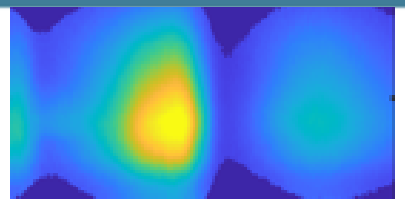
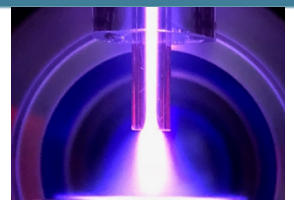
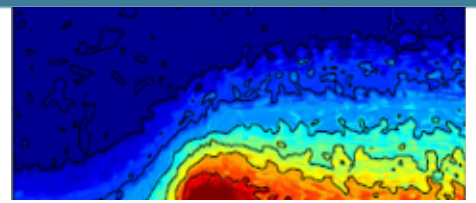
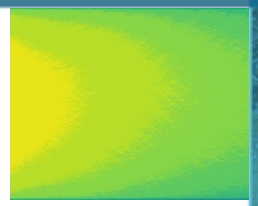
SAND2021-12383C

Sandia National Laboratories

SNL Plasma Research Facility (PRF)

Shane Sickafoose, Brian Bentz, Jonathan Frank, Nils Hansen, Matthew Hopkins, Christopher Kliewer, Amanda Lietz, Dirk van den Bekerom

4-8 October 2021

74th Gaseous Electronics Conference

Huntsville, Alabama

U.S. DEPARTMENT OF ENERGY NNSA

Sandia National Laboratories' Plasma Research Facility is funded by the U.S. Department of Energy's Office of Science, Fusion Energy Sciences.
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SAND2021-XXXXXX C

What We Are: PRF Goals and Approach

Goals:

To continually serve the low-temperature plasma community by providing it access to a growing set of world class capabilities and expertise.

Approach:

Engage with potential collaborators to understand their goals and to help them identify, implement and achieve solutions for their goals by providing access to what our Facility has to offer.

- *Advanced Simulation Capabilities and World-Class High Performance Computing resources*
- *Capability for combined diagnostics simultaneously probing user experiments*
- *Cutting edge* in situ *mass spectrometry*

Continually advance capabilities and techniques to provide new tools for the plasma community to utilize.

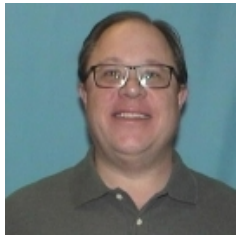
Propose a collaboration at: **www.sandia.gov/prf**

Who We Are: Key Personnel – Core Scientists

- Brian Bentz (bzbentz@sandia.gov)
  - Multi-dimensional interrogation of atomic species, electron densities and electric fields using linear and non-linear spectroscopies

- Jonathan Frank (jhfrank@sandia.gov)
  - Imaging and gas-phase spectroscopy for high-speed, multi-dimensional measurements in plasmas and plasma-assisted reacting flows.

- Nils Hansen (nhansen@sandia.gov)
  - Interrogation of chemistries in reactive environments using high resolution mass spectrometry.



- Matthew Hopkins (mmhopki@sandia.gov)
  - Computational modeling and simulation of non-equilibrium plasma phenomena.

- Christopher Kliewer (cjkliew@sandia.gov)
  - Ultrafast non-linear gas and surface phase spectroscopies.

Our team offers a broad set of skills to serve the community.

Key Personnel (cont.) – Post-Doctoral Appointees

Amanda Lietz (amlietz@sandia.gov)

Computational modeling and simulation of non-equilibrium plasma phenomena.

Dirk van den Bekerom (dvanden@sandia.gov)

Imaging and gas-phase spectroscopy for high-speed, multi-dimensional measurements in plasmas and plasma-assisted reacting flows.

Our team offers a broad set of skills to serve the community.

Differentiating Capabilities

Multiple femtosecond, picosecond, nanosecond and CW lasers for interrogating dynamic plasma and reactive environments

- Neutral species density – LIF, PF-LIF
- Electric Fields (LIF-Dip, EFISH)
- Electron Densities - LCIF
- Multidimensional CARS for gas and surface phase interrogation

High speed imaging and detectors capabilities

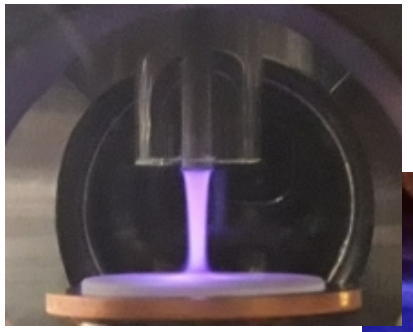
- <200 ps gated cameras, multi-frame framing cameras and high-speed CMOS cameras, streak camera
- VUV to Visible to IR spectrometers

High resolution tandem and molecular beam mass spectroscopy (MBMS) for interrogating gas phase chemistries occurring in multi-atmosphere environments.

