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Seed Electron Generation Mechanisms in the Presence of a Dielectric Particle

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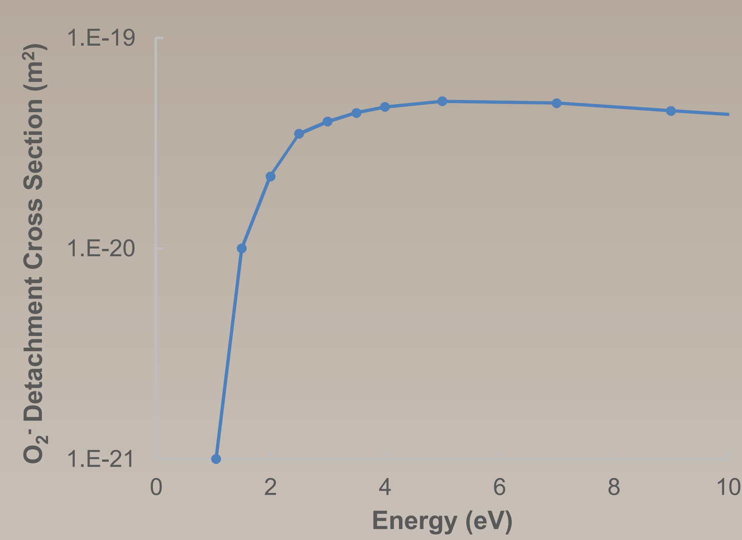
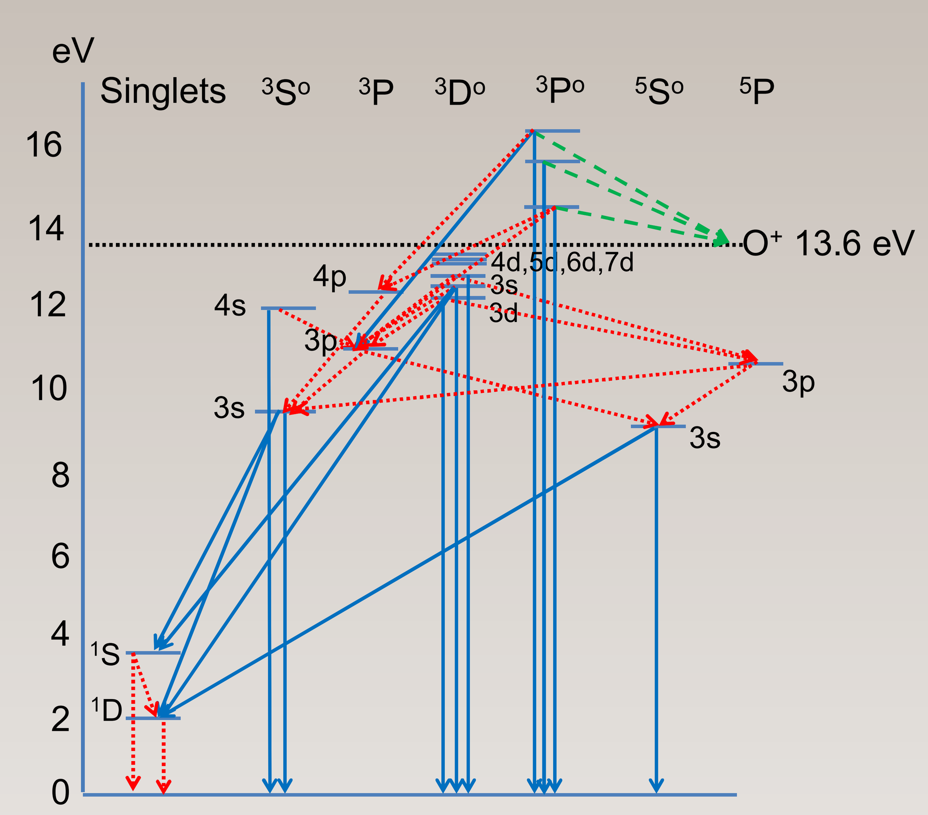
Abstract

