PIC simulations of plasma streamers in atmospheric pressure volume and surface DBDs

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Outline

I. Background

II. PIC/MCC model for streamer simulation

III. Negative/positive streamer mechanism

IV. Plasma streamer propagation in porous catalyst

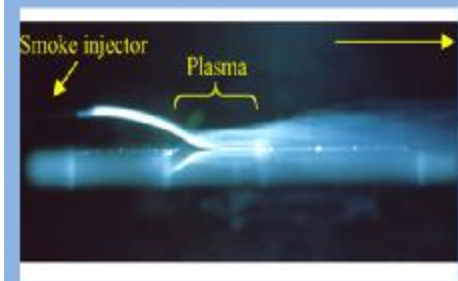
V. Streamer discharge in SDBD

VI. Conclusion

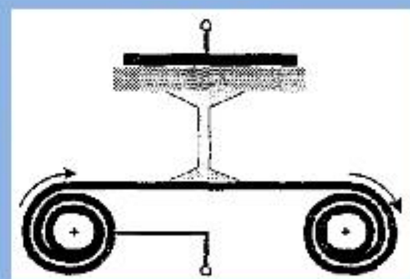
Streamer discharge background

Applications:

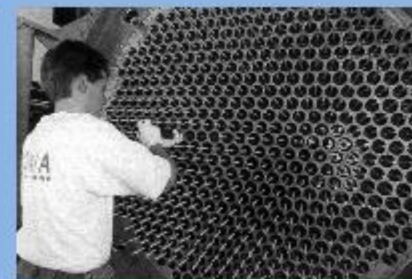
Air flow control



Material processing

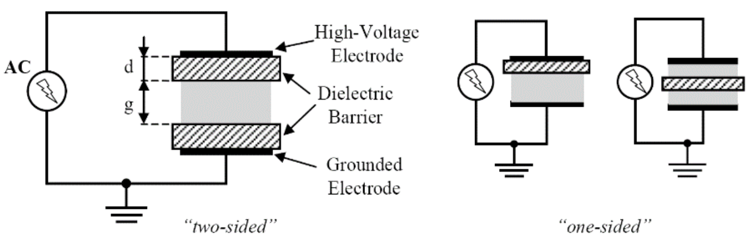


Ozone Generation

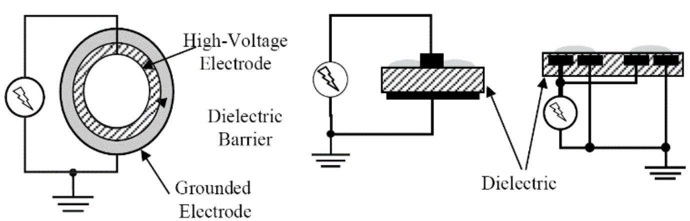


Gas cleaning

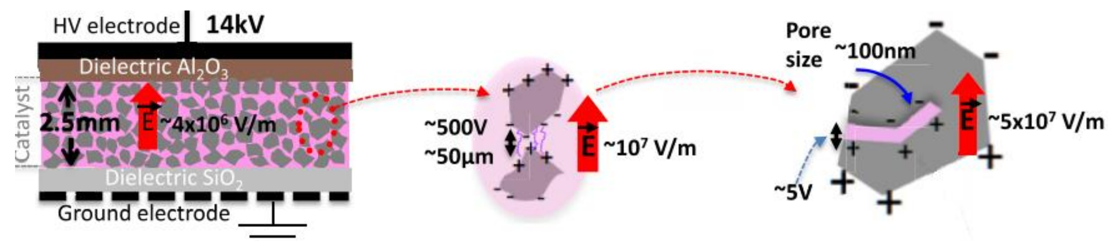
DBD reactors:



Cylindrical Reactor Surface Discharge Coplanar Discharge



Plasma catalysis in packed DBD



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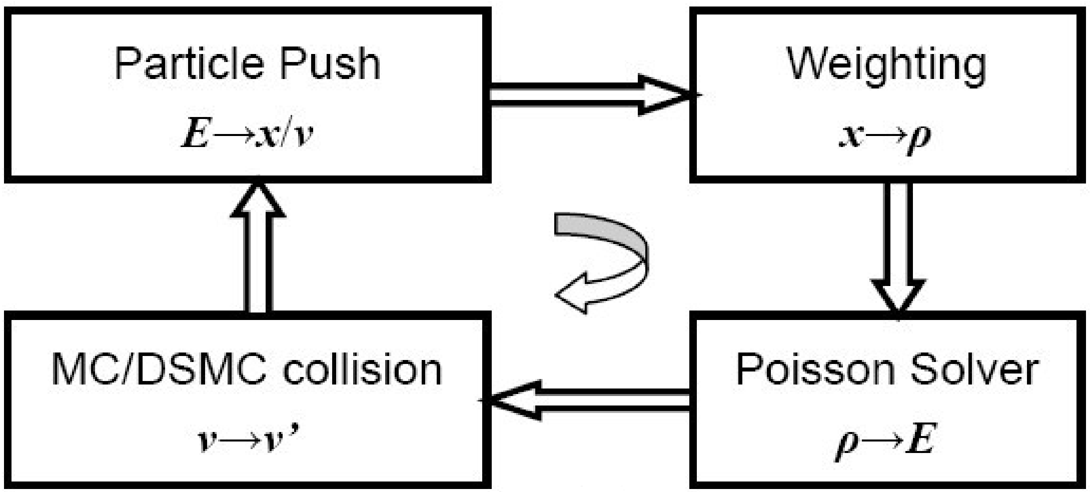
PIC/MCC model (粒子模型）

PIC/MCC flow:



MCC: Null collision method

Max-collision frequency:

$$\upsilon_{\max} = \max_x(n_t(x)) \max_E \left(\sigma_T(\varepsilon) \left(\frac{2E}{m_p} \right)^{1/2} \right)$$

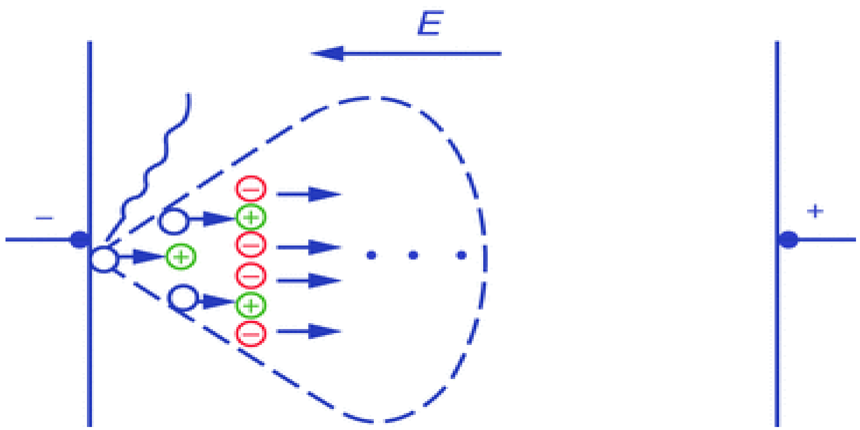
Probability & number:

$$P_{null} = 1 - \exp(-\upsilon_{\max} \Delta t)$$

$$N_{coll} = N_p P_{null} = N_p (1 - \exp(-\upsilon_{\max} \Delta t))$$

PIC/MCC model (粒子模型）

Problems 1:



- **Electrons experience avalanches to form the streamer**
- **The amount of particles increases exponentially**
- **Consuming memory, breaking simulation**

Particle merger:

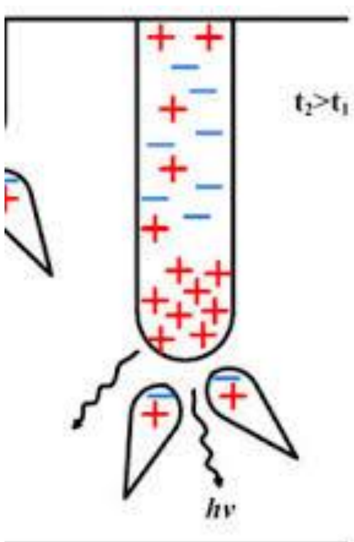
$$m_1 v_{1\alpha} + m_2 v_{2\alpha} + m_3 v_{3\alpha} = m_A v_{A\alpha} + m_B v_{B\alpha},$$

$$m_1 v_{1\alpha}^2 + m_2 v_{2\alpha}^2 + m_3 v_{3\alpha}^2 = m_A v_{A\alpha}^2 + m_B v_{B\alpha}^2,$$

- **Control the particles**
- **Momentum, energy conservation**
- **Combine super-particles when the number of super-particles exceeds a threshold in each cell**

PIC/MCC model (粒子模型）

Problems 2:

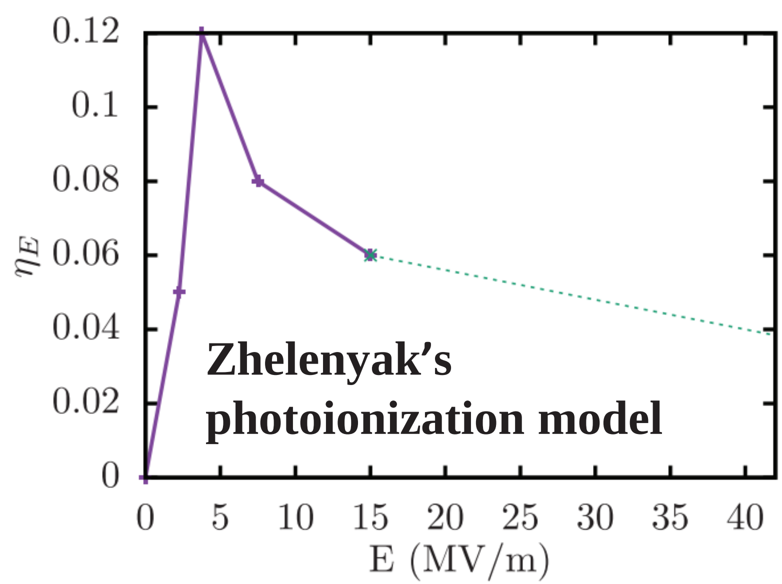


- **Electrons move to the streamer head in positive streamer**
- **Streamer stops when electrons are exhausted in limited geometry**
- **"New particle mechanism?"**