Theoretical/Computational LTP Capabilities

- Aleph and EMPIRE: Massively parallel PIC-DSMC, extensive chemistry and photonic processes
- Aria: multiphase fluid simulation capability being extended to highly collisional plasmas
- 0D global modeling

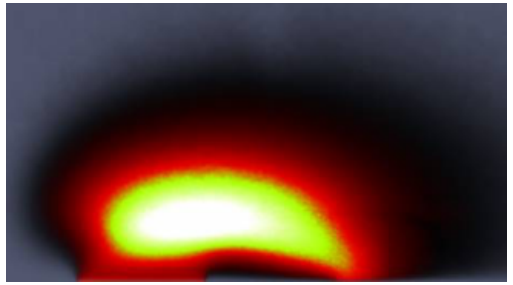
Plane-to-plane ns pulsed discharge for plasma catalysis



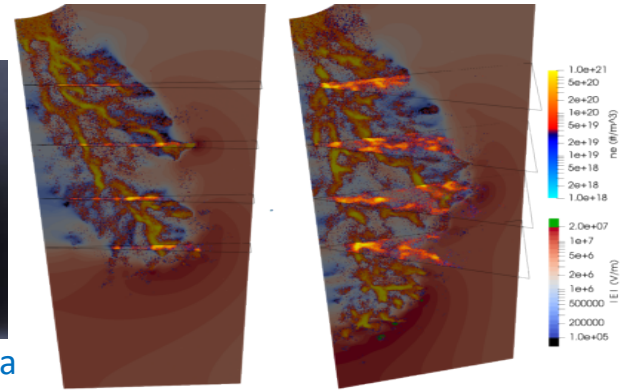
Low-pressure ns pulsed discharge

MBMS – flow reactors with DBD

Plasma-assisted combustion in atmospheric pressure narrow channel



3D image e- density cathode plasma



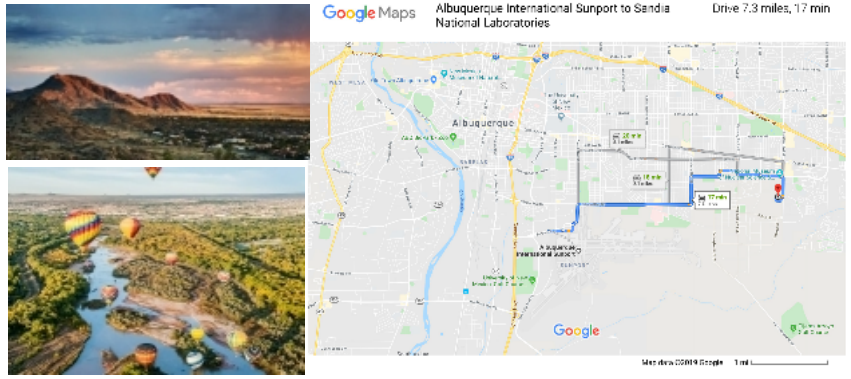
Propose a collaboration at: www.sandia.gov/prf

Access to the Facility

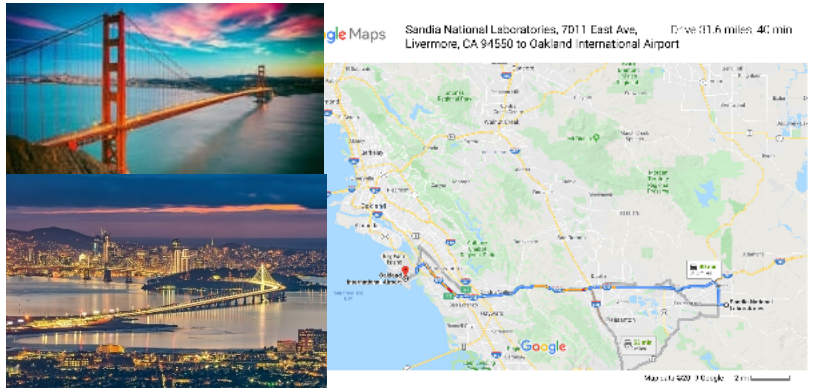
Visitor infrastructure streamlining

- Visitor badging, computer access, data sharing, safety documentation/training
  - Office space for visitors
  - Open network for visitors to access resources
- Working from several existing examples of collaborator engagement at Sandia:
  - Previous Plasma Science Center (DOE FES funded)
  - Center for Integrated Nanoscience and Technology (CINT, DOE BES funded)
  - Combustion Research Facility (DOE BES funded)

Sandia New Mexico



Sandia California



We will work with collaborators to ensure streamlined access to our sites

SNL Plasma Research Facility Status

PRF hosted 10 collaborations in the last year

- Seven experimental
  - North Carolina State University - completed
  - University of New Mexico - completed
  - University of Notre Dame - completed
  - University of Minnesota - completed
  - Princeton University (2) – one completed, one in process
  - The Ohio State University – in process
- Three modeling/simulation
  - University of Michigan – wrapping up
  - Modern Electron, LLC. – wrapping up
  - Applied Materials, Inc. – in process

