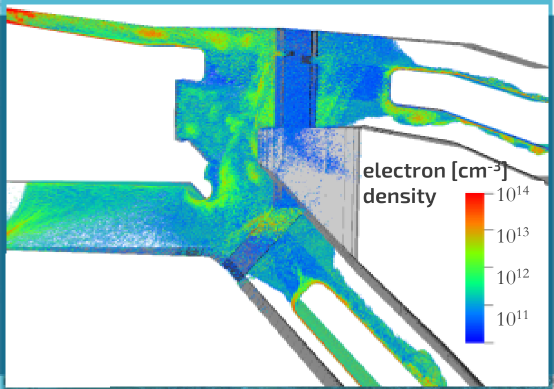
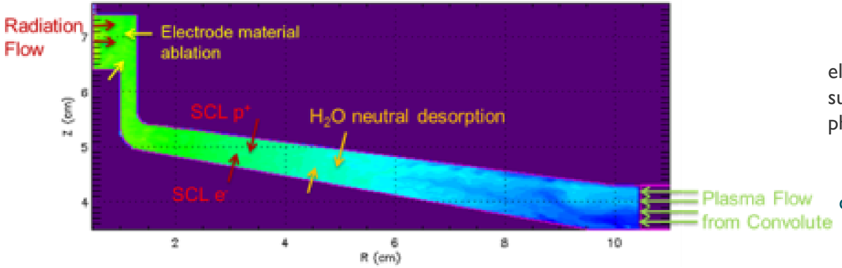
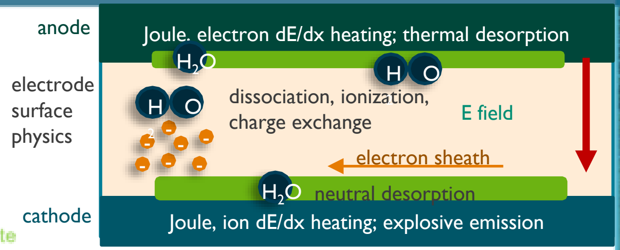
SAND2021-14385C

First principles model of electrode plasma formation in MA-scale accelerators







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Modeling electrode plasma formation is required in simulations of MA-scale transmission lines.

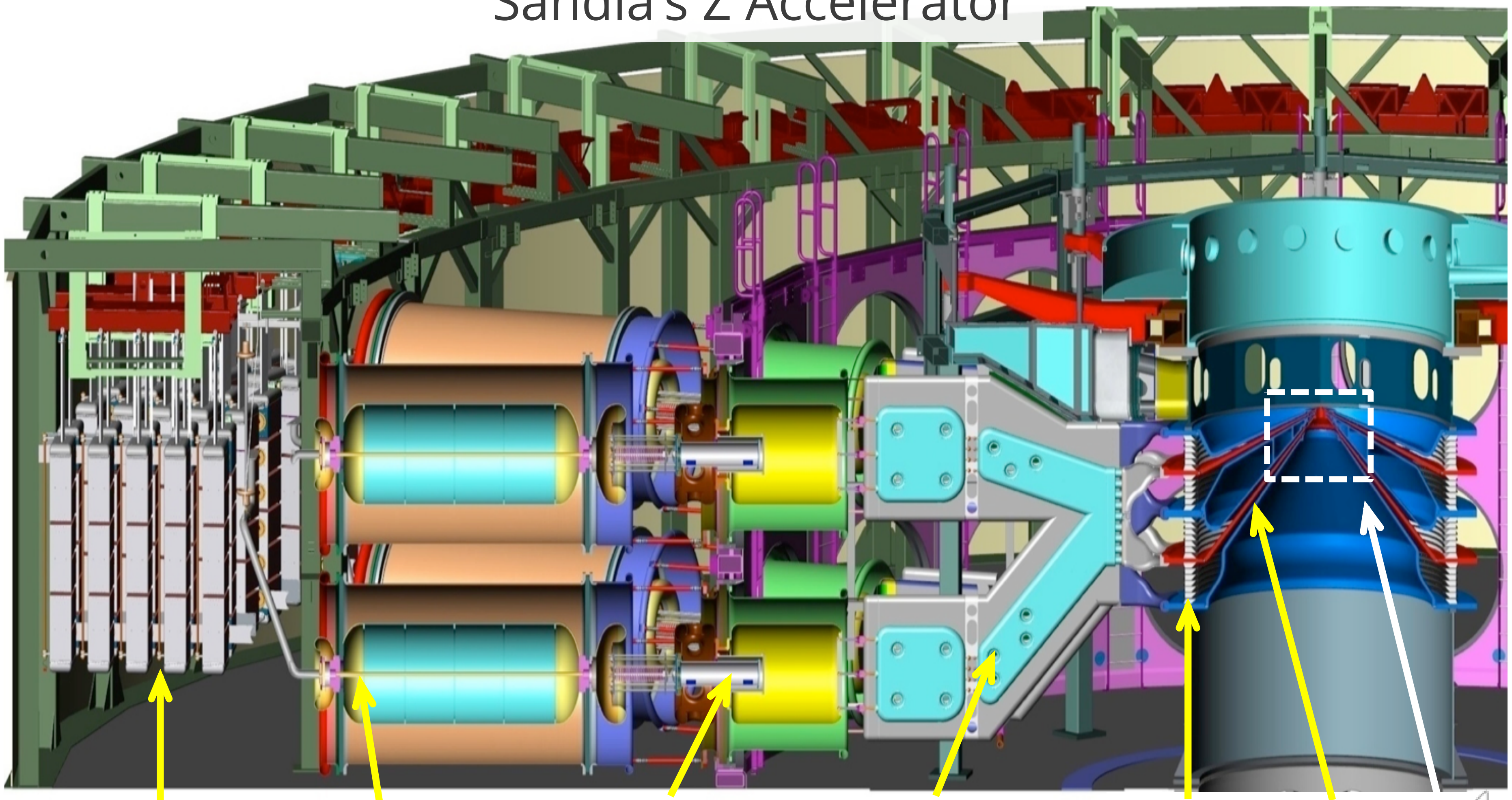
Outline

- Motivation of model using Sandia's MA-scale Z Accelerator
- Discussion of how plasma formation is presently modeled
- Description of the first-principles breakdown model
- Demonstration that the present, simplified model is sufficient at the MA scale
- Outline future work

In multi-MA accelerators, such as Sandia's Z Machine, electrode surface plasmas may impact efficiency.

