Space Propulsion and Power

Integrity ★ Service ★ Excellence

8 March 2013

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Air Force Research Laboratory

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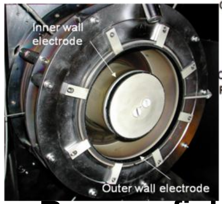
Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std Z39-18

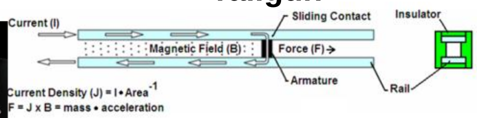
Space Propulsion and Power Portfolio

Research to Understand, Predict, and Control Complex interactions of the Matters in Space Propulsion Systems

Electric thrusters

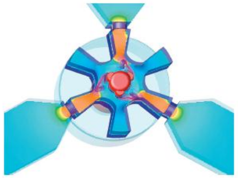


railgun

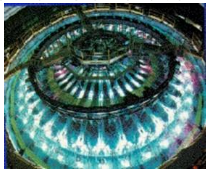


Micro plasmas

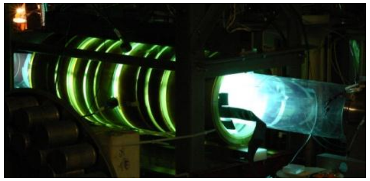
magnetron



Sandia Saturn Pulsed Power Generator

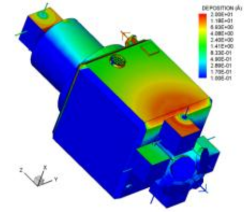


Reverse field configuration



Coupled Materials and Plasma Processes Far From Equilibrium

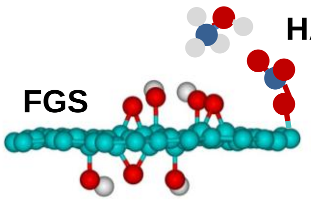
Satellite contamination

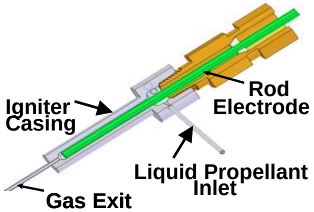


DUAL- MODE PROPULSION - micro chemical thruster

HAN

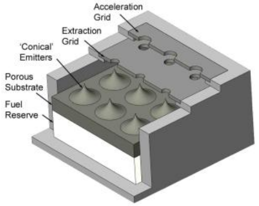
FGS



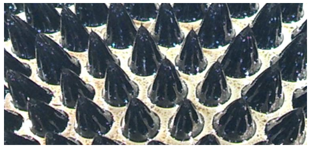


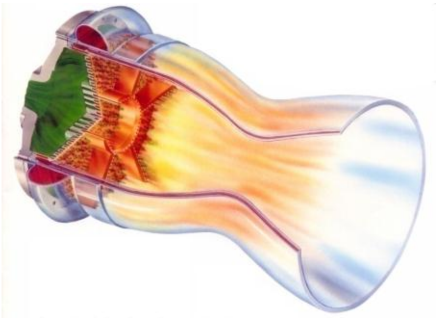
Electrosprays

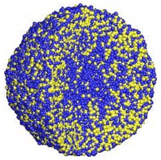
Electrospray propulsion



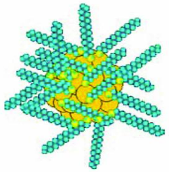
ionic-liquid ferrofluid



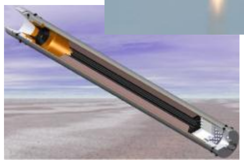




Novel Energetic Materials



Reduced Basis and Stochastic Modeling of high pressure combustion dynamics



Program Interactions and Trends

AFRL/RQ

NASA

Joint Workshop, Dec 2011

Coupled Materials and Plasma Processes Far From Equilibrium

Sayir (RTD)

Luginsland (RTB)

AFRL/RQ

NASA

Electrosprays

Berman (RTE)

Bedford/ONR

Office of Naval Research

Joint Contractors Mtg, Aug 2012

Hawkins/AFRL/RQ

Petris/DTRA

Palaszewski / NASA

Pagoria/LLNL

Lawrence Livermore National Laboratory

Novel Energetic Materials

Sayir (RTD)

Berman (RTE)

Anthenien/ AFOSR

AFRL/RQ

NASA

Reduced Basis and Stochastic Modeling of high pressure combustion dynamics

Fahroo (RTA)

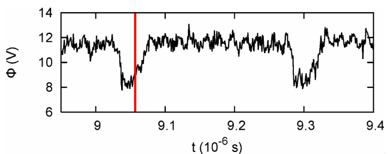
Darema (RTC)

Li (RTE)

Coupled Materials and Plasma Processes Far From Equilibrium-Material / Plasma Coupling

Sheath Potential Instabilities

~4 MHz

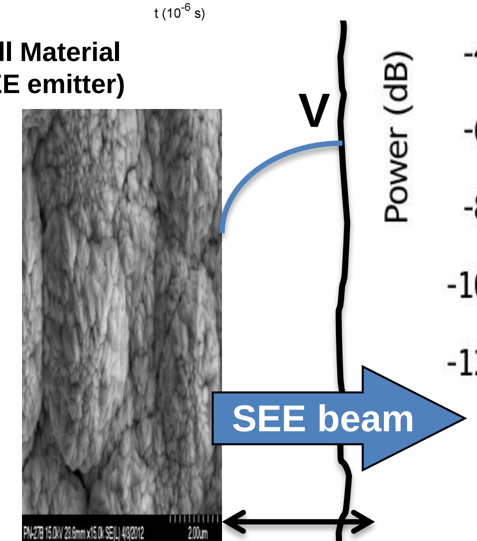


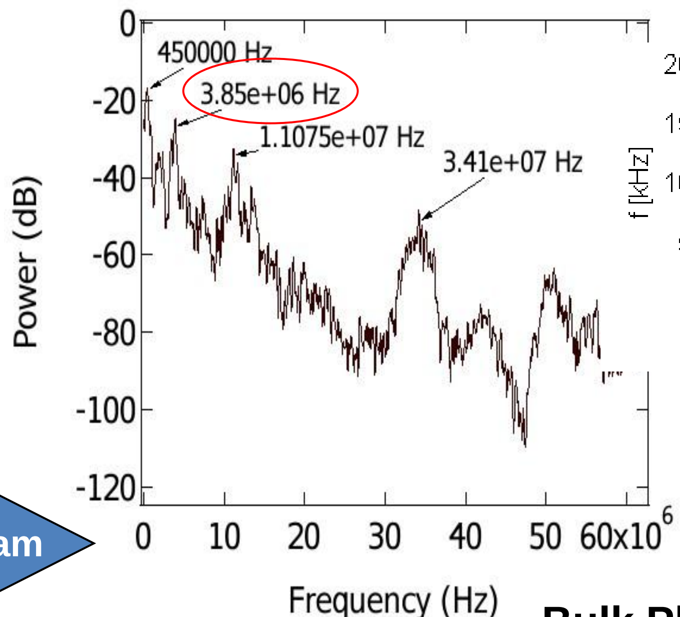
High Frequency Bulk Plasma Oscillations

Inverse Cascade

Coherent structures

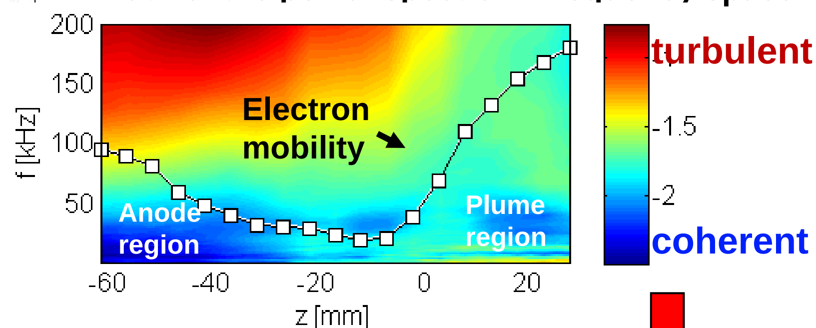
Wall Material (SEE emitter)



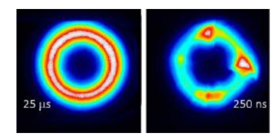


Bulk Plasma

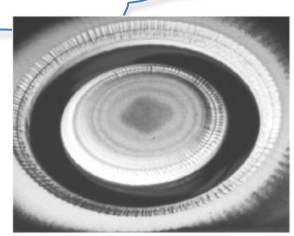
width of the power spectra in frequency space

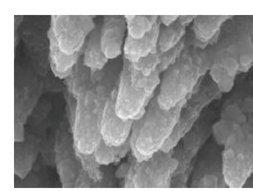


magnetron



Coherent instability in Hall Thruster





Why do we care?

- Change the particle & energy fluxes !
- Change the stability and lifetime of device !
- Change the characteristics (SSA) of device !

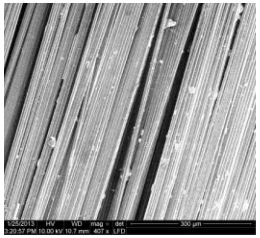
Wall Material Experiments (Raitses, Princeton)

Wall Architectures Have Significant Effects on Secondary Electron Emission (SEE) and Discharge Behavior

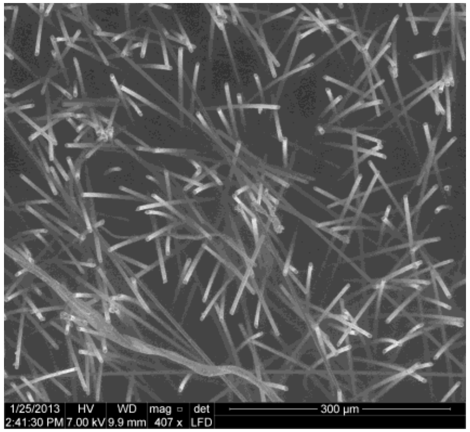
Scanning Electron Microscope Images

"Black" regions – No SEE; "White" regions - SEE

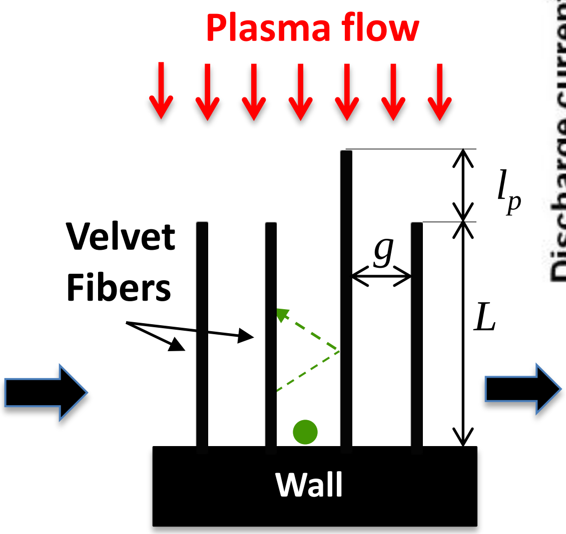
Velvet fibers on the surface strong SEE from fibers



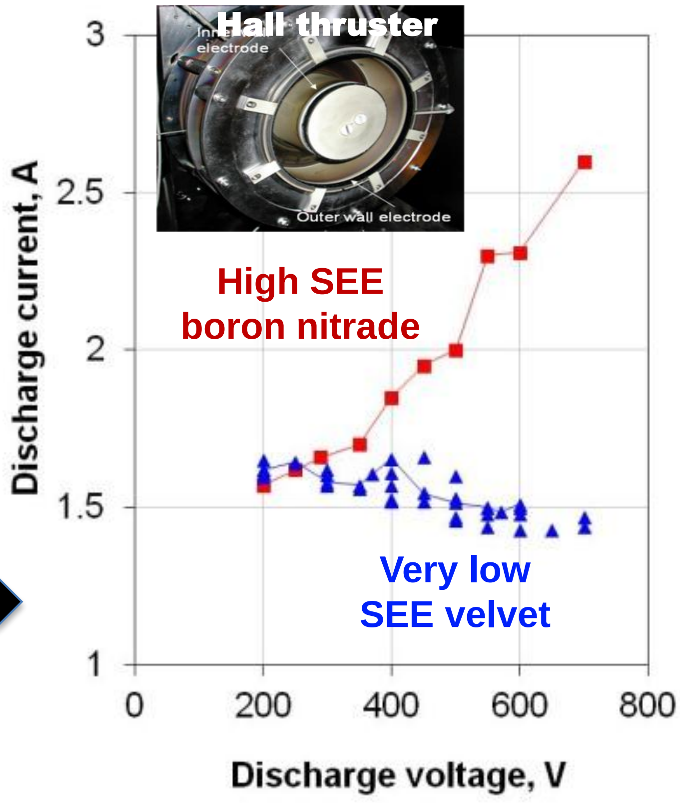
Velvet fibers perpendicular to the surface–No SEE except from fiber tips



To avoid field emission leading to arcing g, $l_p < \lambda_D$



Velvet suppresses SEE, reducing current at high voltages, leading to very high efficiencies

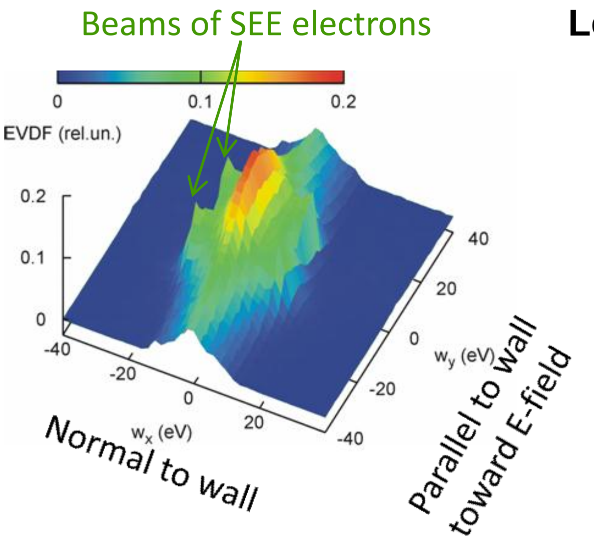


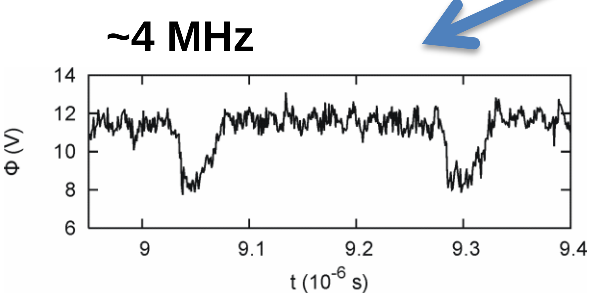
•Need to take into account spatial /temporal variations of plasma scale, λ_D (Debye length), due to plasma design and instabilities