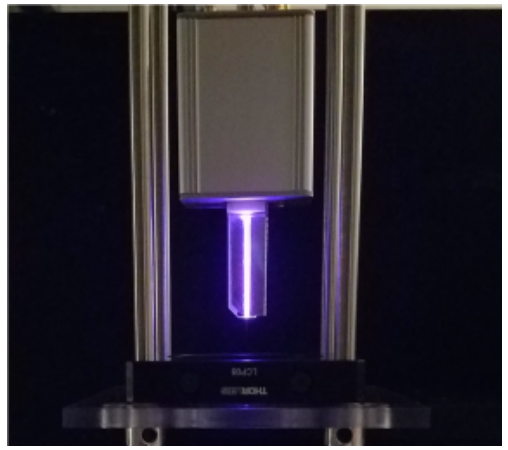
Six collaborations set to start shortly

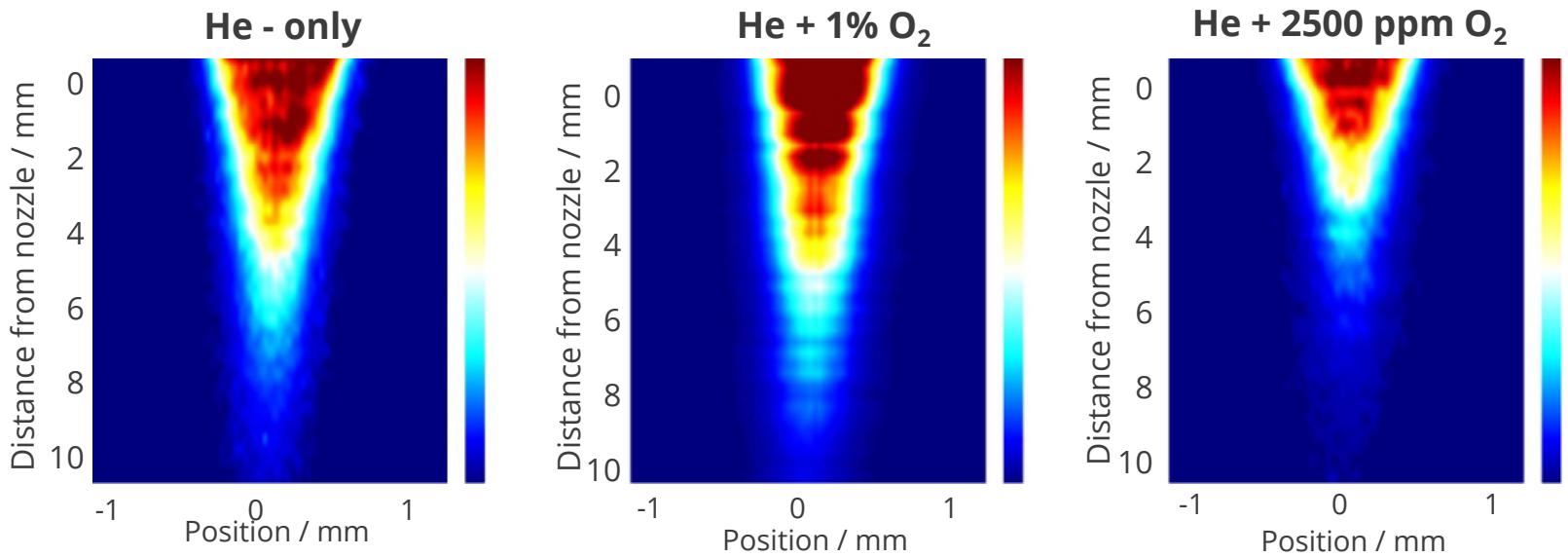
- Three experimental
  - Georgia Tech
  - University of South Carolina
  - University of Alabama, Huntsville
- Three modeling/simulation
  - University of Tartu
  - PPPL and Tech-X, Inc.
  - University of Alabama, Huntsville

Four collaborations included DOE Office of Science Graduate Student Research (SCGSR) Awardees.

- Lucas Beving, University of Michigan
- Brayden Myers, North Carolina State University
- Christopher Burger, Princeton University
- Madeline Vorenkamp, Princeton University

Absolute Atomic Oxygen Species Densities in the Effluent of the COST Reference Source





Spatially resolved TALIF signals of atomic oxygen, normalized to counts per second, in the effluent of the COST jet operated with admixtures of helium-only, helium with 1% oxygen, and helium with 2500 ppm of water

Collaborators:

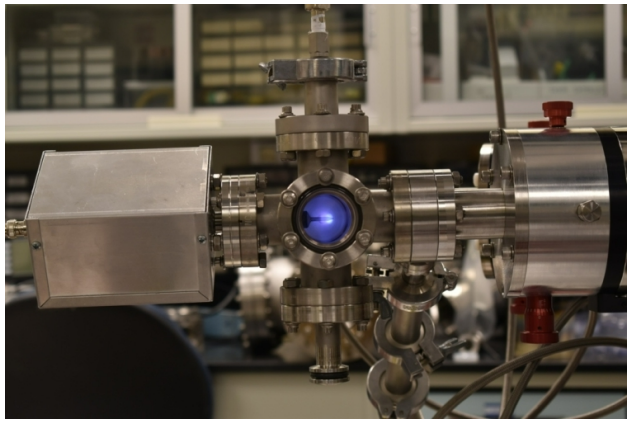
- Katharina Stapelmann, Brayden Myers, North Carolina State University
- PRF PI - Ed Barnat

Brayden Myers, Edward Barnat, Katharina Stapelmann,"Atomic oxygen density determination in the effluent of the COST Reference Source using *in situ* effective lifetime measurements in the presence of a liquid interface," J. Phys. D: Appl. Phys. **54**, 455202.