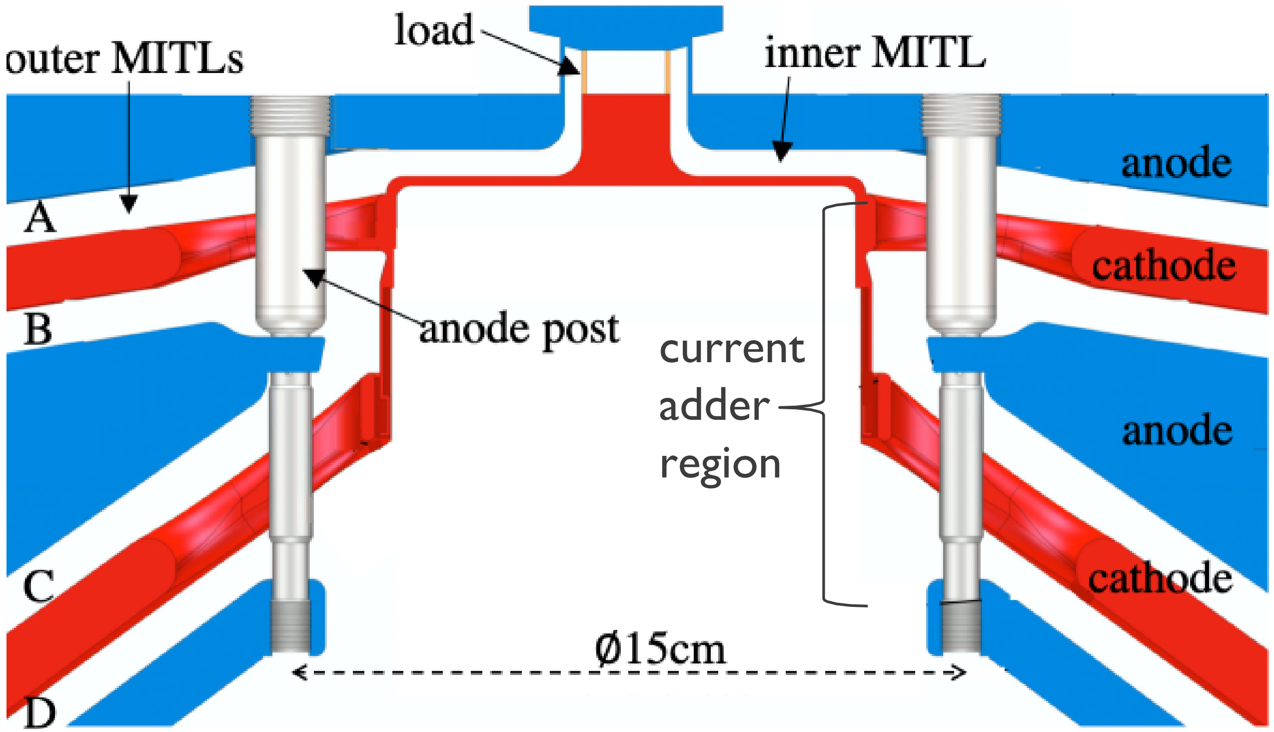
- 36 pulsed-power modules are connected in parallel to four radial "outer" magnetically insulated transmission lines (MITLs).
- After the current adder, a single radial "inner" MITL delivers up to 26 MA in 100 ns to the load.
- Charged particle emission and plasma formation are of interest near the load ("simulation volume")

Sandia's Z Accelerator

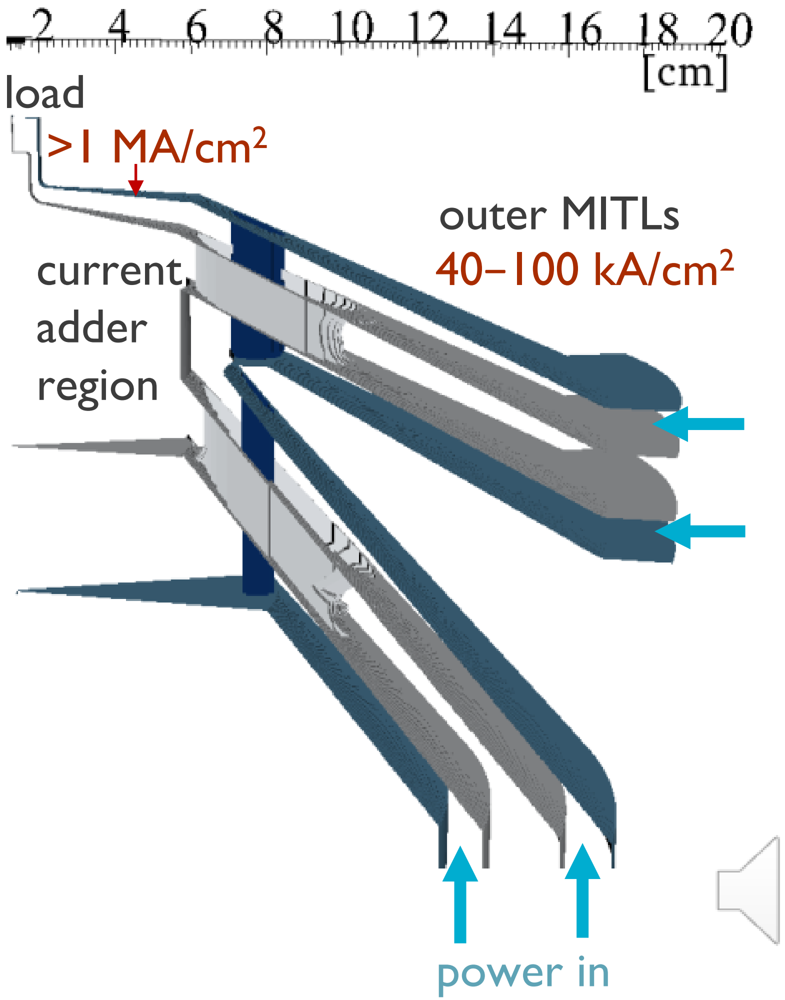


Regions of high current density are modeled kinetically to understand accelerator efficiency.