Particle merger:

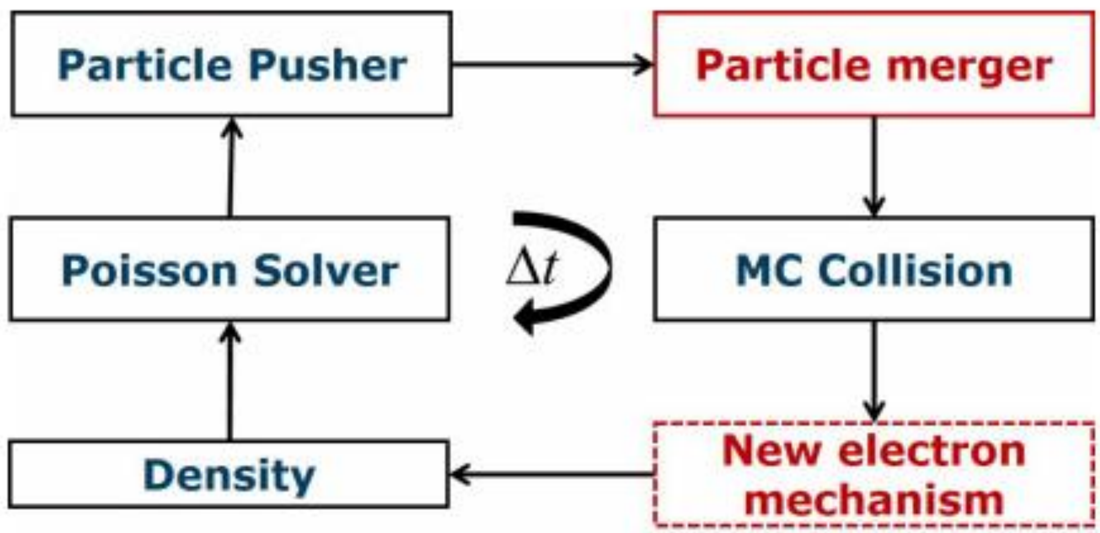
Photon-ionization

N^*_2->O_2



PIC/MCC model (粒子模型）

Improved PIC/MCC flow:



MCC: Null collision method

Max-collision frequency:

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MCC: Null collision method

Max-collision frequency:

$$\upsilon_{\max} = \max_{x}(n_t(x)) \max_{E}\left(\sigma_T(\varepsilon)\left(\frac{2E}{m_p}\right)^{1/2}\right)$$

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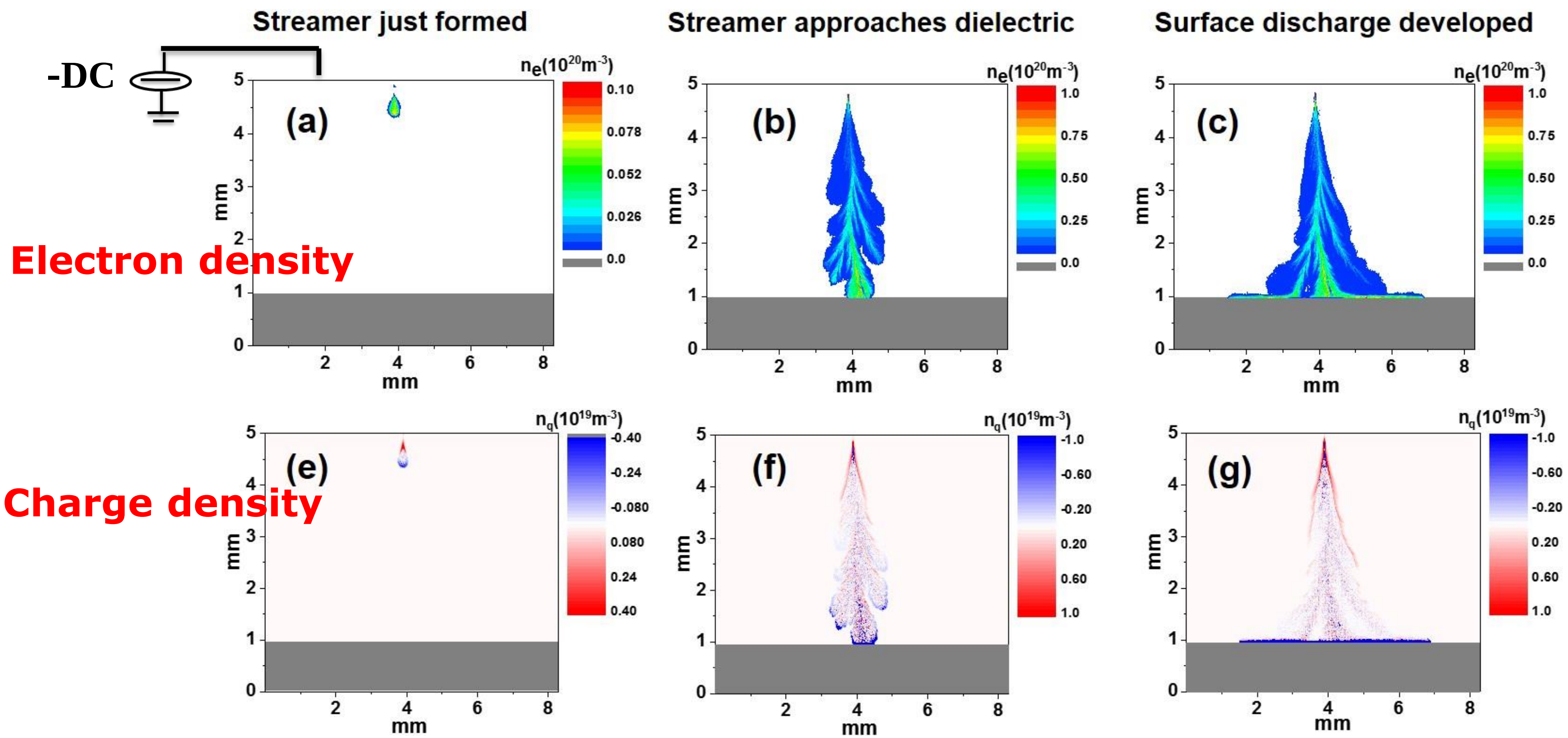
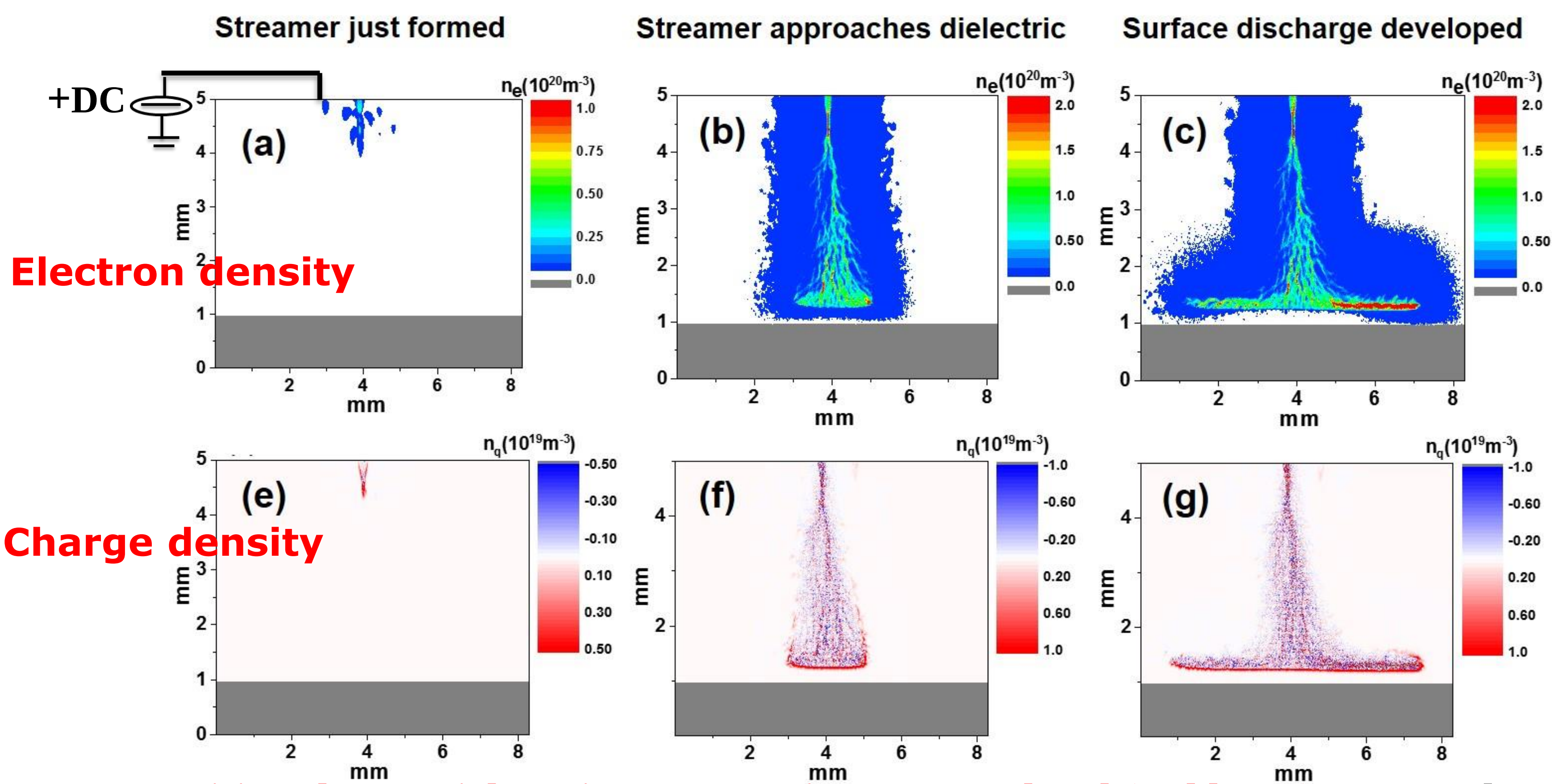
Negative streamer propagations