An electrostatic particle-in-cell (PIC) code which simulates particle-particle collisions using the direct simulation Monte Carlo (DSMC) method has been used to simulate the stochastic initiation of breakdown with dielectric particles present. The simulation model seeds an initial steady state density distribution of electrons and O_2^- in the domain by modeling a switched 10 ns UV light source incident on the dielectric and electrode surfaces (with zero applied potential) as an e^- trickle current that then attaches to O_2 via kinetically modelled collisions. The resultant e^- and O_2^- densities are then added to the neutral background gas mixture as the initial state and the anode potential is increased at 200 kV/μs and O_2^- detachment serves as the primary electron source. The air chemistry model [1] includes standard Townsend breakdown mechanisms (electron-neutral elastic, excitation, ionization, attachment, and detachment collision chemistry and secondary electron emission) as well as streamer mechanisms (photoionization and ion-neutral collisions) via tracking excited state neutrals which can then either quench via collisions or spontaneously emit a photon based on transition-specific Einstein-A coefficients [2, 3]. In addition, photoemission is included for the dielectric and electrode surfaces as pre-computed by a separate Ensemble Monte Carlo code [4]. The present simulation examines the breakdown initiation after a 10 ns UV light source is activated to generate a stochastic initial e^- and O_2^- density distributions and finds that generating the initial electrons from O_2^- detachment results in electron avalanches starting near both the anode and cathode as previously observed in experiments.

Air Chemistry Model

- Details can be found in [1]
- Assume N_2 and O_2 are dominant species for heavy-heavy interactions. Model dry air and neglect N–N, N – O, and O – O interactions.
  - Include elastic (VHS), charge exchange, and quenching heavy-heavy interactions
- Include e-N_2^+ and e-O_2^+ dissociative recombination
- Include O_2^- + M detachment via cross section [5]
  - Self-consistently leads to higher detachment rate in high-field regions
- e-neutral interactions included for N_2, O_2, N, O and metastable states. Use anisotropic scattering model for all electron-neutral collisions.
  - Elastic
  - Ionization: Single (ground and metastable states), double, and dissociative
  - Attachment (3-body and Dissociative)
  - Vibrational and rotational excitation
  - Electronic excitation
- Excited states have probability to radiate a photon based on transition-specific Einstein-A coefficients, quench via collision (assumed P_{quench} = ½) with background neutrals, or, in some cases, auto-dissociate or auto-ionize with state-specific rate
- Photons are modeled as discrete particles that move and stochastically collide through a simulation timestep just like all other particles





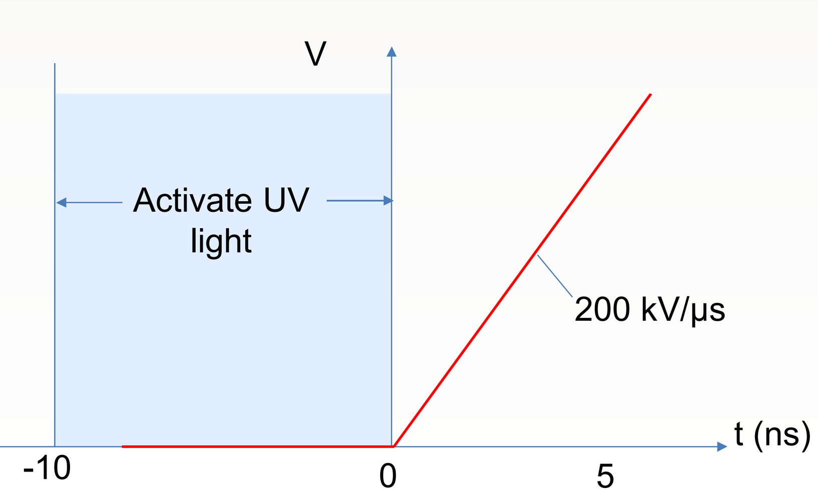
Modeled energy level and transition diagram for atomic O ($^3D^o$ transitions omitted for clarity). Solid blue lines represent radiative decay in which simulation photons are generated. Red dotted lines represent decay in which a simulation photon is not generated. Green dashed lines are auto-ionizing states.