Z Accelerator: current adder to the load



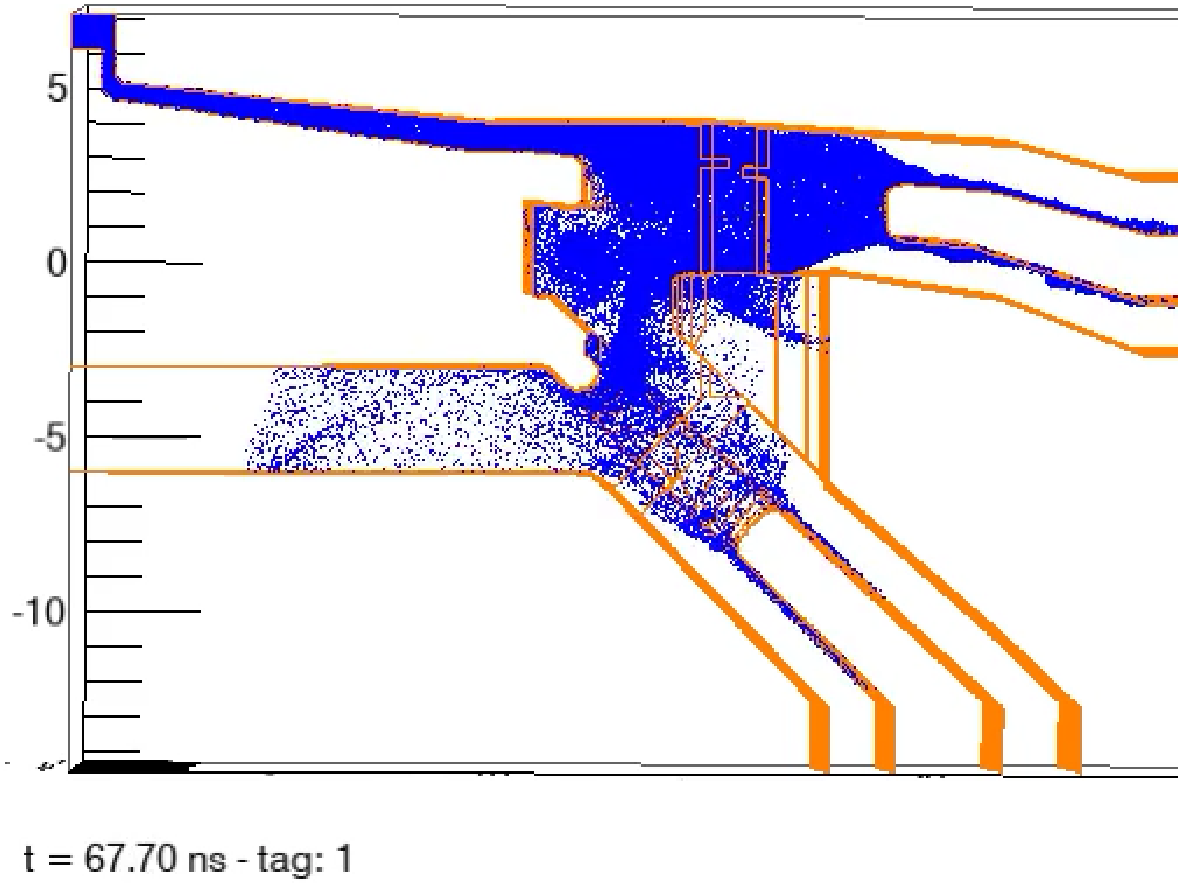
3D particle-in-cell simulation rendering (CHICAGO) of the current adder to the load



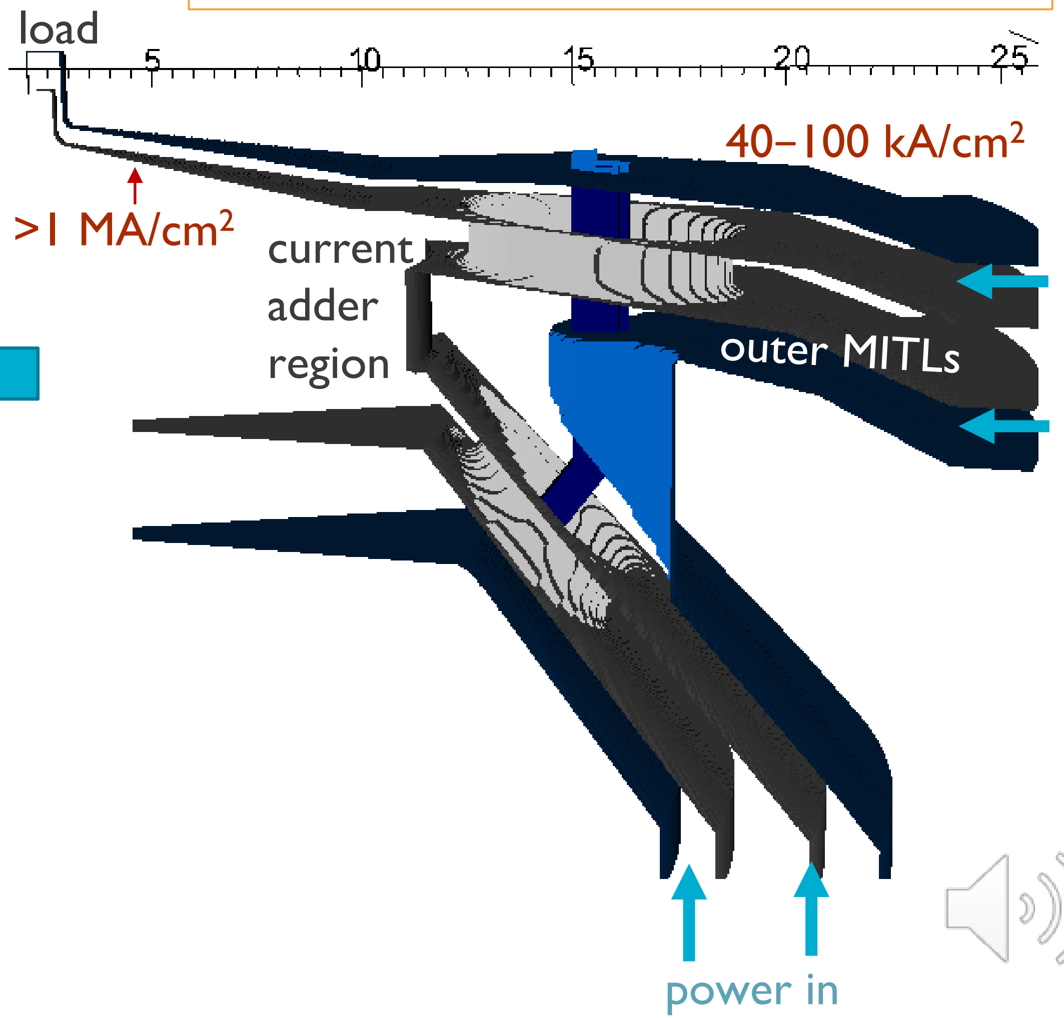
The regions in which $j \lesssim 10^5$ A/cm^2 operate as more traditional MITLs.

Charged particle currents are dominated by E-field emission of electrons governed by Child-Langmuir.

