Kinetic Modeling of Non-Equilibrium Plasmas for Modern Applications

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Kinetic Modeling of Non-Equilibrium Plasmas for Modern Applications

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Outline:

• Plasma Switch for electric grid
• Negative hydrogen ion sources
• Effects of magnetic field on capacitive coupled discharge
• Penning discharge
• Focusing of space-charge dominated beams
• New Collaborative Low Temperature Plasma Research Facilities Open for All Users
High Power Plasma Switch Being Developed by General Electric

Converting electricity between different currents, voltage levels, and frequencies.
Motivation: Developing Plasma Switch for DC to AC Power Conversion

- DC transmission lines are more efficient than AC over distances > 600-800 km. They can transport power between non-synchronized grids and also from alternative sources such as wind/solar plants.

- The plasma switch would serve as a compact, less costly alternative to the bulky assemblies of semiconductor switches now installed in power-conversion systems throughout the grid.

GE HVDC transmission projects, ~ 35 GW to date. More projects by ABB, Siemens.
Back to the History

110Vdc Glass-bulb Mercury Arc Rectifier (early 1900s)

Soviet-designed single-anode HVDC valve for Volgograd-Donbass HVDC project (1959)

133kVdc, 1200A 4-anode HVDC valve for Kingsnorth-Willesden HVDC project (1969)

150kVdc, 1800A 6-anode HVDC valve for Nelson River project in Canada (1970s)
• Largest mercury arc valve ever made

Steel-tank medium voltage industrial rectifier (1930s)
Today’s power converters are large, complex, and costly, in part because high voltages (>300 kV) must be controlled with large numbers of low voltage devices (<10 kV) connected in series.

Gas tube switch could significantly improve, and lower the cost of utility-scale power conversion.
Experiments

- Gas type: Helium
- Cold emissive cathode
- Operating pressure 0.1 to 1 Torr
- Current density 1 to 10 A/cm²
- Anode applied voltage ~ 100kV
- Discharge gap 1.4 cm
- Anode material: stainless steel
- Cathode material: molybdenum

Plasma self-organization in GE plasma switch. T. Sommerer. 8
Performed particle-in-cell simulations and analytical theory to reproduce Paschen curve, including fast ions, electrons, anisotropic scattering and reflection from walls.

Volume production sources of negative hydrogen ions needed for cesium-free operation. A model is required to describe the vibrational kinetics and to predict the negative ion production.

\[ \text{H}_2(\nu) + e (\varepsilon < 2 \text{ eV}) \rightarrow \text{H}^- + \text{H} \]
\[ \text{H}_2(\nu) + e (\varepsilon > 12 \text{ eV}) \rightleftharpoons \text{H}_2(\nu') + e + h\nu \]
\[ \text{H}_2(\nu') + \text{wall} \rightarrow \text{H}_2(\nu) \ (\nu < \nu') \]

Analytical solution (S is the excitation source)

### Negative Hydrogen Ion Sources

- **Electron impact induced processes**
  
  \[
  \begin{align*}
  R_1: & \quad H_2(\nu) + e \rightarrow H_2(\nu') + e \quad \text{(via resonant } H_2^-) \\
  R_2: & \quad H_2(\nu) + e \rightarrow H_2(\nu') + e + h\nu \quad \text{(via } B^1\Sigma_u^+, C^1\Pi_u) \\
  R_3: & \quad H_2(\nu) + e \rightarrow 2H + e \\
  R_4: & \quad H_2(\nu) + e \rightarrow H^+ + 2e \\
  R_5: & \quad H_2(\nu) + e \rightarrow H + H^+ + 2e \\
  R_6: & \quad H_2(\nu) + e \rightarrow H^- + H
  \end{align*}
  \]

- **Vibrational-translational relaxation**
  
  \[
  \begin{align*}
  R_7: & \quad H_2(\nu) + H \rightarrow H_2(\nu') + H \\
  R_8: & \quad H_2(\nu) + H_2(\omega) \rightarrow H_2(\nu \pm 1) + H_2(\omega) \\
  R_9: & \quad H^- + H_2(\nu) \rightarrow H + H_2(\nu - 2) + e
  \end{align*}
  \]

- **Wall relaxation**
  
  \[
  R_{10}: \quad H_2(\nu') + \text{wall} \rightarrow H_2(\nu) \quad (\nu < \nu')
  \]

- **Experimental setup of the source**

  P. Svarnas, S. Aleiferis, Greece
Benchmarking and Validation

Fig. Experimental ECR Hydrogen source

Fig. Simulated Vibrational Distribution Function with 2 codes

Fig. Negative ion measured and simulated as a function of pressure
Effect of weak magnetic field in capacitively coupled discharge

- Good agreement between two codes.
- For $B=15G$ and $30G$, plasma density distribution is asymmetric and shifts towards one electrode. For $B=50G$, plasma density becomes symmetric.
Increased Heating by RF wave

As evident from the EEDF profiles, amount of high-energy electrons is increased when magnetic field is applied.
ExB Penning-Type Plasma Discharge to Study Low Temperature Magnetized Plasma and Its Applications

Team: Yevgeny Raitses, Igor D. Kaganovich, A. Powis, Valentin Skoutnev, Eduardo Rodriguez, Andrey Smolyakov

Plasma set up with a convenient access for optical and probe diagnostics to study electron kinetic, turbulence and structure formation in plasmas relevant to ion beam plasma source, soft-plasma processing of materials, sputtering magnetrons, plasma thrusters (http://htx.pppl.gov/penning.html).