- Only 20 charge species are artificially placed near the DC source, as seeds
- Plasma streamer develops from the avalanche of seeds after a certain distance
- A negative charge-rich region (blue layer) appears around the streamer head, (a strong electric field) accelerates the front electrons to move forward
- Negative streamer finally arrives at the dielectric, and charge the dielectric surface, inducing an extra electric field along the surface, and a surface discharge

<u>"Horizontal electric field is caused by surface charging"</u>

Positive streamer propagations

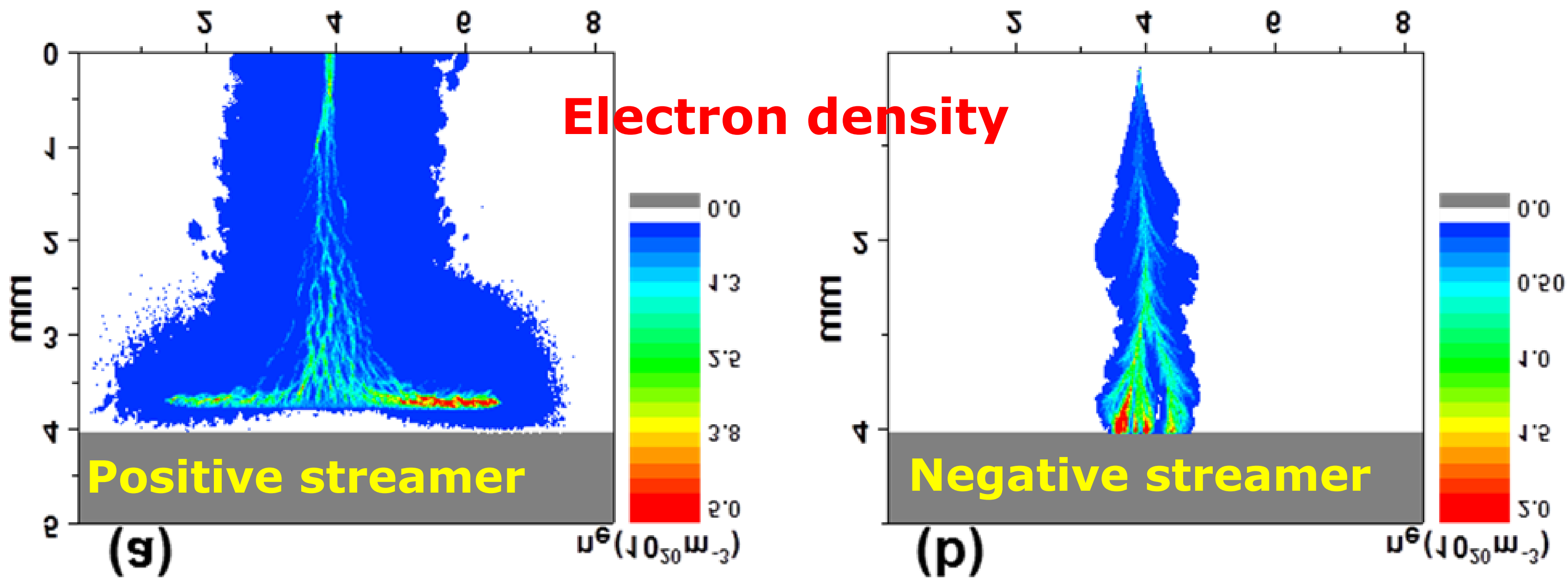


- A positive charge-rich region appears in streamer head (red layer), strong electric field
- The strong electric field induces avalanches of free electrons near the streamer head toward the charge region, facilitating the streamer propagation and branching
- When the streamer approaches the dielectric, it develops horizontally and floatingly

Conditions: <u>enough free electrons + enough travel space for the free electrons</u>

<u>"Horizontal electric field is caused by spatial positive charge"</u>

Influence of surface charging



After removing the surface charging:

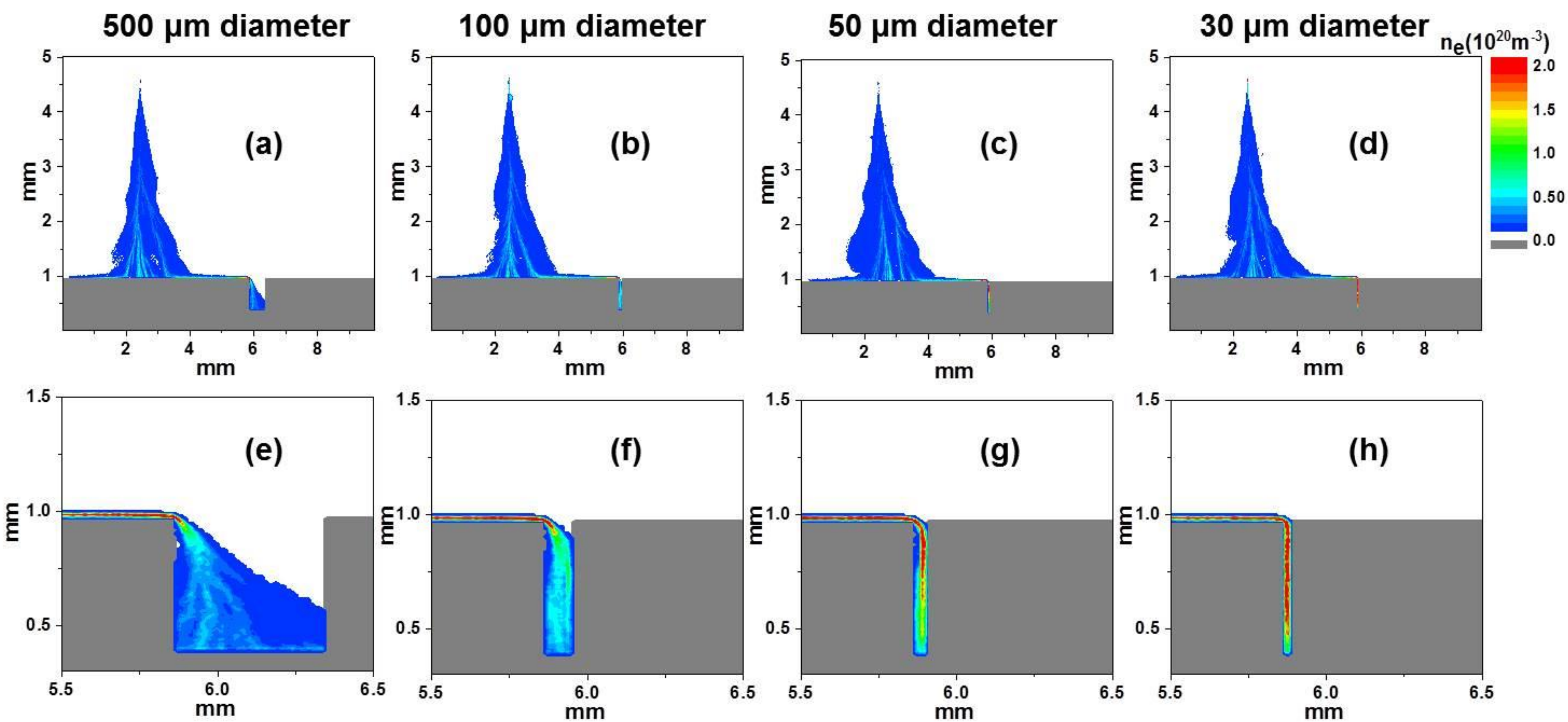
- **The positive streamer can still develop above the dielectric**
- **The negative streamer can not spread at all, as no horizontal electric field**

Emphasize:

“Horizontal electric field is caused by spatial positive charge” in positive streamer