Animation of electron macroparticles demonstrates traditional MITL flow only in the outer MITLs



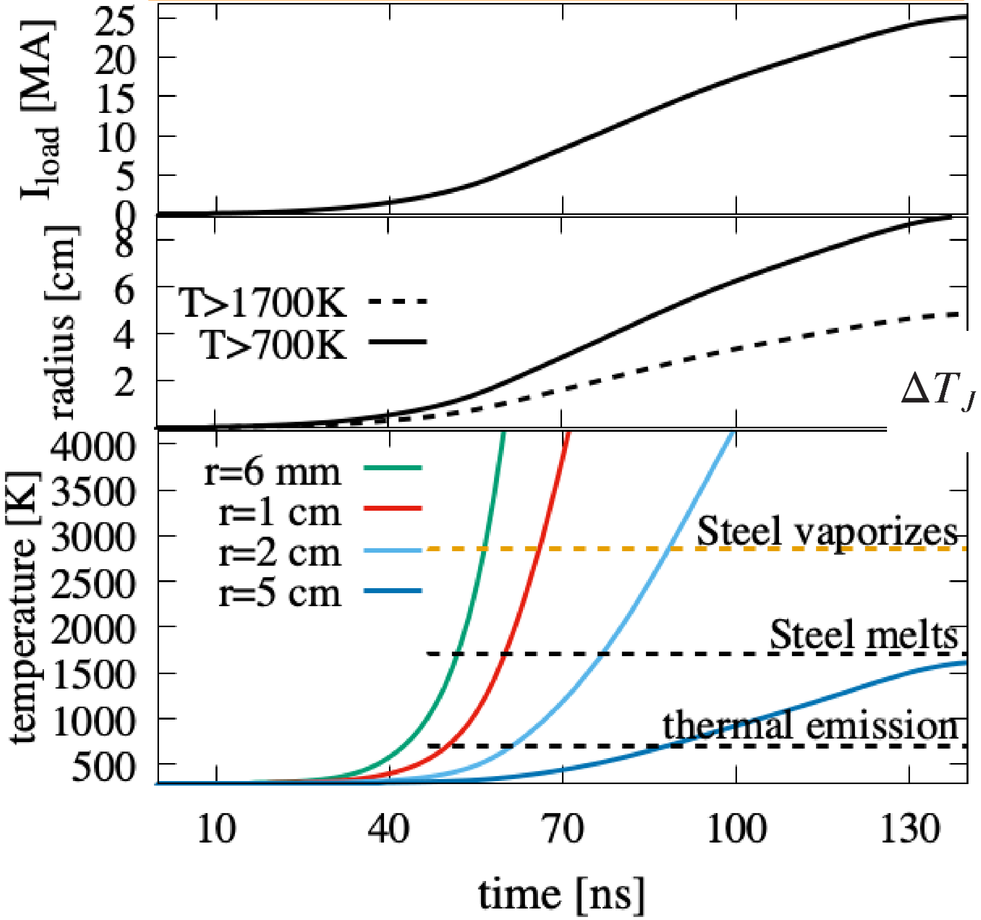
3D particle-in-cell simulation rendering (CHICAGO) of the current adder to the load



On the Z Accelerator, plasmas rapidly form on the electrode surfaces near the load.

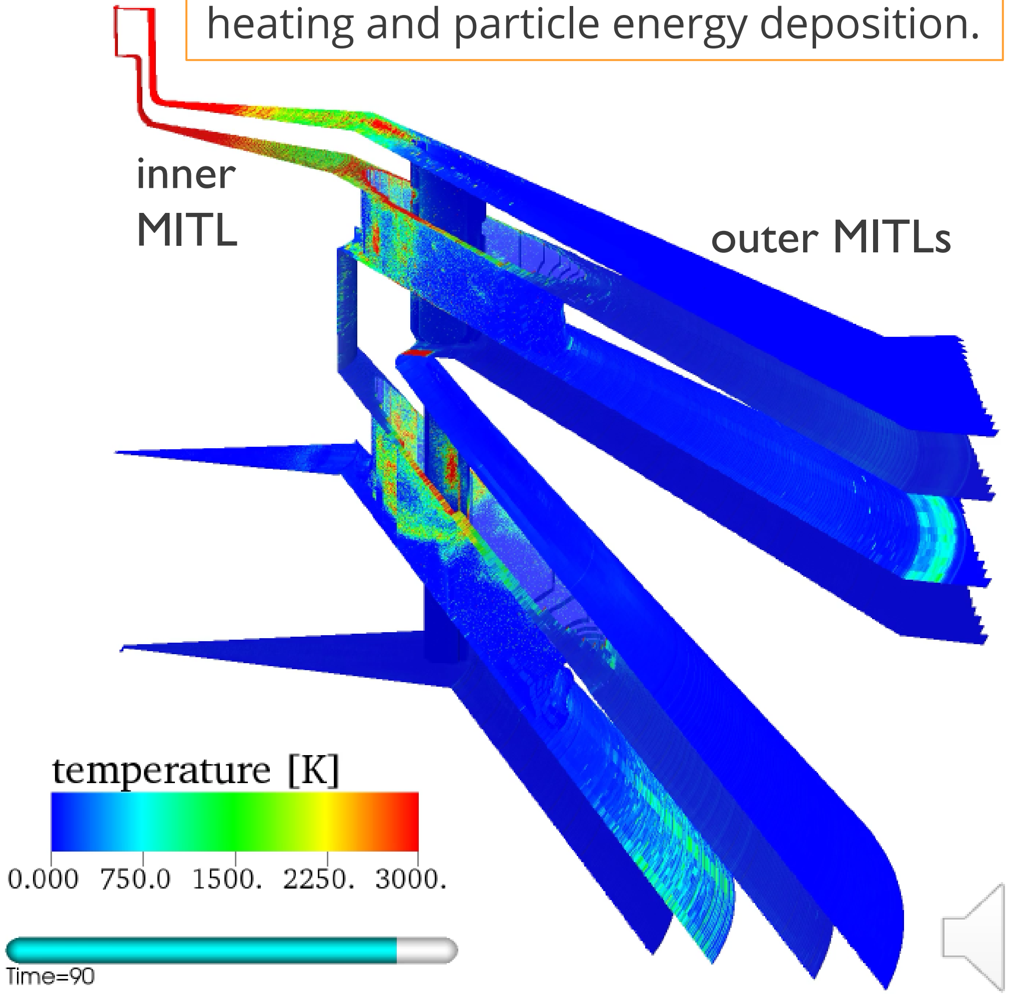
- Thermal emission of ions (T >700 K) occurs in the inner MITL.
- Electrode melt occurs near the load and is actively being explored.

