Sibley School of Mechanical and Aerospace Engineering

ASTRA lab
Advanced Space Transit and Architectures

Multiscale Modeling of Molecular Ion Beams and Beam-Surface Interactions

Michigan Institute for Plasma Science and Engineering

September 27, 2023

Prof. Elaine Petro
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Director, **Cornell ASTRAlab**

Introduction

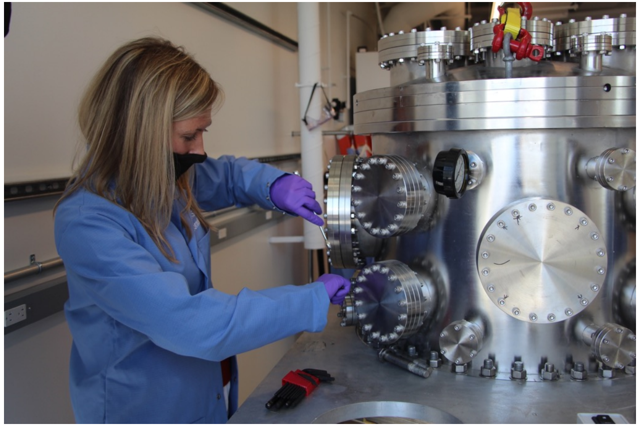
Cornell MAE Assistant Professor (July 2020 – present)
ASTRAlab Director

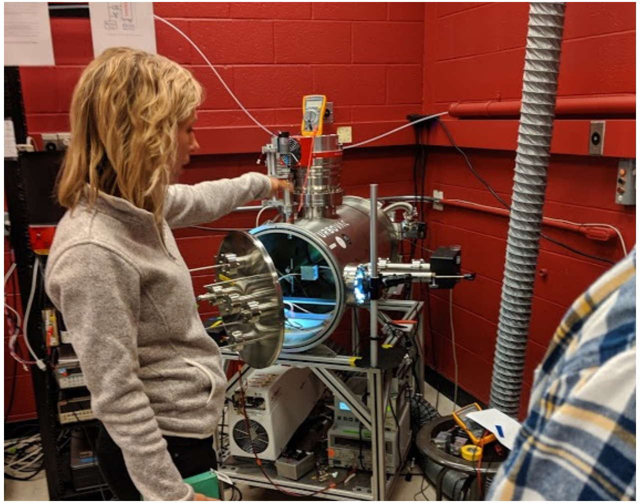
MIT Post-Doctoral Researcher (2019-2020)
Dept. of Aeronautics & Astronautics
Space Propulsion Lab, MIT SmallSat Center

Univ. of Maryland (B.S. 2010, M.S. 2015, Ph.D. 2019)
Dept. of Aerospace Engineering
Space Power and Propulsion Lab

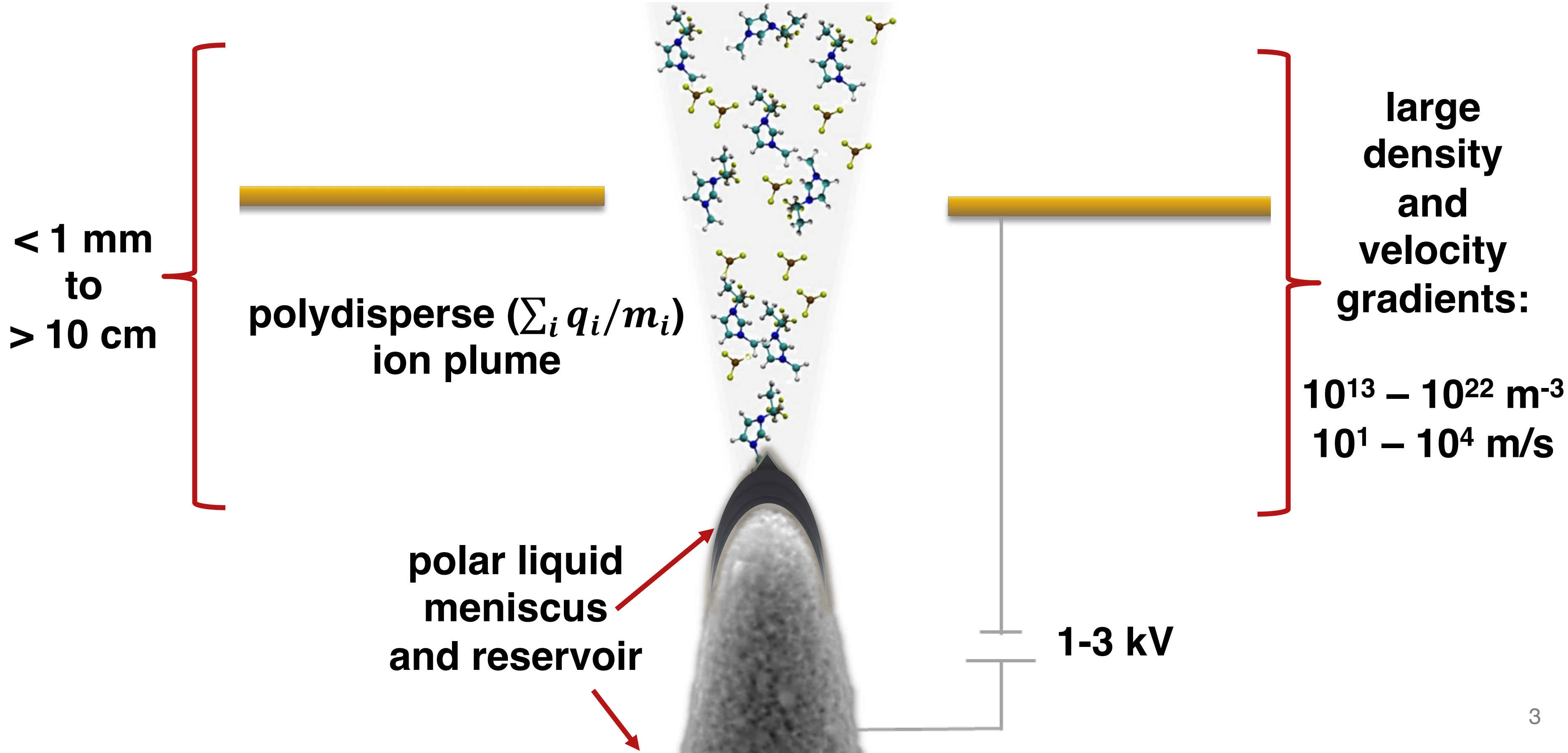
Previous Employment: NASA Goddard, Lockheed Martin

Research Interests:
plasma and ion beam science, plasma simulation, plasma instrumentation, molecular plasmas, spacecraft electric propulsion, small satellite propulsion, sustainable satellite architectures



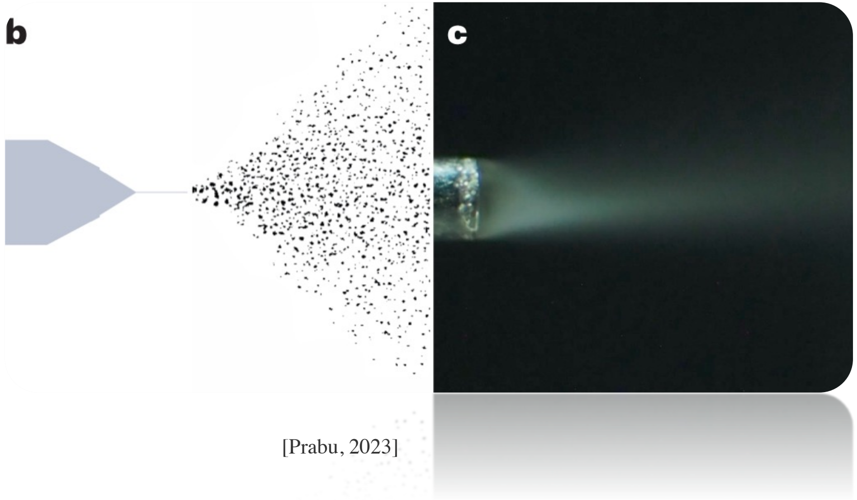


electrosprays: molecular ion beams



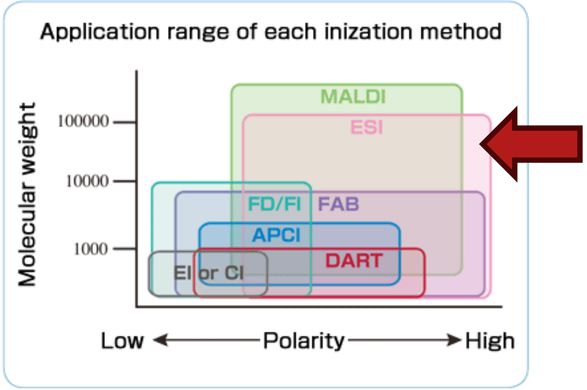
applications of electrospray ion beams

electrospray ionization mass spectrometry (since ~1980s)



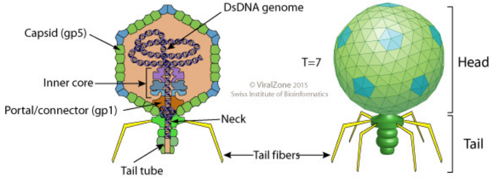
[Prabu, 2023]

https://www.jeol.com/products/scientific/lcms/DART.php



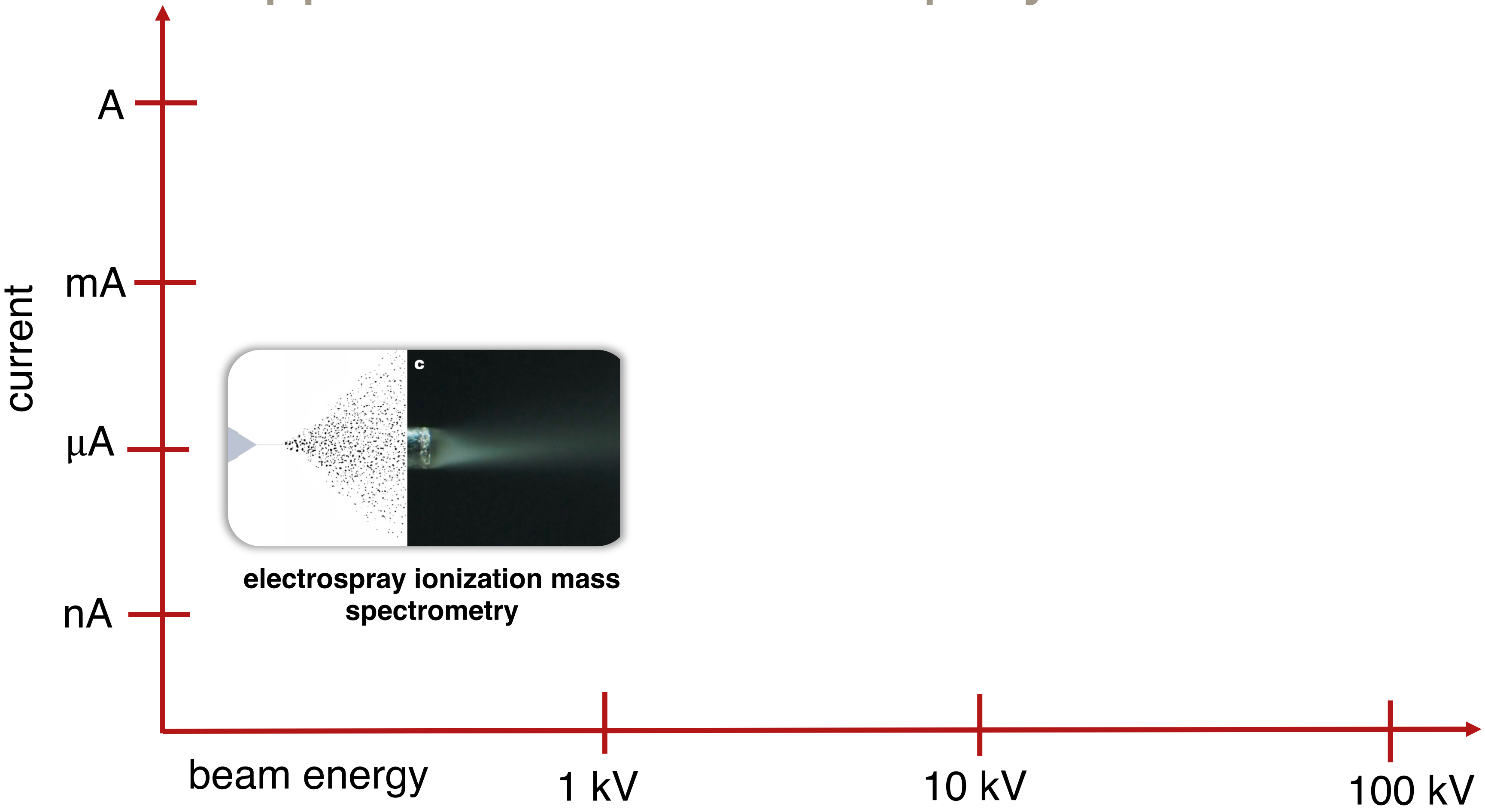
intact virus (10^6 amu)