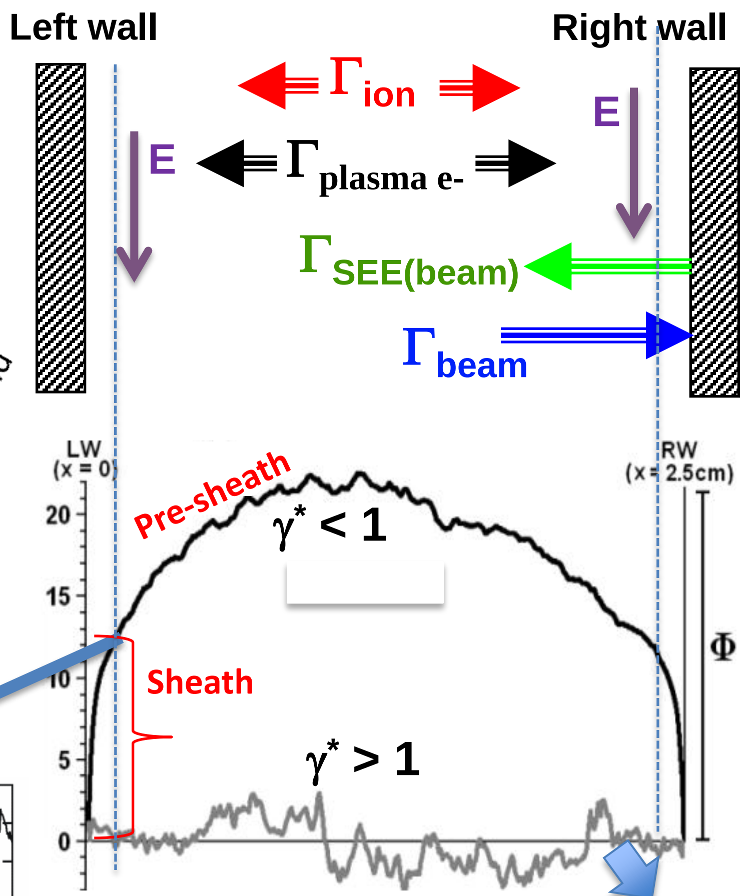
- Y. Raitses, I. D. Kaganovich, A. Khrabrov, D. Sydorenko, N. J. Fisch, A. Smolyakov, IEEE Transactions on Plasma Science 39, 995 (2011)

Modeling of plasma-wall interaction (Kaganovich, Princeton)

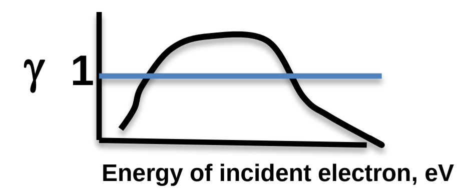
Kinetic simulations revealed a new regime of plasma-wall interaction with a very strong secondary electron emission







- SEE yield is the number of secondary electrons emitted per incident primary electron



- **Effective secondary electron emission γ^* accounts for non-Maxwellian effects**

- Experimentally validated by N.Claire and F. Doveil, Aix-Marseille Université/CNRS

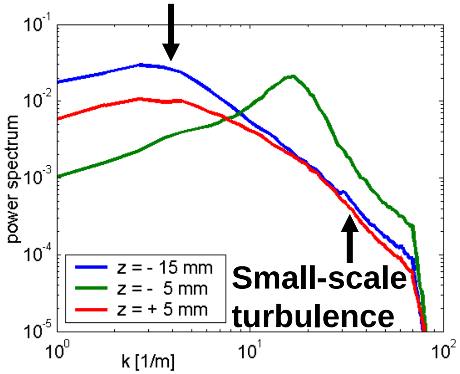
- **electrons acquire enough energy from the electric field parallel to the wall, causing , $\gamma^* > 1$**
- **Sheath collapse leads to extreme wall heating by plasma and plasma losses (bad)**

- M. D. Campanell, A.V. Khrabrov, I. D. Kaganovich, Physics of Plasmas 19, 123513 (2012)

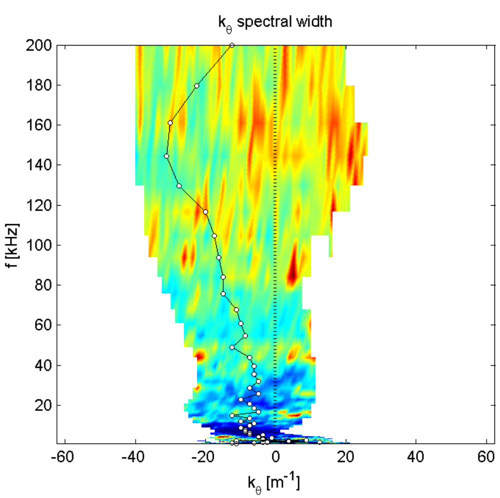
Small-Scale Turbulence and Inverse Cascade Generating Large Scale Coherent Structures for Hall discharges (magnetron similar)

- Generated by nonlinear coupling between fast-growing unstable higher frequency modes and lower frequency modes
- These large-scale fluctuations correlate to measured transport properties

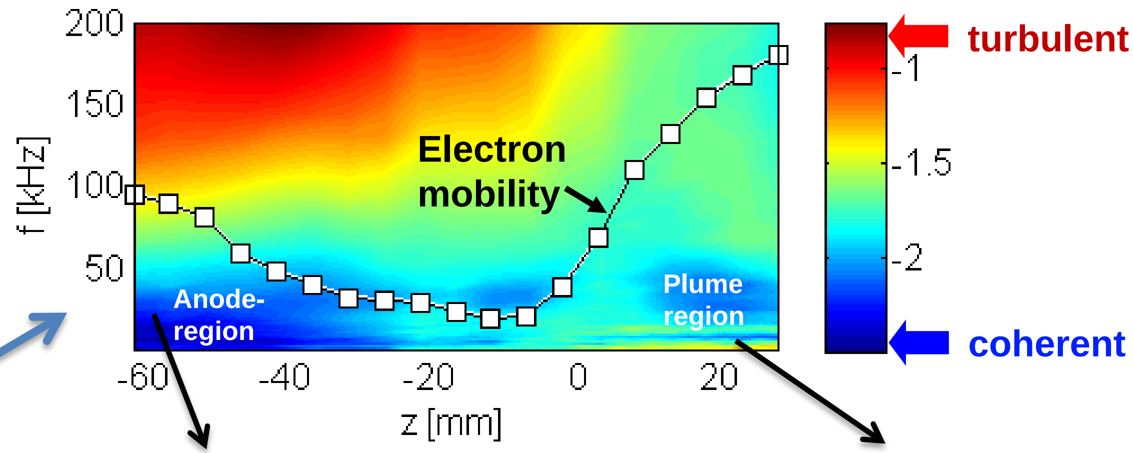
Large-scale fluctuations



Fluctuation Dispersion – k(theta)

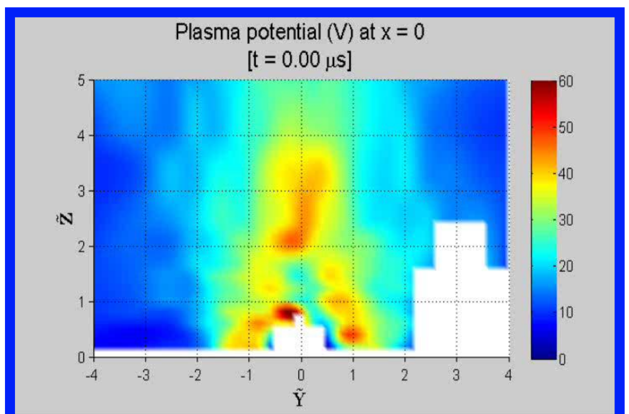


width of the power spectra in frequency space



High turbulence + coherent structures (spoke?)

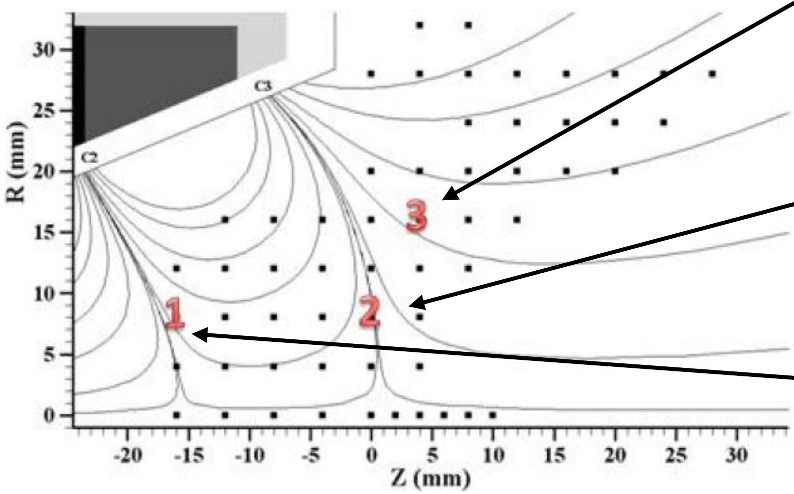
Just coherent structures (drift waves?)

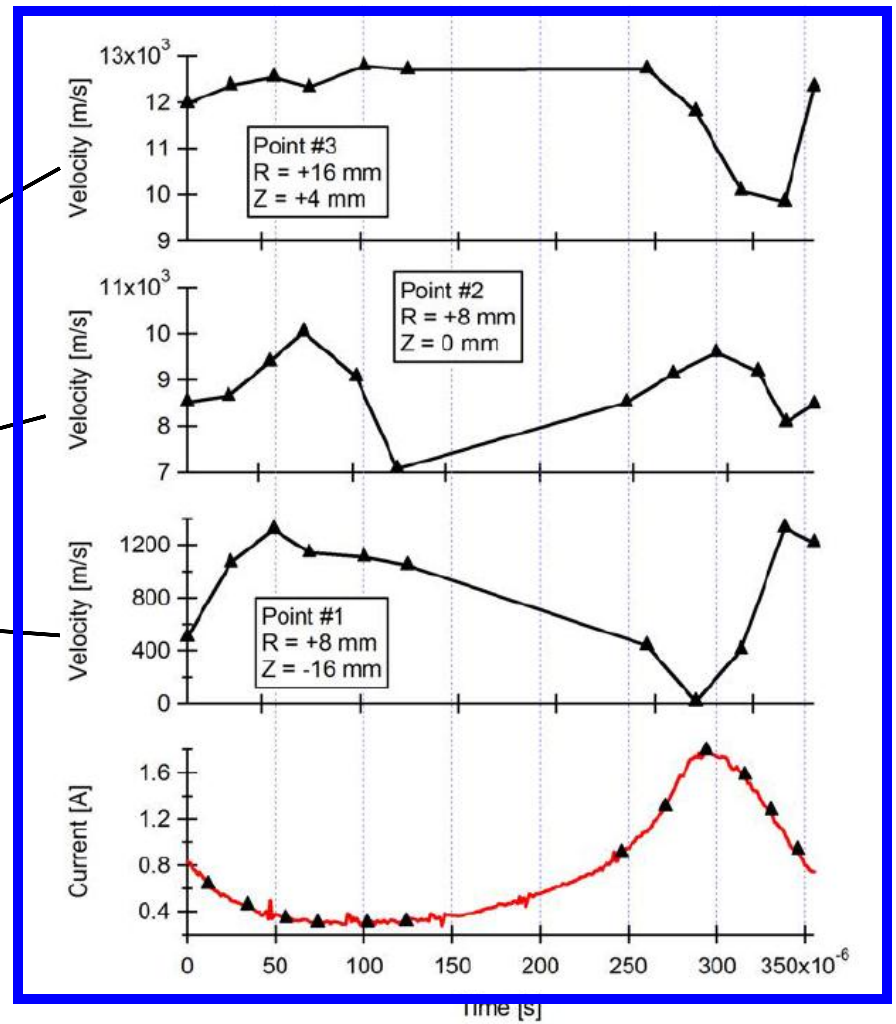


Successfully synchronized continuous wave laser induced fluorescence to coherent structures in plasmas

- N. A. MacDonald, M. A. Cappelli, and W. A. Hargus, Rev. Sci. Instruments 83, 113506 (2012)

- **Time-Synchronized continuous wave LIF Measurements of Velocity – First Results**





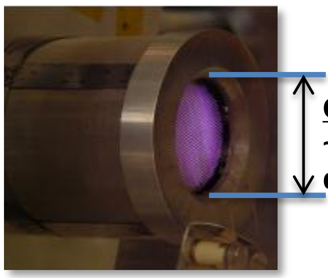
- **Velocity fluctuations vastly different depending on probed location in magnetized plasma**
- **Physical probes can only measure the average velocity!**

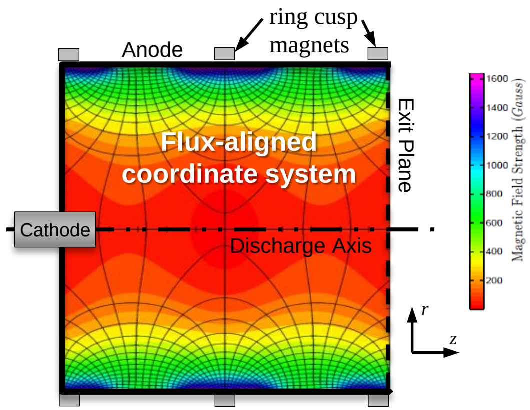
Wirz / UCLA- YIP- Center of Excellence (Univ. of Michigan)

Self-consistent analytical theory used to optimize micro plasma source

- **Critical research for in-space propulsion, plasma-enhanced combustion, plasma aerodynamics, small scale sensors, directed energy devices, plasma processing …**