Joule heating is calculated downstream from the adder region.



$$\Delta T_J(t) \approx \frac{\vartheta \mu_0 H^2(t)}{2c_v} \; ^*$$

Surface temperatures rise due to Joule heating and particle energy deposition.



*H. Knoepfel, *Magnetic Fields* (John Wiley and Sons, 2000).

In present Z simulations, desorbed electrode surface contaminants are assumed ionized.[1-4]

Experiments indicate that the main surface contaminants are CO, H_2O, H_2, and CO_2.[5]

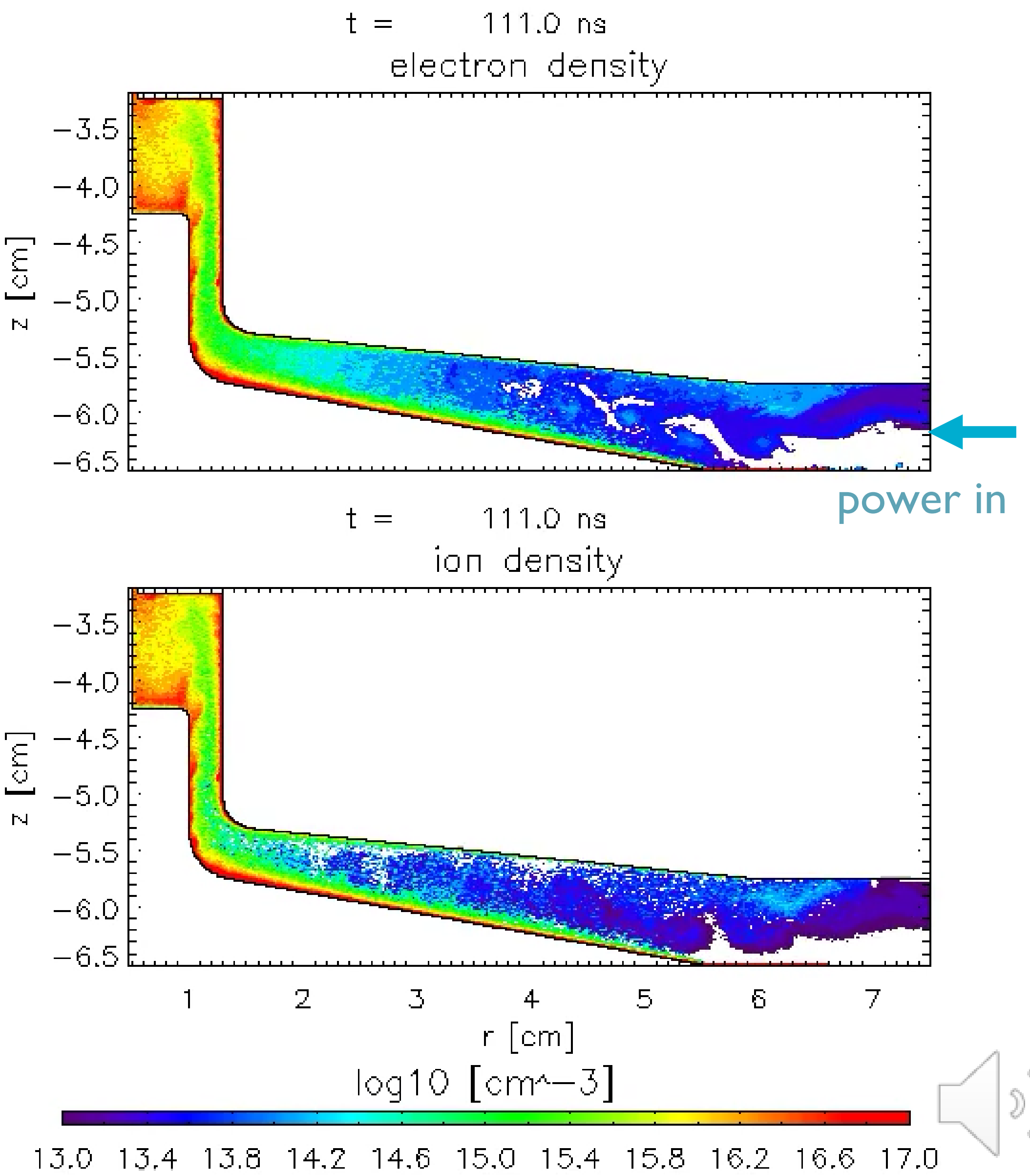
Simulations include three particle emission mechanisms:

1. electrons from Child-Langmuir emission at 240 kV/cm
2. protons from thermal emission at 700 K
3. assuming H_2O, neutral desorption (number of contaminants in a surface cell):

$$\frac{dn(t)}{dt} = -\nu_{th} n(t)\ e^{-E'(n)/(k_B T(t))}$$

Followed by rapid ionization within 2 cells of the surface:

$$H_2O \rightarrow 2H^+ + O^+ + 3e$$

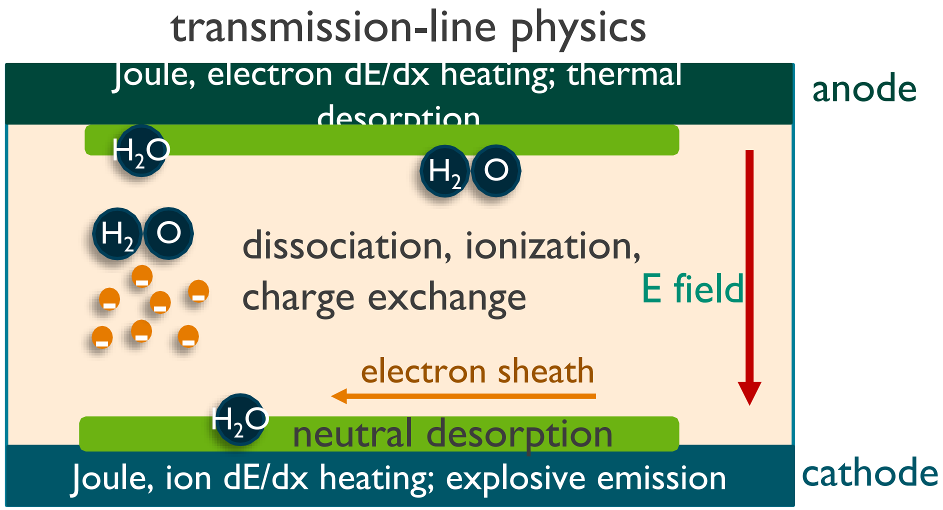


1) Welch, et al. Phys. Rev AB **22**, 070401 (2019).
2) Bennett, et al. Phys. Rev AB **22**, 120401 (2019).
3) Welch, et al. Phys. Rev AB **23**, 110401 (2020).
4) Bennett, et al. Phys. Rev AB **24**, 060401 (2021).
5) Gomez, et al. Phys. Rev ST-AB **20**, 010401 (2017).