Dielectric Model

- Field solve accounts for relative permittivity and surface charging of the dielectric
- Charged particles and photons incident on the dielectric have electron emission yields defined as functions of the incident particle energy
  - Ensemble Monte Carlo code [3] used to pre-compute photoemission yields vs. wavelength for a fixed applied field (the emission yield includes the contribution from enhanced tunneling) using DFT calculations to obtain TiO_2 band structure.
  - The precomputed yields are constant during the PIC simulation – they do not vary with field or the dielectric surface charge.

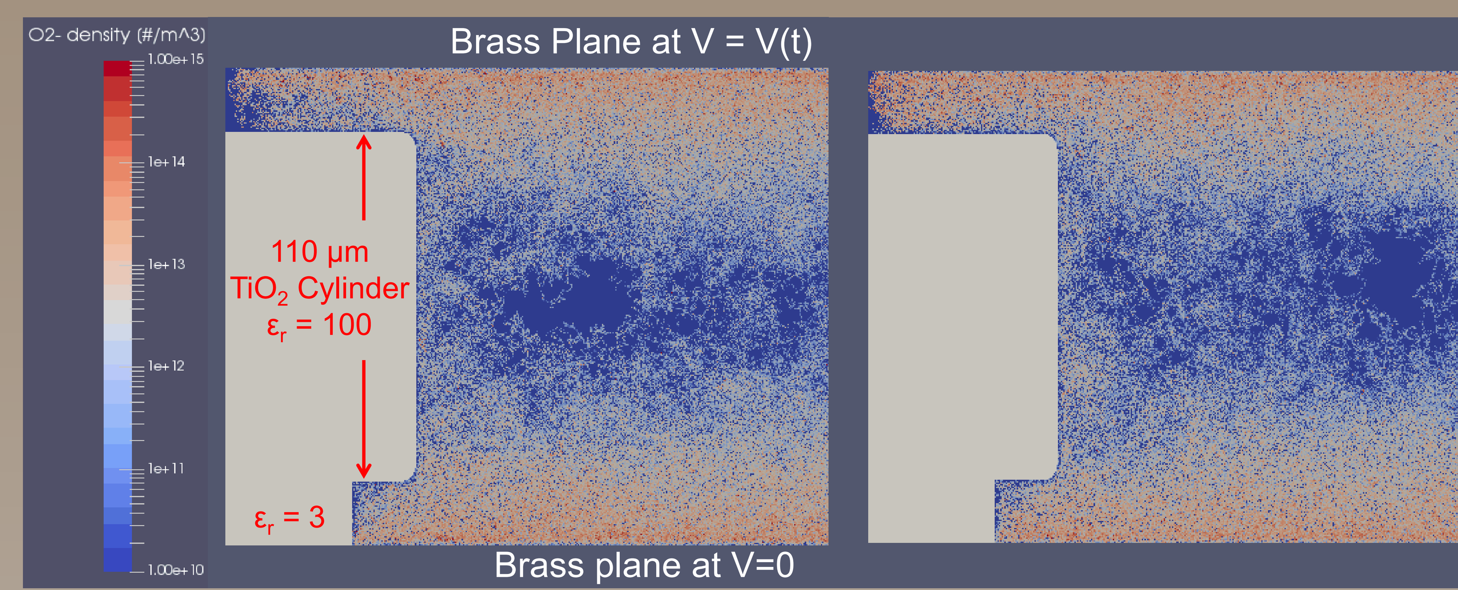
Initial Charged Particle Model

- 2D Axisymmetric simulation of a 600 Torr, air-filled 150 μm gap with 110 μm TiO_2 (ε_r = 100) cylinder between the electrodes
- Activate UV light source for 10 ns with no applied potential and then ramp anode voltage at 200 kV/μs
  - UV light source modeled as e^- flux with T_e = 0.1 eV
  - Electrode flux = 10^{19} #/m³ and Dielectric flux = 10^{18} #/m³
- Electrons diffuse through the background neutral gas and attach to O_2 through 3-body collisions