Enterobacteria phage P22

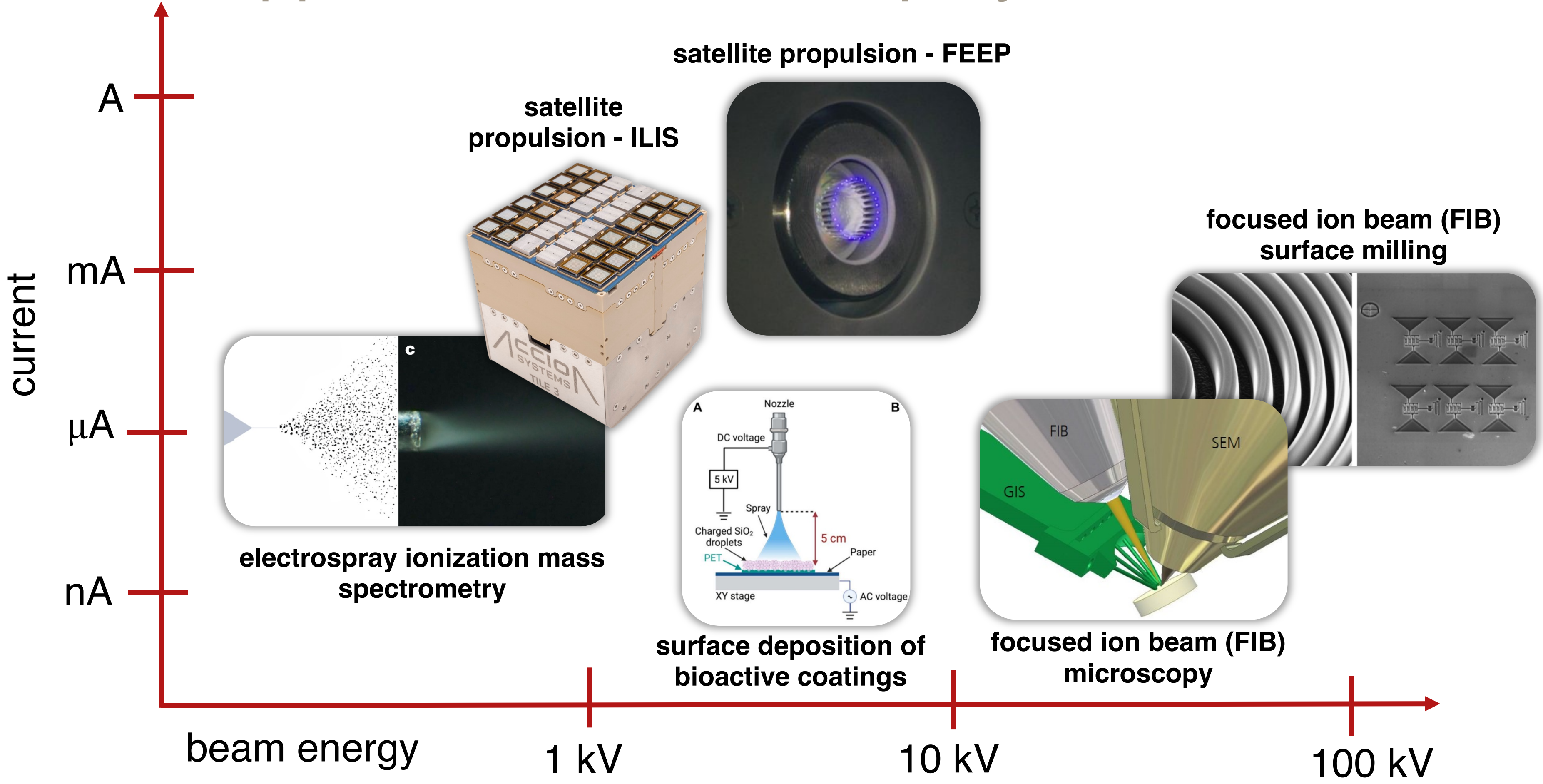


[Keifer, 2016]

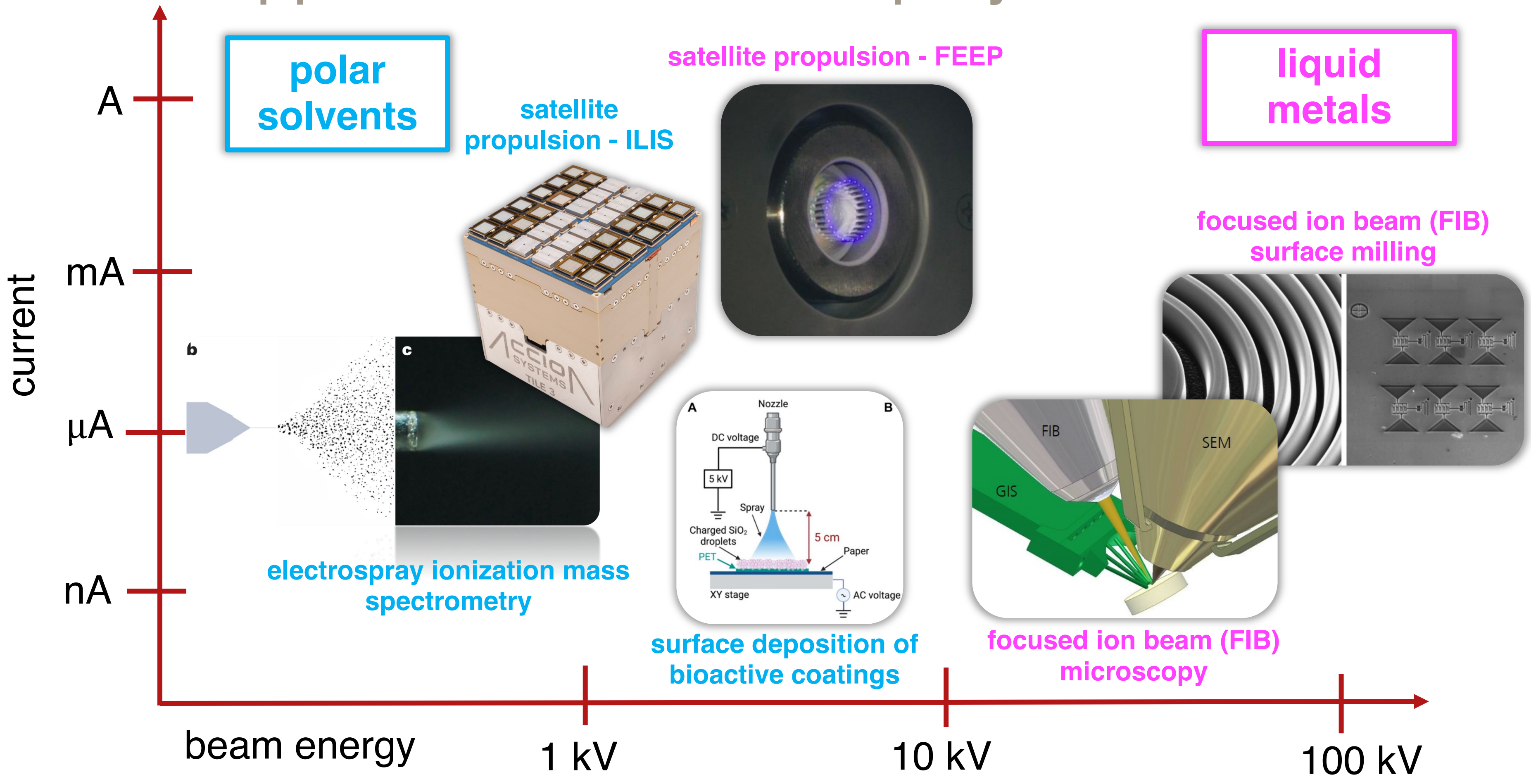
applications of electrospray ion beams



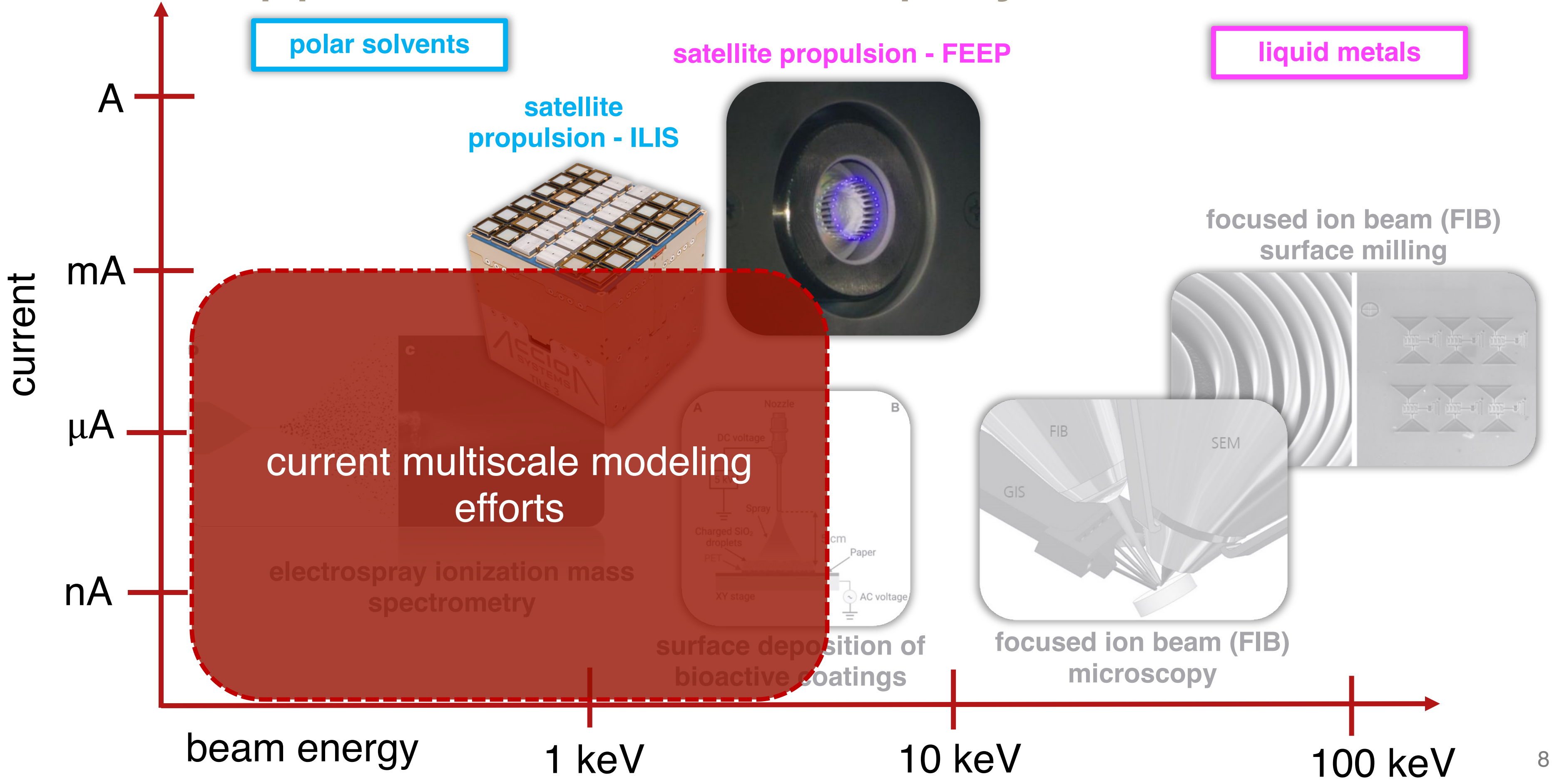
applications of electrospray ion beams



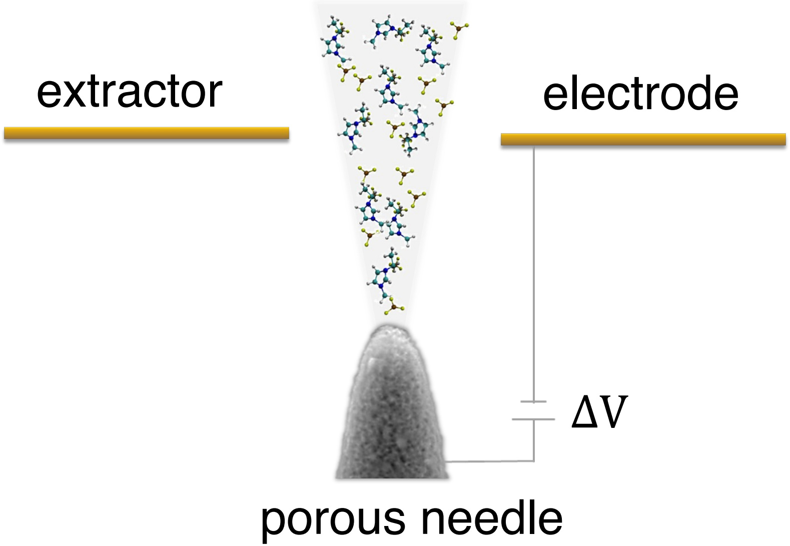
applications of electrospray ion beams



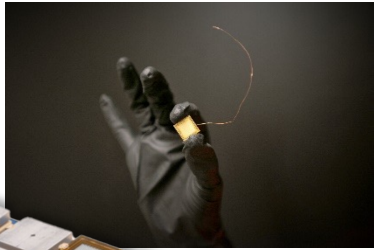
applications of electrospray ion beams



electrospray thrusters

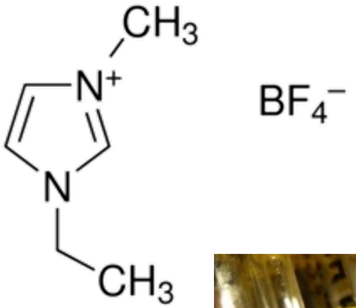


> 50,000
ion plumes
in parallel

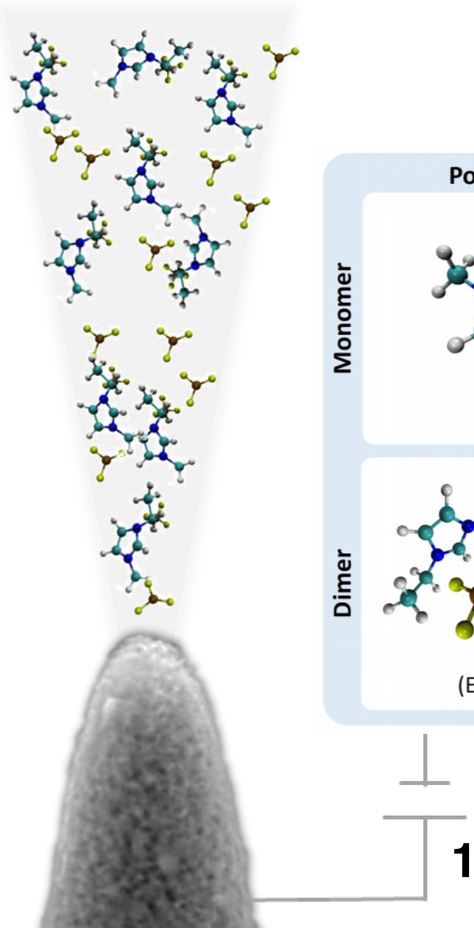


[1] http://www.satnews.com/story.php?number=1771211614
[2] https://www.21stcentech.com/gizmos-gadgets-scalable-ion-engine-transform-space-travel/