We are testing the range of validity for assuming full ionization using kinetic models of breakdown in a coaxial transmission line.

- The simulations track the desorption of neutral surface contaminants and their subsequent dissociation and ionization.

- As in present Z models:
  - Joule/particle-impact heating
  - field-stress/thermal emission
  - Arrhenius Eq. desorption



- Additional relevant particle models :

thermal dissociation

$H_2O \rightarrow H_2 + O$

attachment

$e + H \rightarrow H^-$

$e + O \rightarrow O^-$

ionization: dissociative, electron/ion impact

$\mathbf{e} + H_2 \rightarrow 2e + H^+ + H$

$e + H \rightarrow 2e + H^+$

$e + O \rightarrow 2e + O^+$

$H^+ + H \rightarrow e + 2H^+$

$H^+ + H_2 \rightarrow e + H^+ + H_2^+$

$H + H_2^+ \rightarrow e + H^+ + H_2^+$

$O^+ + H \rightarrow e + O^+ + H^+$

$O^+ + H_2 \rightarrow e + O^+ + H_2^+$

$H + H \rightarrow e + H^+ + H$

$H + H_2 \rightarrow e + H^+ + H_2$

$H + H_2 \rightarrow e + H + H_2^+$

charge and momentum exchange

$H^+ + H_2 \rightarrow H + H_2^+$

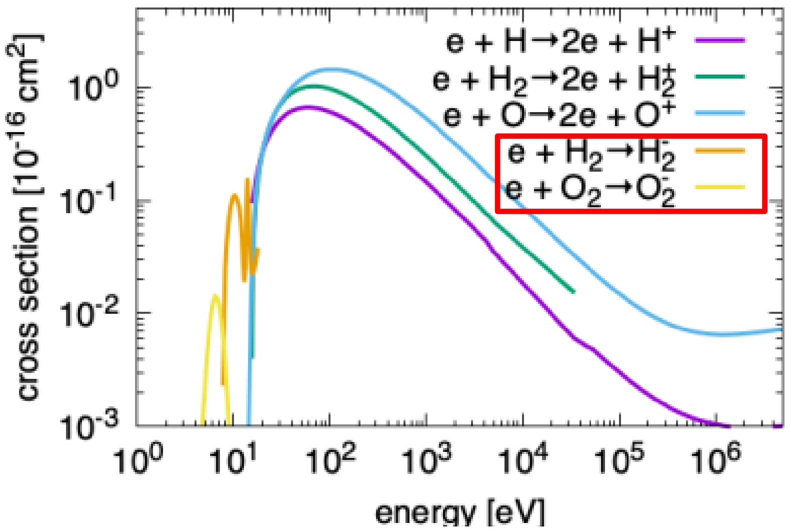
$H + H_2^+ \rightarrow H^+ + H_2$

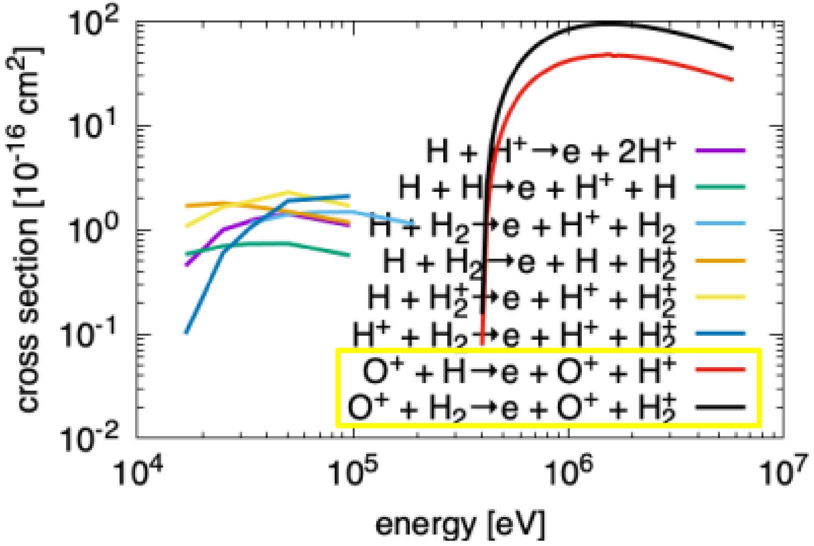
$H^+ + H \rightarrow H + H^+$

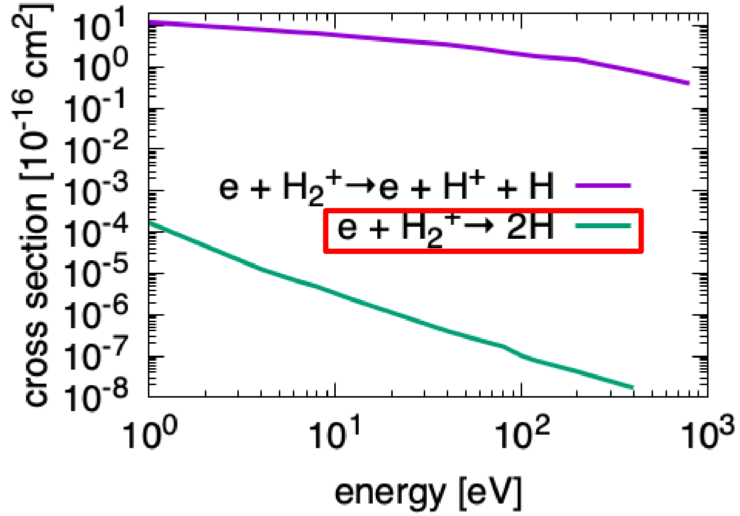
$e + H_2^+ \rightarrow e + H^+ + H$

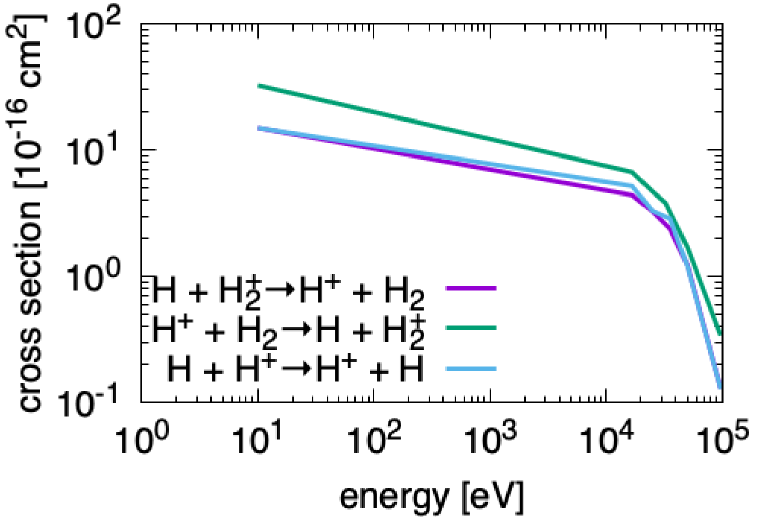
$e + H_2^+ \rightarrow e + 2sH$

Particle species with small interaction probabilities may be excluded from the models.