![Diagram of ExB Penning-Type Plasma Discharge](image_url)
Structures and anomalous transport in ExB plasmas

- We performed integrated experimental and modelling studies applying time-resolved diagnostics and kinetic simulations supported by theory.
- Spoke is nonlinear stage of Simon-Hoh instability and is complex rotating structure where plasma fills only part of chamber with turbulent flow inside spoke.

A high-perveance, 38 keV Ar+ ion beam was propagated through the plasma. The effects of charge neutralization were inferred from the transverse beam profile.

Charge neutralization fraction of 98% was measured → transverse electrostatic potential of the ion beam reduced from 15 V to 0.3 V. A. Stepanov et al, Matter and Radiation at Extremes, 78 84 (2018).
Simulations of Accumulation of Cold Electrons

Numerical study of the charge neutralization process of an ion beam with 2D ES PIC. The results show that the process of charge neutralization by electron injection is comprised of two stages. During the first stage, the self-potential of the beam is higher than the temperature of injected electrons ($Te/e$). At the second stage, hot electrons escape from the ion beam, while cold electrons are slowly accumulated. As a result, self-potential can be much lower than $Te/e$ and scales as

$$\Delta \varphi = C \sqrt{\Delta \varphi_0 T_e/e}$$

Fig. Spatial distributions of electrons and ions at $t=4.3 \mu s$, is $Te=2$ eV.

Fig. Scaling relation between the beam potential and the temperature of injected electrons at different moments.

C. Lan, I. Kaganovich submitted PoP (2019)
Formation of Cold Electrons in Plasma Plume

In most of plasma plume simulations it is assumed that plasma is a maxwellian with $T_e \sim$ few eV. This wrong assumption!

→ Selective trapping of the coldest electrons from the plasma into the plume can produce much colder electrons in plume.

Well-known effect in discharges: negative glow

We also observed this effect in experiments and simulations.
Computational Tools at PPPL for LTP Modeling

- **Particle-in-cell codes (2D EDIPIC, 3D PPPL-modified LSP, New Highly Scalable PIC),**
  - state of the art collision models and plasma-surface interaction, validated by numerous benchmarks

- **Fluid codes (3D ANSYS)**
  - implemented sheath models, MHD effects, surface interface

- **Molecular Dynamics (DFT-TB)**
  - (DFT codes: full and tight binding approximation, CMD (classical potentials), KMC –kinetic Monte Carlo, and thermodynamic code for chemical composition.)
Advanced *fs-ps-ns-cw* diagnostics of plasma species, flow, nanoparticles

**Plasma sources**
- Atmospheric pressure plasma: DBD, jets, arcs
- Low pressure LTPs: magnetized, e-beam, DC/RF microscale

**Unique measurements/simulations**
- Plasmas with complex chemistry: *arc discharge*
- 2D CFD simulations (left) and LIF measurements (right)
- 1D, 2D, 3D Kinetic simulations
- Nanoparticles synthesis in arc: modeling, OES and LII measurements
- Atomistic simulations

**PFC properties**
- *fs*- Laser Electronic Excitation Tagging flow measurements
- Laminar flow
- Turbulent flow
- *ns*-discharge in gas bubble
- Streamer in plasma jet

**2D CFD simulations (left) and LIF measurements (right)**
Announcement of Collaborative Low Temperature Plasma Research Facilities (1/2)

The Department of Energy, Fusion Energy Science has funded two collaborative plasma research facilities at PPPL and SNL to offer access to world class capabilities and expertise. These capabilities include:

- Optical interrogation with CW, nanosecond, picosecond and femtosecond laser systems for laser-induced fluorescence, two-photon laser induced fluorescence, laser-collision induced fluorescence, 1D Raman imaging, 2D CARS, tomographic PIV, Thomson scattering, electric field-induced second harmonic generation, multiphoton ionization and microwave scattering,
- High-speed cameras.
- In-situ diagnostics of nanoparticles (size –distribution, chemical composition, charge, velocities)
- Spectroscopic tools: vacuum ultra violet (VUV), visible, Far IR (FTIR), high-resolution mass spectroscopy.
Announcement of Collaborative Low Temperature Plasma Research Facilities (2/2)

These capabilities include:

• Measurements of plasma-induced surface charging and secondary electron emission properties of plasma facing materials
• Massively parallel ES and EM PIC-DSMC, and in-development hybrid and fluid simulation capabilities, for collisionless to high pressure multi-species plasma systems with non-equilibrium chemistry and photonic processes
• Analytical theory support for plasma experiments and simulations, optical calculations
• Support for quantum chemistry calculations relevant to plasma-material interactions and synthesis of nanoparticles

Solicitation for user proposal will be conducted in January
You are welcome to apply, Talk to Y. Raitses, I.D. Kaganovich
New Collaborative Low Temperature Plasma Research Facilities Open for All Users
Thursday, October 24
12:30 p.m. – 1:30 p.m.
Broward Convention Center, Room 301
PCRF LTP diagnostics available at PPPL

- Unique combination of ns/DC diagnostics of low to high pressure plasmas, nanoparticles and secondary electron emission & charging
PCRF LTP diagnostics available at Princeton MAE

Unique fs/ps/ns diagnostics of plasma, gas phase for detailed characterization of moderate to high pressure plasmas, plasma interactions with solids, liquids

- Gas density and temperature, nanoparticle charge, negative ions, structural surface changing
- Flow velocity, density of species
- EEDF, electric field