Micro-scale plasma source



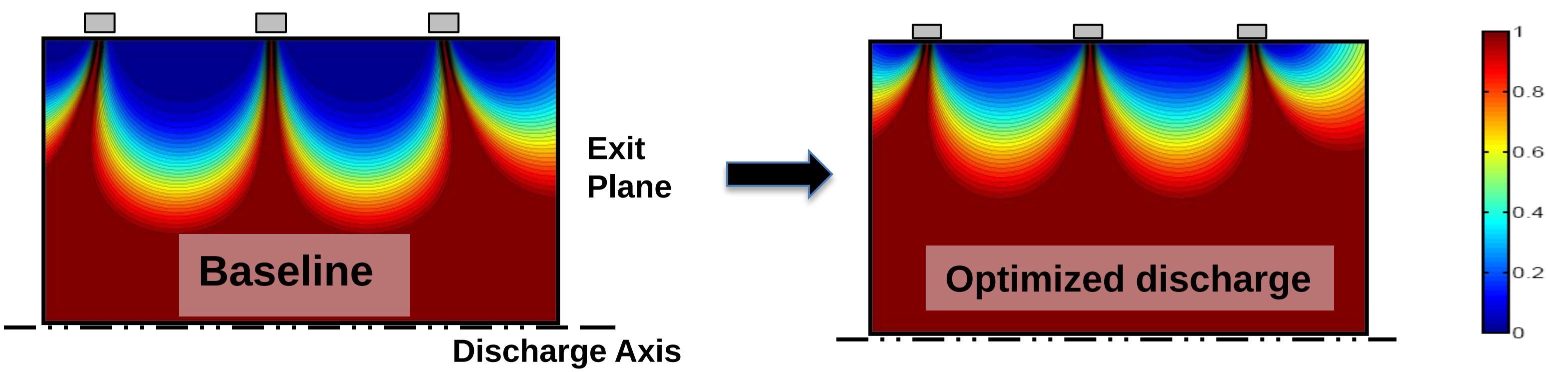


Goal: Develop efficient and stable cusp-confined micro discharge

- **New "stream function" magnetic field analysis developed to predict plasma behavior throughout discharge**

Optimization using analytical theory yields 2X increase in plasma production and stable plasma over baseline

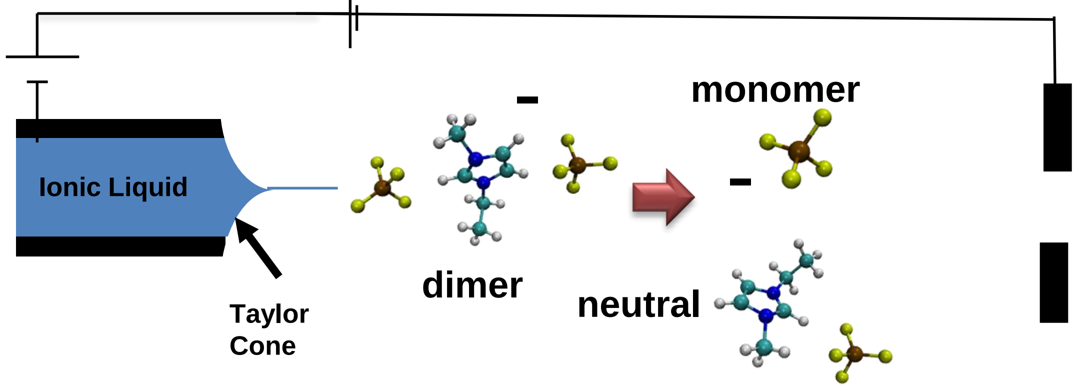
- **Model trends experimentally validated**

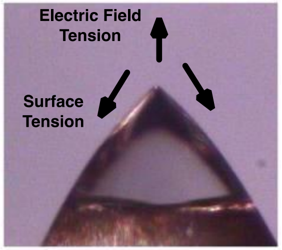


- Mao, H-S., Wirz R. E., *Appl. Phys. Lett.*, accepted Nov 2012

Molecular Dynamics Simulations reveal how to mitigate Fragmentation of Solvated Ions

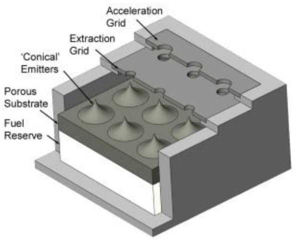
When electric field (or electric pressure) > surface tension + internal liquid pressure



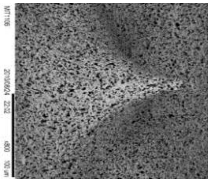


LIQUID TAYLOR CONE

Emitter Array

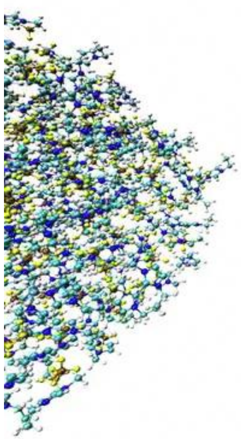


Single Porous emitter

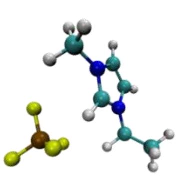
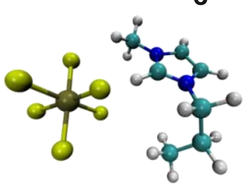


- **If fragmentation occurs, efficiency drops!**

Full-atom MD with E field



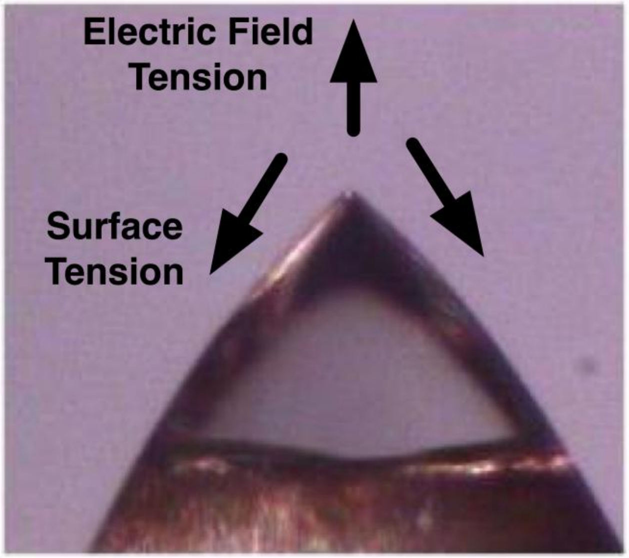
- **MD results suggest the use of complex ions, as there are more degrees of freedom to dissipate internal energy**

EMI-BF_4	vs	PMI-PF_6
		
Less complex dimer 100% fragmentation		More complex dimer 55% fragmentation

Carla S. Perez-Martineza) and Paulo C. Lozano, J. Vac. Sci. Technol. B 30(6), Nov/Dec 2012

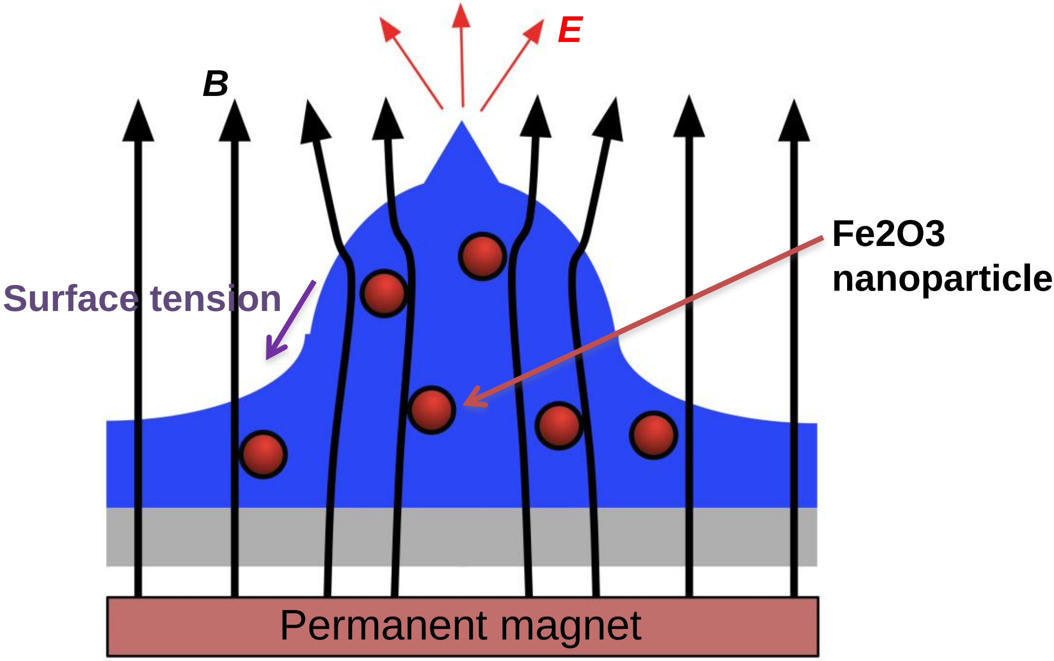
Can we obtain Taylor cone without a physical emitter or capillary?

Taylor cone forming at tip of physical emitter



Physical needle enhances *E*-field – Taylor cone forms.

Taylor cone forming at the peak of Normal Field Instability



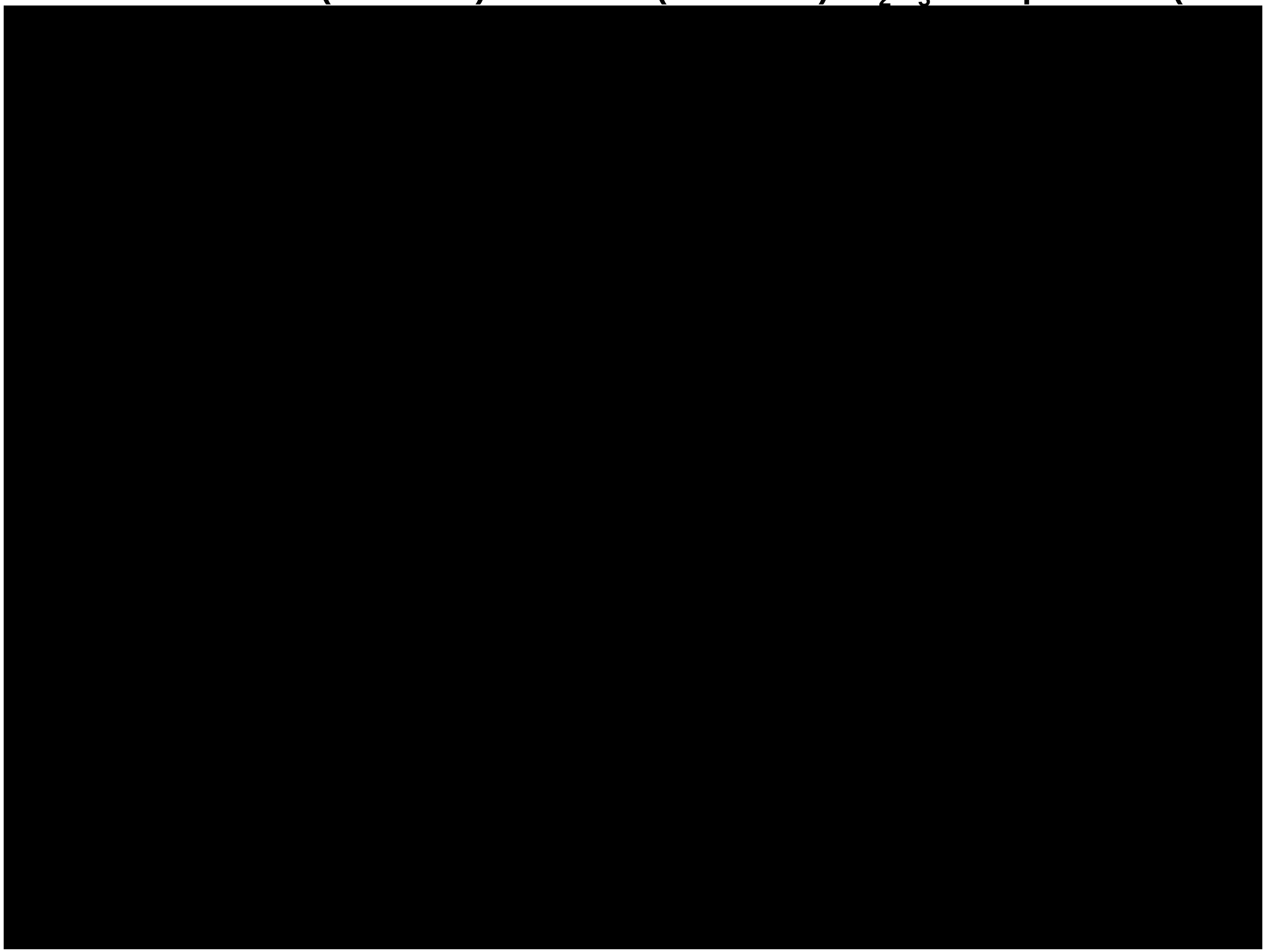
Concentrated *B* at crest attracts more ferromagnetic fluid to crest, amplifying the perturbation into an instability. Crest enhances *E*-field – Taylor cone forms.