ionic liquid ion sources (ILIS)



organic molecular salts



1-3 kV

ion species

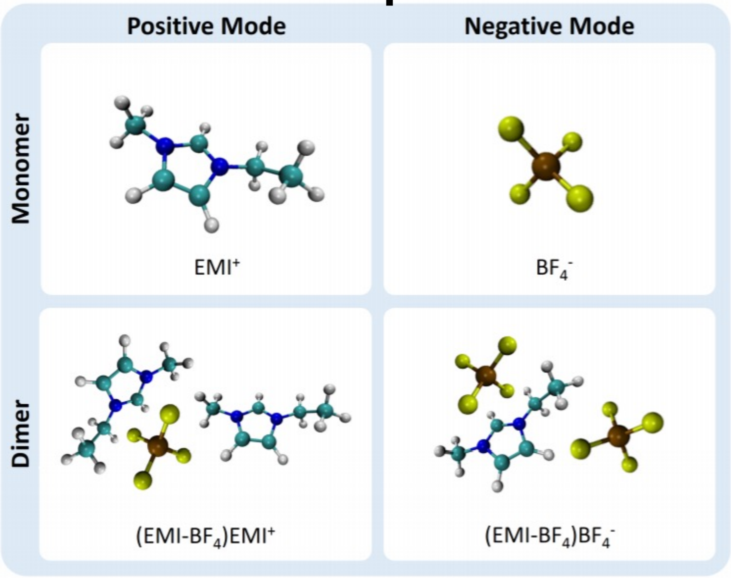
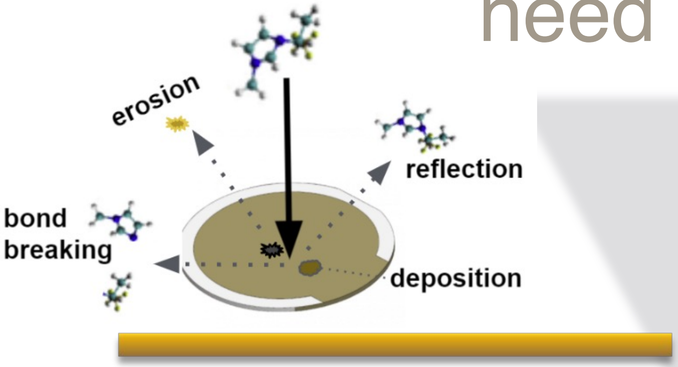
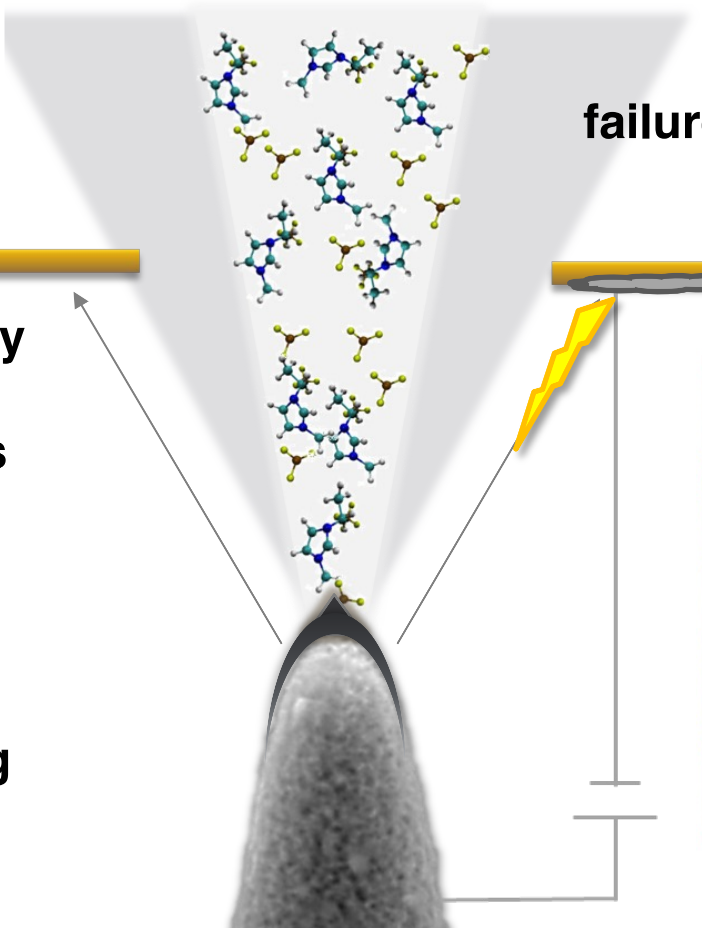


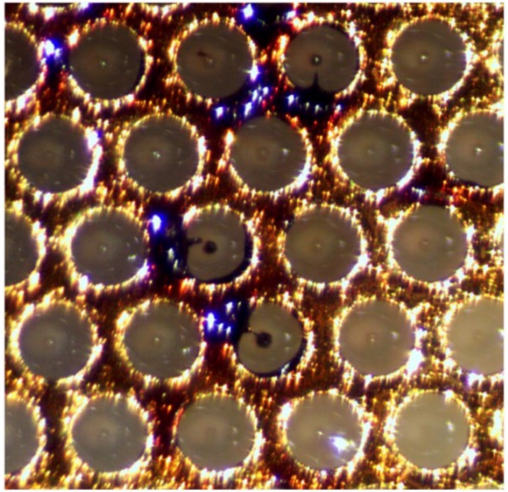
Photo credit: Catherine Miller
https://arc.aiaa.org/doi/pdf/10.2514/6.2016-4551

need for better models





failure due to **propellant arcing**
[Krejci, 2017]



account for **secondary species** from:
- **chamber impacts** [Uchizono, 2021]
- **plume chemistry** [Miller, 2019] [Bendimerad, 2022]

account for **missing mass flux** [Natisin, 2021]

limitations of existing models

50 nm | **100 micron** | **1 mm** | **1 cm** | **1 m**

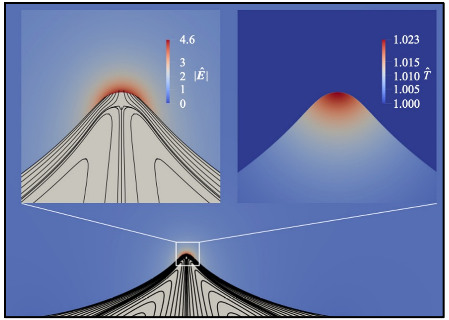
Emission Region

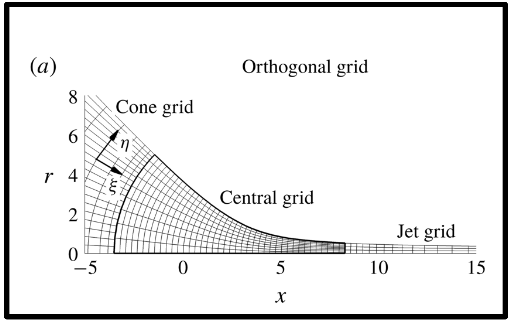
Interacting Beamlets

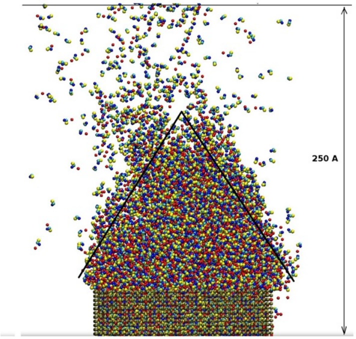
Spacecraft Plume Interactions

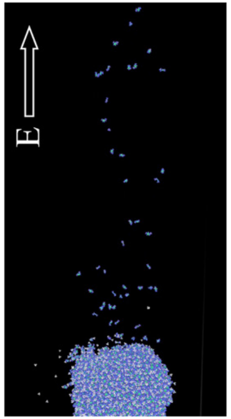
Single Emitter Plume

Multi-Emitter Arrays









Electrohydrodynamic Models [1,2]

I vs. V

Laplacian solution

Molecular Dynamics [3,4]

Particle morphology (q_i/m_i)

Cannot match BCs

[1] Gallud et al. (J. Fluid Mech., 2022), [2] Gamero-Castaño (J. Fluid Mech., 2018),
[3] Mehta & Levin, (Aerospace, 2018) [4] Asher et. al. (J. Applied Phys., 2022)

limitations of existing models

50 nm — 100 micron — 1 mm — 1 cm — 1 m

Emission Region

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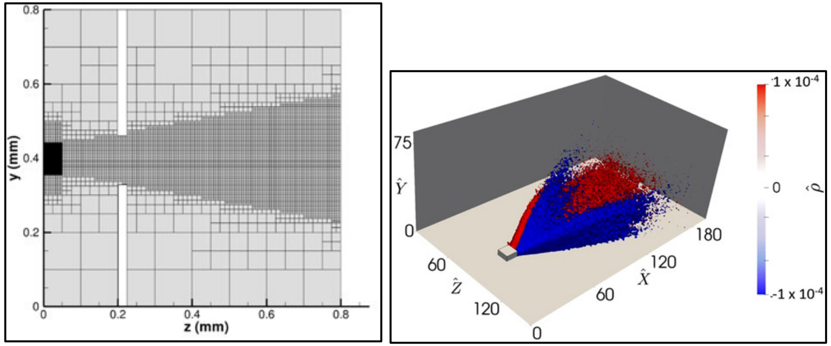
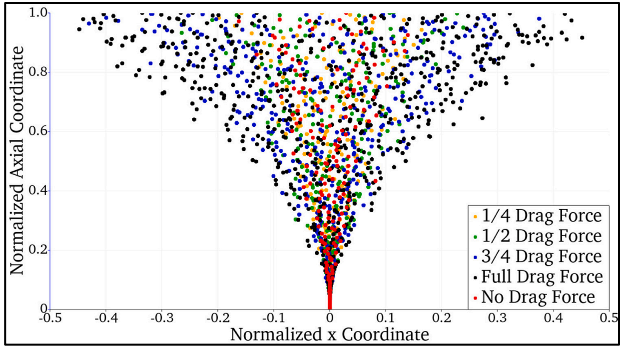


Particle in Cell [1,2]

1 micron resolution

unrealistic injection conditions



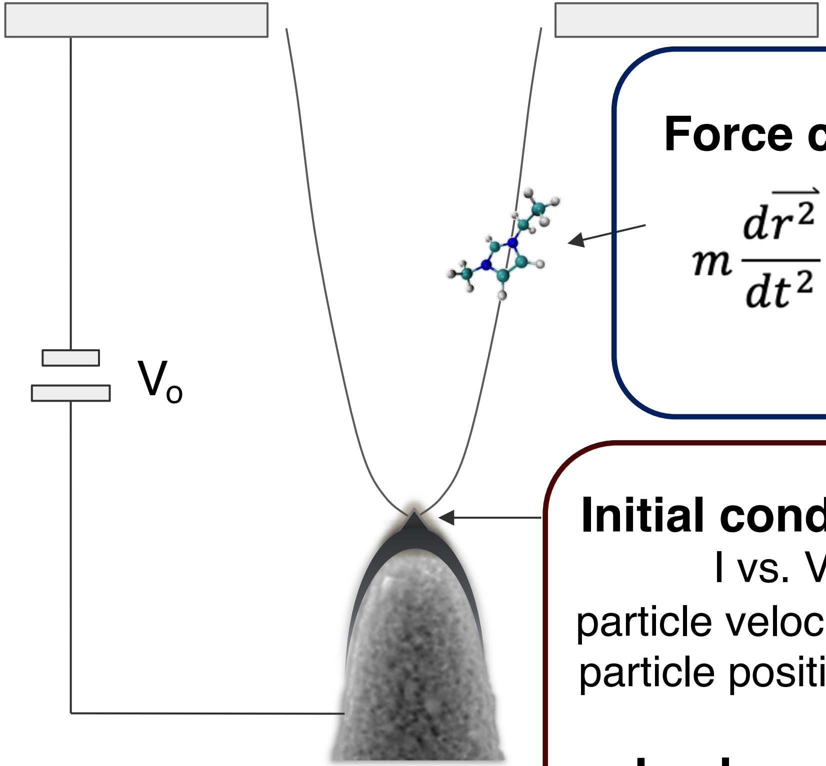
N-Body / Lagrangian Methods [3]

missing Laplacian E-field

unrealistic injection conditions

[1] Nuwal et. al (J. App. Phys, 2021) , [2] Asher et. Al. (J. Applied Phys., 2022), [3] Breddan (J. Aero. Sci, 2022)

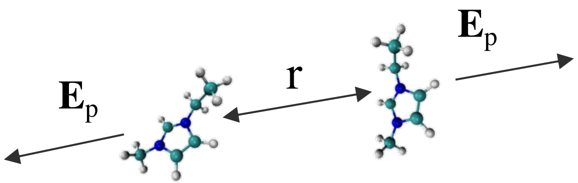
new approach: EHD and n-body



Force computation:

$$m\frac{d\overrightarrow{r^2}}{dt^2} = q(E_L + E_P)$$

Space-charge field: E_p



n-body

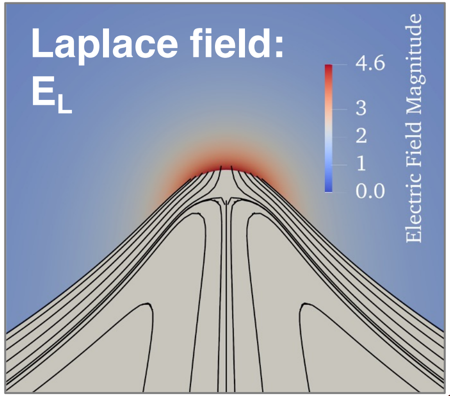
Initial conditions:

I vs. V_o

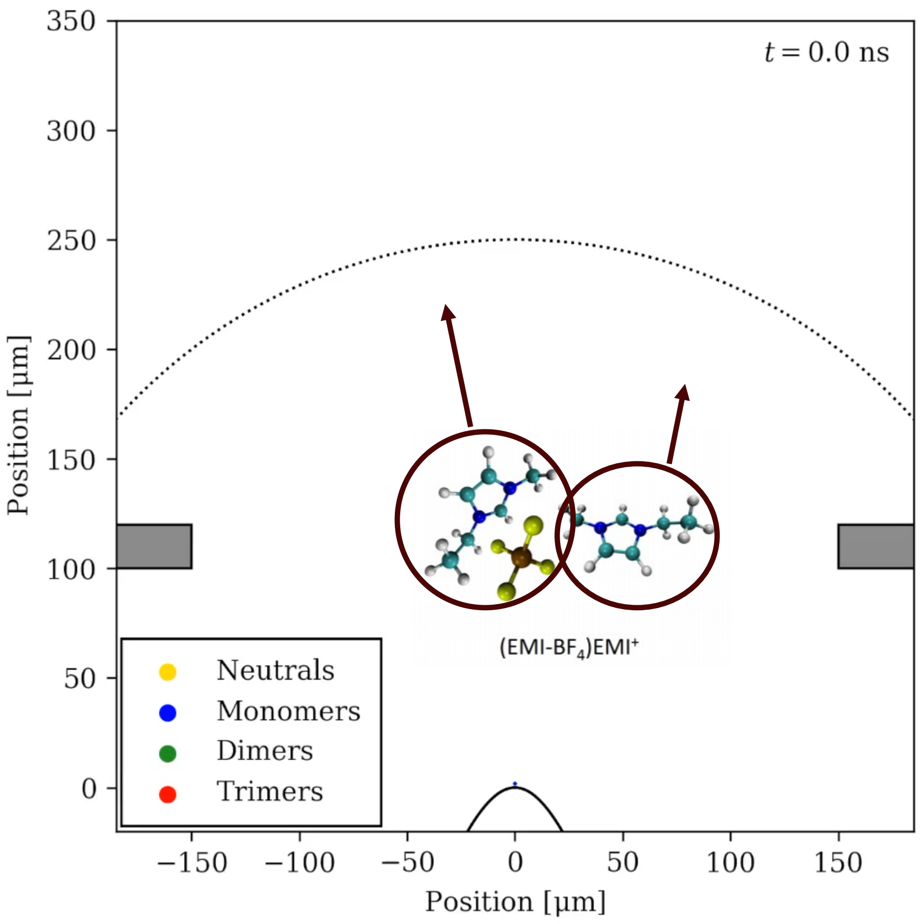
particle velocities ($\vec{v}_o$)

particle positions ($\vec{x}_o$)

Laplace field



EHD

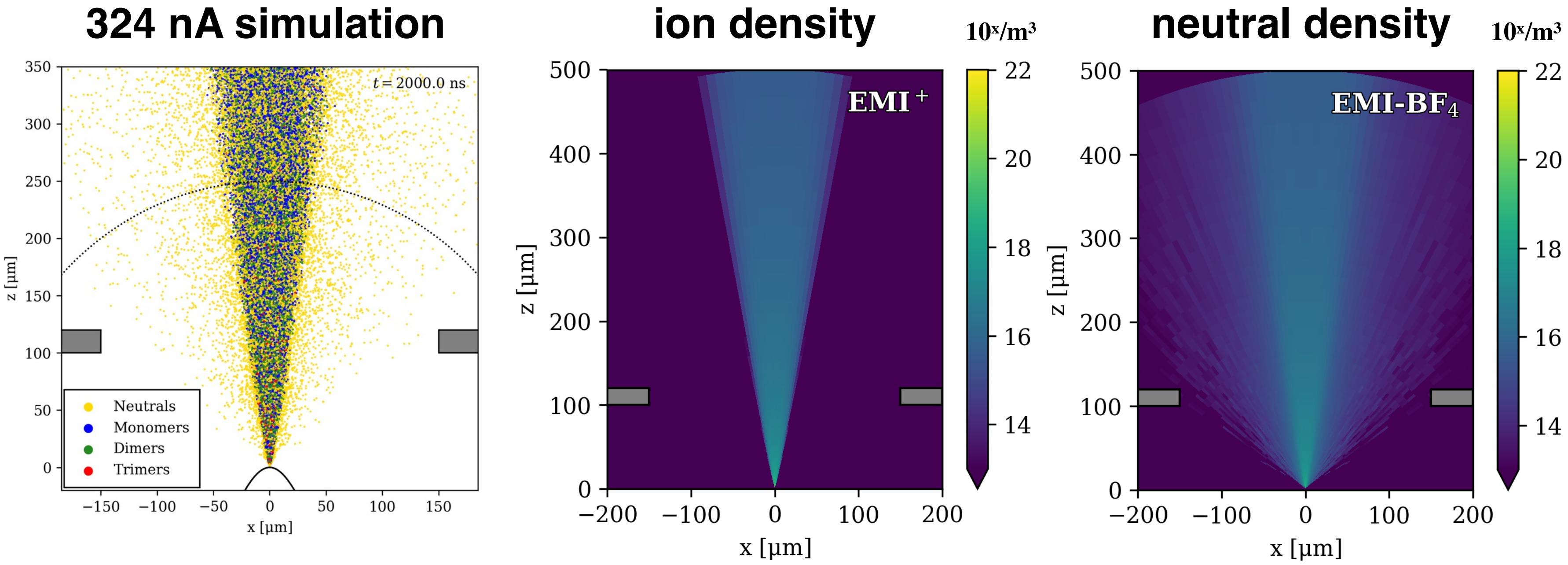


For each particle:

1. Interpolate Laplace field (created by meniscus) with fast tree point search algorithm
2. Compute Coulomb field using Barnes-Hut approximation (**N log N**)
$$\sum_i \frac{q_i \mathbf{r}_i}{|r_i|^3} \approx \frac{\left(\sum_i q_i\right) \mathbf{r}_{CC}}{|r_{CC}|^3}$$
3. Evaluate probability of fragmentation [1]:
$$p = 1 - e^{-\frac{\Delta t}{\tau_m(E)}}$$
4. Integrate trajectory using leapfrog scheme

[1] Schroeder et. al. (J. App. Phys, 2023)

n-body ion beam simulation results



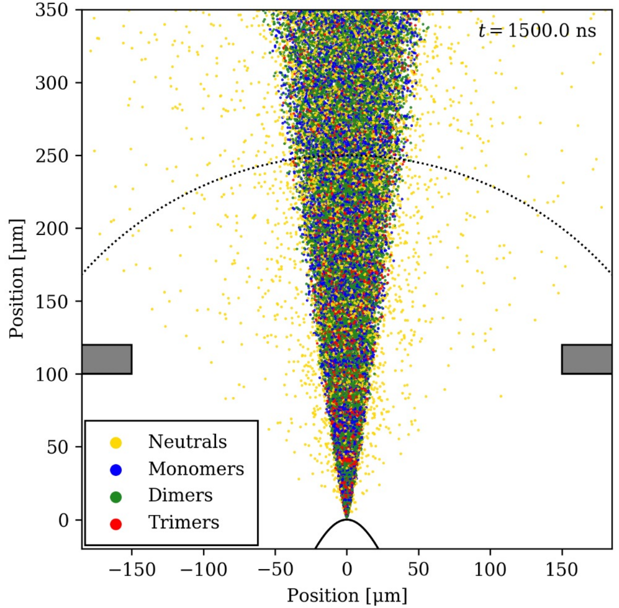
- ~10 orders of magnitude range in particle density within region of interest
- 10^4 - 10^5 particles
- 24 hrs to run on 100 core CPU workstation

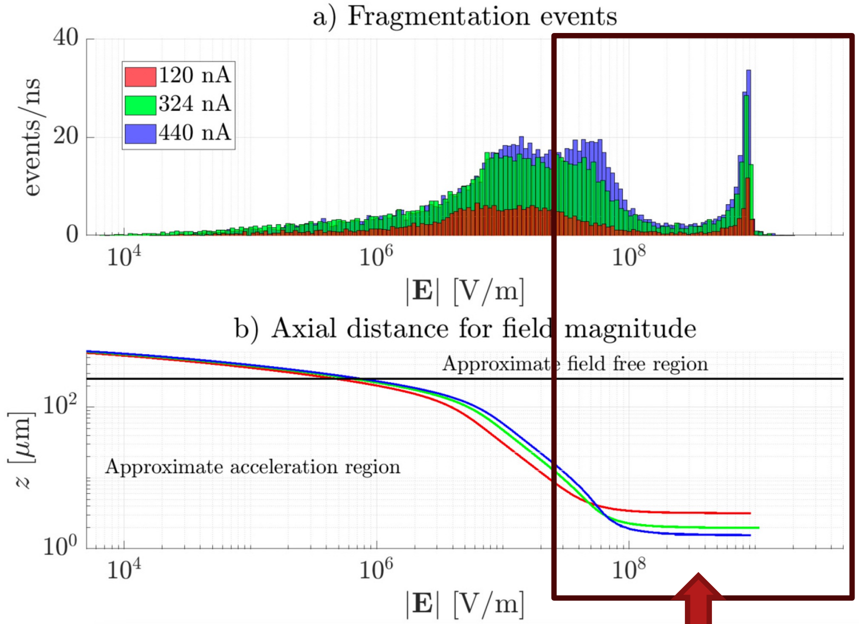
analogous to **low energy neutral particle cloud** on the periphery of **ion engine plumes [2]**

[1] Petro et. al. (J. Appl. Phys. 2022), [2] Gallud et. al. (IEEE Aerospace 2022), Hampl et. al. (J. Elec. Prop. 2022)

n-body ion beam simulation results

324 nA simulation





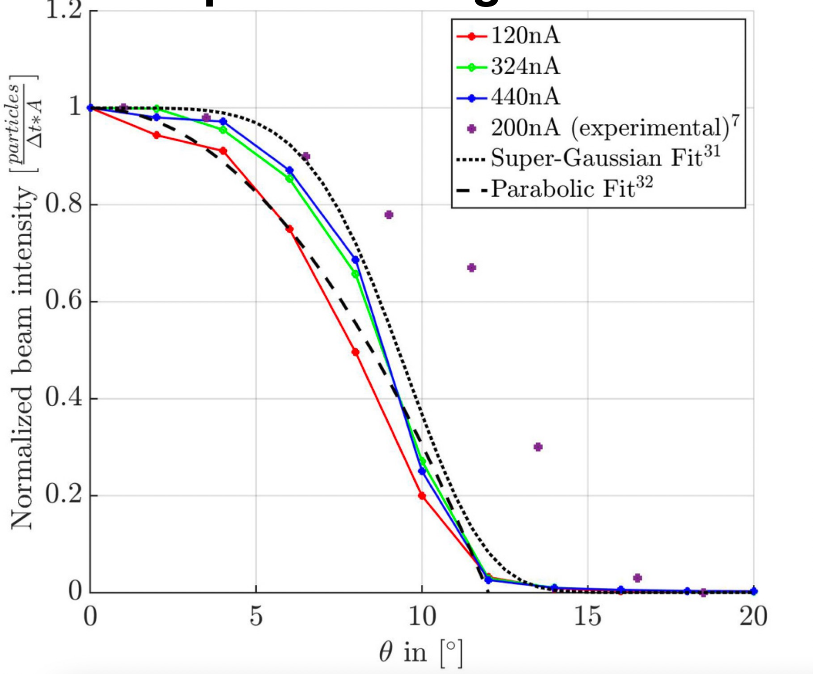
- ~10 orders of magnitude range in particle density within region of interest
- 10^4 - 10^5 particles
- 4 hrs to run on 10 core CPU workstation

Resolving first 5 microns is critical to beam evolution

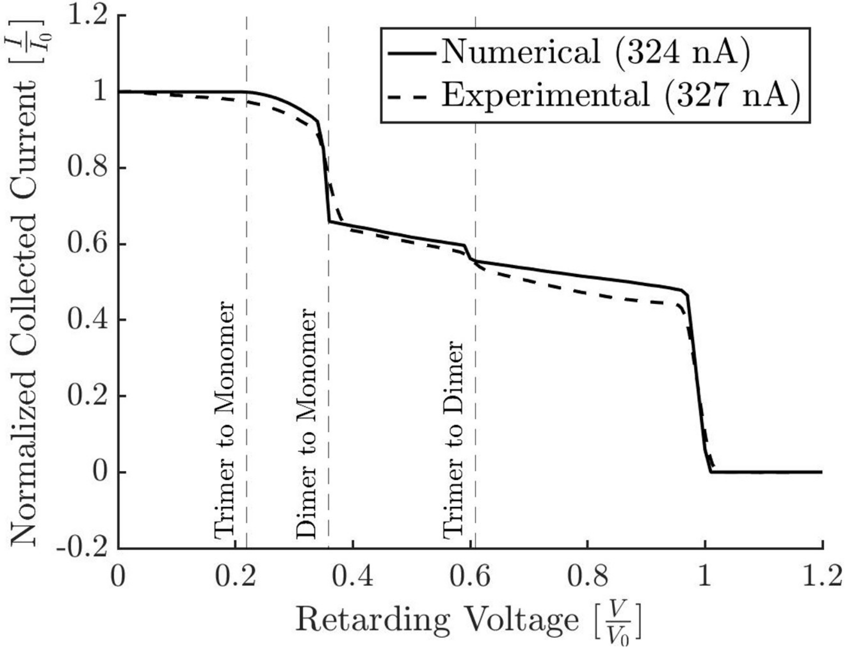
[1] Petro et. al. (J. Appl. Phys. 2022), [2] Gallud et. al. (IEEE Aerospace 2022), [3] Hampl et. al. (J. Elec. Prop. 2022)