“Horizontal electric field is caused by surface charging” in negative streamer

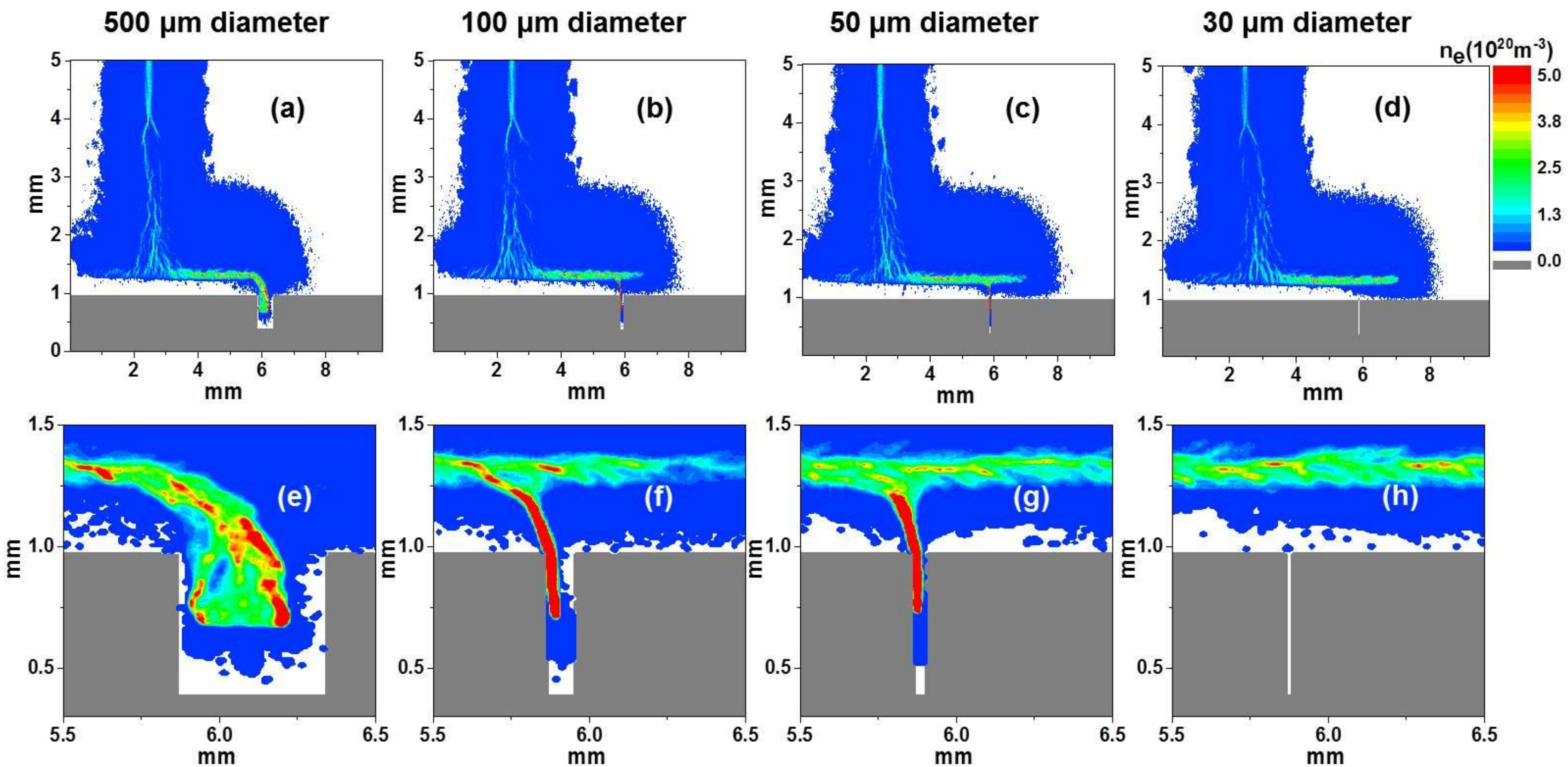
Influence of dielectric pores in negative streamer



- **Negative streamer can climb into the pores, inducing discharge enhancement due to surface charging on the pore sidewall**
- **The discharge enhancement becomes more pronounced at smaller pore diameter (> Debye length)**

Plasma Process Polym. 2021, e2000234

Influence of dielectric pores in positive streamer



- Enhanced discharge can be induced inside the pore as a branch
- Outside the pore, the applied electric field is perpendicular to the dielectric surface, inducing floating surface discharge
- Inside the pore, the applied electric field is parallel to the dielectric surface (pore sidewall), so surface discharge can happen on the sidewall
- 30um pore is too narrow to provide sufficient photoionization and avalanches

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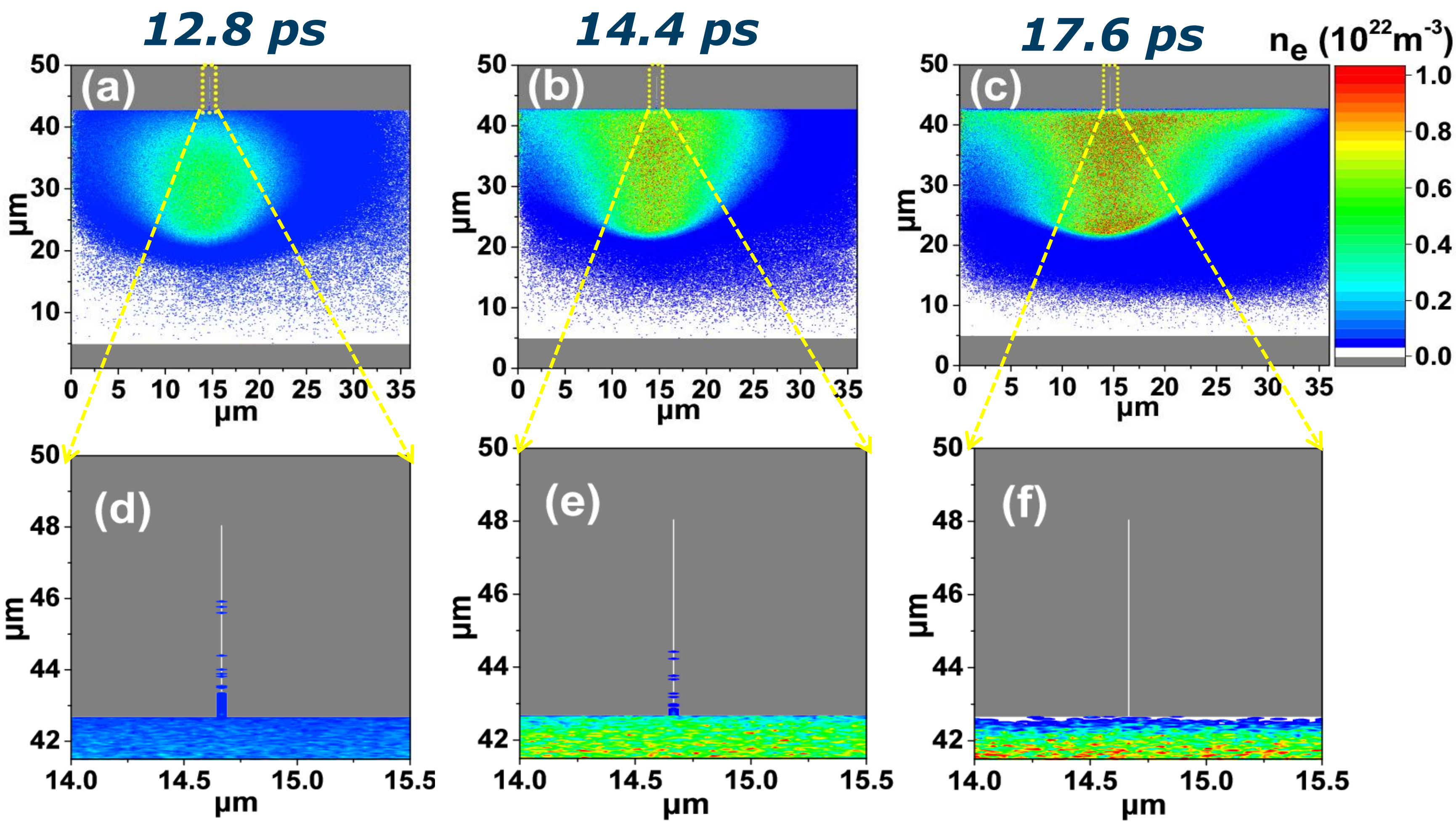
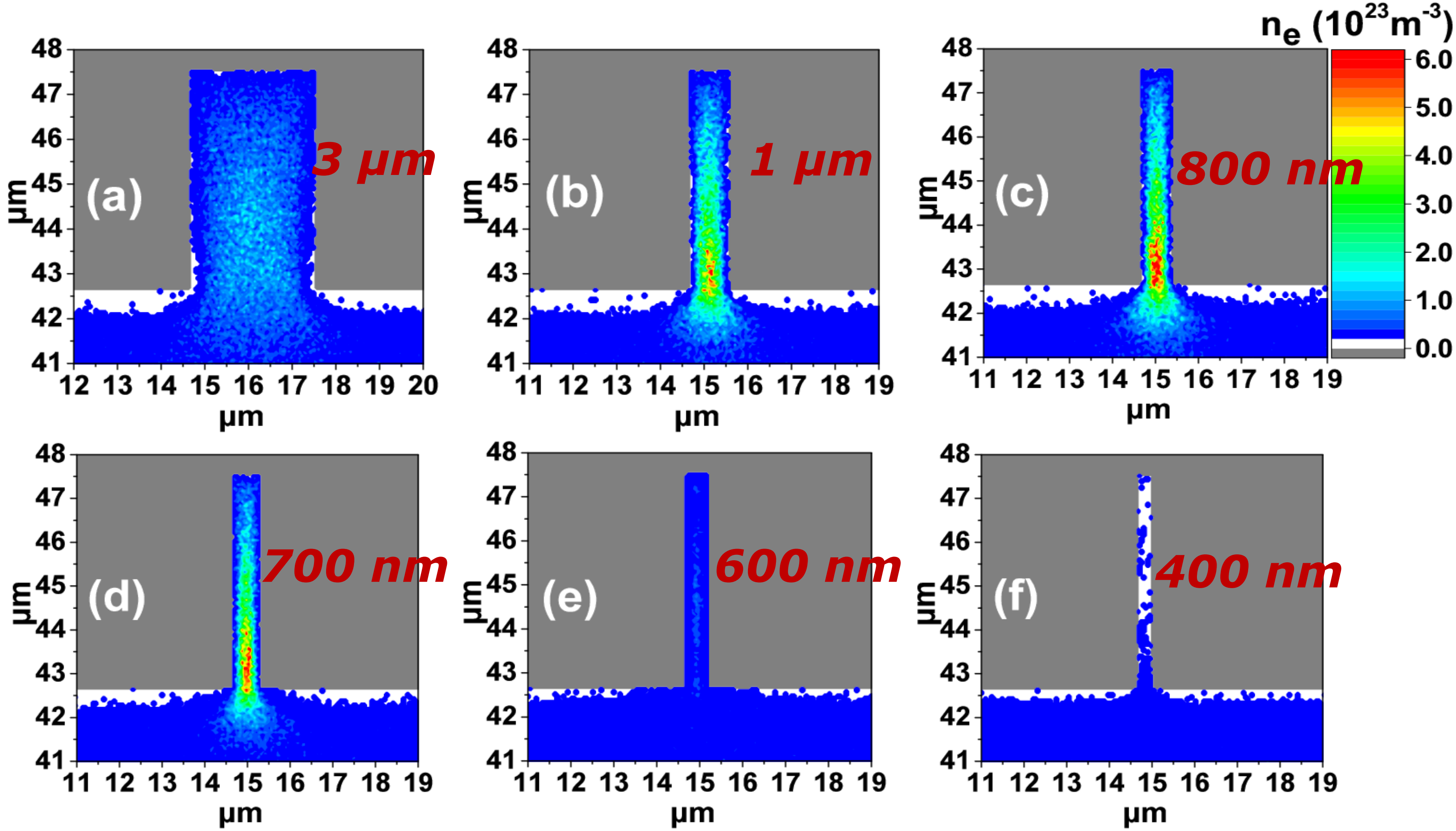
Plasma streamer in 50 nm pore