- **Ionic liquid becomes superparamagnetic with an addition of ferromagnetic Fe_2O_3 nanoparticles!**

Center of Excellence (Univ. of Michigan) – King (Michigan Tech)

First stable ionic-liquid ferrofluid synthesized by Hawkette, et al 2010 (Australia)

- **Ethylmethylimidazolium acetate (EMIM-Ac) with bare (uncoated) Fe_2O_3 nanoparticles (Michigan Tech)**



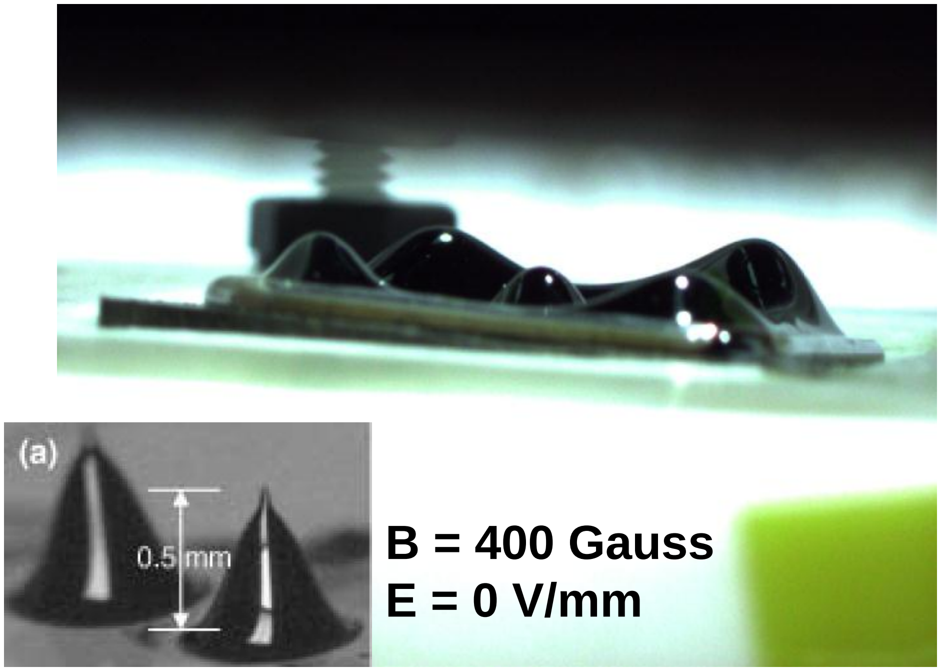
- *Jain, N, Wang, Y, Jones, SK, Hawkett, BS, and Warr, GG, "Optimized steric stabilization of aqueous ferrofluids and magnetic nanoparticles," Langmuir, 26(6), 2010, pp. 4465-4472.*

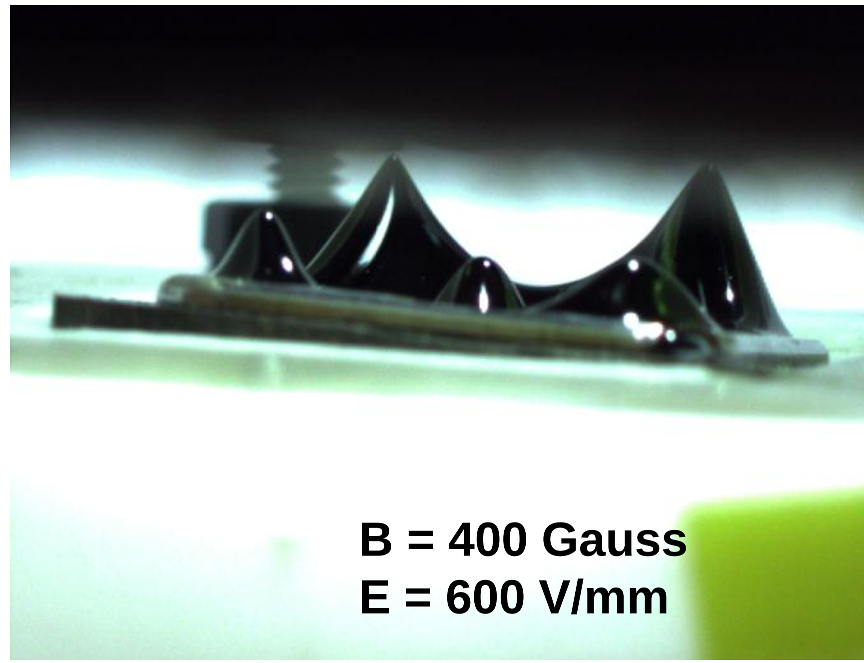
Center of Excellence (Univ. of Michigan) – King (Michigan Tech)

Progress – Normal field Instability with E-field

"Normal field instability" peaks (no electric field) can be rounded or they can be very sharp (shown in inset)

When an electric field is applied these peaks will get even sharper

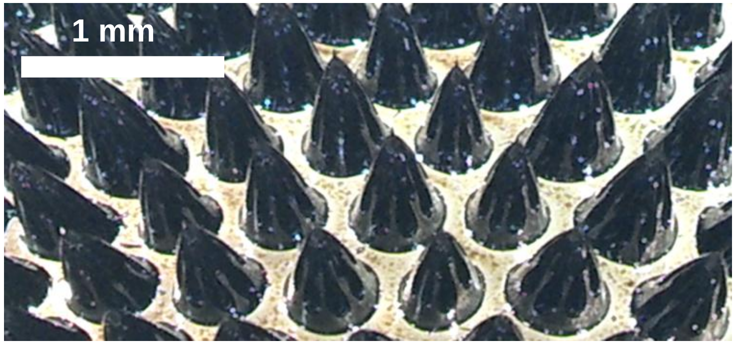




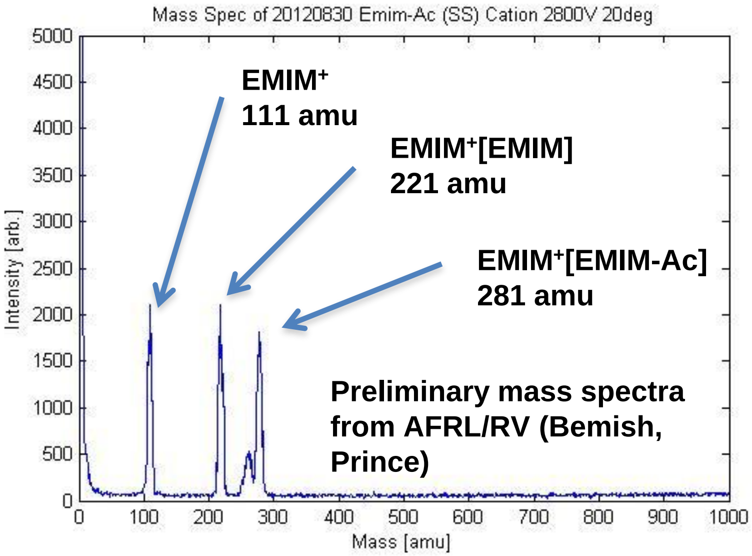
- Weak magnetic field with high-surface-tension ionic liquid ferrofluid shown. Normal-field instability peaks (left) are rounded in this case.
- Application of moderate electric field sharpens peaks due to electrostatic force (right)

Challenges

Q1: Emitter tip density (tips per mm^2) is a function of surface tension, nanoparticle magnetization, and magnetic field. Can we synthesize an "ideal" ILFF for space propulsion that has high thrust density (milli-Newtons per mm^2)?

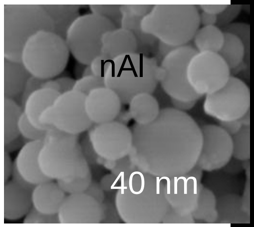


Q2: An ILFF is a complex ferromagnetic, electrically conductive, and non-homogeneous colloidal fluid. What are the velocities of the molecular and macro species emitted when the fluid is electrosprayed and what is the beam divergence?



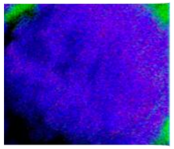
A Brief History of Nanoenergetic Materials

Examples from AFOSR program:

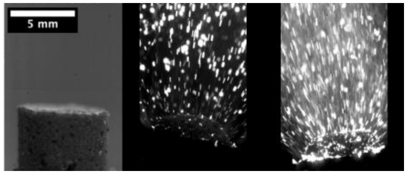


- ***1st Generation***
  - Nanometer-sized Al powder/conventional propellants
  - Some performance gain, variable results

Al + fluoropolymer



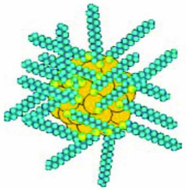
Propellant **w/ Baseline Al** **Modified Al**



- ***2nd Generation - Top down approach***
  - Quasi-ordered nanometer-sized inclusions in energetic matrix
  - Coated nanometer-sized metal powders
  - Controlled oxidation, improved storage lifetime

Nano-Al Encapsulated with Ammonium Perchlorate

- ***3rd Generation - bottom-up approach***
  - Organized multiscale processing to enable the insertion of nanoenergetic materials into larger units
  - 3-dimensional nanoenergetics for reaction control
  - Controlled reactivity, Improved manufacturability/processing

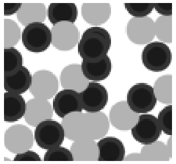


2nd Generation:

Aluminum with nanoscale inclusions of fluoropolymers improves propellant performance (Son/Purdue)

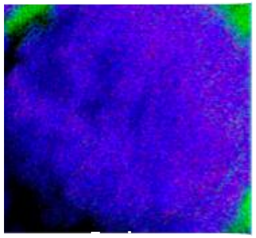
2012

Al + fluoropolymer Powder Mixture

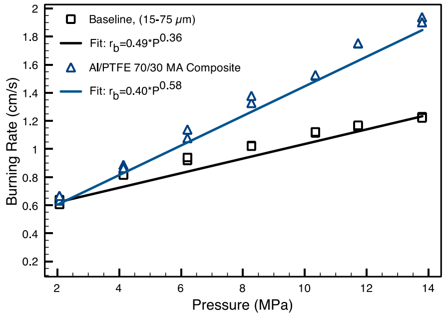


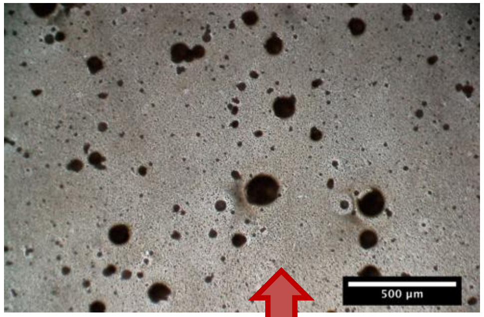
Mechanical Activation

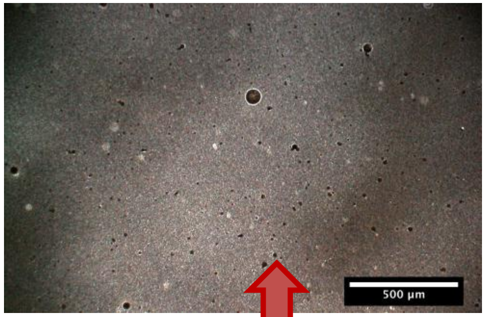
Uniform composition and induced lattice defects (stored energy)

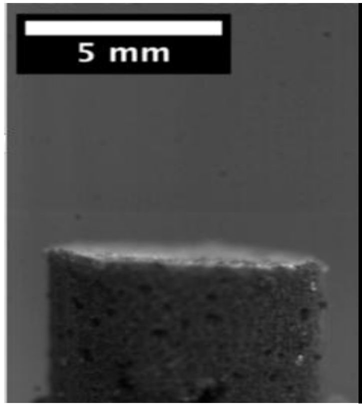


- **Experiments validate the hypothesis that aluminum with nanoscale fluorocarbon inclusions in a solid propellant yield reduced ignition temperature, increased burning rates, and smaller agglomerate size**

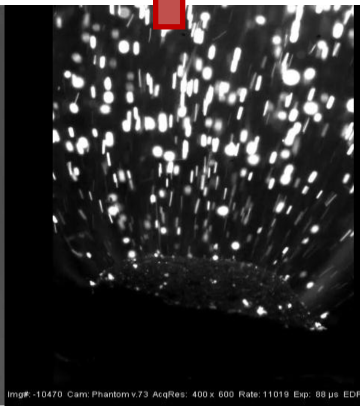




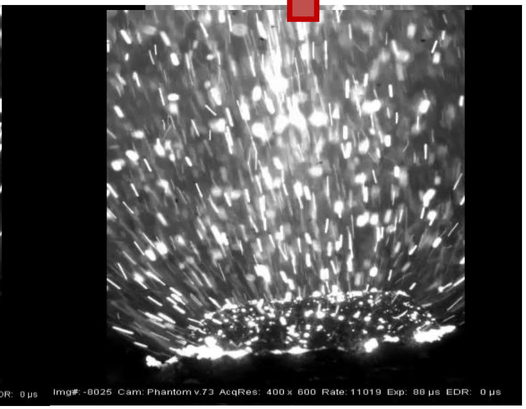




Propellant



w/ Baseline Al



w/ Modified Al

- **Other nano-inclusion materials will be explored, including piezoelectric polymers to achieve smart/functional control of rate or sensitivity**

- **Travis R. Sippel, Steven F. Son, and Lori J. Groven, "Altering Reactivity of Aluminum with Selective Inclusion of Polytetrafluoroethylene through Mechanical Activation" Propellants, Explosives, Pyrotechnics, 2013**

3rd Generation:

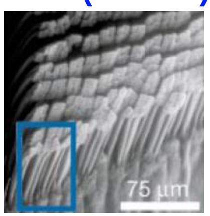
FY 2012 MURI : Smart, Functional Nanoenergetics Design from the atomistic / molecular scale through the mesoscale

biological example of multiscale effects

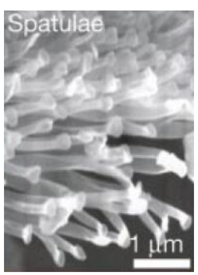
Multiscale Energetic Composites Fabricated on Porous Silicone Substrates (Yetter/ Penn State)

Gecko

Rows of setae from a toe (micron)

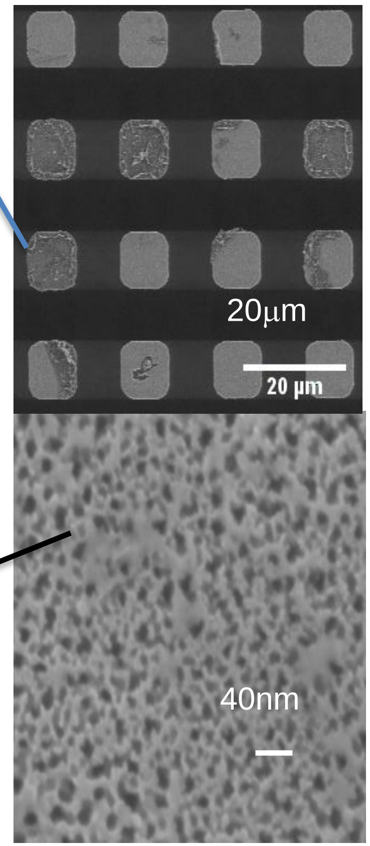


Spatulae (nm)



Autumn, K., *et al.*, Nature, 405, 681-684, 2000

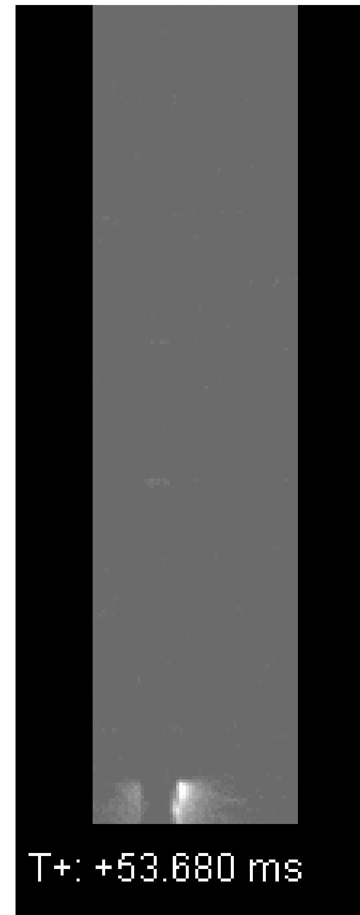
pillars were ~ 35 µm tall and have 8 µm square bases separated by ~8 µm.