- H_2 desorption replaces H_2O.
- O^+ from thermal emission
- O+ did not reach energy for significant H,H_2 ionization

Y.-K. Kim and M.E. Rudd, Phys. Rev. A **50**, 3954 (1994); W. Hwang, Y.-K. Kim and M.E. Rudd, J. Chem. Phys. **104**, 2956 (1996); and Y.-K. Kim and M. E. Rudd, Comments At. Mol. Phys. **34**, 293 (1999).

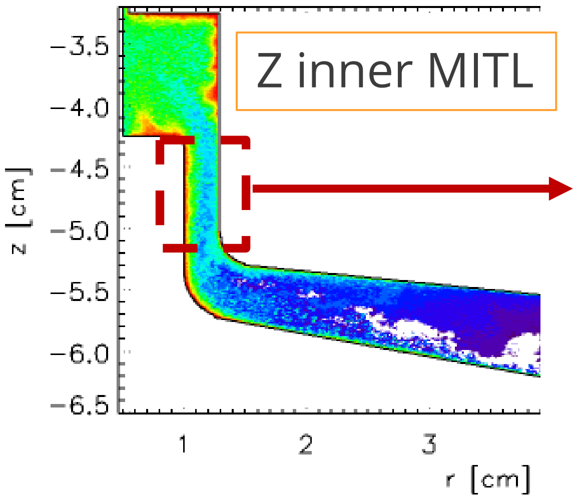
First-principles breakdown models require high resolution and massive numbers of macroparticles.

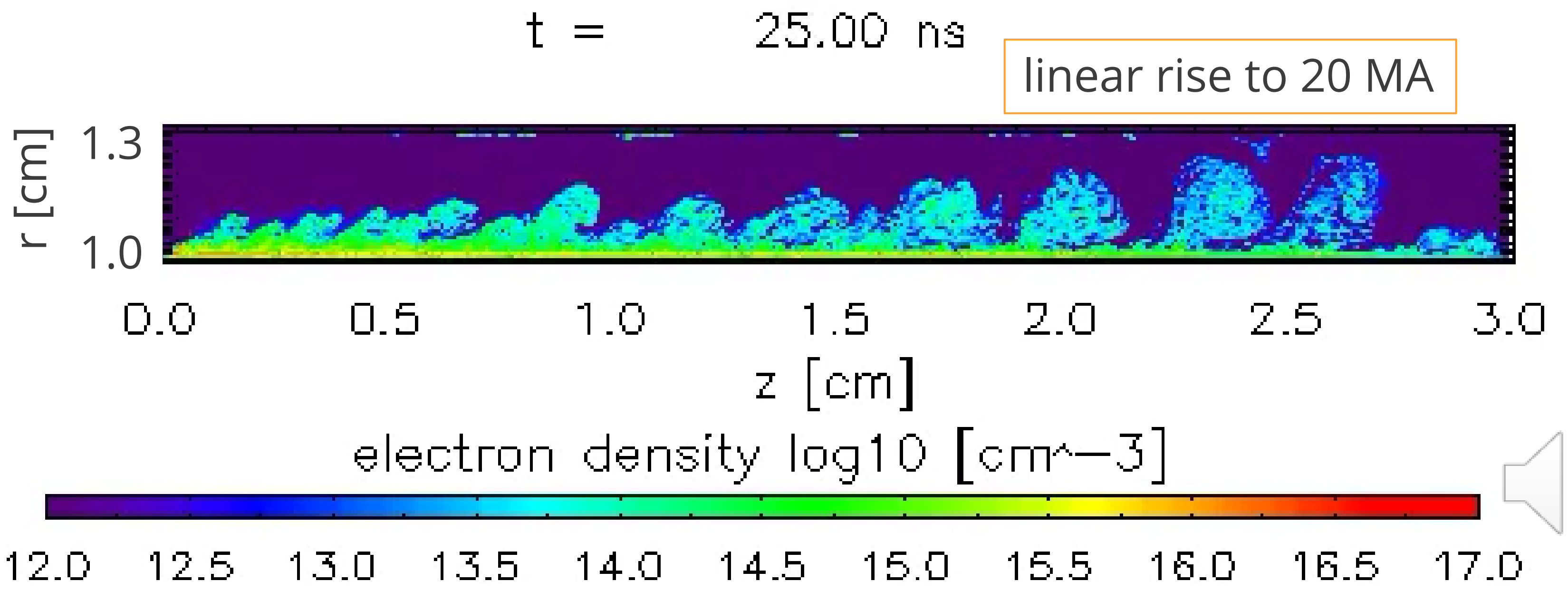
A 2D first-principles model is significantly larger than 3D assumed-ionized models of the Z Accelerator.

Ionization model:
- A coaxial line mimics the inner MITL near the load.
- 1< r< 1.3 cm and 2< r < 2.25 cm
- 4 and 5 μm resolution
- linear, 100-ns pulse rise
- No particle flow from upstream!