Identification of UV/VUV Bands Generated from a Photoionization Source

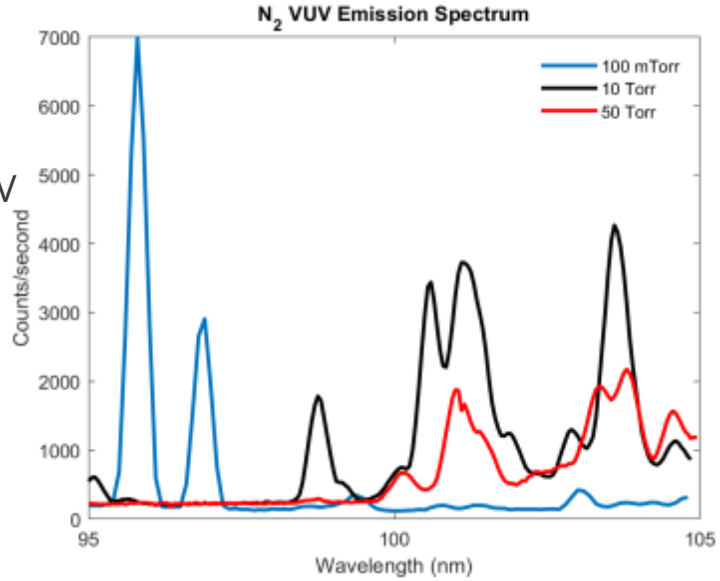
Overview of Project Goals:

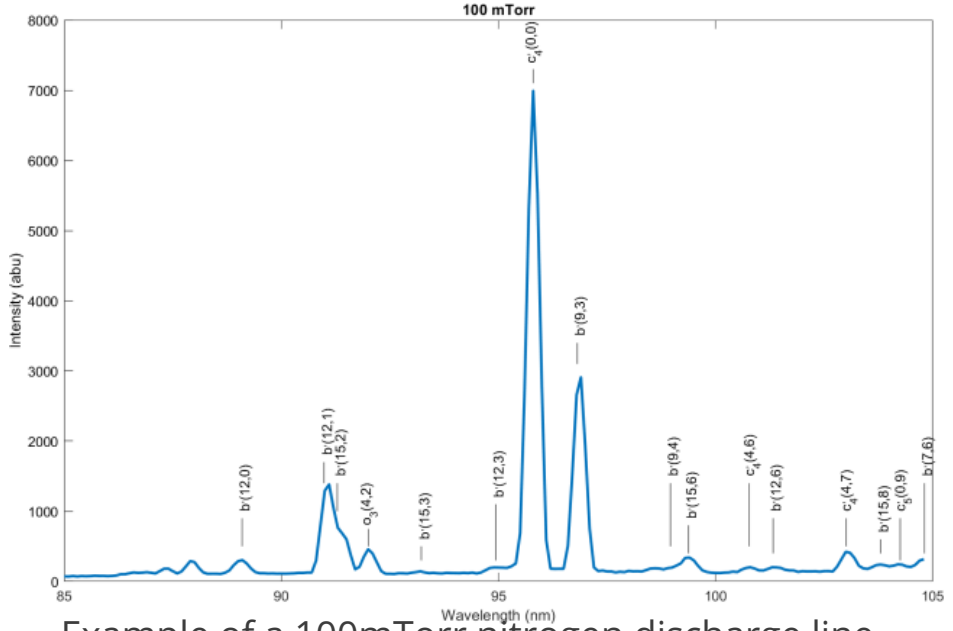
- Measure VUV emission from nitrogen discharge
- Identification of transitions critical to photoionization
- Reassess the photoionization models assumptions and calculations
- Extend model to other gases



Discharge Apparatus: Point to plane geometry

Measured VUV excited nitrogen emission





Example of a 100mTorr nitrogen discharge line identification

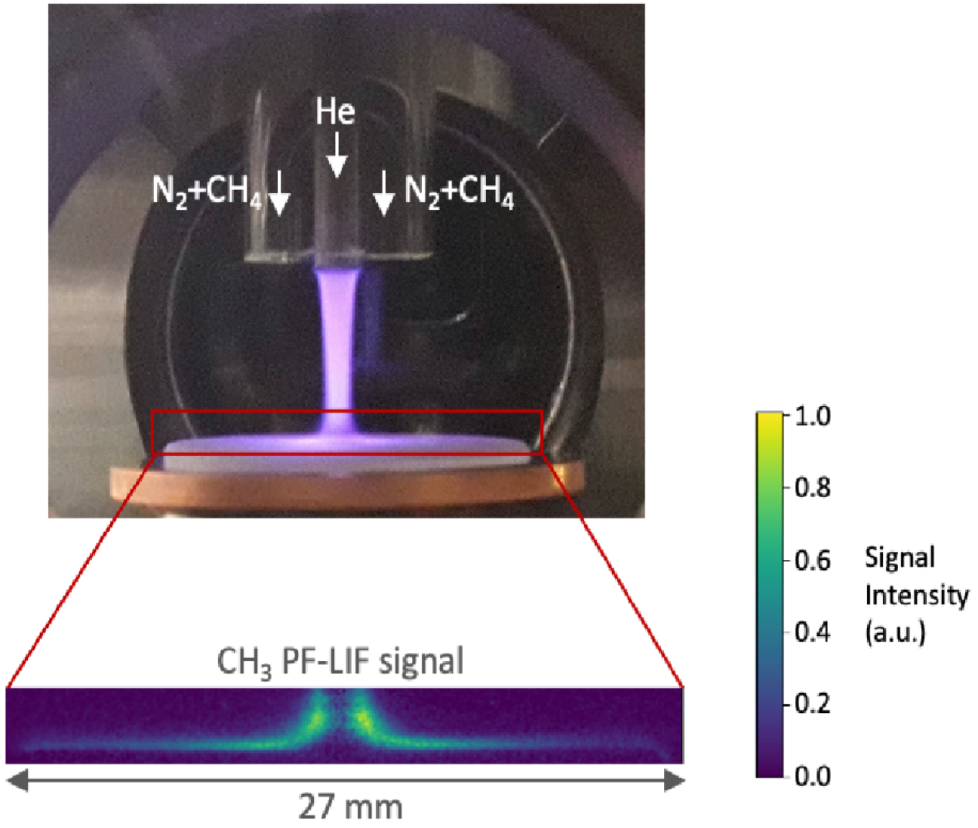
Collaborators

- Justin Smith, Andy Fierro, Jane Lehr
  University of New Mexico
- PRF PI Ben Yee