comparison to experiments

plume divergence

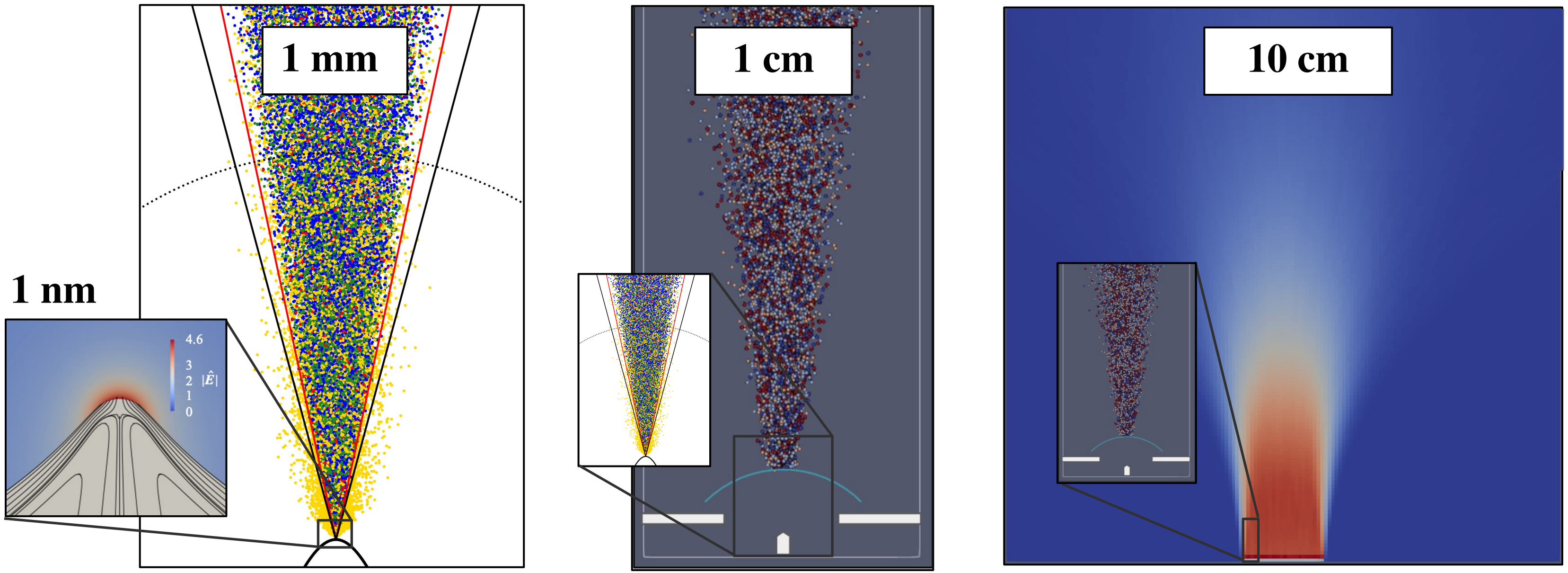


ion energy



Petro et al. (J. Appl. Phys., 2022).
Image credits: Sebastian Hampl (left), Maddie Schroeder (right)

expansion to multi-emitter arrays



N-Body Single Emitter → **Electrospray Ion Source Model** → **500 Emitter Plume Simulation**

[Smith et. al., AIAA SciTech / J. Prop. & Power 2023]

expanding to cm-scale with PIC

50 nm | 100 micron | 1 mm | 1 cm | 1 m

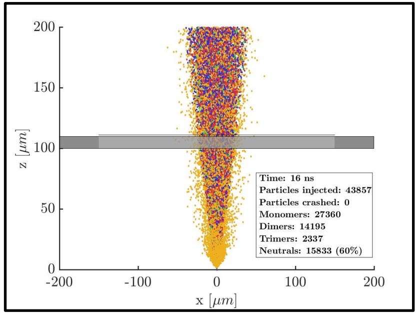
Emission Region

Interacting Beamlets

Spacecraft Plume Interactions

Single Emitter Plume

Multi-Emitter Arrays

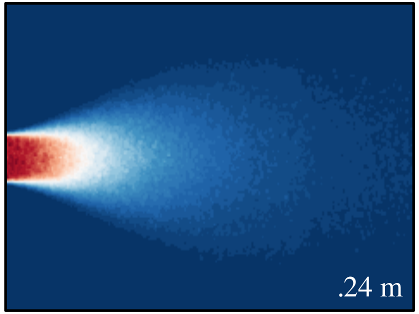


Single Emitter (source model)

~10^5 fold increase in ions

10^9 increase in domain volume

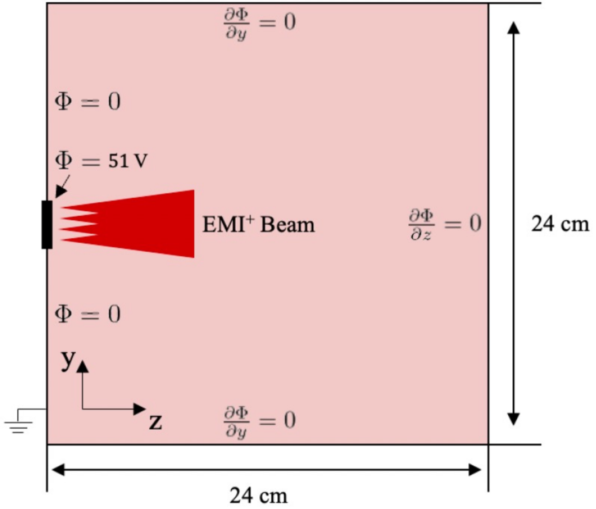
100x increase in time to steady-state



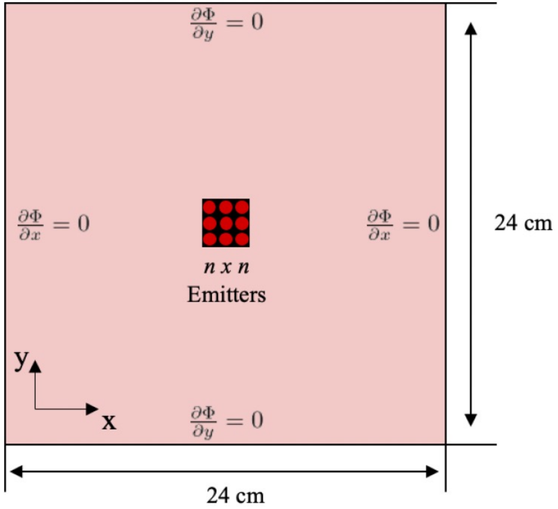
Particle in Cell (array model)

multi-emitter PIC modeling

side view



front view

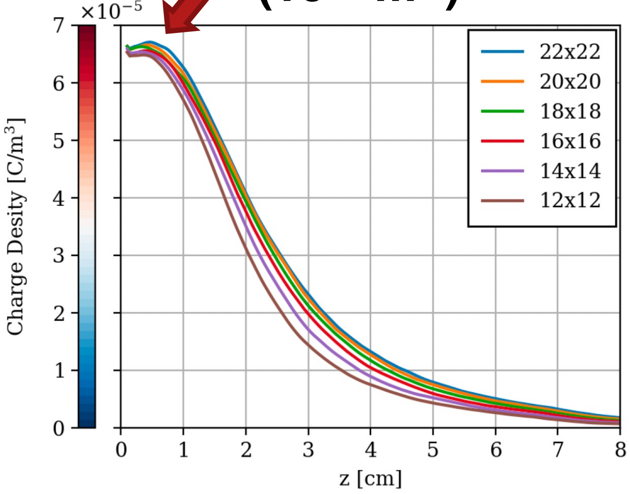


- **~500 ion beams (~200 µA)**
- **400 micron grid spacing**
- **24 x 24 cm domain**
- **time step: 2 ns**
- **simulation time: 2 µs**
- **particle weighting: 100 to 1**
- **peak macroparticle count: 2e6**
- **wall time: 3.5 hrs**

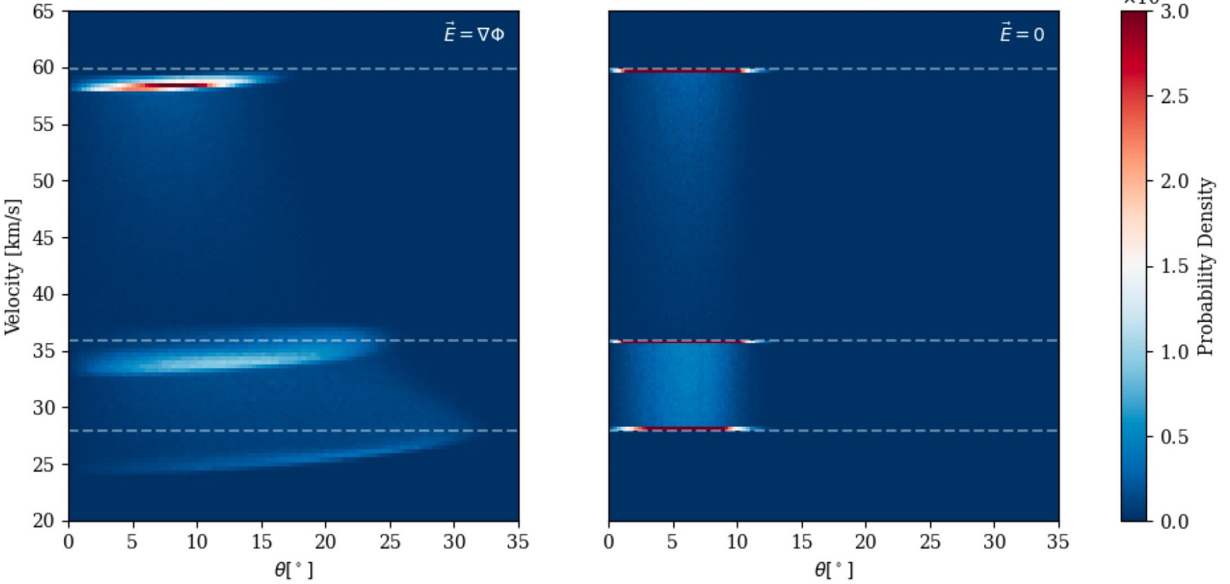
BC matching with n-body simulation → Multigrid Fast Poisson Solver → Ion Cluster Fragmentation → AFRL TURF 'open-access' PIC code

multi-emitter PIC results

region of constant density (10^{14} m^{-3})

