SAND2017-5353C

Kinetic simulation of breakdown for gaps with and without dielectric particles

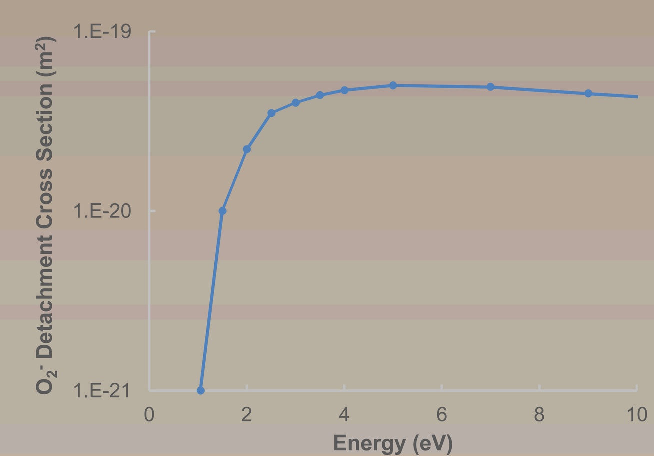
Chris Moore, Andrew Fierro, Roy Jorgenson, Harold Hjalmarson, Ashish Jindal, Matthew Hopkins, Paul Clem, and Laura Biedermann

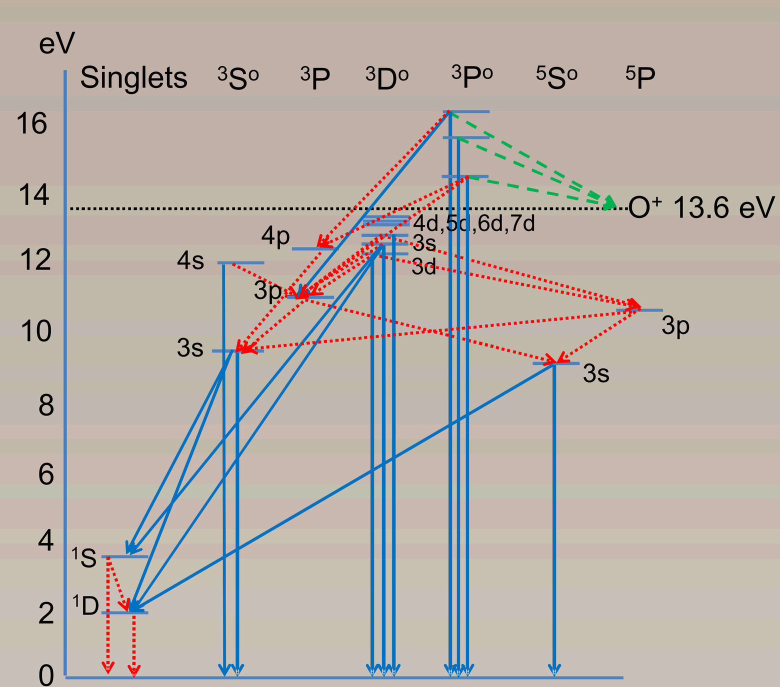
Abstract

An electrostatic particle-in-cell (PIC) code which simulates particle collisions using the direct simulation Monte Carlo (DSMC) method has been used to simulate breakdown initiation with and without a dielectric particle 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) which produces an electron current via photoemission that then attaches to O_2 via kinetically modelled collisions. After 10 ns the anode potential is increased at 250 kV/μs and O_2^- detachment serves as the primary electron source. The present simulations examine the variation in breakdown behavior of an empty gap and a gap with a dielectric particle present between the electrodes. The corner of the dielectric particle is found to enhance the E-field and allow for e^- generation via detachment from O_2^- at earlier times than for the empty gap.