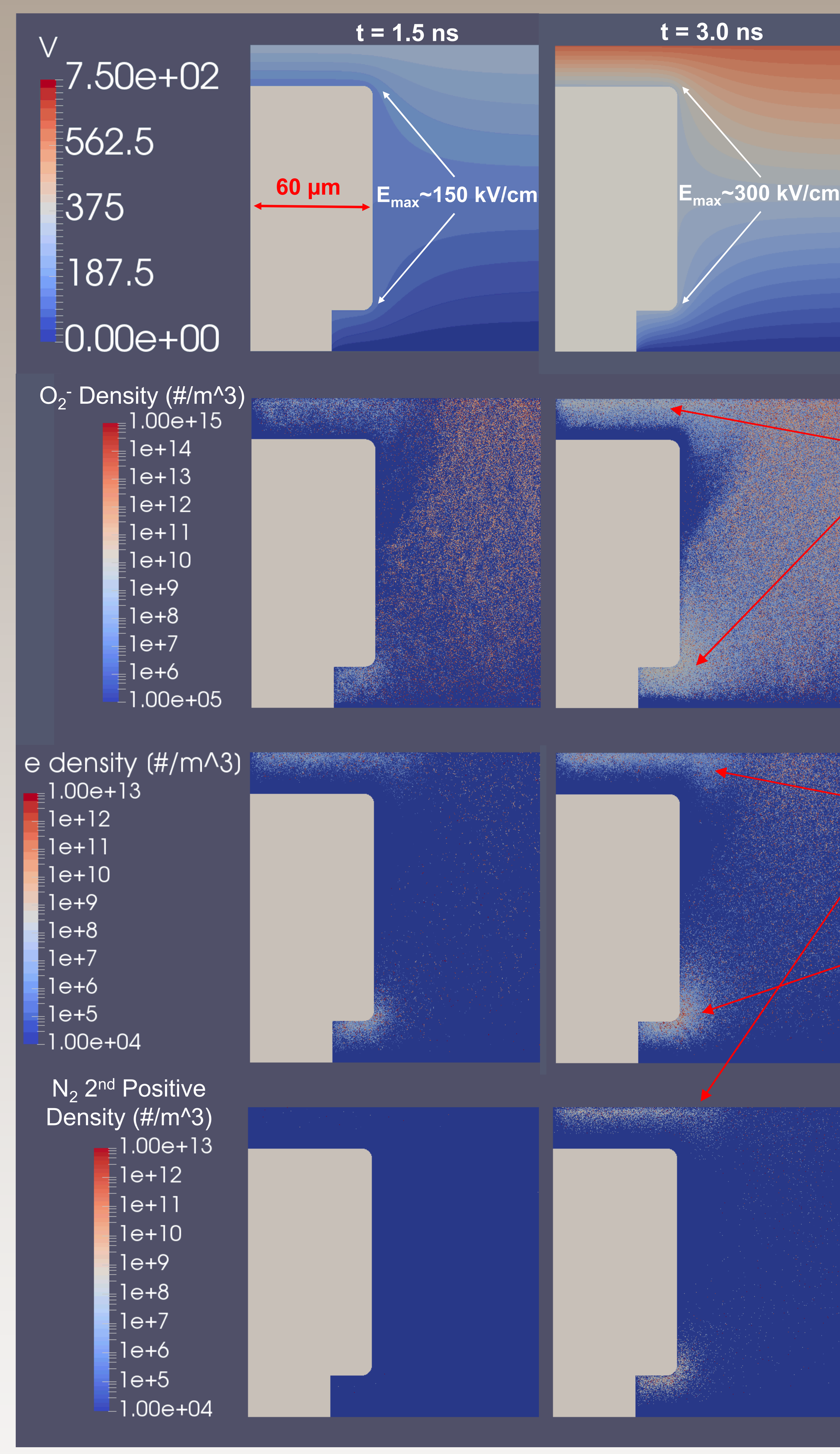


Initial Charged Particle Distributions

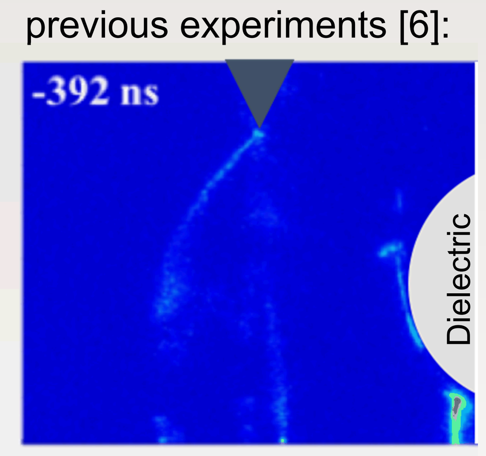
- Simulate initial O_2^- and e^- (not shown) distributions after 10 ns UV flux for input into breakdown sim.
  - Distributions vary with the random number seed (left & right). Leads to variation in the breakdown times



Initiation Results



- Ramp voltage at 200 kV/μs
- Peak E-field at rounded (5μm radius) dielectric corners sufficient to start breakdown
- O_2^- density rapidly evolves as the O_2^- is accelerated by the field and detaches (O_2^- Δx < 10 μm in the gap)
- O_2^- density increases at the dielectric corner near the cathode and in small anode gap at later times due to attachment as avalanche starts
- Initial electrons come almost entirely from detachment of O_2^- that is accelerated in the high-field regions.
- e^- avalanche in high field region between dielectric and anode leads to population of excited states
- e^- avalanche also starts near cathode in the high-field region near the dielectric corner. Not observed with previous models that used less physical initial seed electrons. The behavior is similar to that observed in previous experiments [6]:



Cathode

Conclusions / Future Work

- Continued development of kinetic model for breakdown in the presence of dielectric particles that includes Townsend mechanisms, excited states, O_2^- detachment, photoionization, and photoemission