- Plasma can slightly penetrate into small pores at the beginning (12.8 ~ 14.4 ps)
- Sheath develops fast after the streamer arrives at the dielectric
- Plasma bulk will be pushed away by the sheath, and no plasma penetration into the pores any more

Plasma streamer in larger pores

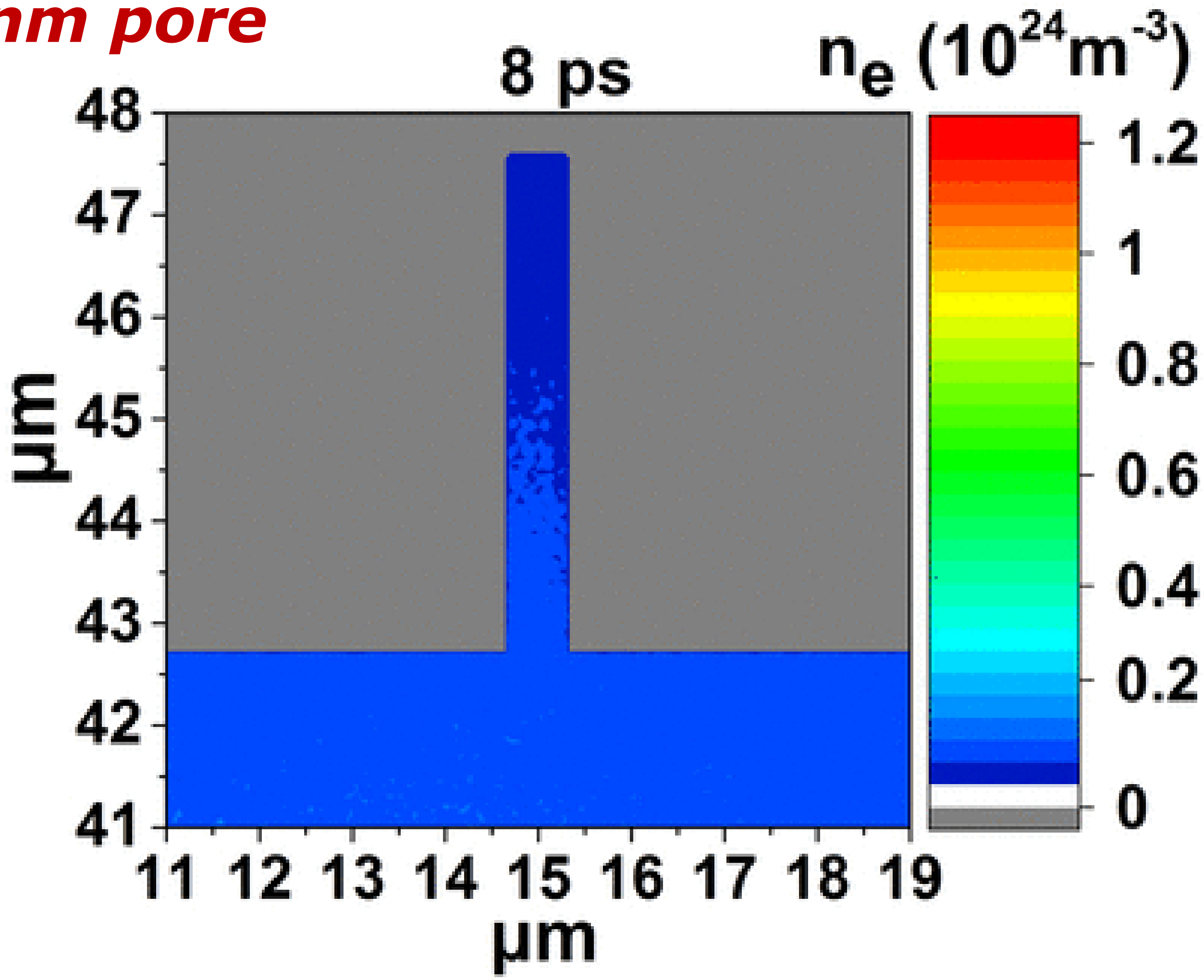


- Plasma properties before pores: λ_{de}~600nm
- Discharge can be significantly enhanced for bigger pore size (>600 nm)
- Maximum density appears at 800 nm pore

