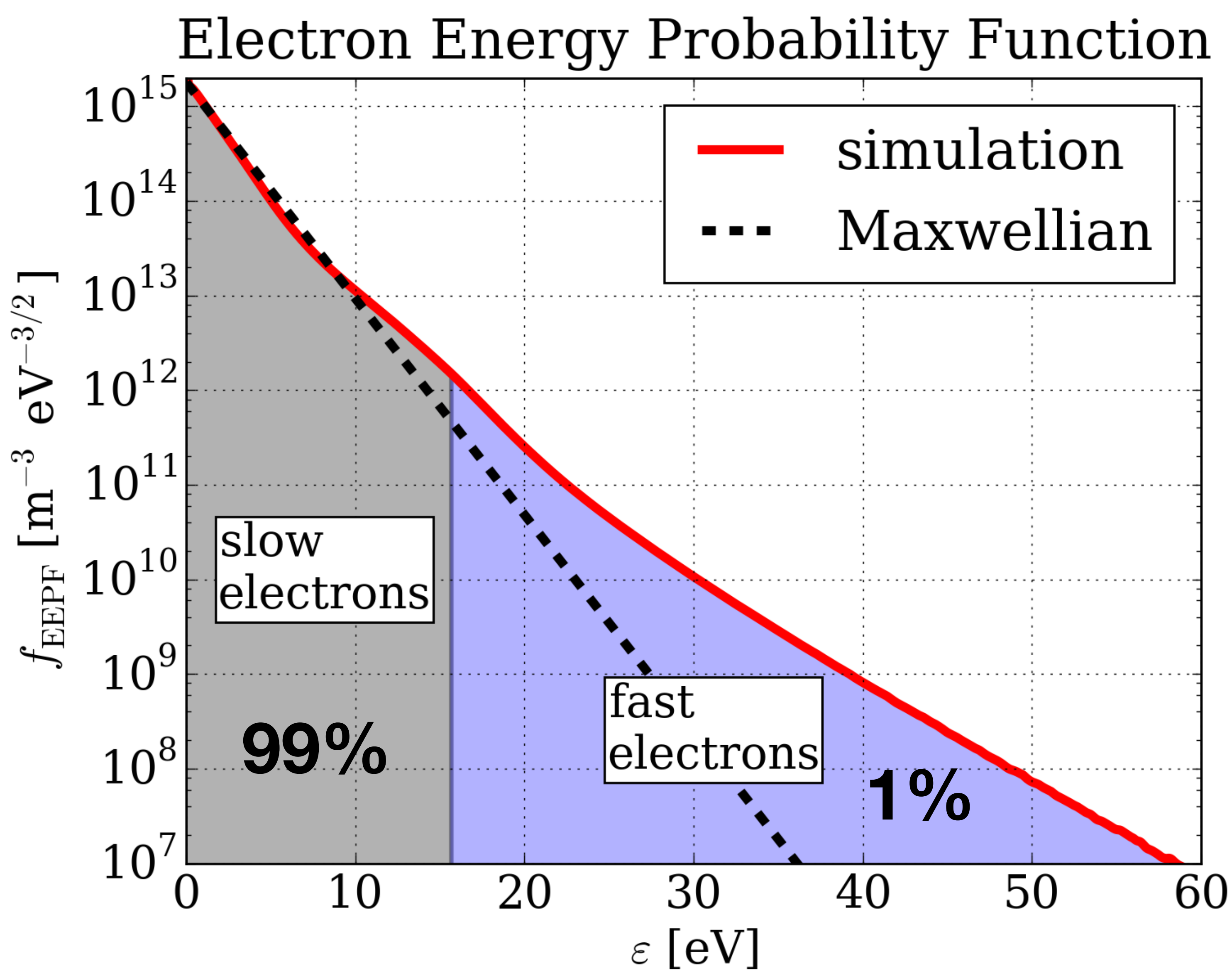
# Distribution Function

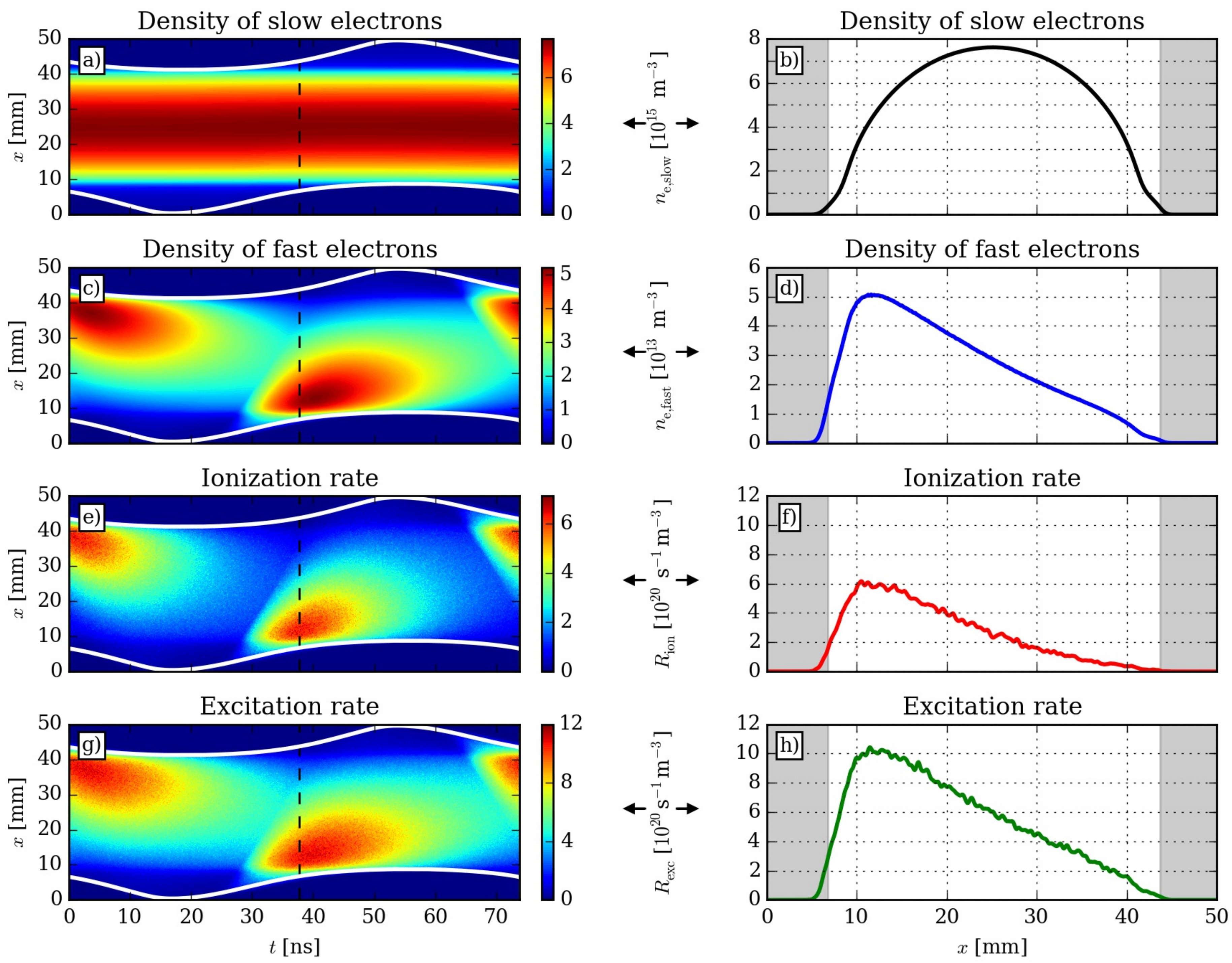



- non-Maxwellian distribution due to the anisotropy
- significant difference compared to a Maxwellian distribution (at higher energies)
- divide electrons into different energy groups, ionization threshold of argon is 15.7 eV
- 99 % of slow electrons (E < 15.7 eV), only 1% of fast electrons (E > 15.7 eV)

# Fast Electrons and Inelastic Collisions

- it's always important to understand and control the dynamics of the fast electrons ($E > 15.7$ eV), even if they just represent less than 1 % of all electrons (use the link to the movie on the next slide)
- slow energetic electrons (a and b) are only modulated in the plasma sheath and represent most of the electron population (99 %), however they can not support the discharge via ionization
- fast electrons (c and d), also called beam electrons, are generated during sheath expansion and penetrate collisionlessly into the plasma bulk due to the low pressure ($p = 3$ Pa)
- the dynamics of the ionization rate (e and f) indicate the same dynamics of the density of fast electrons
- the excitation rate (g and h) demonstrate a similar behavior and can be linked to experimental results of phase resolved optical emission spectroscopy (PROES)