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 $e\text{-}N_2^+$ and $e\text{-}O_2^+$ 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, Attachment, Excitation (electronic, vibrational, rotational)
- 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



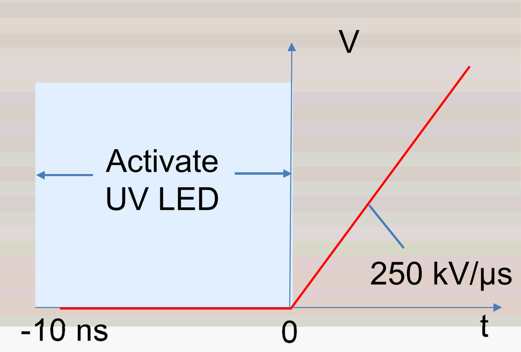


Modeled energy level and transition diagram for atomic O ($^3D^o$ transitions omitted for clarity). Solid blue lines represent radiative decay in which simulation photons are generated. Red dotted lines represent decay in which a simulation photon is not generated. Green dashed lines are auto-ionizing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

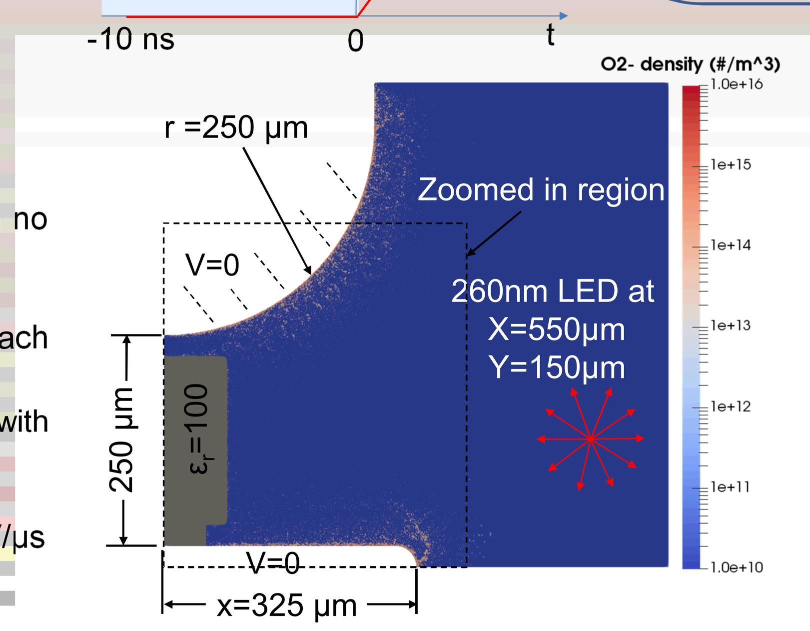
Dielectric Model

- Field solve accounts for relative permittivity
- 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] pre-computes photoemission yields vs. wavelength for a fixed applied field (the emission yield includes the contribution from enhanced tunneling). TiO_2 band structure obtained using DFT
  - The precomputed yields are constant during the PIC simulation – they do not vary with field or the dielectric surface charge.