Pore Diameters ~ 20nm and filled with oxidizer $Mg(ClO_4)_2$

Direction of Propagation, 40 mm

Side View - Reaction Propagation

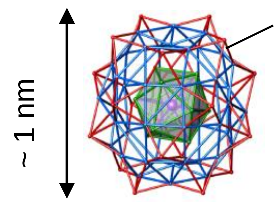


- V.K. Parimi, S.A. Tadigadapa, and R.A. Yetter, J. Micromechanics and Microengineering, 22, 5, 2012

Third Generation:
Organized Multiscale Energetic Al Composites for Combustion Control

Step 1: Generation of passivated Al clusters

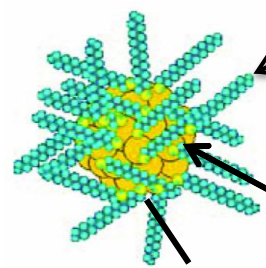
Al-77 Cluster



Pyrophoric and extremely fast reacting Al particle

Metalloid Al clusters modeled after Schnöckel aluminum cluster chemistry (Ecker, A., Weckert, E., Schnockel, H., Nature 1997, 387, 379)

Nanoscale passivated Al Cluster using ligands



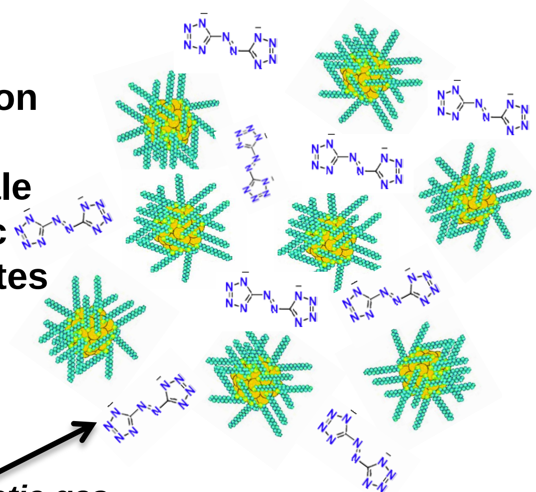
provide additional energy during combustion

Bond energy at ligand head controls IGNITION TEMPERATURE of cluster

Nanoscale passivated Al clusters to be evaluated as additives to liquid fuels & propellants

Step 2: Generation of mesoscale energetic composites

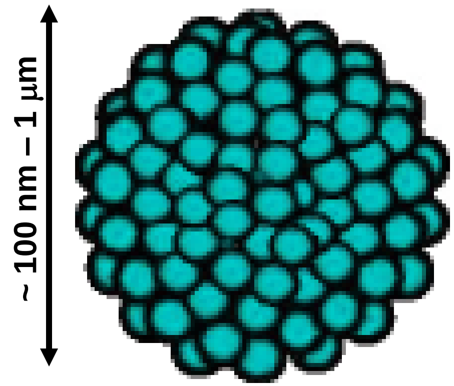
Aerosol of Al cluster and gas generator molecules



Energetic gas generators with large ΔH of combustion

Aerosol based self assembly – a bulk manufacturing process

Mesoscale composite of Al cluster and gas generator for incorporation in solid and liquid propellants



disassemble and release ***highly dispersed*** reactive nanostructures at a predetermined pressure and temperature for **controlled combustion**

Gasification and decomposition temperatures of gas generator molecules control s energy and temperature of mesoparticle disruption

Summary and New Research Areas

Coupled Materials and Plasma Processes Far From Equilibrium

Control of Coherent Structures:

- **Stable Plasma Propulsion with extended lifetime**
- **Plasma Photonic Crystals**

Electrosprays

Novel Energetic Materials

- **Non-Equilibrium Plasmas in Liquid Propellants**
- **Miscible liquid boranes in propellants**
- **Transformable Energetic Materials via co-crystallization or molecular blending**

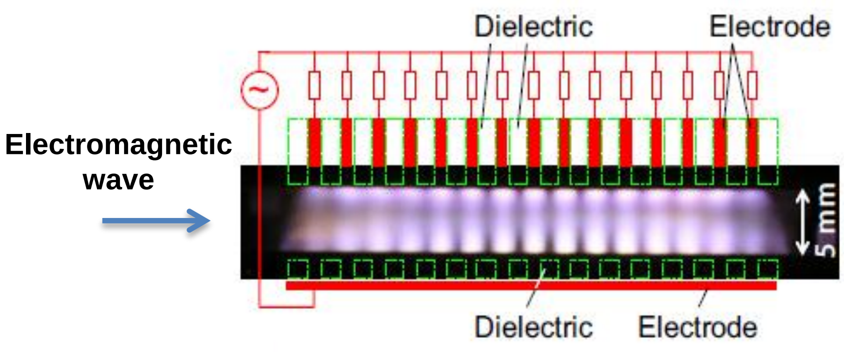
Reduced Basis and Stochastic Modeling of high pressure combustion dynamics

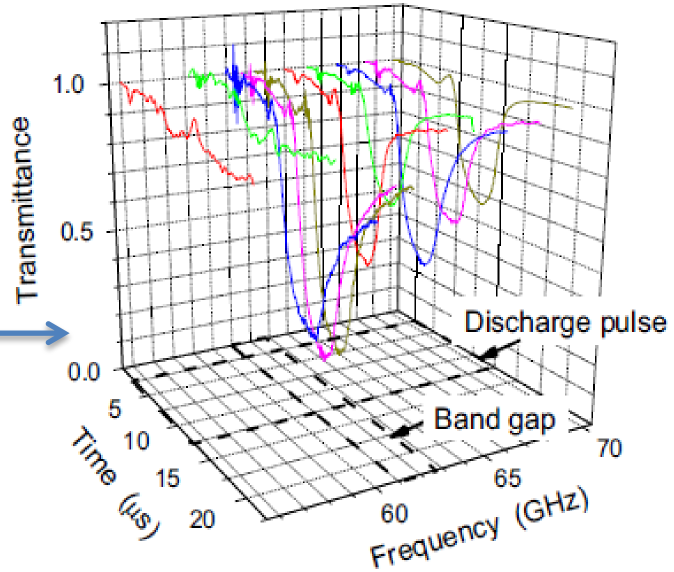
- **Quantum Lattice Modeling for Multiphase reacting flows**

Space Propulsion and Power - New Research Areas

Control of the Coherent Periodic Microstructures in plasmas may lead to reconfigurable THz Plasma Photonic Crystals

From micro plasmas

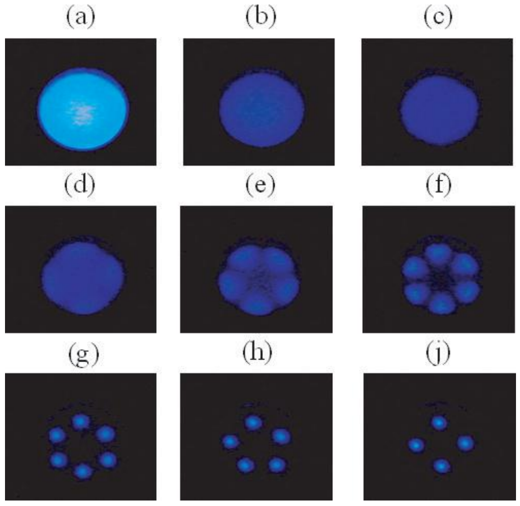




Advantages of using Plasma Photonic Crystals :

- Tunability : variable Refractive Index and Band Gap
- Reconfigurable structure : variable crystal Geometry/Symmetry
- Inherent Nonlinearity : Harmonic Wave Generation

From bulk coherent structures



CHALLENGES:

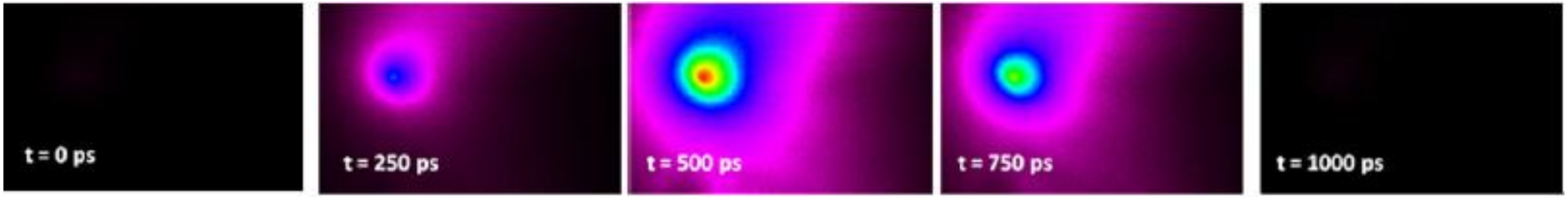
- Can researchers achieve plasma crystal lattice scale to THz electromagnetic wavelength with a plasma frequency close to electromagnetic frequency ?
- Can researchers generate and stabilize coherent organized microstructures from large otherwise uniform dense plasmas ?

Space Propulsion and Power - New Research Areas

Non-equilibrium plasmas in liquid propellants

Recently, non-equilibrium plasmas have been formed in liquid water without formation of gas bubbles yielding propagation velocities of 5000km/s for *low energy nanosecond discharges*

(Starikovskiy et al., *Plasma Sources Sci. and Technol*. 20, 1, 2011).



Impact:

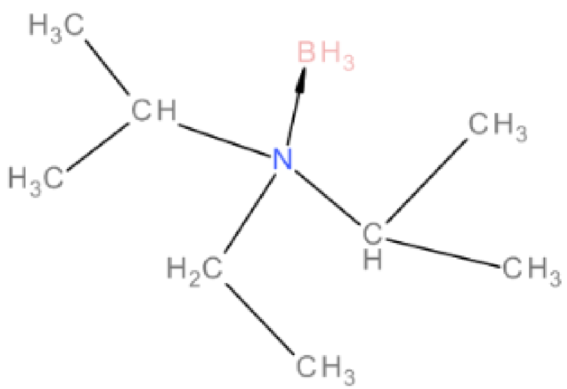
The formation of highly ionized channels in condensed media without void formation may create "liquid plasma" applications for ignition assistance, in-situ propellant modification, and accelerated combustion.

Challenge:

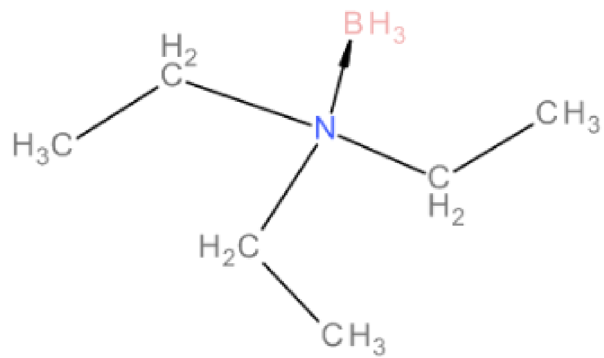
However, the roles of low energy non-equilibrium discharges with propellants and models for describing discharges in dense media are poorly understood

Miscible liquid Boranes in RP1 (kerosene)

Borane-N,N diisopropyl ethylamine complex



Borane-triethylamine complex



Impact: low-toxicity and combustion instability control

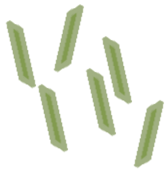
Challenges:

- A fundamental study is needed to synthesize optimal amine-boranes and/or other borane molecules that are miscible in RP-1 with coupled simulation and feedback from small-scale characterization to develop optimal propellants and additives
- Applicable to ionic liquids?

Transformable Energetic Materials

Example: Co-Crystallization

Material A

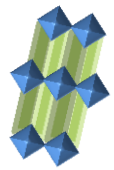


high sensitivity
good performance

Material B

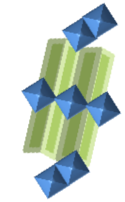
low density
poor performance

co-crystallization



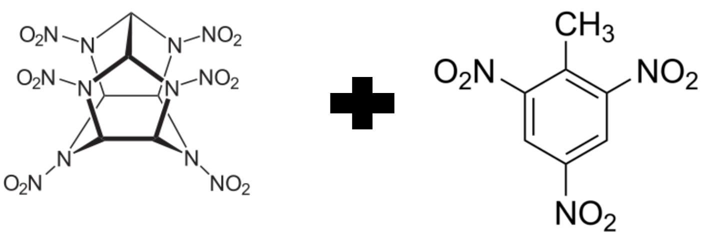
low sensitivity
good performance
propellant
ability to transform when stimulated

Application of "switching" energy (electro-magnetic, heat, light, etc.)



sensitized materials

Insensitive cocrystal of CL-20 and TNT



Heat activation

more sensitive material

Bolton, O.; Matzger, A.J. Angew. Chemie Int. Ed. 2011, 50, 8960-8963

Challenges:

- **Can we engineer green energetic materials that can transform (e.g. from propellant to explosive, or even in situ modification)?**
- **Can we model and predict transformations and necessary stimuli?**

Space Propulsion and Power - New Research Areas

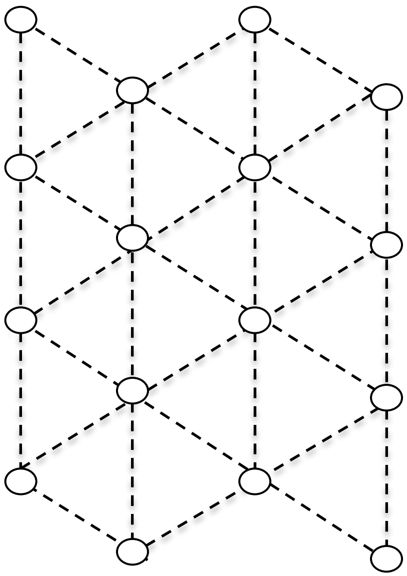
Quantum Lattice Algorithms for the Simulation of Multiphase/Multicomponent Fluid Phenomena

Classical computer bit: 0 or 1

Quantum qubit: $|q\rangle = a|0\rangle + b|1\rangle$ **(quantum state)**

Quantum advantage: instantaneous result, noiseless, unconditionally stable, reversible

One or more qubits can be arranged on lattice sites (here 2-D)



System state at time t $\quad |\mathrm{Y}(x_1,\ldots,x_n;t)\rangle$

System evolves in time by

$$|\mathrm{Y}(x_1,\ldots,x_n;t+t)\rangle = \hat{S}\hat{C}|\mathrm{Y}(x_1,\ldots,x_n;t)\rangle$$

where $\hat{S}$ **is a streaming operator (flow)**
$\hat{C}$ **is a collision operator (fluid interactions)**
both implemented via quantum gates

Algorithm can be run on quantum or classical computers

Shown by Yepez[1] to reproduce the lattice Boltzmann equation, a popular CFD methodology.

[1]Yepez, J., "Quantum Lattice-Gas Model for Computational Fluid Dynamics," *Physical Review E*, Vol. 63, 2001, p. 046702.