# Electron Beams and Inelastic Collisions




**Link to Movie 5**

# Concept of this Investigation

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- Chapter 1: Interaction between field and particles
- Chapter 2: Current densities and current conservation
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- Chapter 4: Concept of the kinetic electron temperature
- Chapter 5: Mechanism of electron power absorption

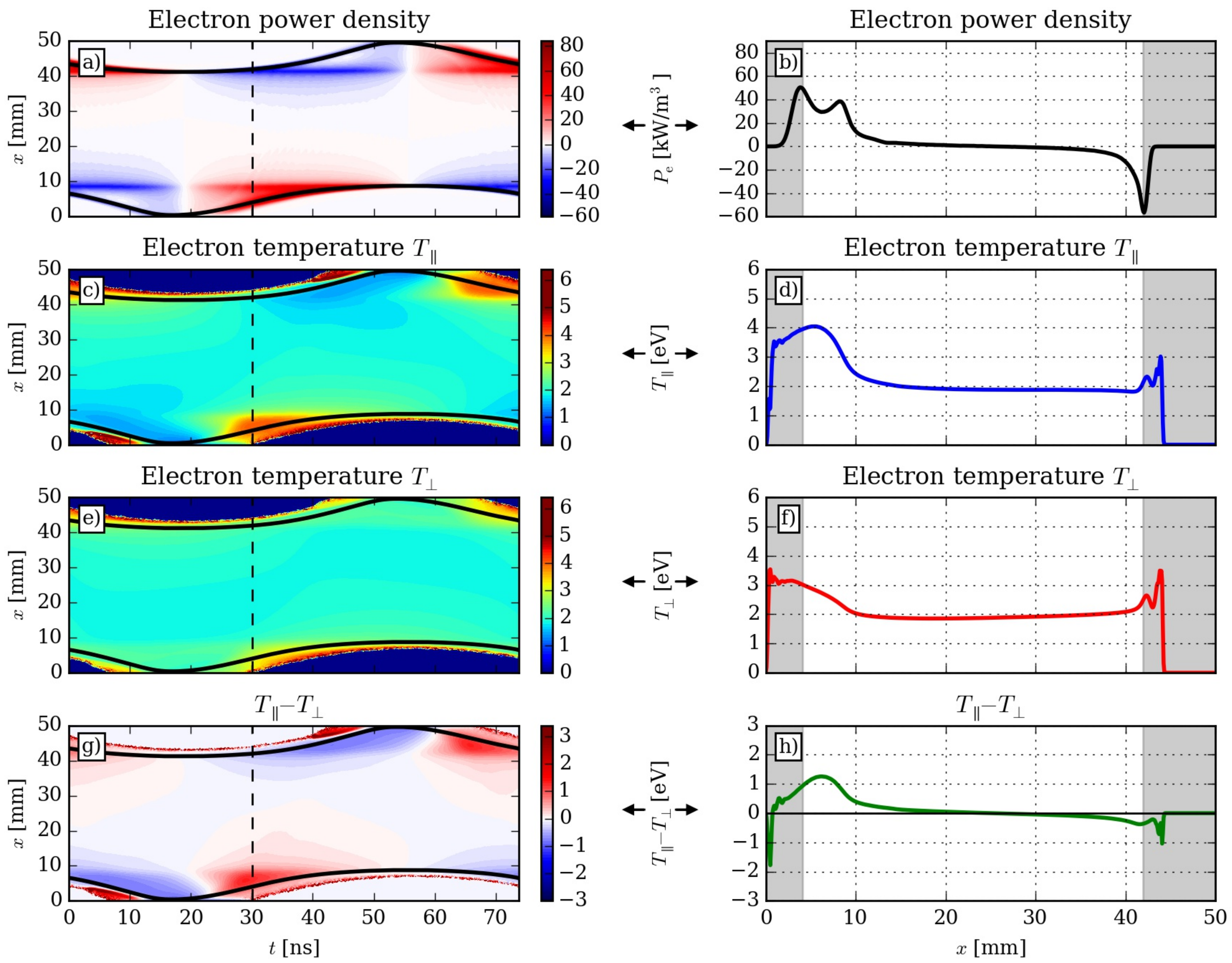
# Heating vs. Power Absorption

- the mechanism of electron power gain and loss can be studied by the electron power density (a and b on the next slide): $P_e = j_e \cdot E$
- most of the power absorption happens during sheath expansion and in the ambipolar electric field in front of the sheath edge
- the term heating (change of the temperature) can be studied by introducing the concept of the kinetic electron temperature which is based on the pressure tensor