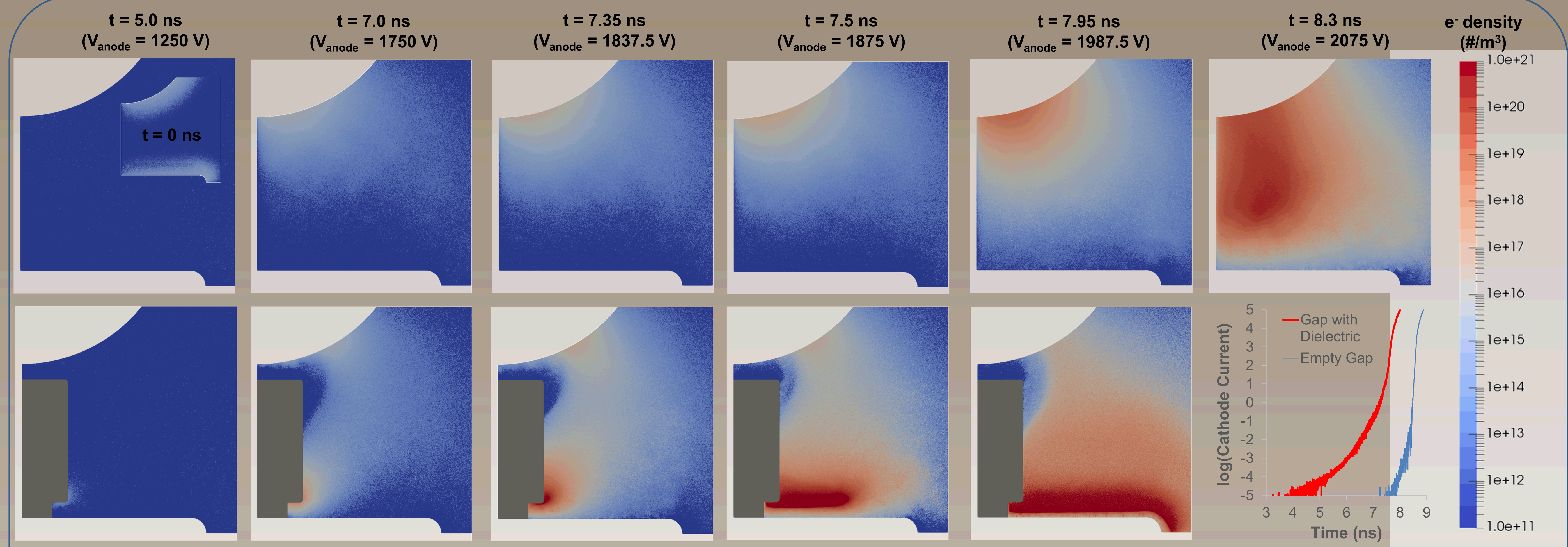
Initial Charged Particle Model



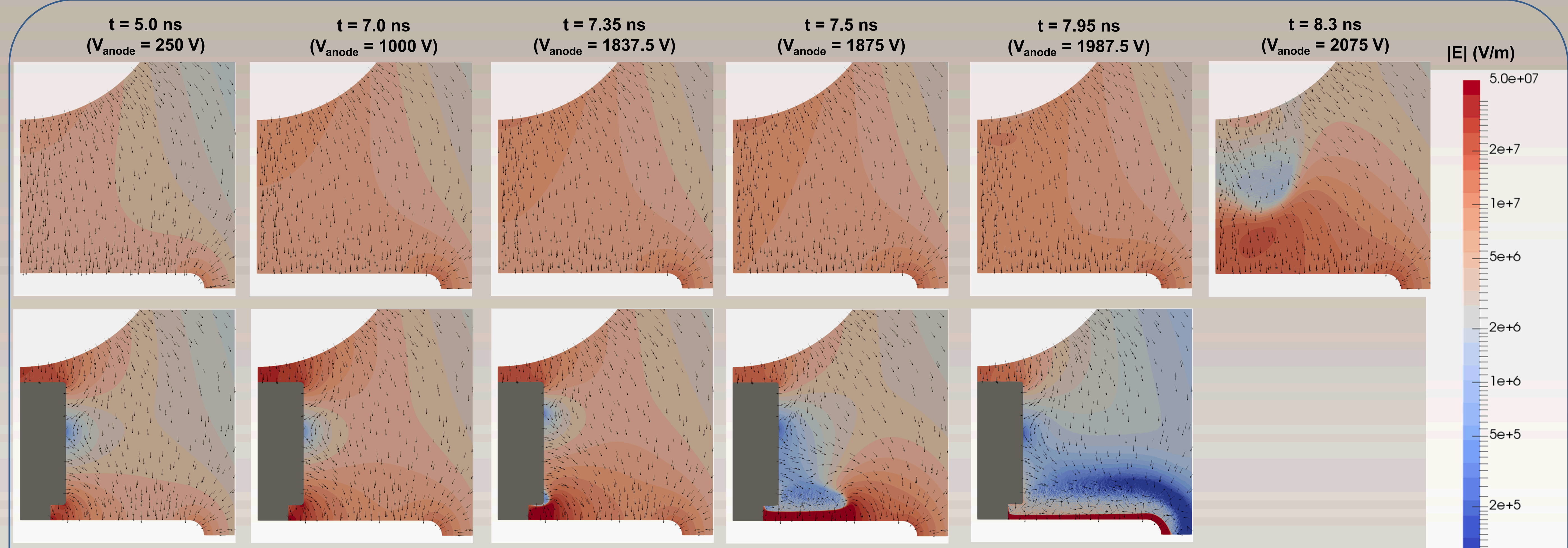
- 2D simulation of a 600 Torr, air-filled hemisphere-to-plane 250 μm gap with 200 μm TiO_2 (ε_r = 100) cylinder on top of a 25 μm dielectric (ε_r = 3) spacer between electrodes.
- Δx = 0.235 μm (λ_D ~ 0.1 μm in streamer channel)
- Δt = 5×10^{-14} s (ω_{pe}^{-1} ~ 10^{-12} s; ν_{col} ~ 10^{-12} s; Δt_{CFL} ~ 10^{-13} s)
- Activate isotropic, 260 nm UV LED light source for 10 ns with no applied potential. Intensity of 1.6 mW/cm² on axis.
- Electrons diffuse through the background neutral gas and attach to O_2 through 3-body collisions
  - Gives initial density distribution for e^- & O_2^- which varies with random number seed
- Turn off LED after 10ns and ramp the anode voltage at 250 kV/μs