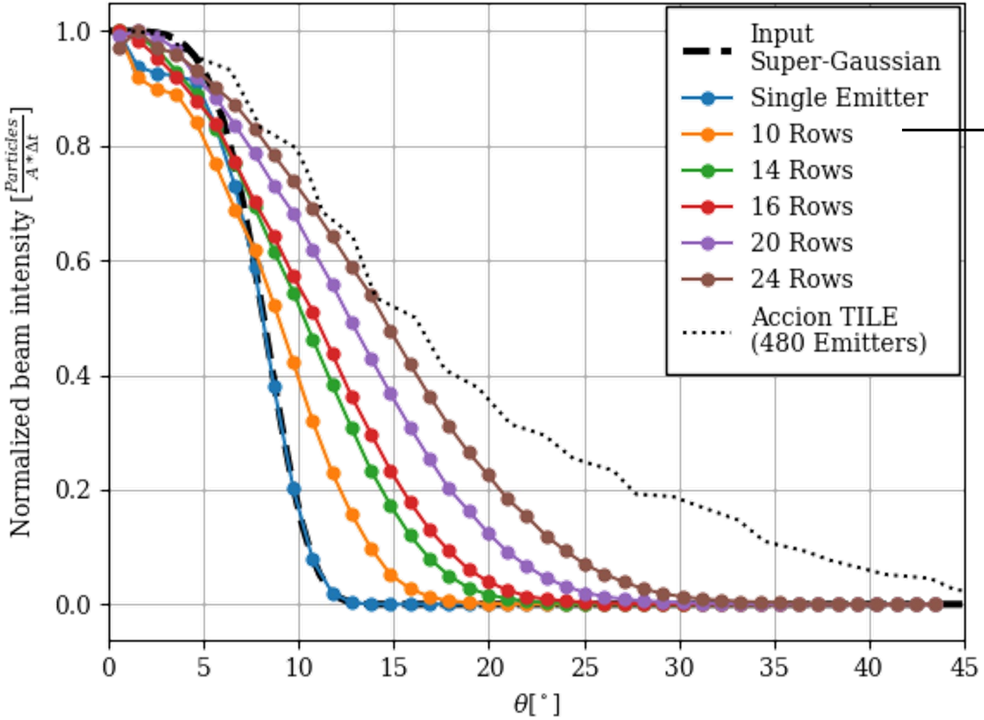


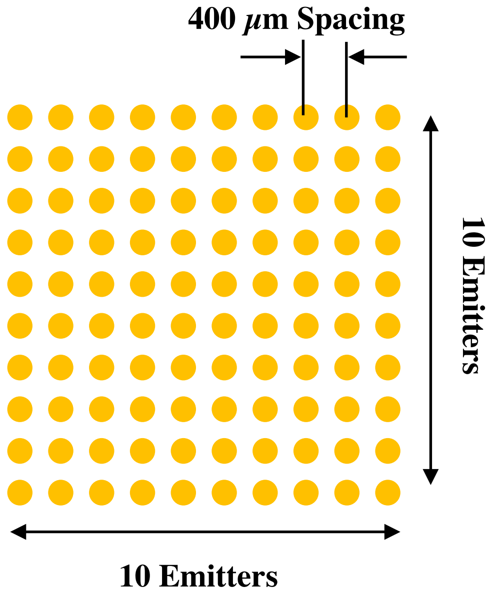
space charge **ballistic**



space charge induces beam spreading out to 30 degrees

comparison to experiments

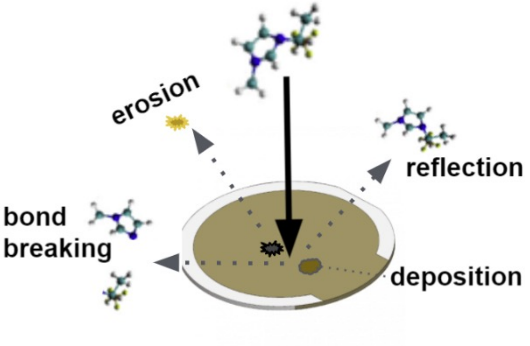


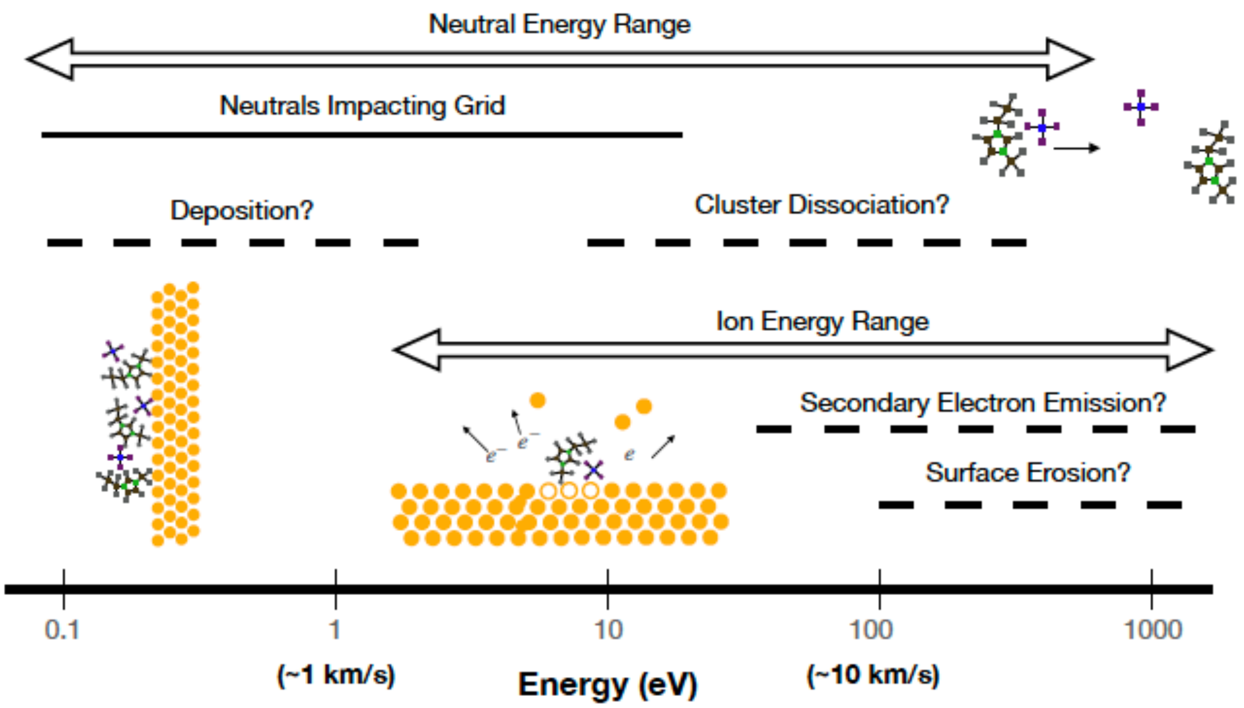


- **significant improvement in divergence model over other approaches**
- **missing large angle scattering**

Petro, E. et. al "Characterization of the TILE electrospray emitters," AIAA Propulsion and Energy 2020 Forum, 2020, p. 3612.

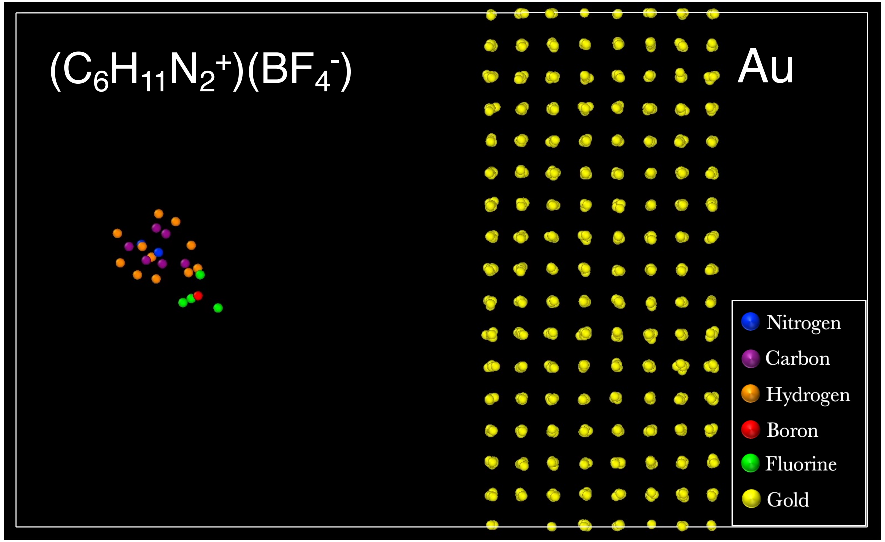
both n-body and PIC models predict collisions



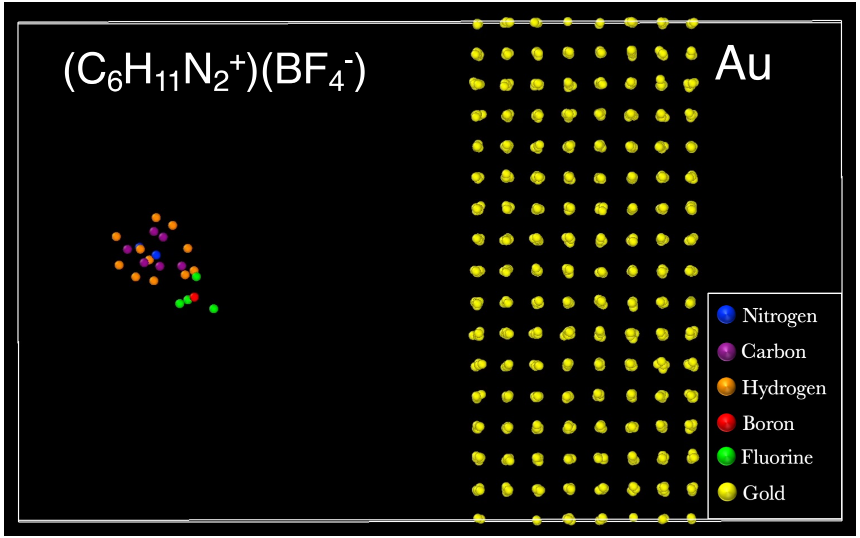


PhD Student: Rafid Bendimerad

analysis of surface impacts
(non-reactive molecular dynamics)



1 eV, 1 km/s, reflected intact

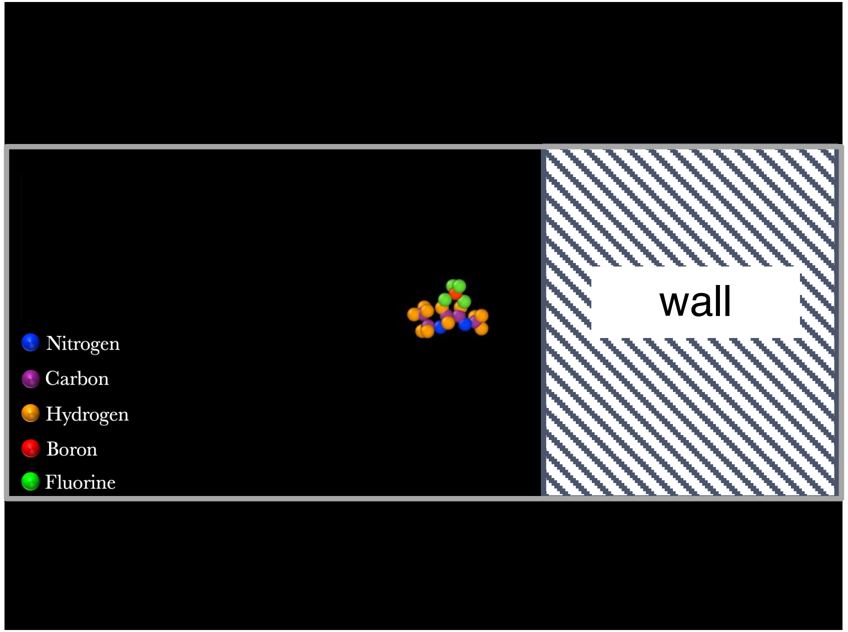


25 eV, 5 km/s, ionic ‘bond’ breaks

[Bendimerad & Petro, J. Elec. Prop 2022]

PhD Student: Rafid Bendimerad

analysis of surface impacts
(reactive molecular dynamics)



EMIBF4-wall collisions at 100 eV

Initial molecule:

$$\mathrm{EMI-BF_4} \equiv (\mathrm{C_6H_{11}N_2}^{+})(\mathrm{BF_4}^{-})$$

Surface collision products:

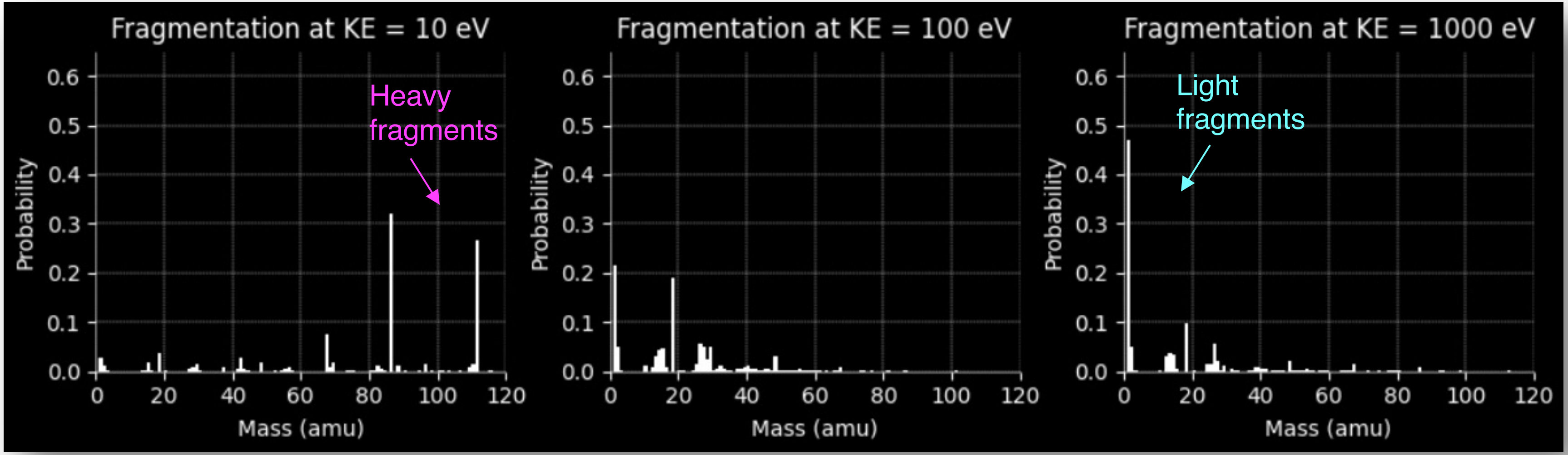
$$\mathrm{C_2H_5}\,;\mathrm{CHN}\,;\mathrm{CHN};\mathrm{CF}\,;\mathrm{CH}\,;\mathrm{BF_2};\mathrm{F}\,;\mathrm{H_2};\mathrm{H}$$

[Bendimerad & Petro, J. Elec. Prop 2022]

PhD Student: Rafid Bendimerad

analysis of surface impacts
(reactive molecular dynamics)

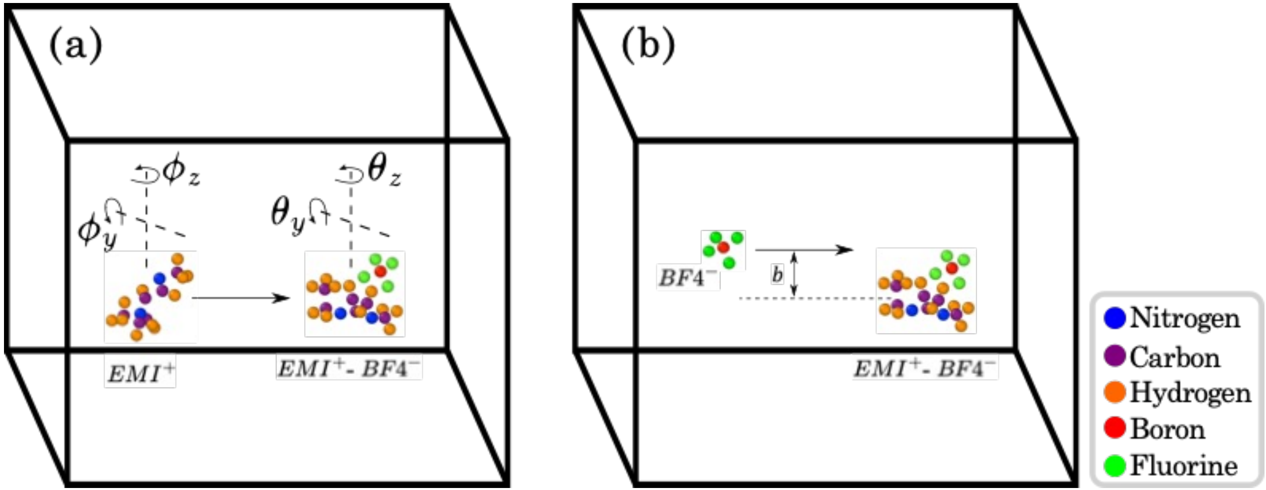
simulated mass spectra for EMIBF4-wall collisions at 300K



[Bendimerad & Petro, J. Elec. Prop 2022]

PhD Student: Abu Tahsin

modeling inter-particle collisions
reactive Molecular Dynamics (MD)



2 sets of simulations : EMI-neutral and BF_4-neutral collisions
variable parameters:

- Angles of rotation: ϕ_y, ϕ_z and θ_y, θ_z
- Impact parameter: b
- Impact energy

[Bendimerad et al., AIAA SciTech 2023]

PhD Student: Abu Tahsin

modeling inter-particle collisions
reactive Molecular Dynamics (MD)