$$T_{||} = m_e \left( < v_{||}^2 > - u_e^2 \right) \qquad T_{\perp} = m_e < v_{\perp}^2 >$$

- the parallel temperature (c and d) increases during sheath expansion
- the perpendicular temperature (e and f) temporally lags behind and it needs a certain time to redistribute the energy due to collisions
- the difference of both temperatures (g and h) is an indicator for the anisotropy of the system (nearly isotropic in the center of the discharge T = 1.9 eV)

# Kinetic Electron Temperature




**Link to Movie 6**

# Concept of this Investigation

- Chapter 1: Interaction between field and particles
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# Mechanism of Electron Power Absorption

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- the detailed analysis of the electron power absorption can be done by using the so called Boltzmann term analysis
- the fundament is the momentum balance equation which can be rearranged by solving it for the electric field

**momentum balance in x-direction:**

$$m_\mathrm{e}\frac{\partial(n_\mathrm{e}u_\mathrm{e})}{\partial t}+m_\mathrm{e}\frac{\partial(n_\mathrm{e}u_\mathrm{e}^2)}{\partial x}=-en_\mathrm{e}E-\frac{\partial p_{xx}}{\partial x}-\Pi_\mathrm{c}$$

**solving for the electric field:**

$$E=\underbrace{-\frac{m_\mathrm{e}}{n_\mathrm{e}}\left(\frac{\partial(u_\mathrm{e}n_\mathrm{e})}{\partial t}+\frac{\partial(n_\mathrm{e}u_\mathrm{e}^2)}{\partial x}\right)}_{E_\mathrm{in}}\underbrace{-\frac{1}{en_\mathrm{e}}\frac{\partial p_{xx}}{\partial x}}_{E_\mathrm{pr}}\underbrace{-\frac{1}{n_\mathrm{e}e}\Pi_\mathrm{c}}_{E_\mathrm{Ohm}}$$