THE UNIVERSITY OF NEW MEXICO

In Situ Measurements of Formaldehyde and Methyl Radical in Plasma-Assisted Catalytic Methane Conversion

Development of new 2D photo-fragmentation laser-induced fluorescence (PF-LIF) capability in nanosecond pulsed plasma discharges



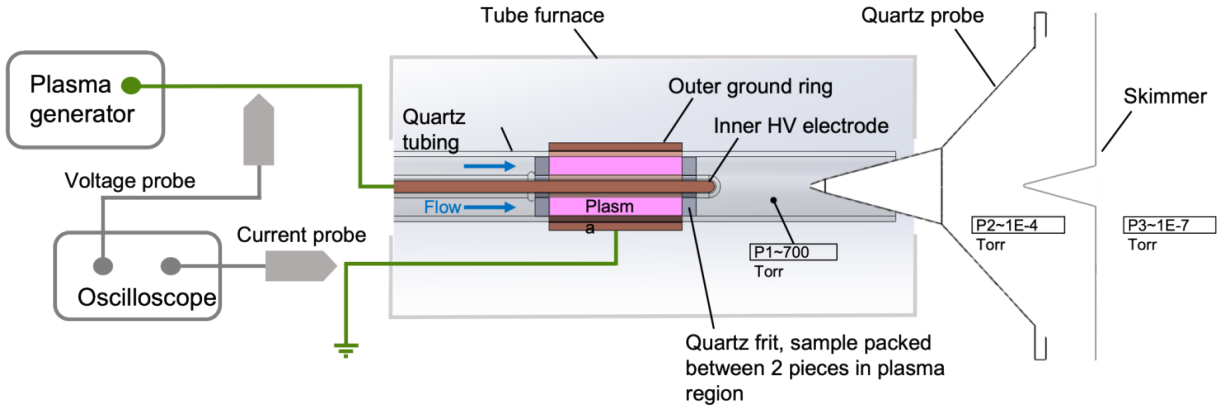
Collaborators:

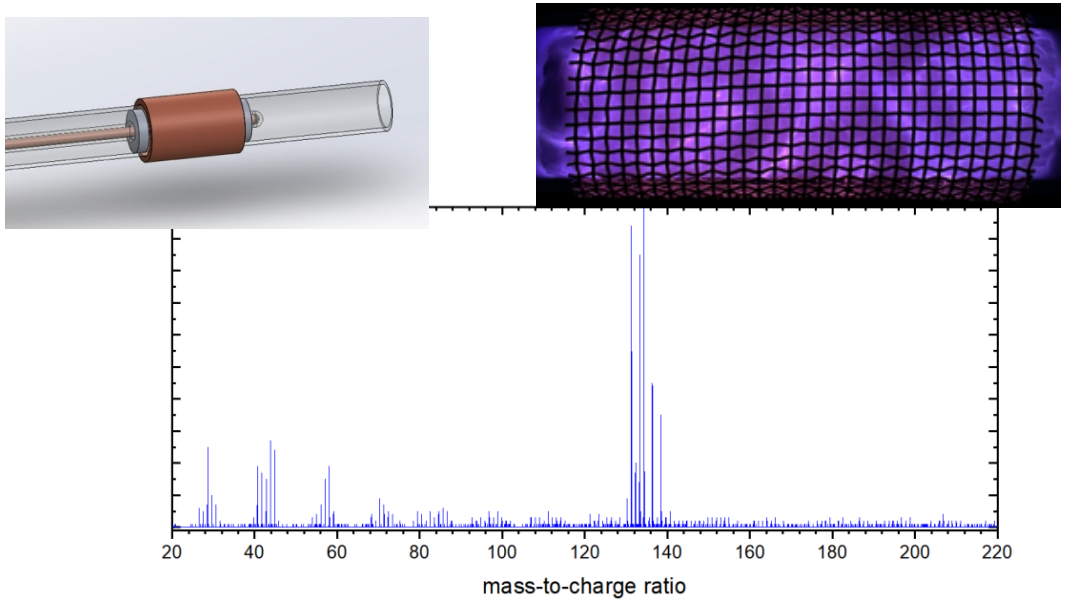
- Caleb J. Richards, The Ohio State University
- Igor V. Adamovich, The Ohio State University
- PRF PI Jonathan H. Frank,
- PRF Dirk van den Bekerom

Data Collection on-going.