- Generate initial "seed" electrons by modeling electron current due to UV light
- Unlike prior simulations that artificially seed electrons, current model results in initiation and excited state buildup near the cathode similar to prior experiments
- Run multiple simulations to later times and observe breakdown
- Perform validation experiments
  - Investigate effect of decreasing O_2:N_2 ratio – Expect increased shot-to-shot variability in breakdown times

References

[1] C. Moore *et al.*, "Development of Kinetic PIC-DSMC Model for Breakdown in the Presence of a Dielectric", ICOPS, Banff, 2016

[2] C. Moore *et al.*, "Development and Validation of PIC/DSMC Air Breakdown Model in the Presence of Dielectric Particles," Pulsed Power Conference, Austin, TX, 2015.

[3] A. Fierro *et al.*, "Discrete Photon Implementation for Plasma Simulations," Physics of Plasma, 23, 013506, 2016.

[4] H. Hjalmarson *et al.*, "Calculations of Photoemission from Rutile," APS Meeting, San Antonio, TX, 2015.

[5] A. Ponomarev and N. Aleksandrov, "Monte Carlo simulation of electron detachment properties for O_2^- ions in oxygen and oxygen:nitrogen mixtures," PSST **24**, 035001, 2015.

[6] S. Feathers, A. Fierro, S. Beeson, J. Stephens, A. Neuber, "Fundamental investigation of microsecond breakdown near a high permittivity dielectric," IEEE International Pulsed Power Conference, Austin, TX, 2015.

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