Plasma Sources Sci. Technol. 27 (2018) 035009

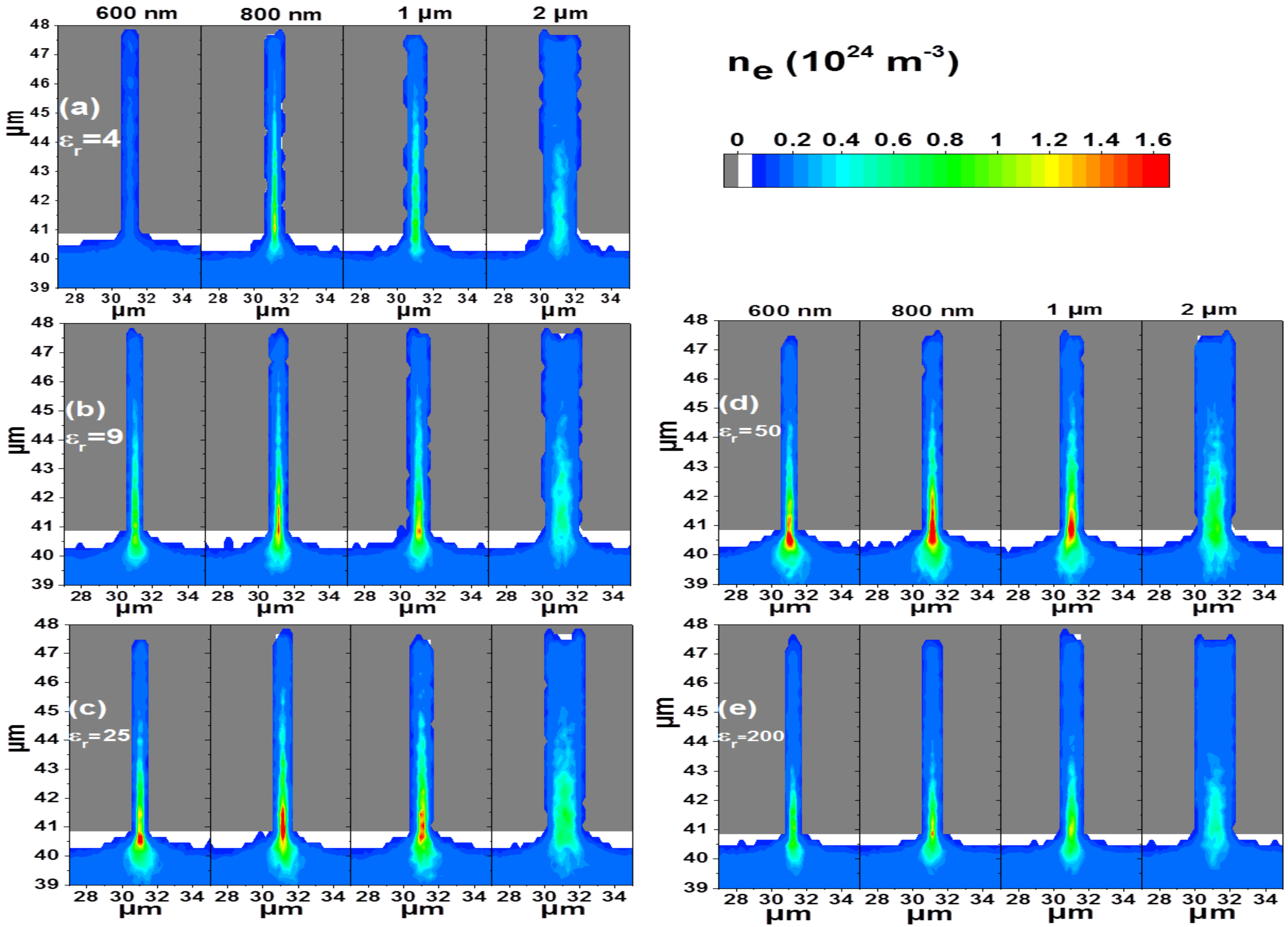
Discharge enhancement inside the pore

700 nm pore



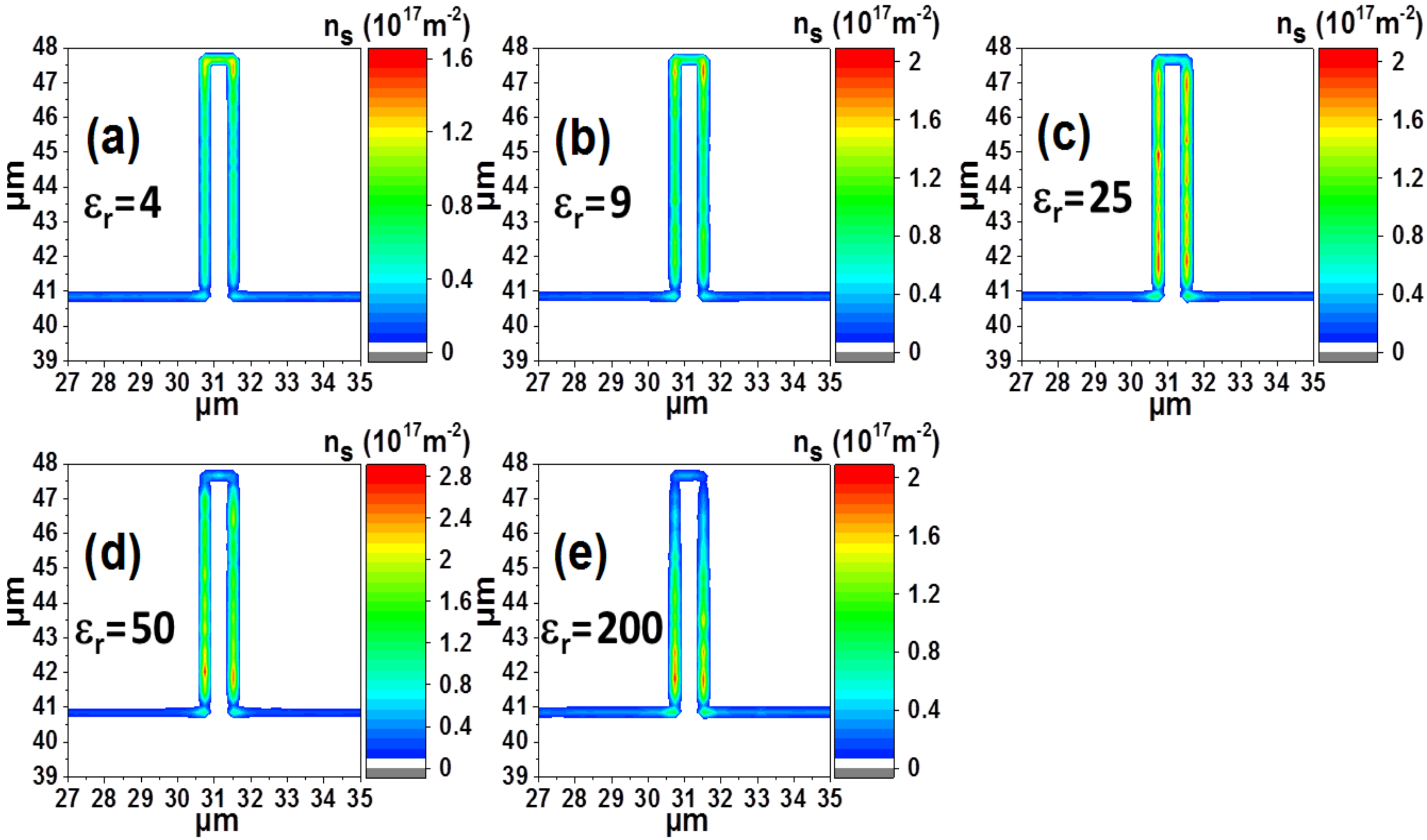
- **Electron charge the sidewall, and induce an extra electric field**
- **Discharge inside the pore is enhanced -- surface discharge**

Surface charging effect: dielectric constant ε_r



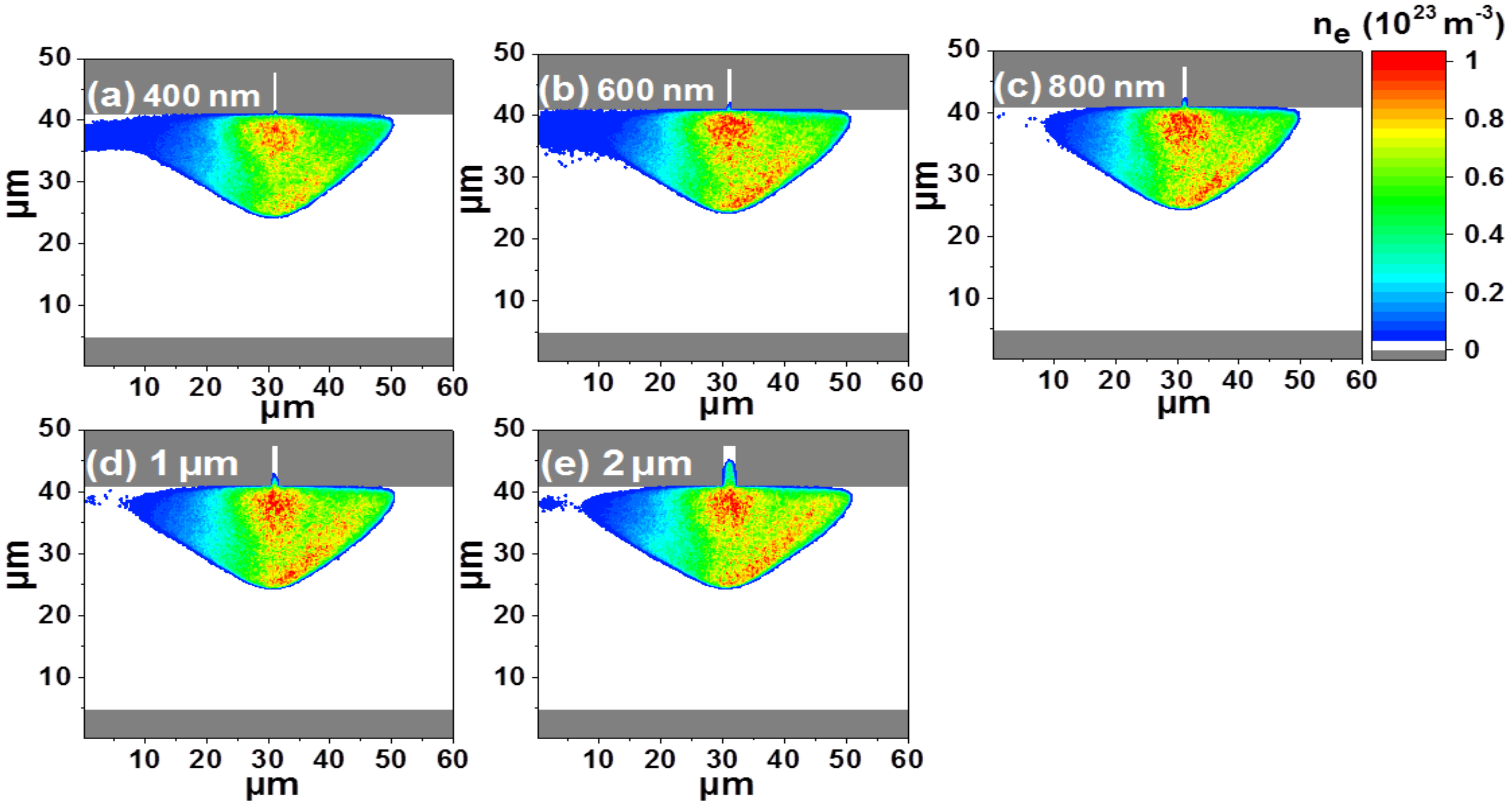
- The maximum plasma density first increases, but then decreases when rising ε_r
- The length of the streamer slightly reduces upon rising ε_r

Importance of surface charging



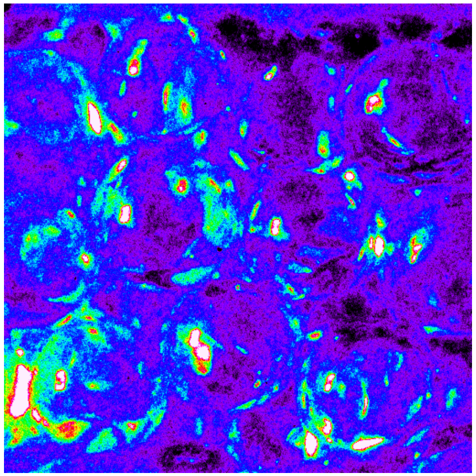
- The electrons will charge the pore sidewalls, when the streamer arrives at the pore
- The non-uniform charging induces an extra (surface) electric field, and accelerates the streamer
- Dielectric material is more easily polarized at larger ε_r, which reduces the surface electric field

Can plasma penetrate in pores with metallic coating (infinite ε_r)?

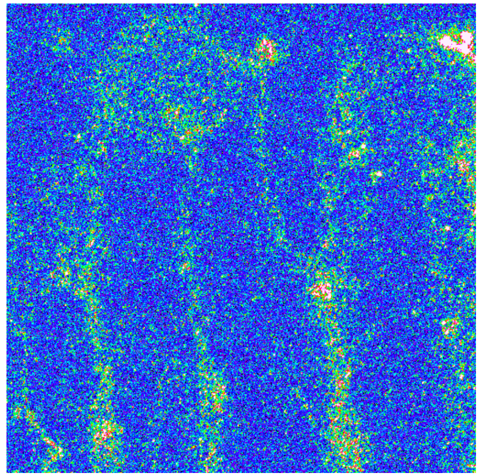


- Streamer is difficult to propagate into the pores with metallic coating
- More plasma can diffuse into larger pores, but there is no discharge enhancement
- No surface discharge, no discharge enhancement

Experimental validation (ICCD)

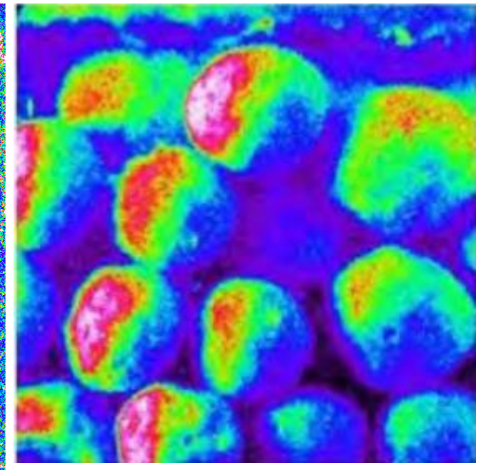


before discharge

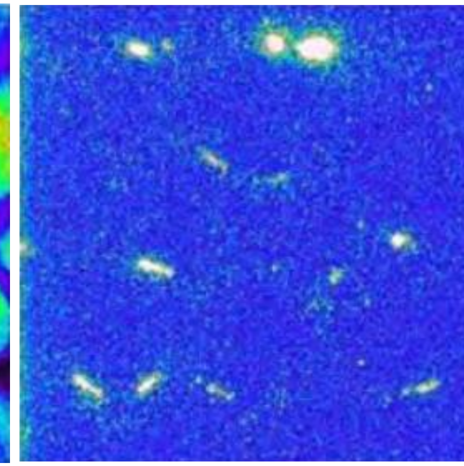


during discharge

Glass (ε_r=5), Voltage = -11.1 kV



before discharge



during discharge

$BaTiO_3$ (ε_r=2600)*,Voltage = -7.5 kV

- **There are obvious enhanced plasma streamer in the pores between pellets at low ε_r**
- **Intense discharge happen at the contact points of the beads, no surface discharge**
- **The experimental results validate our simulations in a large degree**