Results



- Initial background e^- density present near the electrodes due to photoemission. These e^- are swept out of the gap while the field is still too low to result in breakdown
- After ~5ns the field near the dielectric corner is sufficient to cause significant O_2^- detachment and supply initial e^- in the high-field (and thus high α) region
- In contrast, O_2^- detachment in the empty gap (with lower E) is significantly slower and leads to more scattered seed e^-
- After 7ns significant e^- avalanche starts near cathode in the high-field region near the dielectric corner and leads to 2nd positive excitation.
- In the empty gap e^- densities are highest near the anode as would be expected from seed e^- avalanching back to the anode
- The gap with a dielectric particle breaks down in under 8ns after the e^- density expands from the dielectric corner along the cathode (see below) and then the e^- avalanche to the anode
- The empty gap breaks down in ~8.5ns via a positive streamer (see the E-field exclusion in the channel and enhancement ahead of the streamer head below)



- The field is increasing in time as the anode voltage is increased
- A sub-sample of E-field vectors are plotted on top of the E-field magnitude contours to give directional information
- Since the dielectric does not span the gap, the potential drop is almost entirely in the small (25 μm) gap between the dielectric and the anode
- E_y << E_x along the side of the dielectric due to its large permittivity not allowing it to support a large field parallel to the surface (like a metal).
- At 7.35ns e^- produced via photoionization along the cathode in the vicinity of the dielectric corner will stream back to the corner; e^- produced along the side of the dielectric stream into the dielectric
- After 7.35ns it appears that a streamer travels along the cathode surface given the field exclusion and enhancement (as well as the photoionization upstream, not shown). However, it is unclear how much the expanding e^- density is affected by more O_2^- detachment further out along the cathode as the potential increases such that the local field then exceeds a critical value.

Conclusions / Future Work

- Unlike prior simulations that artificially seed electrons, current model results in initiation and excited state buildup near the cathode when a dielectric particle is present in the gap. A positive streamer was still observed for an empty gap initialized via seed electrons from O_2^- detachment.
- The presence of field enhancement at the dielectric corner allowed for earlier production of the initial seed electrons and thus the gap with a dielectric particle broke down earlier in time given the same voltage rise time.
- Run multiple simulations (and vary O_2:N_2 ratio) and observe variance in breakdown time for the empty gap vs. a gap with a dielectric particle

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.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.