THE OHIO STATE UNIVERSITY
COLLEGE OF ENGINEERING
Non-Equilibrium Thermodynamics Laboratory

Studies of plasma generated active species on low temperature fuel oxidation





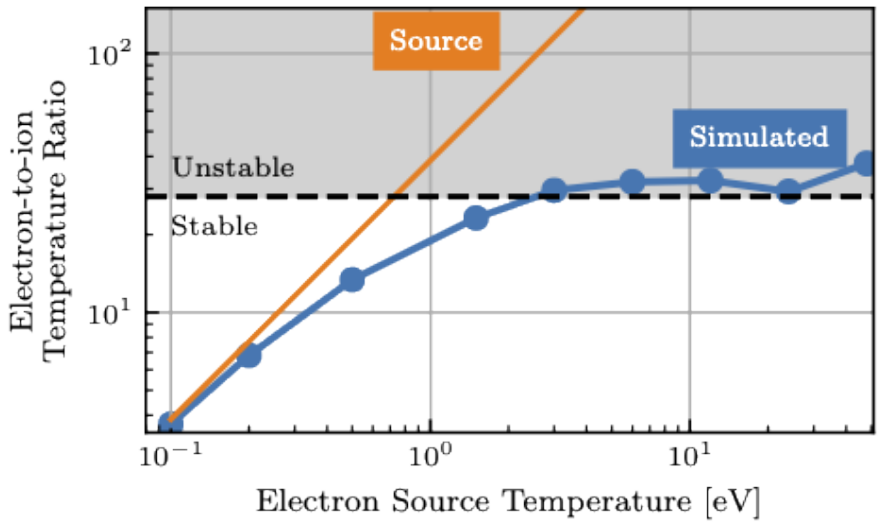
- Important for developing plasma-assisted combustion, chemical looping, catalysis and plasma surface interactions
- Mass spectrometry is a perfect analytical tool to study complex reaction networks and chemical processes.
- Mass spectrometry allows for the detection of all intermediates/products simultaneously without prior knowledge of their identity
- Molecular-beam approach allows for detection of short-lived reactive species
- Multi-dimensional data space can be explored, i.e. as a *function of time, residence time, temperature, electron (photon) energy.*

Collaborators (chemical looping)

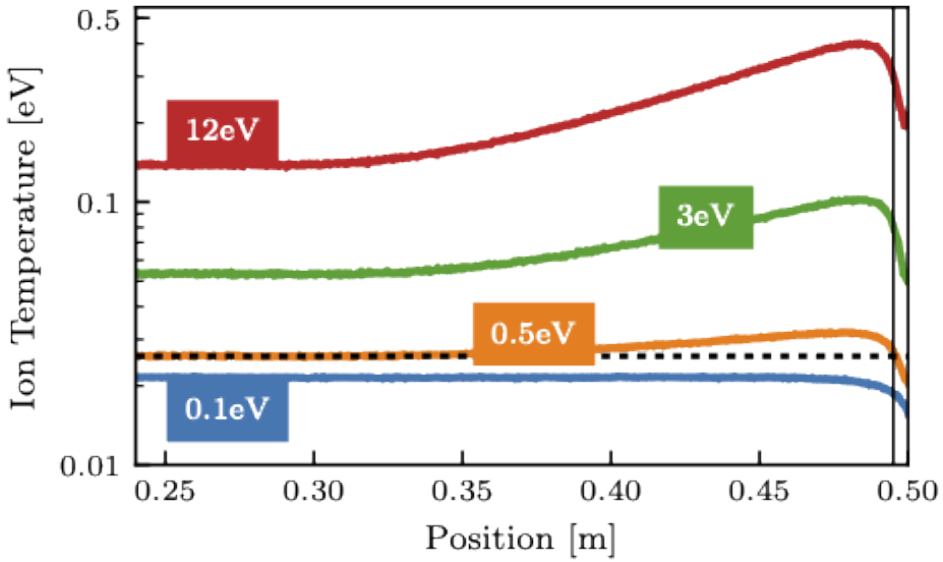
- Christopher Burger, Princeton University, SCGSR
- Yiguang Ju, Princeton University
- PRF PI - Nils Hansen

PRINCETON UNIVERSITY

Tests of a proposed sheath instability mechanism using Aleph



Source vs. steady-state electron temperatures for various source electron temperatures. As can be seen, the steady state temperatures are limited to the temperature at the instability threshold.



When the instability is present, significant pre-sheath heating occurs and causes bulk plasma ion temperatures to increase as well.

Collaborators

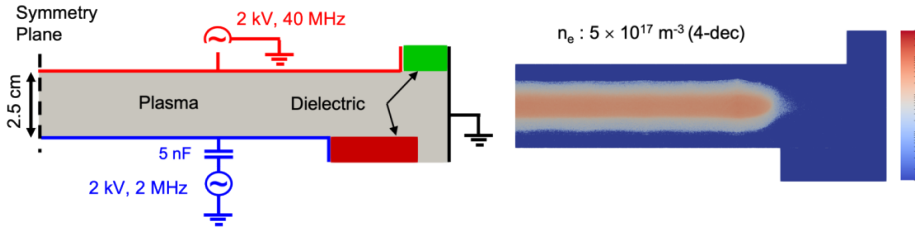
- Lucas Beving, University of Michigan, SCGSR
- Scott Baalrud, University of Michigan.
- PRF PI - Matt Hopkins