Chemical Engineering Journal 334 (2018) 2467–2479

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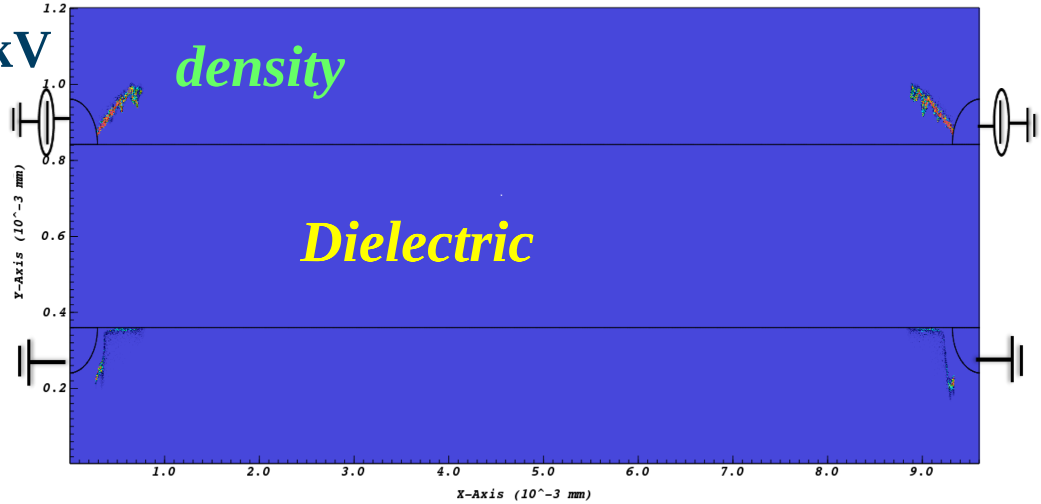
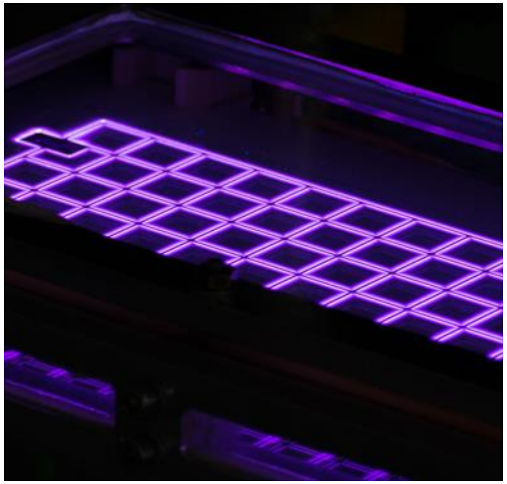
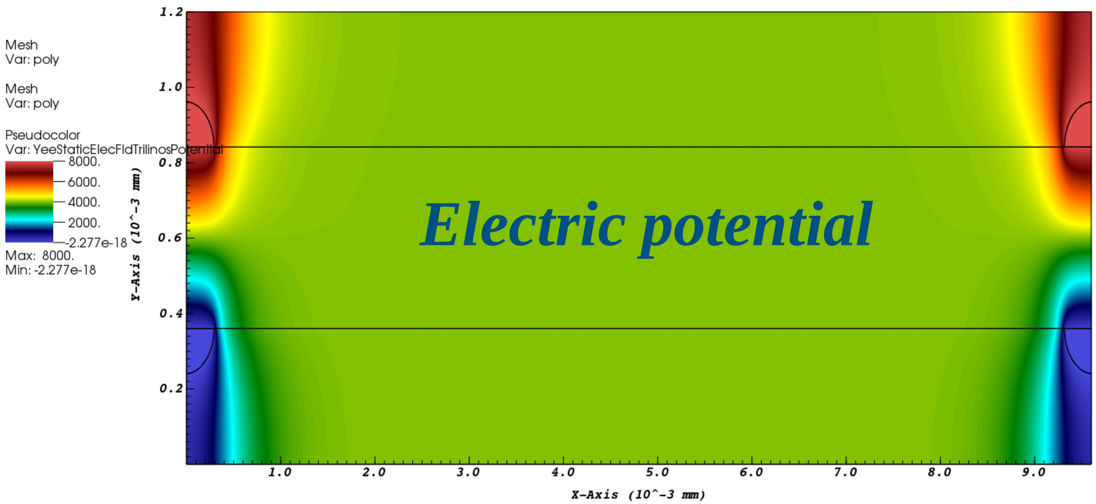
Streamer discharge in SDBD

DC: 8 kV



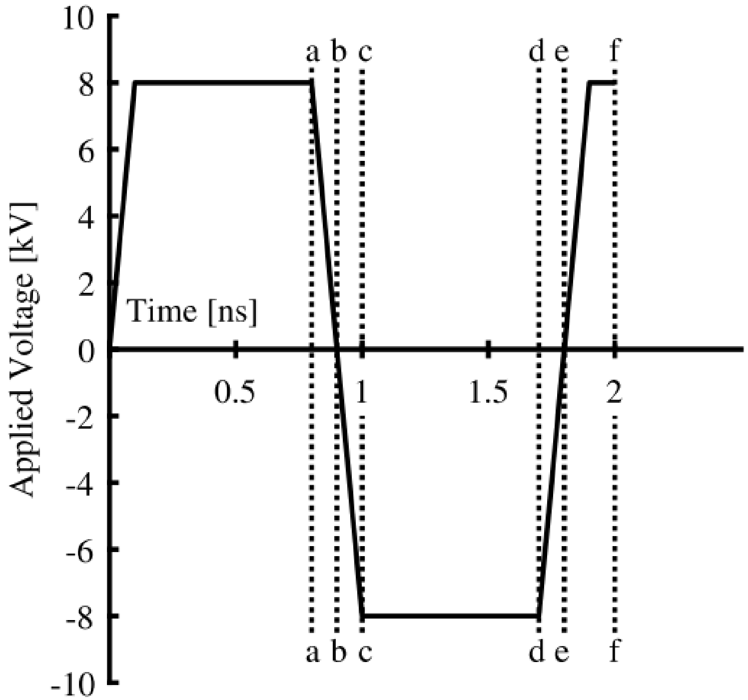


Experimental photo
(from R T Nguyen-Smith,
Ruhr-Universität Bochum)

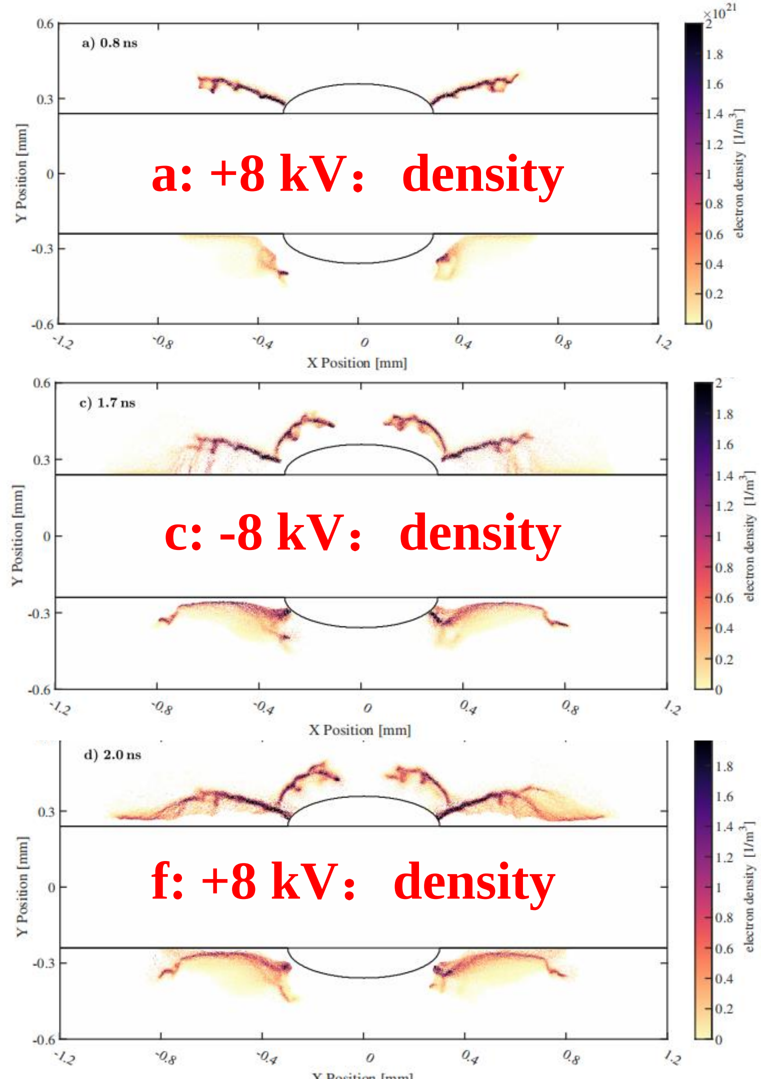


- Discharge happen at both sides
- Electric potential drops significantly along the r direction, which is the reason for short streamer length
- Simulating a small region near the electrode is enough for accuracy