Five types of collisional processes observed

1. Pure momentum exchange

2. Ionic Fragmentation

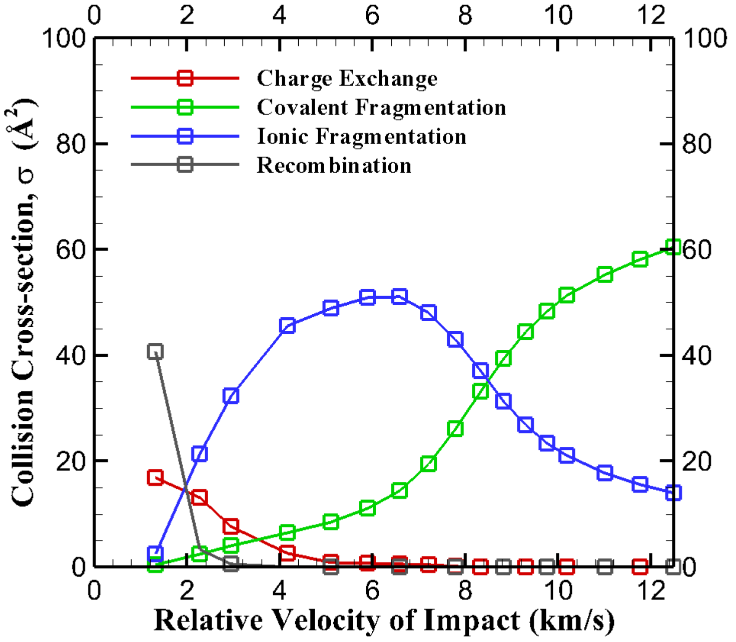
3. Covalent Fragmentation

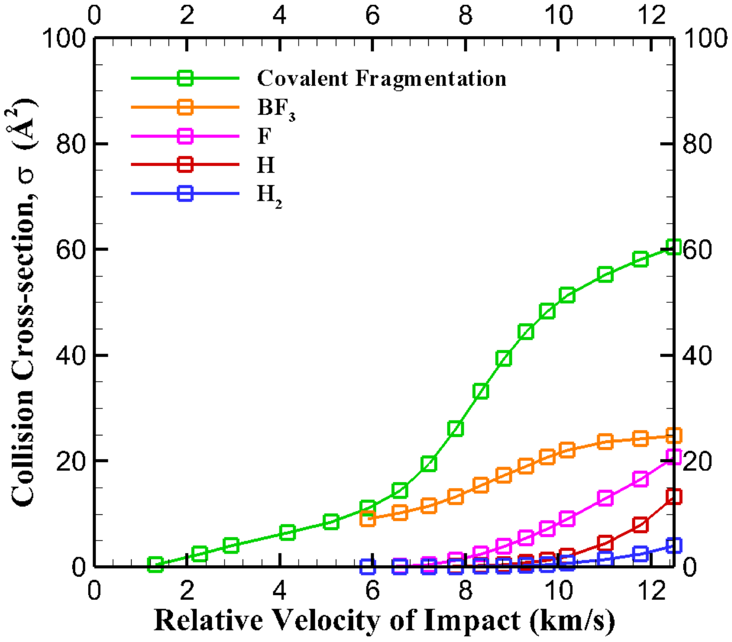
4. Charge Exchange

5. Recombination

PhD Student: Abu Tahsin

inter-particle collision cross-sections





[Tahsin et. al., AIAA SciTech 2024]

summary – multiscale modeling

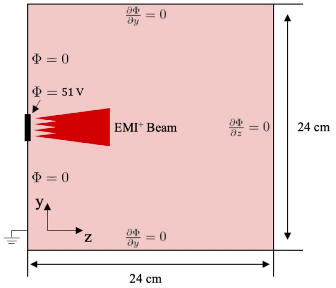
current

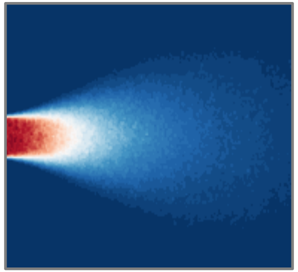
mA

µA

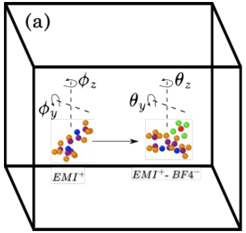
nA

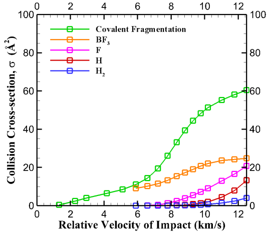
500 emitter array PIC

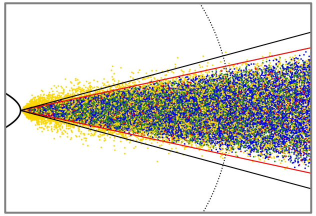




MD collisions







single emitter
n-body + EHD

beam energy

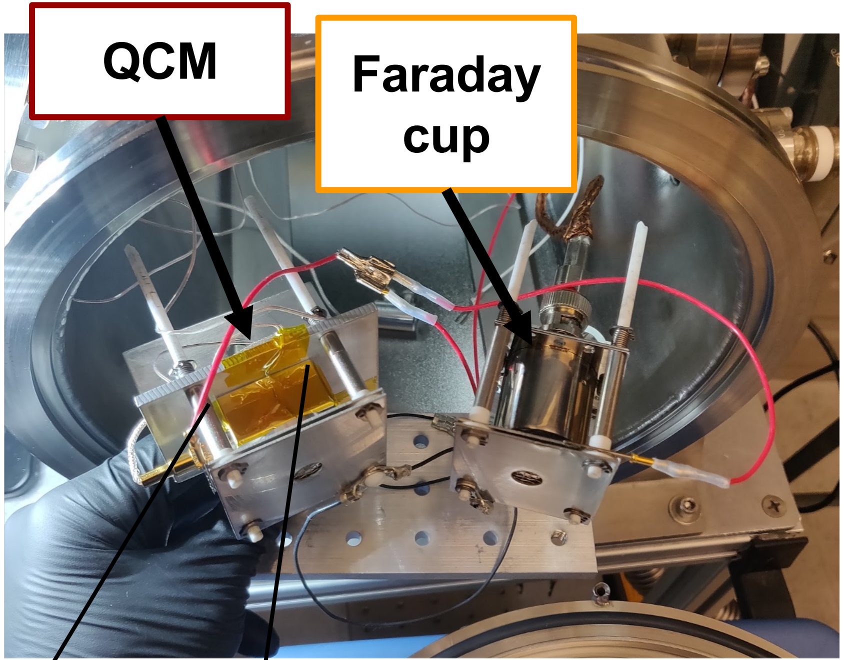
1 keV

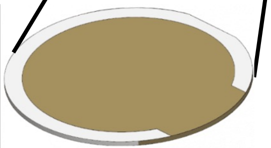
2 keV

3 keV

complimentary experimental efforts

can we measure propellant accumulation in-situ?



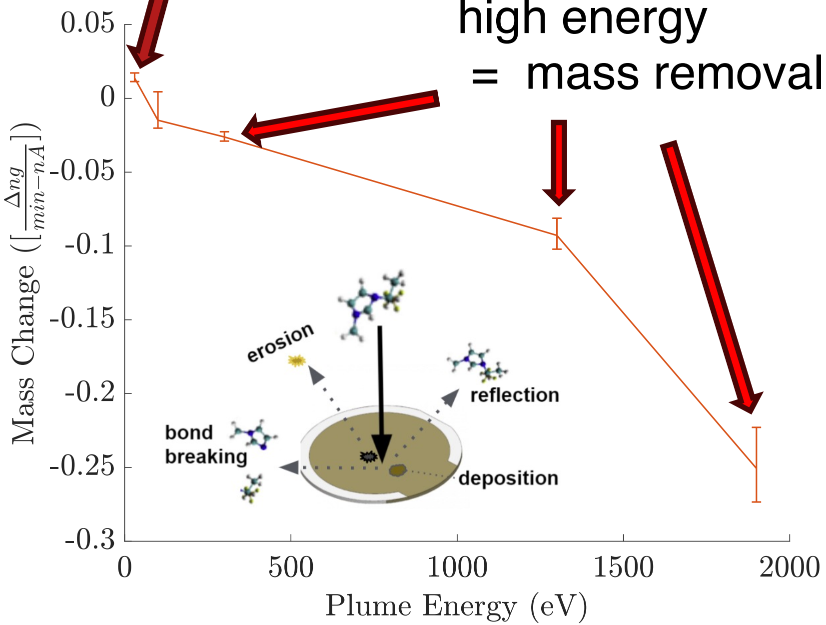


6 MHz gold coated quartz-crystal
(14 mm / 8 mm exposed)

[Geiger et. al., IEPC2022]

low energy = mass deposition

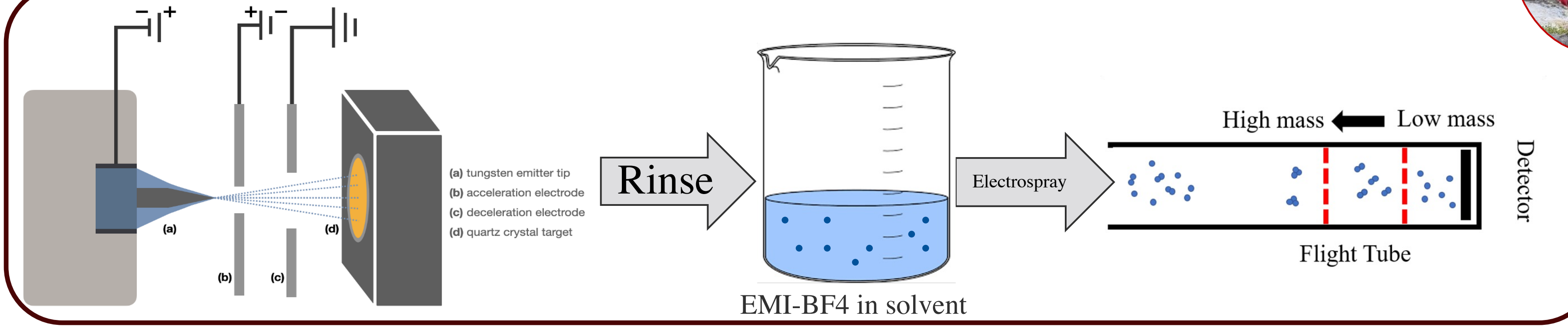
high energy = mass removal

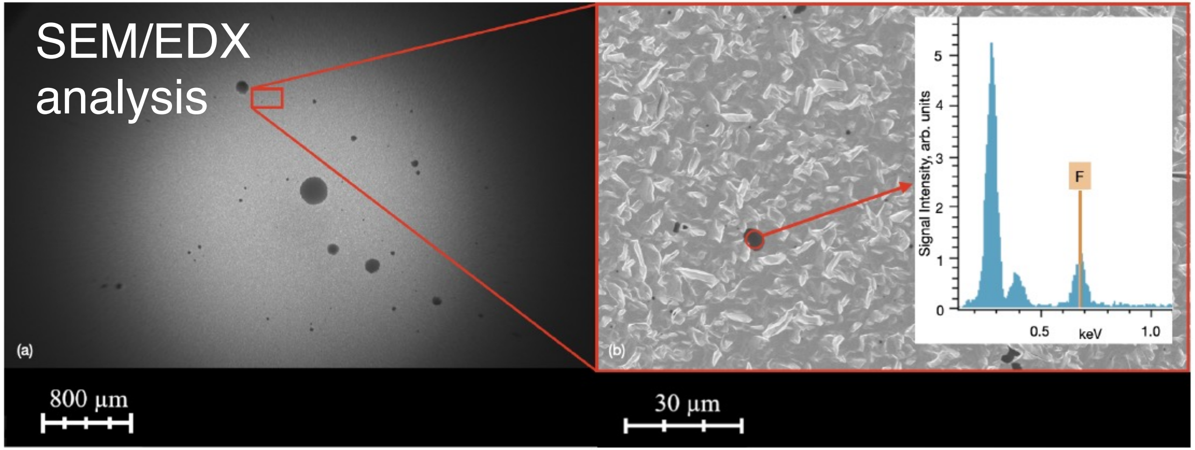


how can we characterize surface deposition?

non-volatile residue (NVR) analysis

[Bell et. al., AIAA SciTech 2023]





	Deposition (picograms)	% of Emitted Mass
Low (30 eV), 4 hours	342	0.016%
High (2700 eV), 17 hours	765	0.0012%