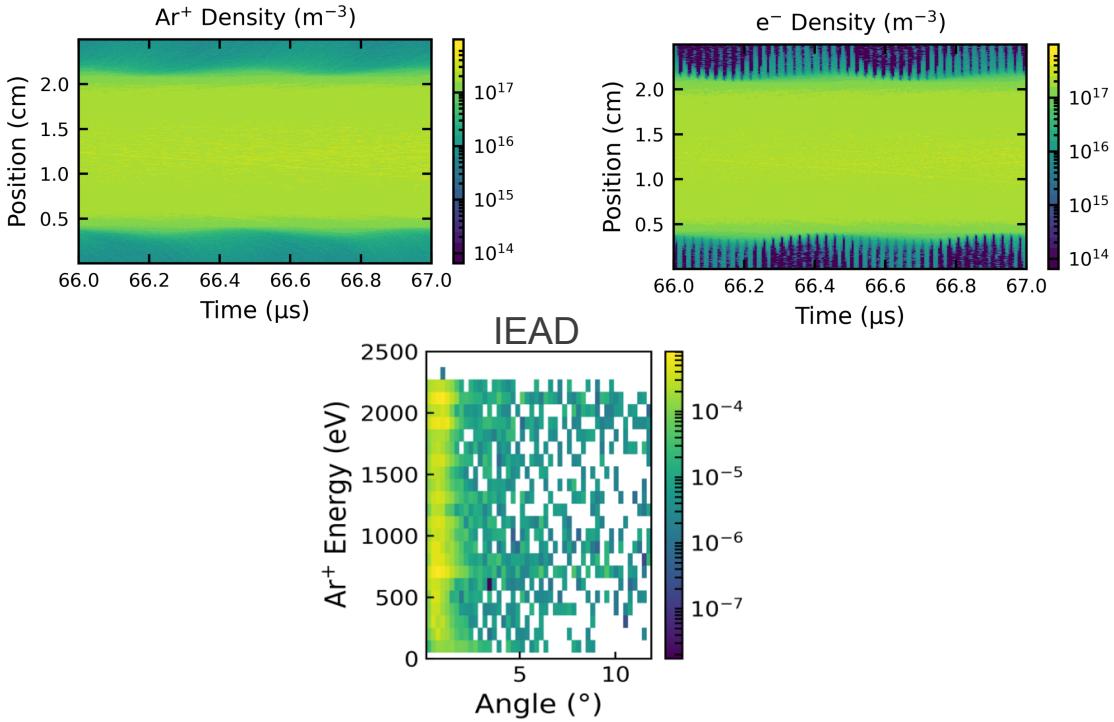
74th GEC - Session ET44.00003 : Simulations of ion heating in the presheath due to ion-acoustic instabilities*

Lucas P. Beving, **Matthew M. Hopkins**, Scott D. Baalrud, "Simulations of ion heating in the presheath due to ion-acoustic instabilities," (Phys. Plasmas, submitted PRF publication).

UNIVERSITY OF MICHIGAN

Particle-in-a-Cell modeling of low pressure (<10 mTorr) high bias (>2000 V) dual-frequency capacitively coupled plasmas





High aspect ratio etching, requires computationally intense conditions:

- Low pressures – fluid/hybrid models fail.
- High voltages - fast electrons constrain timestep

Accessing relevant time scales and fidelity requires advanced parallel simulation and computational method capabilities – Aleph enables these studies

Collaborators:

- Shahid Rauf, Kenney, Applied Materials, Inc.
- PRF PI Amanda Lietz,
- PRF co-PI Matt Hopkins

APPLIED MATERIALS®

Publications

Brayden Myers, **Edward Barnat**, Katharina Stapelmann,"Atomic oxygen density determination in the effluent of the COST Reference Source using *in situ* effective lifetime measurements in the presence of a liquid interface," J. Phys. D: Appl. Phys. **54**, 455202.

Lucas P. Beving, **Matthew M. Hopkins**, Scott D. Baalrud, “Simulations of ion heating in the presheath due to ion-acoustic instabilities,” (Phys. Plasmas).

Recent and Upcoming Presentations

48th International Conference on Plasma Science – Sept. 2021

- 2D Imaging of Methyl in a N_2/CH_4 Nanosecond Pulsed Plasma by Photo-Fragmentation Laser-Induced Fluorescence – **van den Bekerom**, Huang, Richards, Adamovich, **Frank**

74th Gaseous Electronics Conference – Oct. 2021

- Imaging of Methyl Radical in a Plasma Jet by Photo-fragmentation Laser-Induced Fluorescence - **van den Bekerom**, Huang, Richards, Adamovich, **Frank**
- Student Excellence Award Finalist: Electric field measurements of piezoelectric direct discharge plasmas using electric-field induced second harmonic (E-FISH) generation. Yang, **Barnat**, Im, Go.
- Simulations of ion heating in the presheath due to ion-acoustic instabilities – Beving, **Hopkins,** Baalrud.

American Vacuum Society 67th International Symposium & Exhibition – Oct. 2021

- Two-dimensional particle-in-cell modeling of low pressure, high voltage capacitively coupled Ar plasmas. **Amanda M. Lietz**, Peng Tian, Jason Kenney, Shahid Rauf, **Matthew M. Hopkins.**

Bold are PRF Scientists

Work with us: 3rd Facility Proposal Call

Propose a collaboration at: www.sandia.gov/prf

Open of PRF Proposal Call	October 12, 2021
Close of PRF proposal Call	December 17, 2021
External Reviews	~ 1 month
Notification of Principal Investigators	February 4, 2022

Call timing is aligned with PPPL PCRF

Contact us to ensure projects are well-aligned with our capabilities:

- Brian Bentz (bzbentz@sandia.gov)
- Jonathan Frank (jhfrank@sandia.gov)
- Nils Hansen (nhansen@sandia.gov)
- Matthew Hopkins (mmhopki@sandia.gov)
- Christopher Kliewer (cjkliew@sandia.gov)
- Shane Sickafoose (smsicka@sandia.gov)

Acknowledgements

Sandia National Laboratories' Plasma Research Facility is funded by the U.S. Department of Energy's Office of Science, Fusion Energy Sciences.