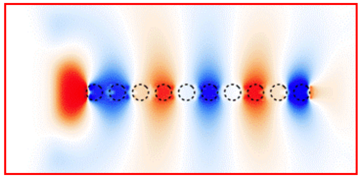
BACK-UP SLIDES

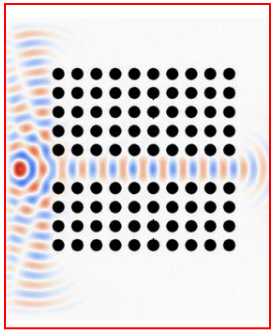
Plasma Metamaterials and Plasma Optics

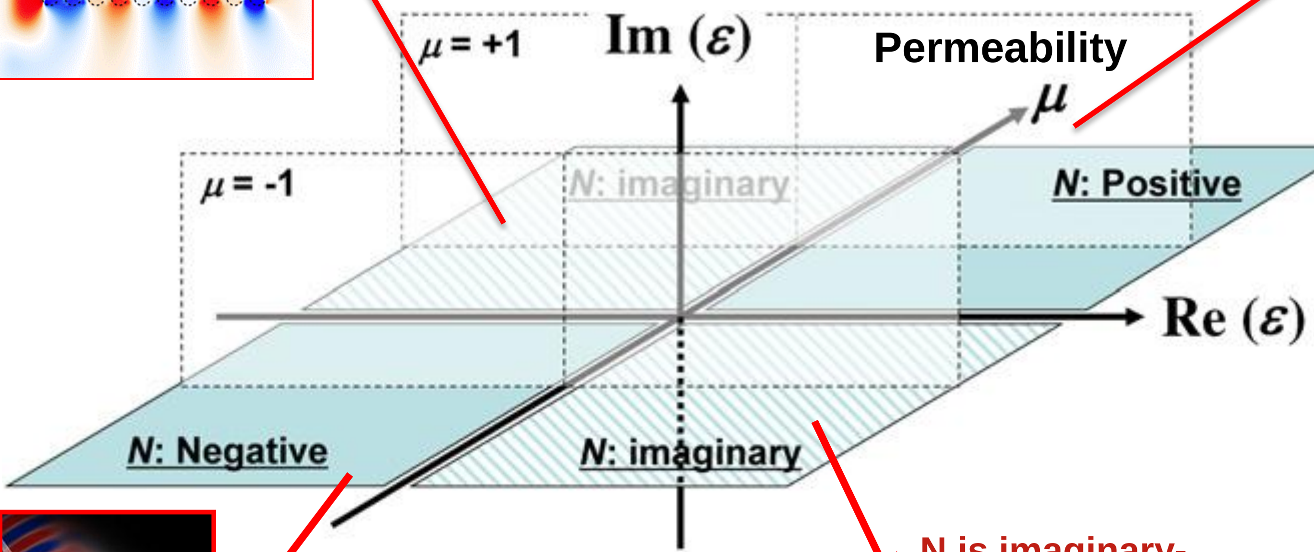
- **plasma metamaterials, we can use the effects of *Im(ε)***

Refractive index N is imaginary -
Bulk Electromagnetic waves cannot propogate
But surface plasmons possible

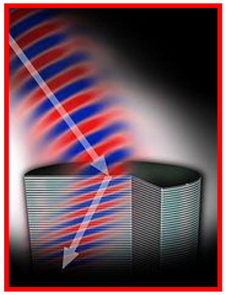
Refractive index N > 0
Low density collisionless
Plasmas – photonic crystals with
tunable band gaps possible







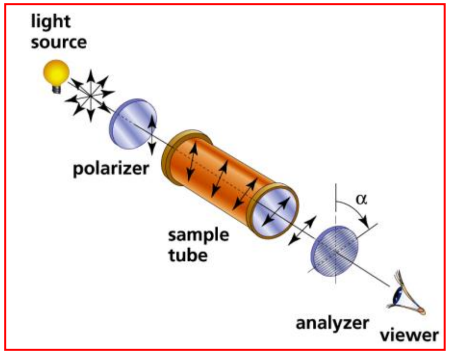
Real part of emissivity



http://en.wikipedia.org/wiki/Negative_index_metamaterials

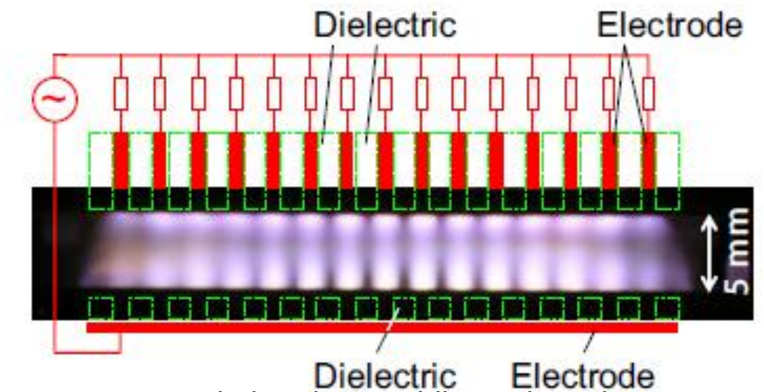
N is negative -
Metamaterial causes light to refract, or bend, differently than in more common positive refractive index materials

N is imaginary-
Gyrotropic material (with imposed magnetic fields), leading to Faraday rotation and Optical Kerr effect, one-way waveguides



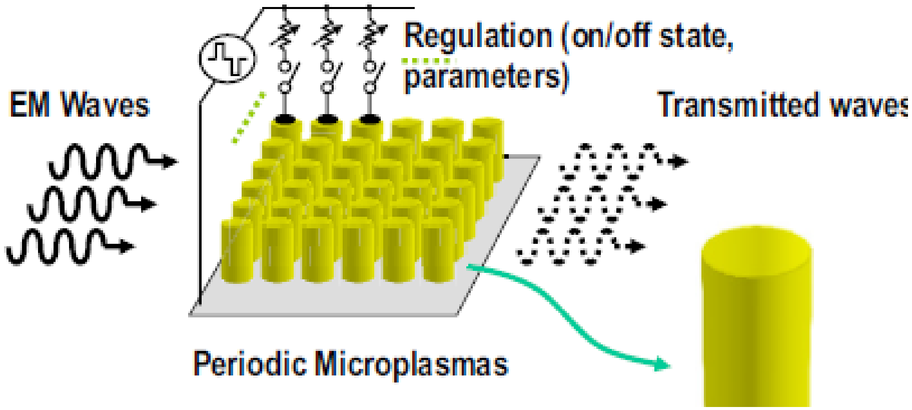
Plasma Photonic Crystals

A plasma photonic crystal (PC) is an array of plasma structures which have the unique ability to control the propagation of EM waves

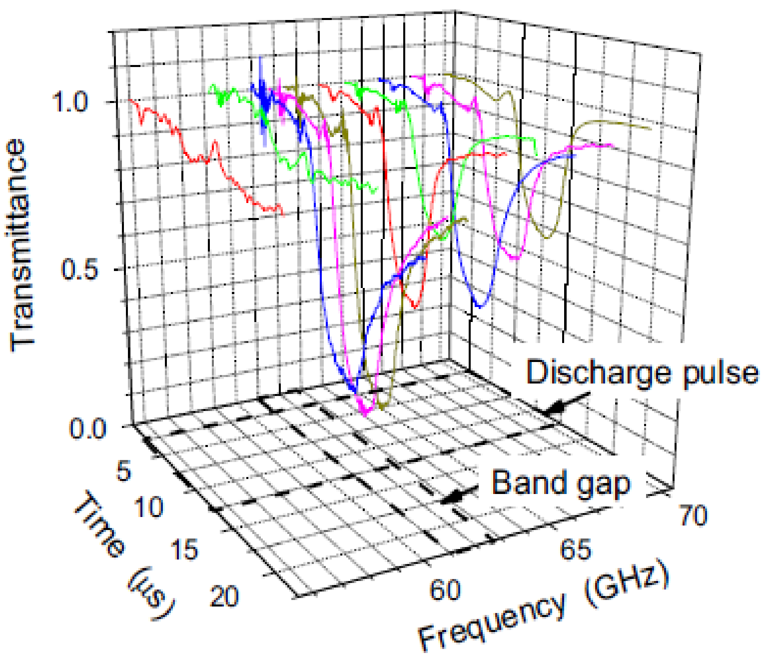


O. Sakai and K. Tachibana (2012)

Novel EM response can be obtained such as wave guiding, and spectral filtering



O. Sakai and K. Tachibana (2012)



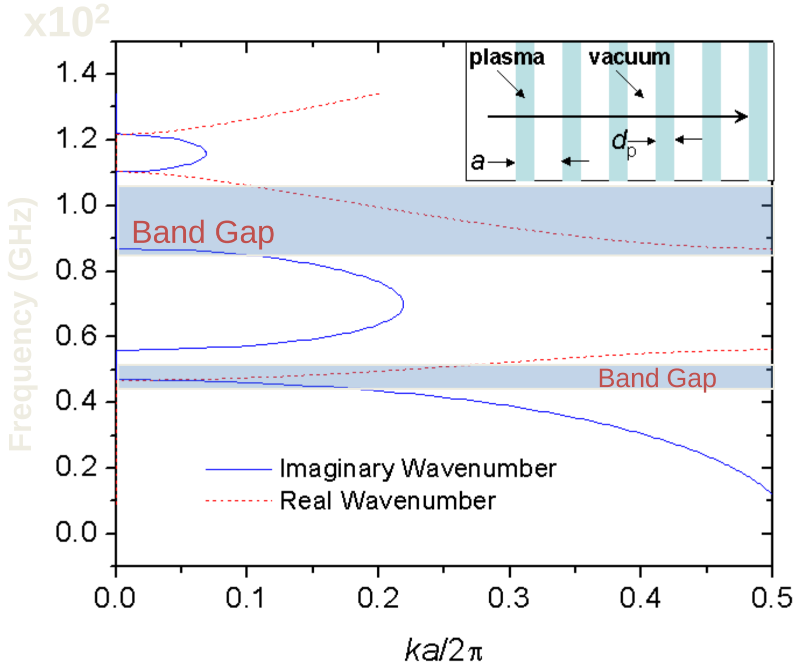
Plasma Photonic Crystals

State-of-the art PPC's are designed for controlling several mm-wavelength radiation (tens of GHz)

- Plasma scales ~ several mm's
- Plasma densities ~10^{13} cm^{-3}

Propagation bands and bandgaps appear near cut-offs and resonances (e.g., plasma frequency)

Future trends and applications seek to control or manipulate higher frequencies – hence higher plasma densities and smaller plasma scales



Normal incidence dispersion in a 1D plasma-air photonic crystal. The inset shows the configuration. The plasma density is $n_e = 10^{14}$ cm^{-3}, $d_p = 1.20$ mm and lattice parameter, $a = 3$ mm.

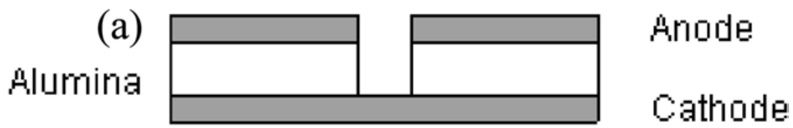
Terahertz EM Wave Manipulation →

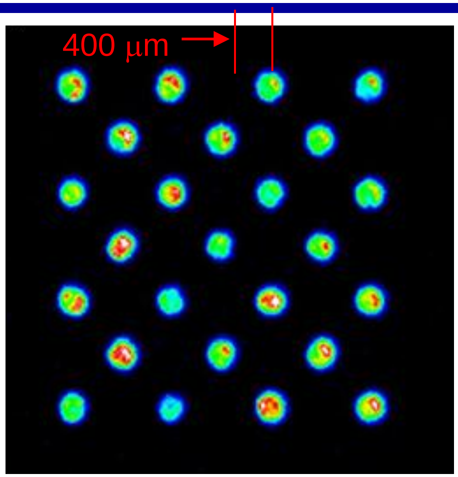
$$n_e \approx 10^{15} - 10^{16} cm^{-3}$$

$$a \approx d_p \approx 0.1\, mm$$

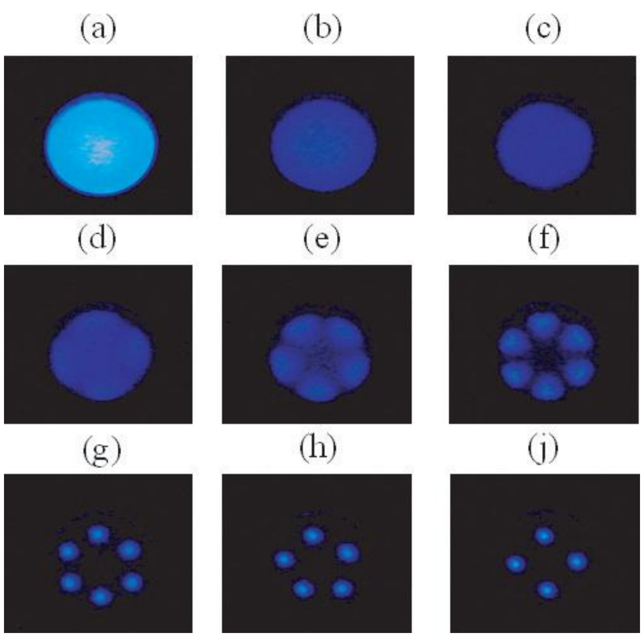
Plasma Photonic Crystals

Externally generating an array of microplasmas (using hollow anode discharge arrays, for example) will become increasingly difficult, particularly for the smaller scales and higher plasma densities needed for controlling THz and FIR waves





Martin et al (2012)



Takano and Schoenbach (2006)

Plasmas (and magnetized plasmas in particular) constitute highly non-linear and naturally unstable systems.

Seemingly uniform plasmas (see top left figure to the left) can be “coaxed” into self-organizing into regular patterns

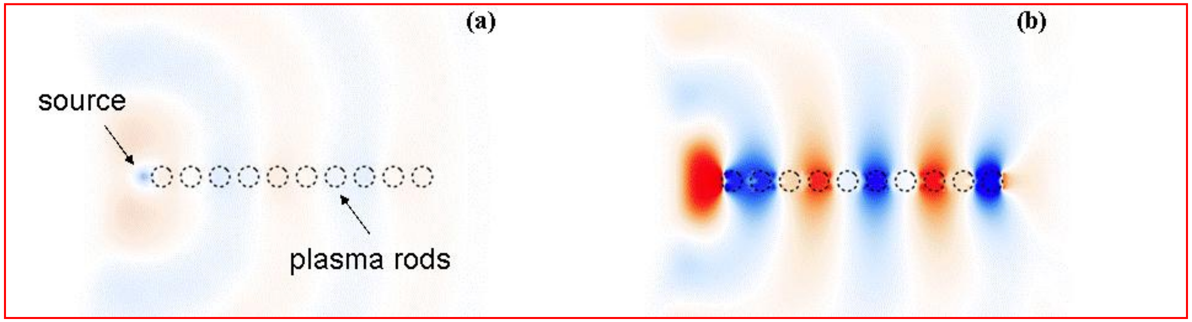
Challenge:

Can researchers generate and stabilize coherent organized microstructures from large otherwise uniform dense plasmas ?