NVR can quantify, SEM/EDX can resolve spatial features

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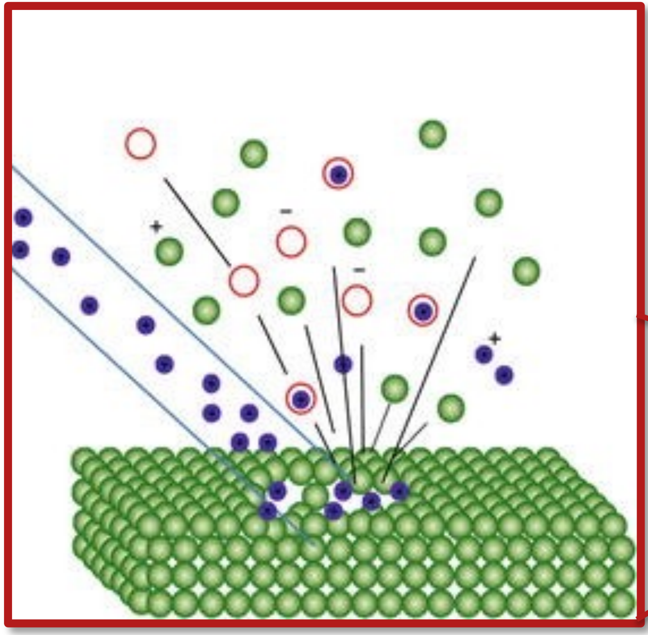
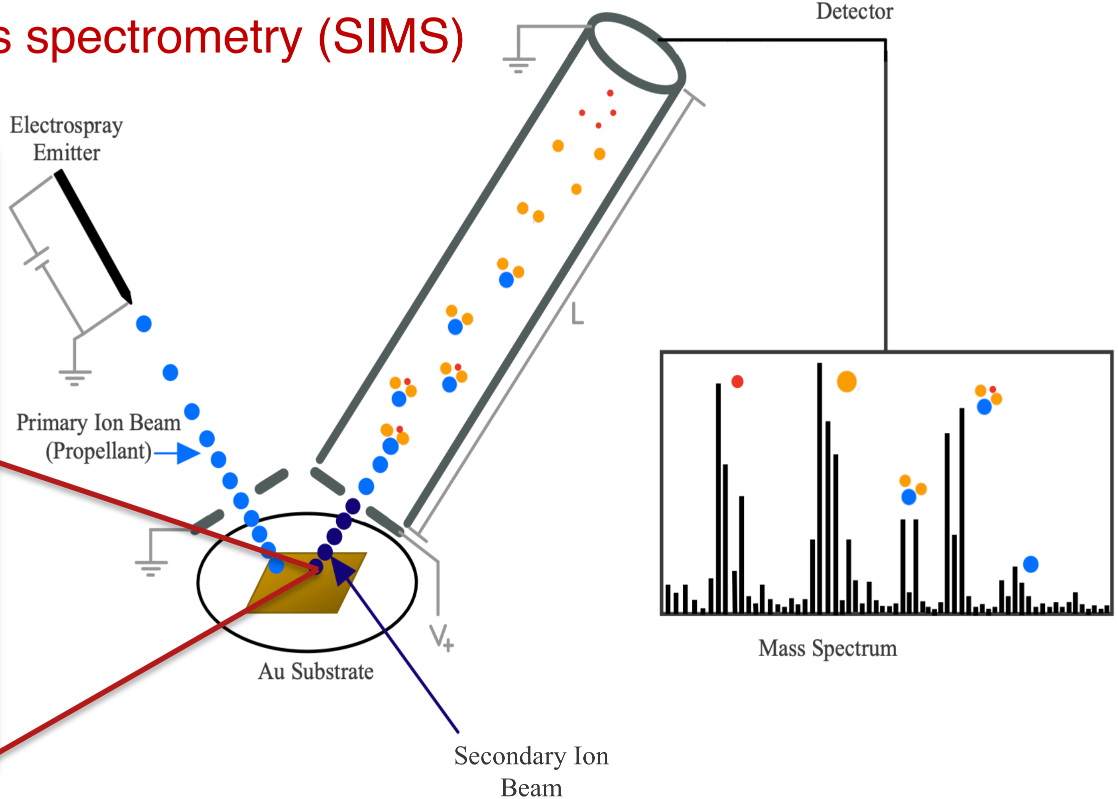
California Institute of Technology

can we characterize surface impact byproducts with ESI-SIMS?

secondary ion mass spectrometry (SIMS)

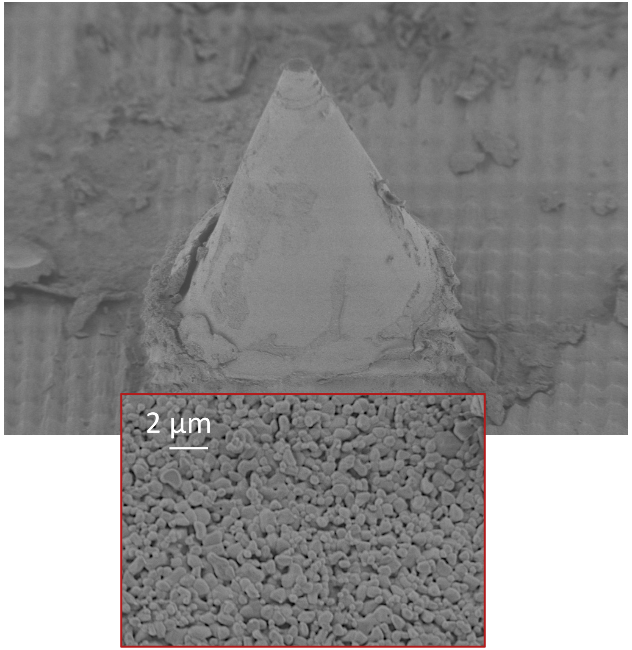
[Liang et. al, 2013]

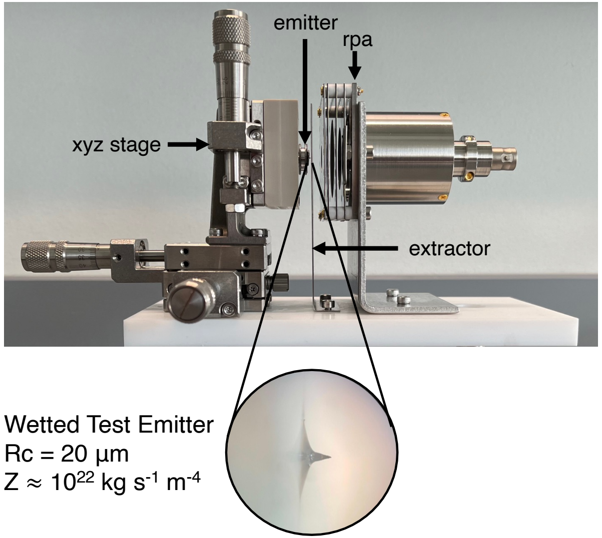




can we use nanoscale AM to make better electrospray emitters?

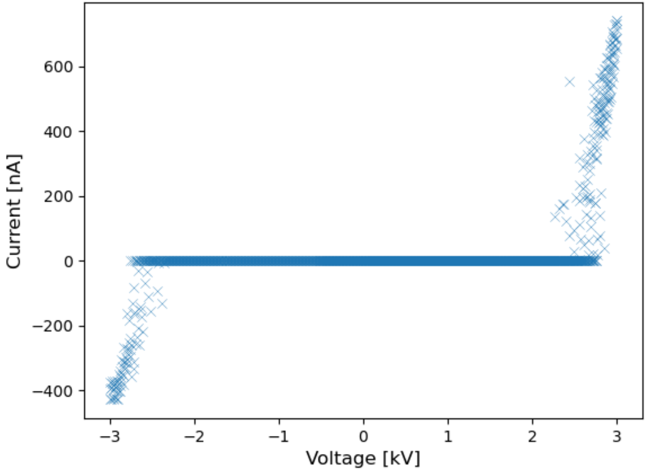
porous alumina





Wetted Test Emitter
Rc = 20 µm
$Z \approx 10^{22}$ kg s^{-1} m^{-4}

I vs. V

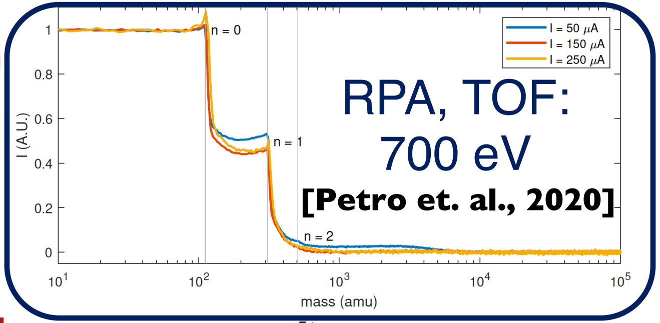


[Chamieh et. al., AIAA SciTech 2023]

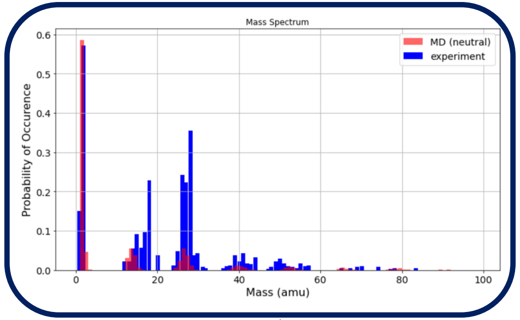
Collaborator: Prof. Sadaf Sobhani (Cornell)

PhD Students: Luke D'Cruz, Suhail Chamieh

summary – experimental validation



RPA, TOF:
700 eV
[Petro et. al., 2020]



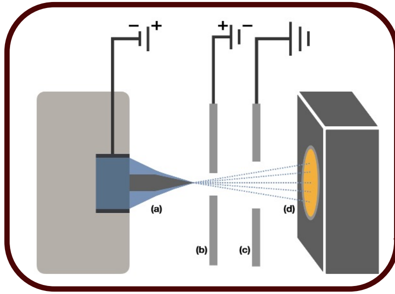
RGA:
100 eV
- 1 keV

[Shaik et. al., AIAA SciTech 2024]

current: mA, μA, nA

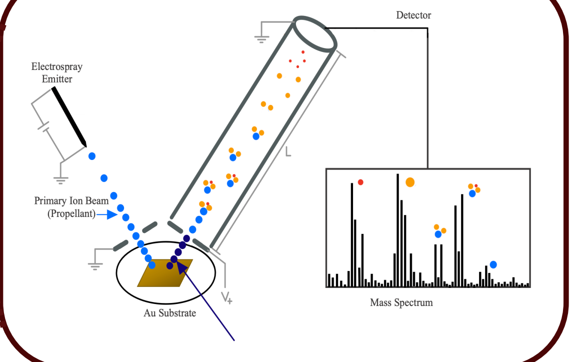
emitter arrays
100 μA

QCM, SEM, NVR:
30 eV - 2 keV



single emitter
100 nA

SIMS: 2-4 keV



beam energy: 1 keV, 2 keV, 3 keV

2018 – 2023 MIT / Cornell Team

EHD + nbody “SOLVEiT” Team:

Paulo Lozano (PI, MIT)

Elaine Petro (PI, Cornell University)

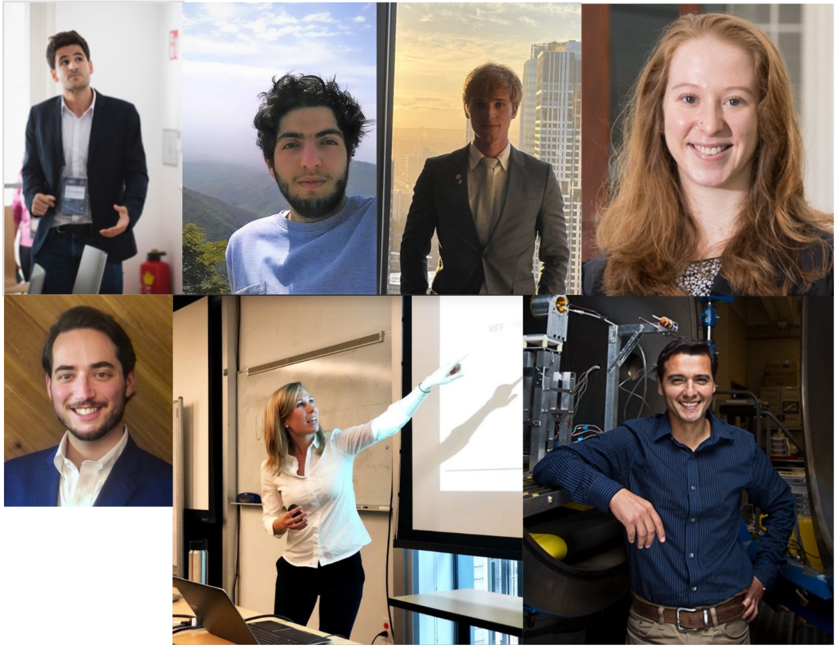
Ximo Gallud (PhD Student, MIT)

Madeleine Schroeder (MS/PhD Student, MIT)

Rafid Bendimerad (PhD Student, Cornell University)

Sebastian Hampl (MSc Student, McGill University)

Adler Smith (PhD Student, Cornell University)



Previous students:
Carl Geiger (PhD Student, Cornell University),
Joey Schmidt (now PhD, UT Austin), Kofi Blake (now PhD),
Adi Mehrotra (now PhD), Humberto Caldelas (now PhD, MIT)

PhD Students


Carl Geiger


Rafid Bendimerad


Giuliana Hofheins

Abu Taqui Md Tahsin


Stefan Bell


Luke D’Cruz

Post Doc


Zach Ulibarri

M.Eng


Max Luo


Drake Moorewood


Emily Harmon


Marshall Waggoner

Undergraduates


Adam Yonas


Justice Starks

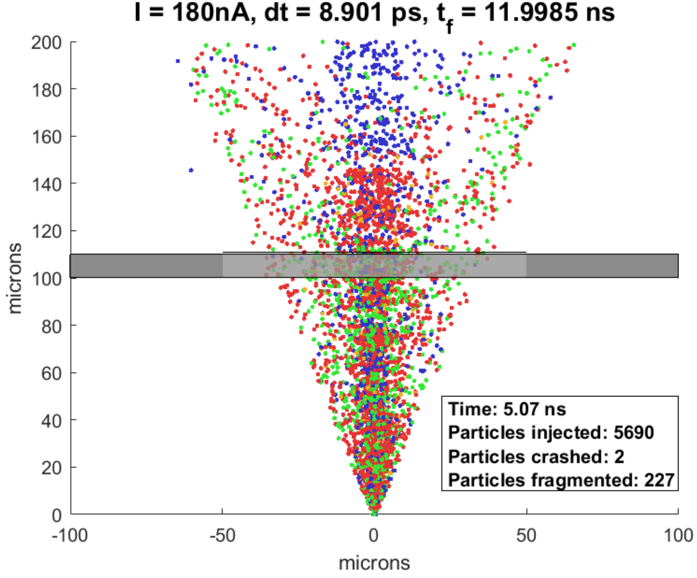

Adler Smith

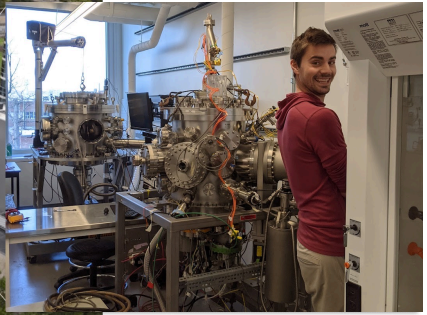

Jack Meyer


Aastha Bagree

Some of the researchers who have contributed to this work!

Thank you!





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