Streamer discharge in SDBD

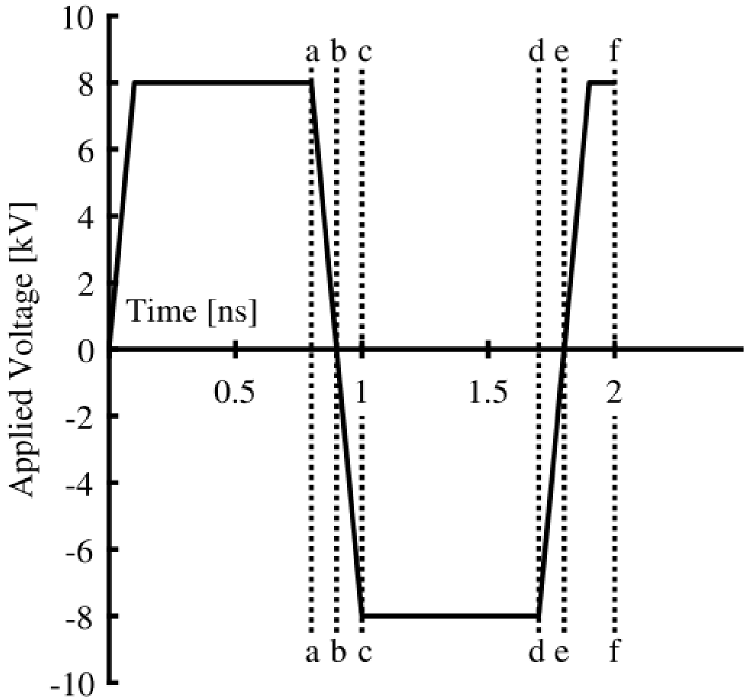


waveform

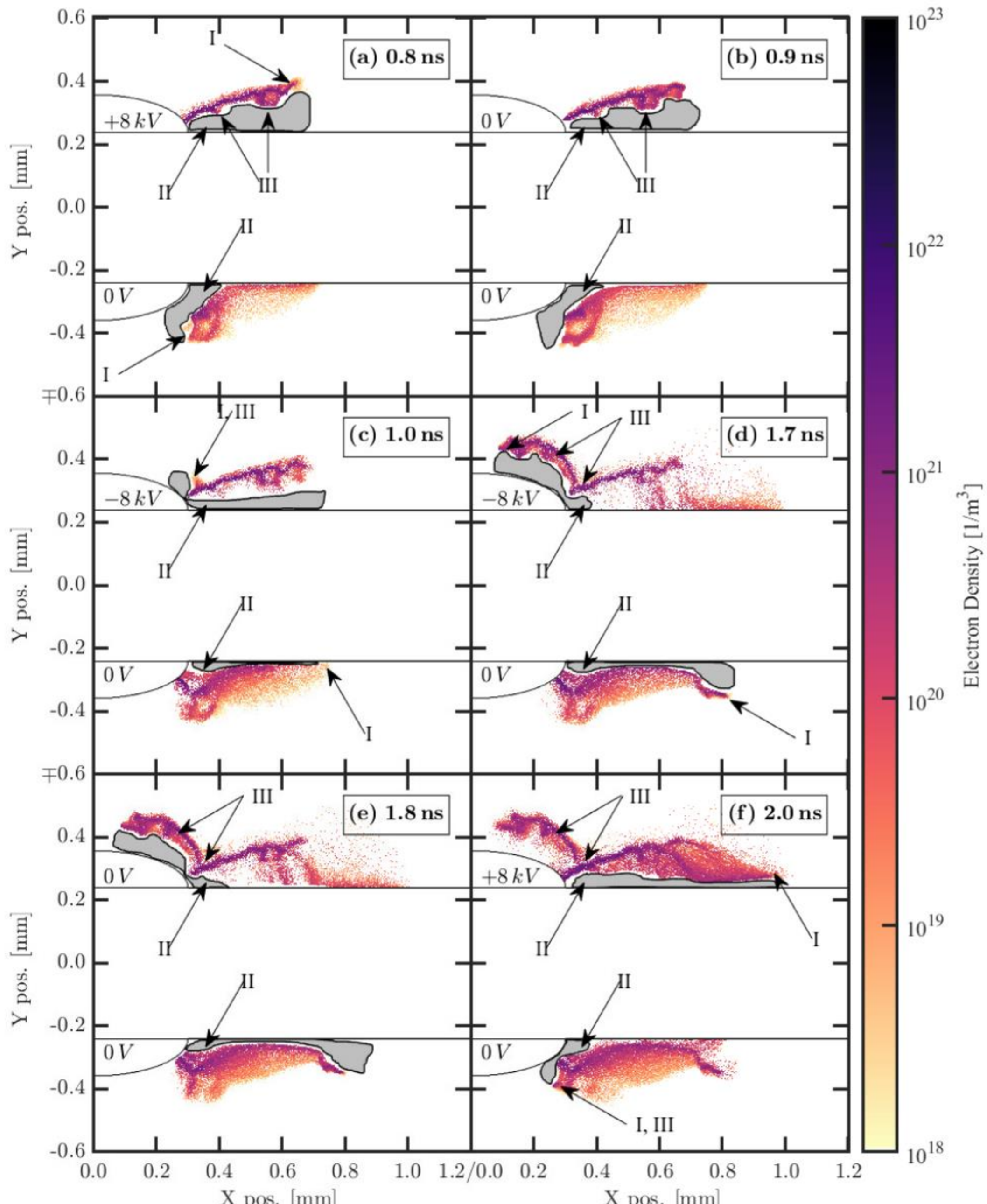


- Positive streamer is floating, negative streamer can develop on the dielectric
- Voltage reversal converts the streamer polarities (negative ↔ positive)
- A much stronger streamer branch is induced within short time at the top

Streamer discharge in SDBD - details



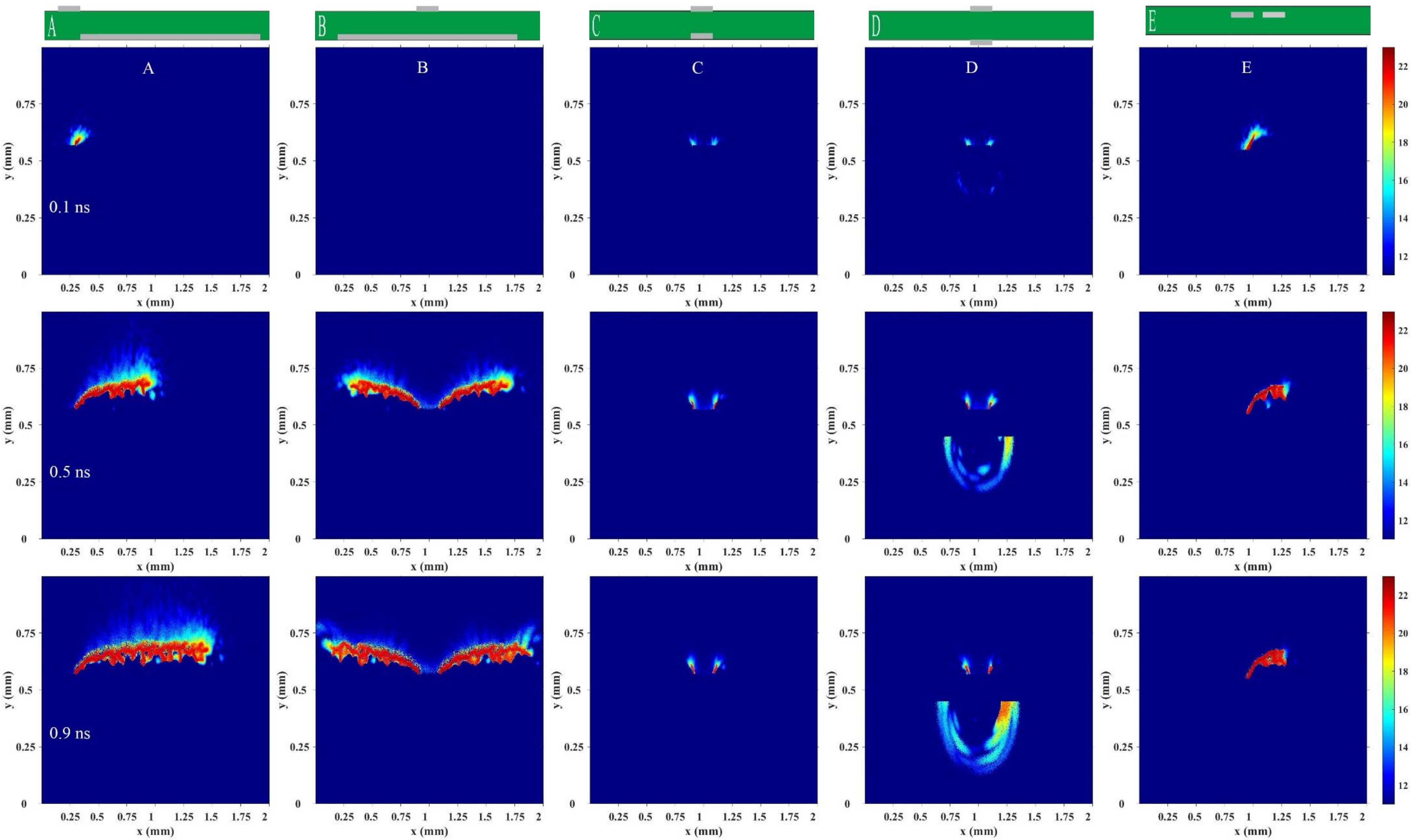
waveform



ACCEPTED BY PLASMA SOURCES SCI. TECHNOL.

Streamer discharge in various SDBD

Electron density: Positive dc voltage



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Conclusion

- Modified PIC/MCC flow is needed for streamer simulation
- Positive surface streamer is floating
- Negative surface streamer develops along the surface
- Debye length is an important criterion for plasma penetration into catalyst pores
- Surface charging plays important role for plasma streamer propagation in dielectric pore
- Polarization of material will localize the discharge
- Waveform and configuration affect the streamer propagation in SDBD

Thank you!

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