U.S. DEPARTMENT OF ENERGY

THE UNIVERSITY OF NEW MEXICO

APPLIED MATERIALS®

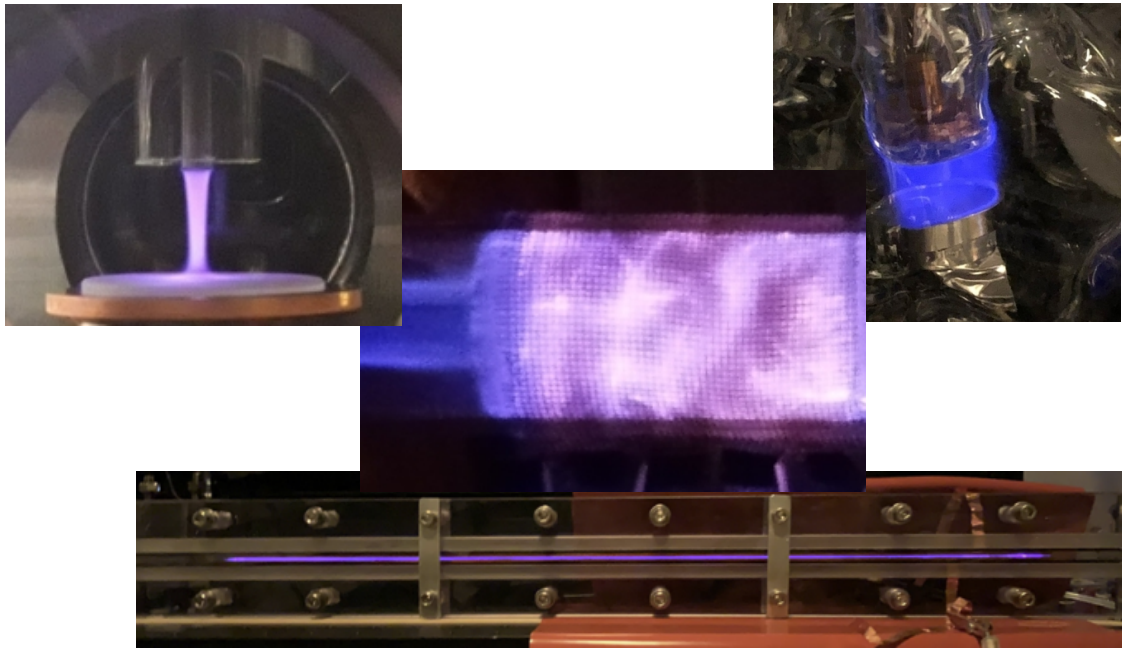
UNIVERSITY OF MICHIGAN

PRINCETON UNIVERSITY

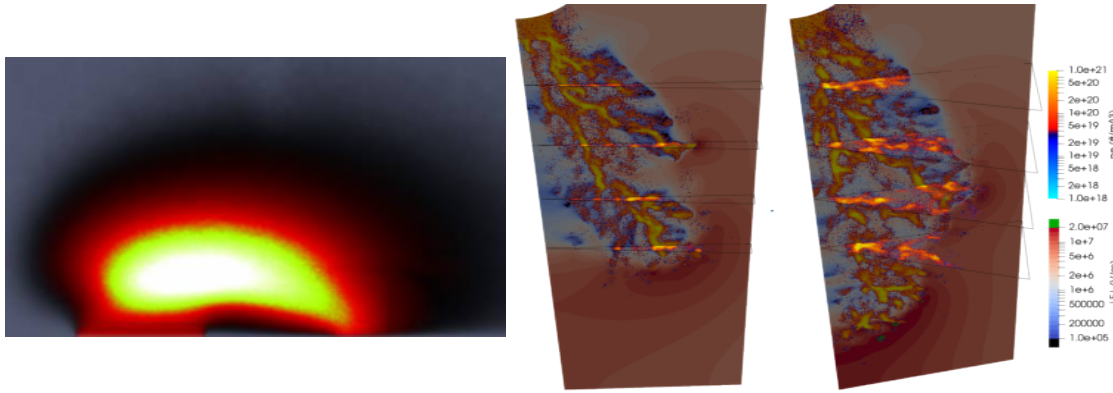
THE OHIO STATE UNIVERSITY
COLLEGE OF ENGINEERING
Non-Equilibrium Thermodynamics Laboratory

Sandia Low-Temperature Plasma Research Facility (PRF)

- **Experimental Capabilities:**
  - Femtosecond, picosecond, nanosecond and CW lasers.
  - Diagnostics for measuring various neutral species densities (MBMS, LIF, PF-LIF), electric fields (LIF-Dip, EFISH), electron densities (LCIF), and temperatures (CARS).
  - High speed detectors for imaging and spectroscopy
  - Plasma generating capabilities from vacuum to atmospheric pressure.



- **Computational Capabilities:**
  - Aleph and EMPIRE: Massively parallel PIC-DSMC, extensive chemistry and photonic processes
  - Aria: multiphase fluid simulation capability being extended to highly collisional plasmas
  - 0D global modeling



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