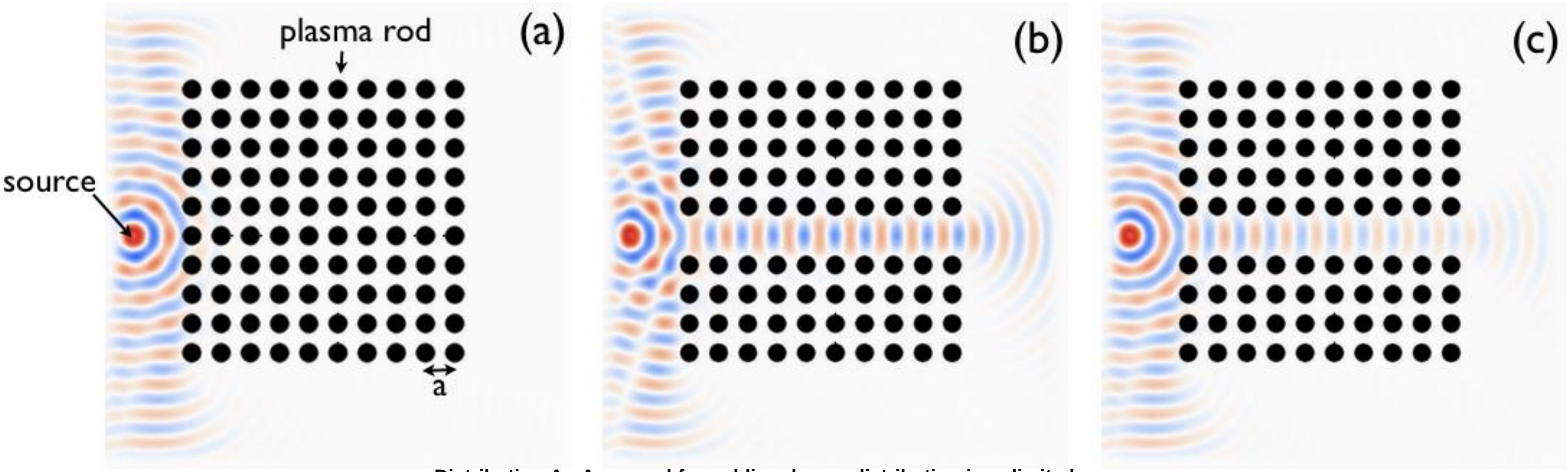
Plasma Photonic Crystals

Through self-organization of coherent periodic microstructures of high plasma density – several high bandwidth reconfigurable THz wave devices can be constructed:

Directional wave radiation through plasmon resonances

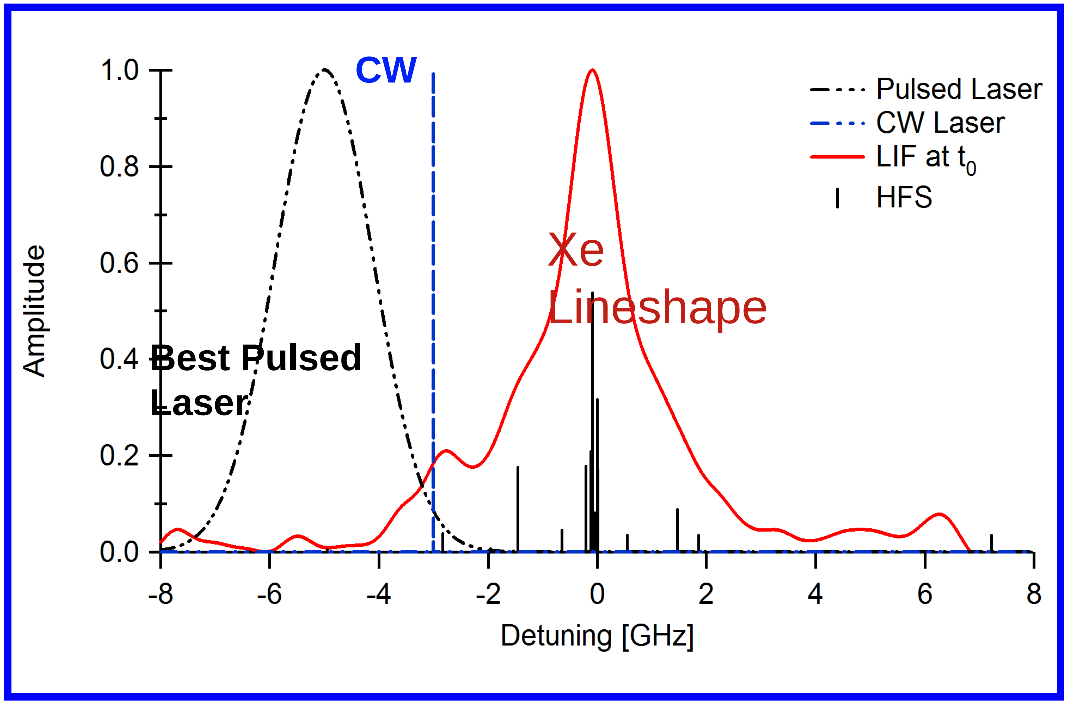


Directional wave guiding through mid-band defect wave localization



continuous wave versus pulsed laser-induced fluorescence

Pulsed lasers are transform-limited, cannot resolve distributions in moderately warm plasmas of relatively heavy species (e.g., argon, krypton, xenon)



Must use ultra-narrow continuous wave laser sources to resolve Doppler-broadened and shifted spectral lines in heavy ions!

- **Mazouffre / CNRS used continuous wave laser source, was unsuccessful synchronize drifting phases in the coherent plasma fluctuations**

Cappelli / Stanford successfully synchronized continuous wave laser induced fluorescence to coherent structures in heavy ion plasmas

- **Laser is chopped at frequency < coherent fluctuation frequency and individual sample-held signals are passed through digital lock-in amplifier to pull out time-synchronized LIF lineshapes as laser is scanned in wavelength**

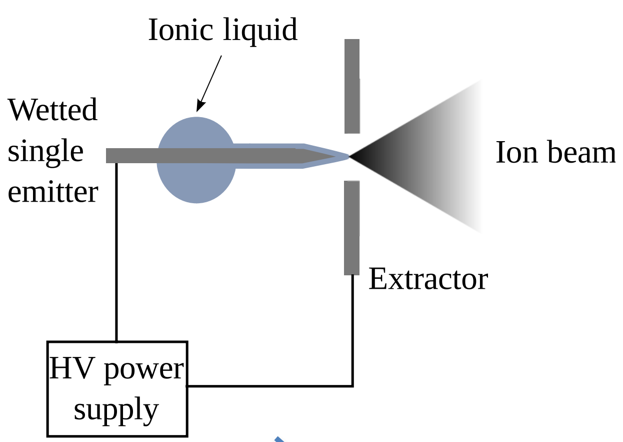
Electrosprays, dual-mode propulsion (Lozano-MIT-YIP)

Analytical Model reveals distal Contact as a solution for Electrochemical Degradation of Emitter Tips

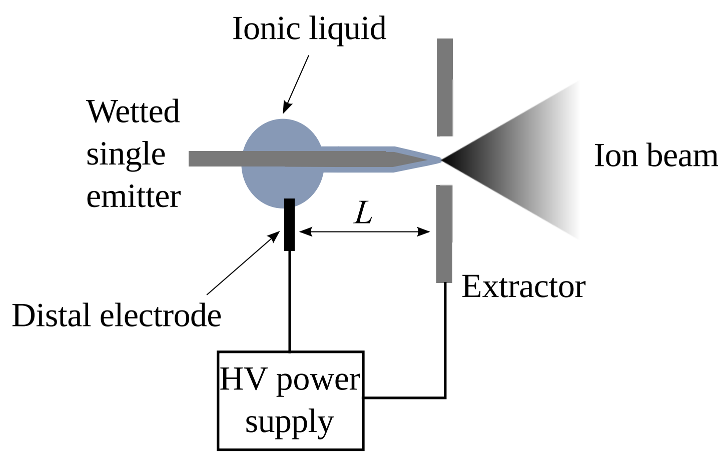
•When a single polarity is extracted in the pure ionic regime, counter ions accumulate in a double layer of charge and could produce corrosion of the emitter if its potential increases beyond the electrochemical window limit

•Voltage alternation incapable of removing electrochemical degradation at the tip apex, where the double layer potential grows faster than its upstream diffusion.

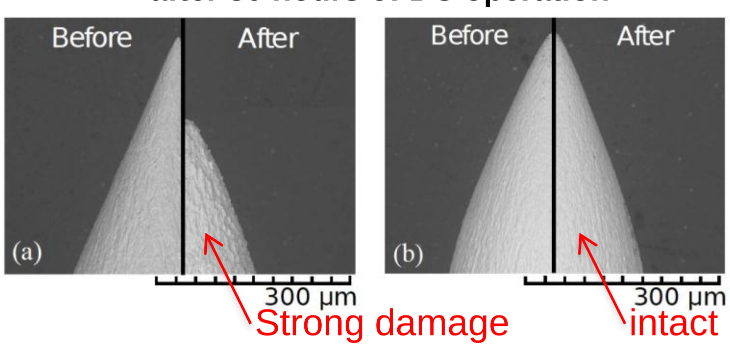
Direct contact



Distal contact



after 80 hours of DC operation



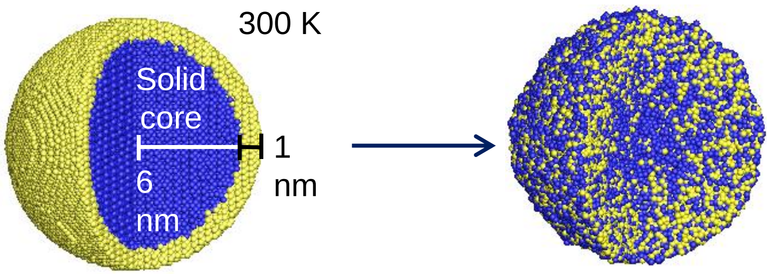
- **In addition to removing electrochemistry from the tip, this configuration allows for emitter manufacturing using dielectric materials.**

2nd Generation: Thermo-Chemical Behavior of Nickel/Aluminum Core-Shell Particles

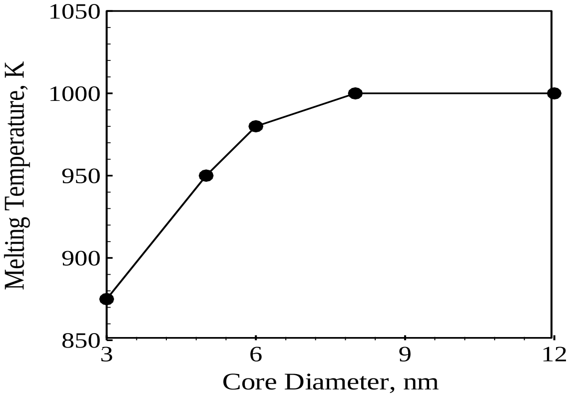
- Ignition of aluminum particles may be assisted by design of coating. Examples are Ti/B and Ni/Al particles.
- ***What is the influence of the core-shell design on ignition?***

Molecular dynamics calculations are performed to investigate particle designs.

Ni coated Al Particle

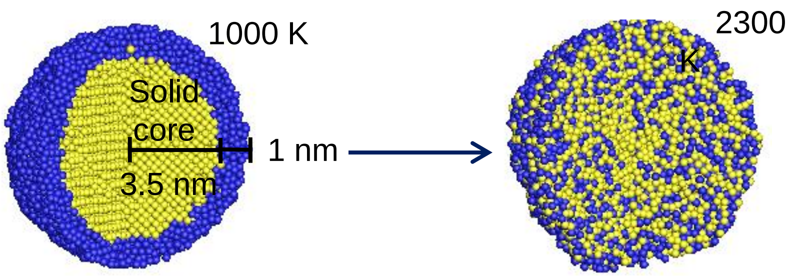


Aluminum Core MP

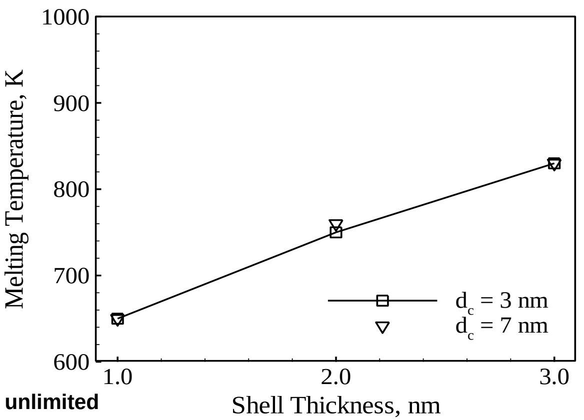


Ni shell exerts cage-like effect and raises MP of core; ignition only after core melting

Al coated Ni Particle



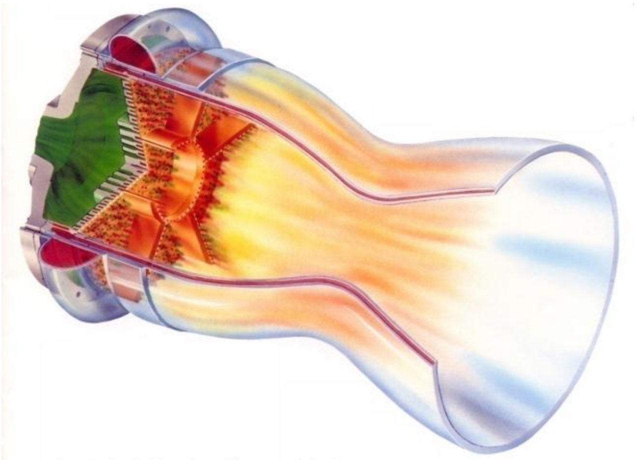
Aluminum Shell MP



Surface pre-melting of Al shell implies lower ignition temperature of Al-coated Ni particles.