# Mechanism of Electron Power Absorption

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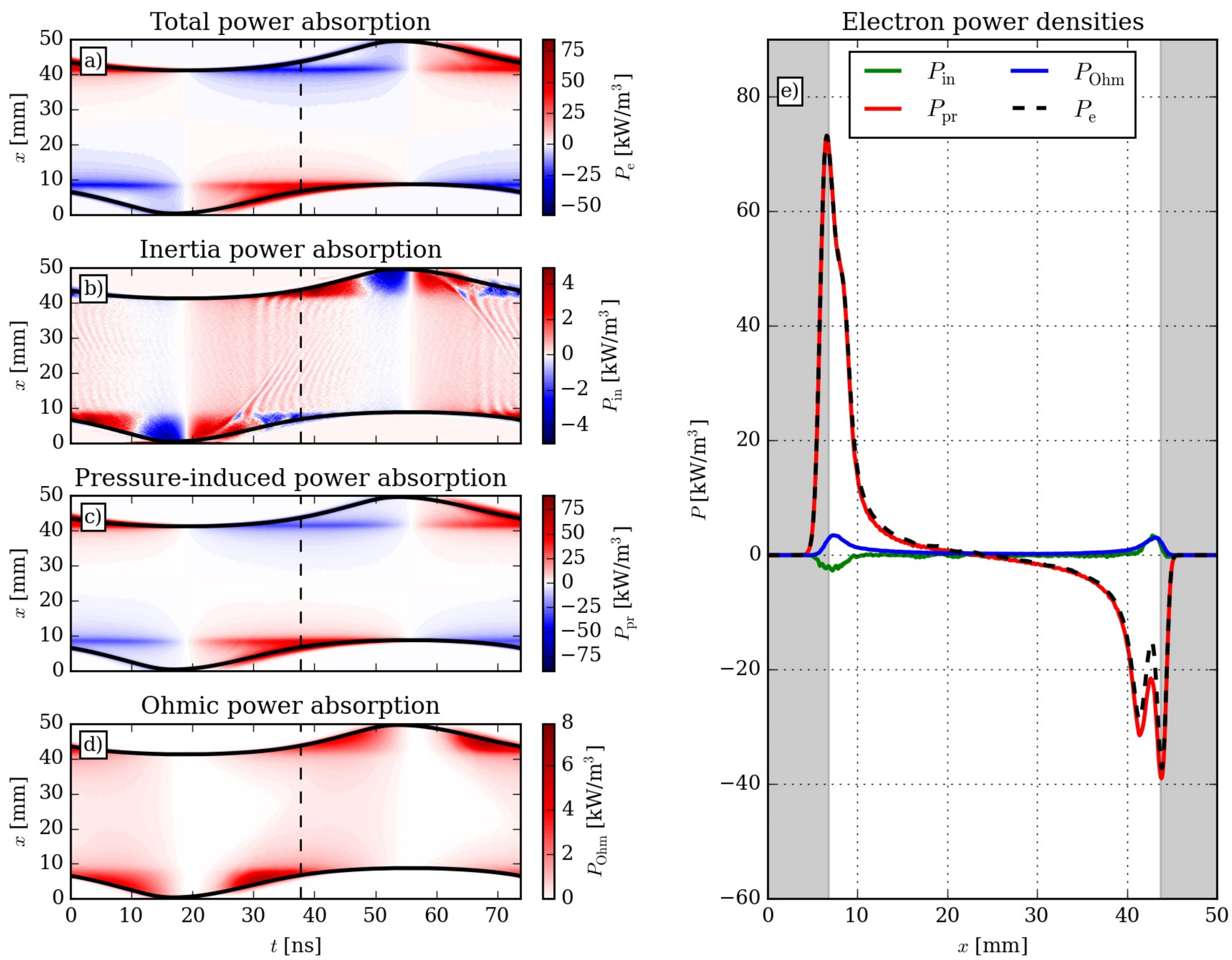
- multiplying by the electron current density leads to 3 power absorption terms
- every individual term can be obtained from the PIC/MCC simulation

**multiply by the electron current:**

$$\underbrace{j_e E}_{P_e} = \underbrace{\underbrace{j_e E_{\rm in}}_{P_{\rm in}} + \underbrace{j_e E_{\rm pr}}_{P_{\rm pr}}}_{P_{\rm collsionless}} + \underbrace{\underbrace{j_e E_{\rm Ohm}}_{P_{\rm Ohm}}}_{P_{\rm collisional}}$$

- the inertia term (b and green line in e) contributes only weakly to the power absorption (in total (time and spatio averaged) less than 0.1 %)
- the pressure heating term (c and red line in e) is the most dominant term with positiv and negativ values (in total 63 %)
- the Ohmic heating term (d and blue line in e) is always positiv but the amplitudes are weak (in total 37 % because it has only positive values)

# Mechanism of Electron Power Absorption




**Link to Movie 7**

# Mechanism of Electron Power Absorption

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**more information about the electron power absorption by Máté Vass**

**Session PW2: Capacitively Coupled Plasmas II**
1:00 PM–2:30 PM, Wednesday, October 7, 2020

Chair: Xiaopu Li, Applied Materials

**Abstract: PW2.00001 : Electron power absorption in capacitive RF plasmas based on a moment analysis of the Boltzmann equation**
1:00 PM–1:30 PM Live

# Conclusion

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- CCRF discharges at low pressures ($p < 3$ Pa), work in a very nonlocal regime
- the ambipolar electric field plays an important role
- electrostatic waves are excited during sheath expansion (interplay between the conduction and displacement current density)
- additionally, the sheath expansion generates electron beams which lead to a pronounced anisotropy in the distribution function
- these electron beams are important for the ionization process even if they only represent less than 1 % of the electron population
- the concept of the kinetic electron temperature (parallel and perpendicular) indicates that electron power absorption and electron heating are physically two different mechanisms
- the Boltzmann term analysis shows how the electrons gain and lose their energy due to inertia, pressure and Ohmic effects