A Paradigm Shift in High Pressure Combustion Dynamics Prediction and Control: Analytics and Dynamic Data Driven Modeling and Validation

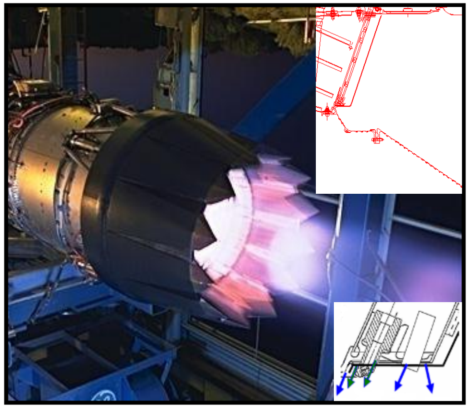
•Great Challenge Example: In a High Pressure/Temperature, Two-Phase, Turbulent, Acoustically – Excited Environment, investigate Amplification

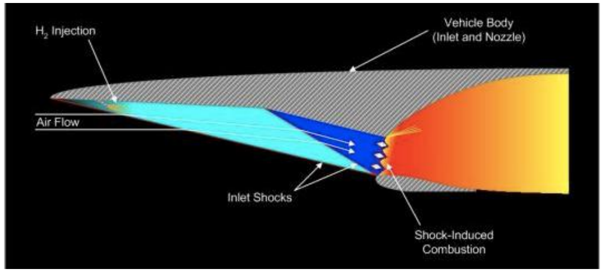


•High amplitude and high frequency acoustic instabilities can lead to local burnout of the combustion chamber walls and injector plates

Processes:

- Jet Break-up
- Atomization
- Vaporization
- Supercritical States
- Turbulence
- Compressibility
- Combustion
- Acoustic Field
- Boundary Interactions





SCIENTIFIC CHALLENGE:

- Modeling and Simulations of highly complex, nonlinear, multi-physics, multi-scale stochastic phenomena
- Current state of the art methodologies are not adequate to address the challenges in this domain ➔ new mathematics and computational methods are needed

State of the Art Modeling

History of modeling efforts (ALL DETERMINISTIC)

↓

Galerkin's Method / perturbation expansions of Navier Stokes

↕

Unit problems (injector flow, atomization, drop vaporization, spray combustion etc.)

↓

Large Eddy Simulations with subgrid Models

Why these modeling efforts are not sufficient?

- ***Stochastic modeling*** **is essential to capture the complex physical phenomena -> very challenging problem since current stochastic models only look at simplified problems**
- **The problem cannot be addressed using only simulations, or experiments**
- **Use of experimental data is essential to validate models and codes, but it should not be done *aposteriori* as it is done today**
- **Consistency of models with data is a major issue**
- **Hard to get data, either too much data, or too little ---→ need a new mathematical framework to bring together data, experiments and simulations in a dynamic, feedback manner**

Any model, by definition, involves stochastic behaviors

(PERTURBATION EXPANSION EXAMPLE)
classical wave equation for combustion instability:

model uncertainties (the model has many approximations and assumptions) including intrinsic stochastic behaviors in the real physics

$$L(P') = \partial P'^2 / \partial t^2 - \overline{C}^2 \partial P'^2 / \partial x^2 = f(\overline{M}, Q, NL)$$

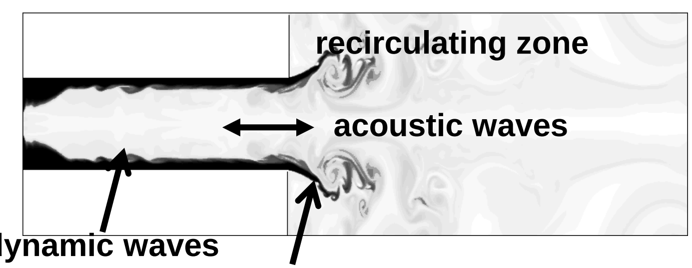
Combustion noise

Parameter uncertainty
random fluctuation of speed of sound due to temperature uniformity and fluctuation

Source term uncertainty
turbulence-induced random combustion response, acoustic damping, shear-layer instability

Parametric Variability- Uncertainties at the Boundary Conditions:

PROPER ORTHOGONAL DECOMPOSITION revealed that Kelvin-Helmholtz wave motion and the acoustic waves must be accounted as the boundary conditions for the chamber dynamics simulation



Experimental uncertainty (dynamical data sampling):

When the inlet flow condition fluctuates stochastically, the flame switches from one recirculation region to other (bifurcation)

Compressible LES Equations + Reduced Basis Model

Stochastic modeling requires many realizations. LES alone is too costly. So, a combined LES-Reduced Basis Model approach fits best.

Mass

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i}{\partial x_i} = 0$$

Momentum

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_i\tilde{u}_j + \bar{p}\delta_{ij} - \bar{\tau}_{ij} + \tau_{ij}^{sgs}\right) = 0$$

Energy

$$\frac{\partial \bar{\rho}\tilde{E}}{\partial t} + \frac{\partial}{\partial x_i}\left[\tilde{u}_i(\bar{\rho}\tilde{E} + \bar{p}) - \bar{\tau}_{ij}\tilde{u}_j + \bar{q}_i + H_i^{sgs} + \sigma_i^{sgs}\right] = 0$$

Species

$$\frac{\partial \bar{\rho}\tilde{Y}_k}{\partial t} + \frac{\partial}{\partial x_i}\left(\bar{\rho}\tilde{u}_i\tilde{Y}_k - \bar{\rho}\tilde{V}_{i,k}\tilde{Y}_k + Y_{i,k}^{sgs} + \theta_{i,k}^{sgs}\right) = \bar{\dot{w}}_k \qquad where: k = 1, N_s$$

Subgrid Stress Flux $\tau_{ij}^{sgs} = \bar{\rho}\left(\widetilde{u_i u_j} - \tilde{u}_i\tilde{u}_j\right)$

Subgrid Enthalpy Flux $H_i^{sgs} = \bar{\rho}\left(\widetilde{Eu_i} - \tilde{E}\tilde{u}_i\right) + \left(\overline{u_i P} - \tilde{u}_i\bar{P}\right)$

Subgrid Viscous Work $\sigma_i^{sgs} = \left(\overline{u_j\tau_{ij}} - \tilde{u}_j\overline{\tau_{ij}}\right)$

Subgrid Species Flux $Y_{i,k}^{sgs} = \bar{\rho}\left(\widetilde{u_i Y_k} - \tilde{u}_i\widetilde{Y_k}\right)$

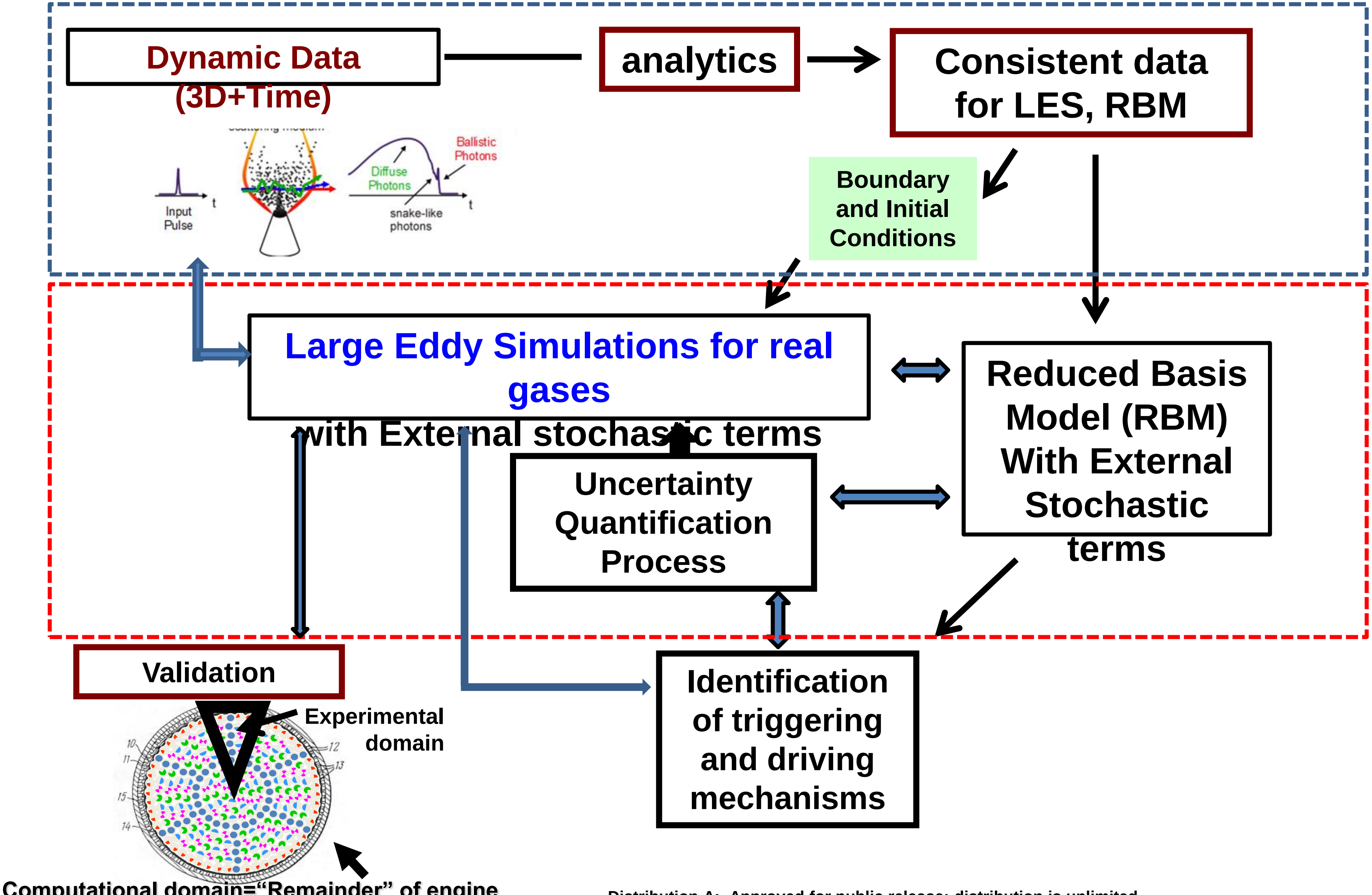
Subgrid Mass Diffusion Flux $\theta_{i,k}^{sgs} = \bar{\rho}\left(\widetilde{V_{i,k}Y_k} - \widetilde{V_{i,k}}\widetilde{Y_k}\right)$

Arrhenius term $k = Ae^{-E_a/RT}$

Stochastic at Every Scale

- **Molecular (atomistic) to micro scales (Angstrom-microns)**
  - Uncertainty in kinetics, transport properties
  - Kinetics interactions with fine-scale turbulence
- **Meso-scale (100 micron-mm)**
  - Small-scale turbulence-kinetics coupling
  - Uncertainty in coupling to large-scales
- **Macro-scale (cm-m)**
  - System level responses and nonlinear feedback effects
  - Uncertainty in boundary conditions
- Insufficient data will lead to uncertainty due to incomplete system characterization – Closures needs to include Uncertainty Quantification (UQ) in the model
- **Possible UQ Methods:**
  - **Polynomial Chaos, Stochastic Collocation, Bayesian Approaches for Inverse Modeling and Data Assimilation, Sparse Sampling Methods, etc. ➔ The underlying problems are multiscale and high-dimensional. Dealing with the curse of dimensionality is a major challenge.**

Dynamic Data Driven Strategic Simulation & Modeling

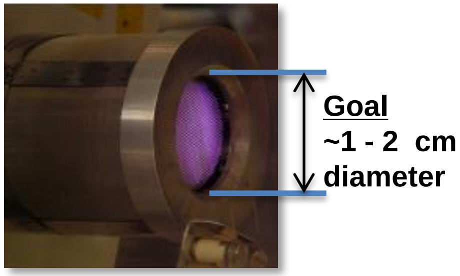


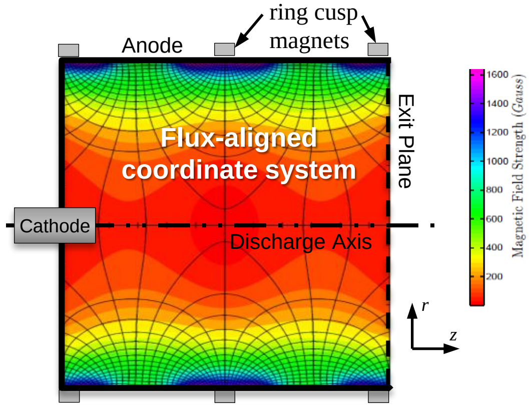
Wirz / UCLA- YIP- Center of Excellence (Univ. of Michigan)

Self-consistent analytical theory used to optimize micro plasma source

- **Critical research for in-space propulsion, plasma-enhanced combustion, plasma aerodynamics, small scale sensors, directed energy devices, plasma processing …**

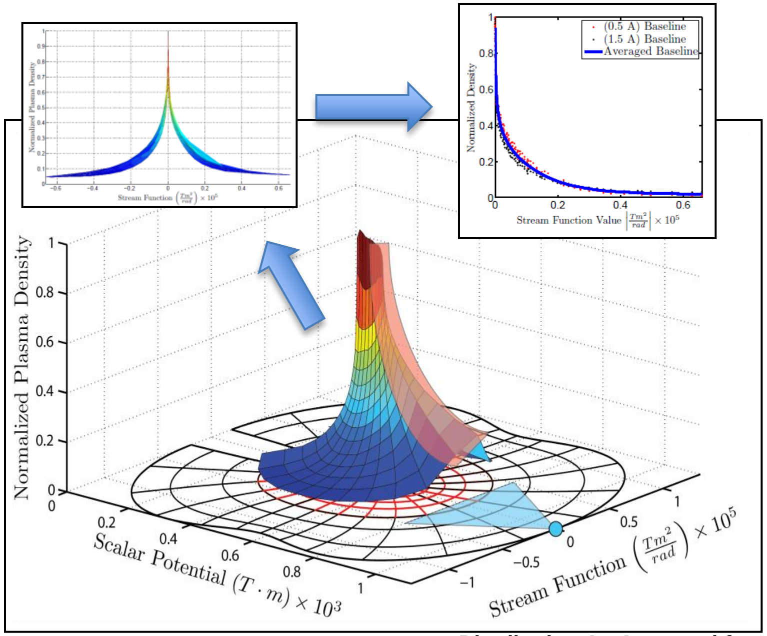
Micro-scale plasma source





Goal: Develop efficient and stable cusp-confined micro discharge

- **New "stream function" magnetic field analysis developed to predict plasma behavior throughout discharge**



Optimization using analytical theory yields 2X increase in plasma production over baseline

- **Model trends experimentally validated**