2D coax:	3D Z model:
3,750,000 cells	26,217,000 cells
1,511,956,530 particles	3,712,364 particles
at 35 ns	at 35 ns

run on NNSA high performance compute platforms



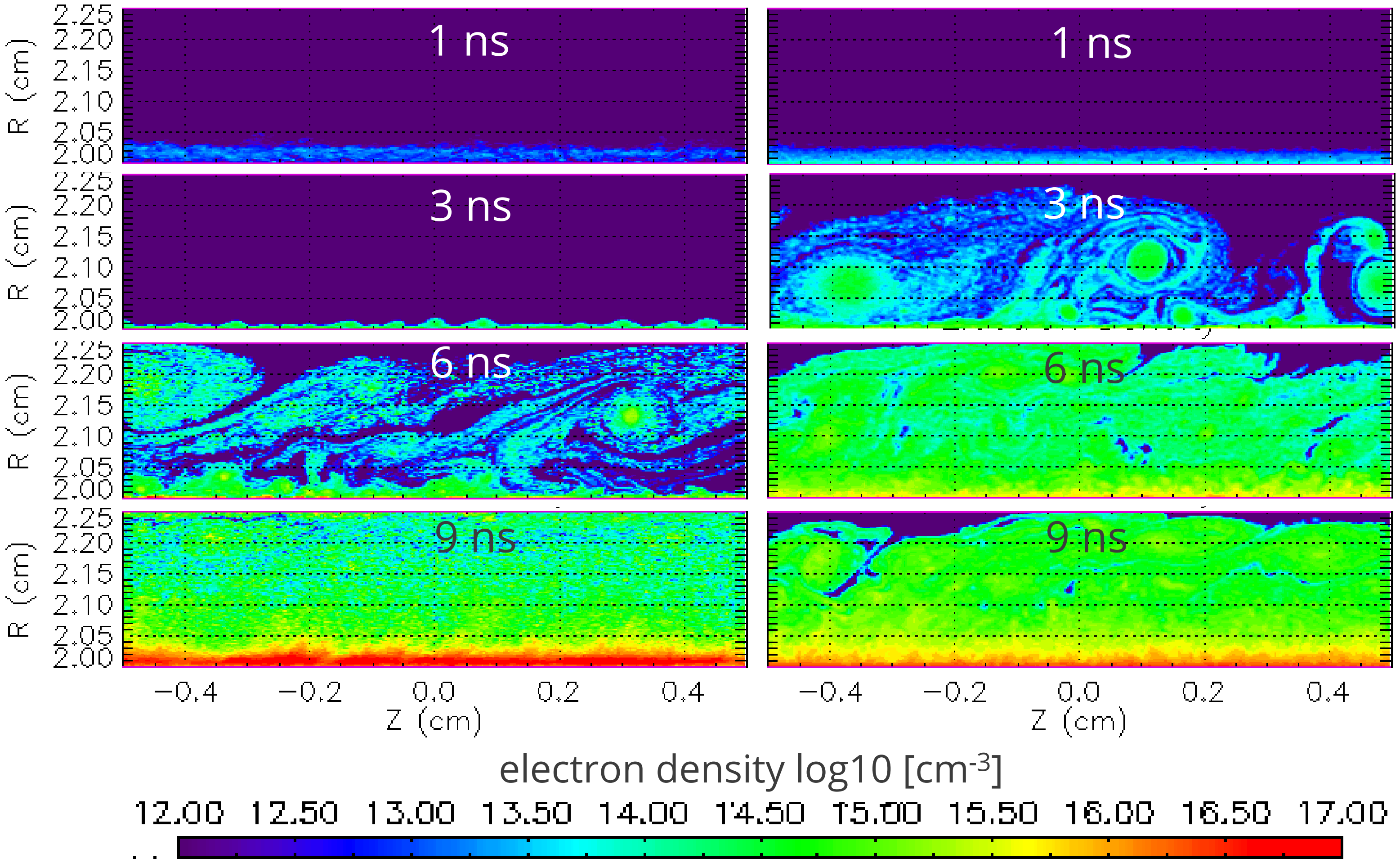


Ionization occurs in nanoseconds

For a linear rise to 20 MA, the density distributions from the ionization model are similar to the fully ionized model 3 ns earlier.

Desorbed neutral H_2, kinetic breakdown. 5 μm resolution.

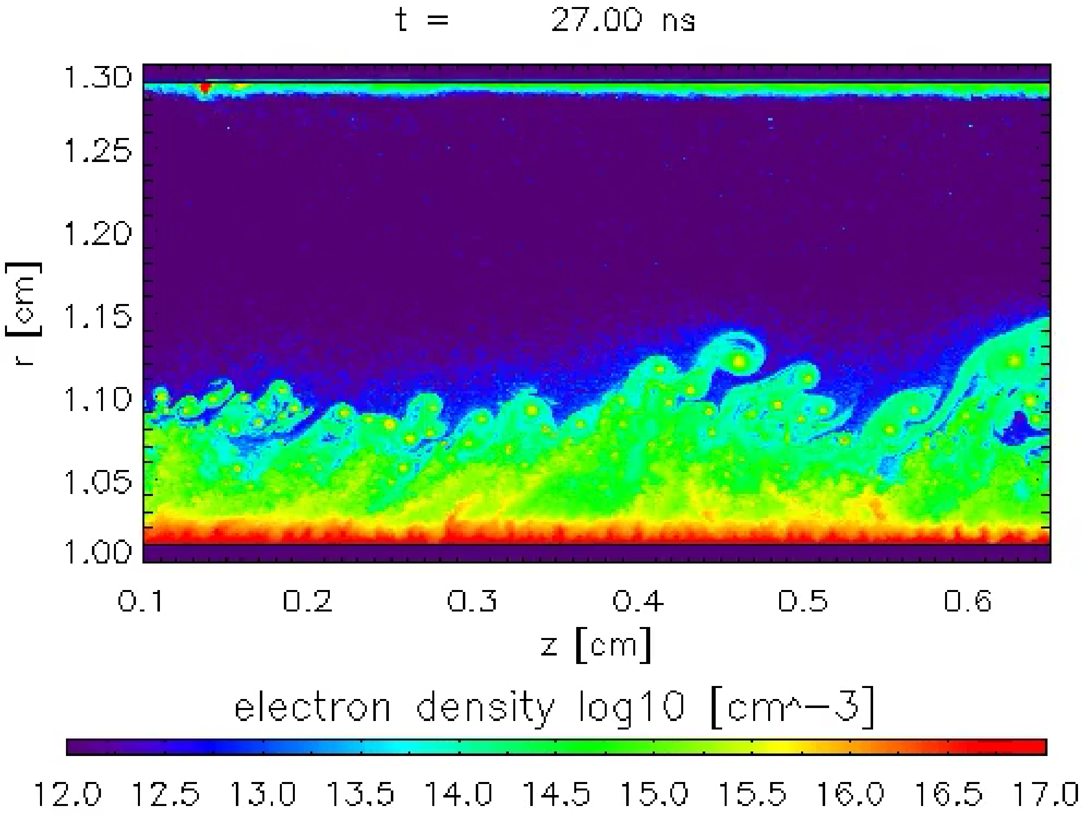
Desorbed Fully Ionized $2H^+$, O^+ 25 μm resolution.



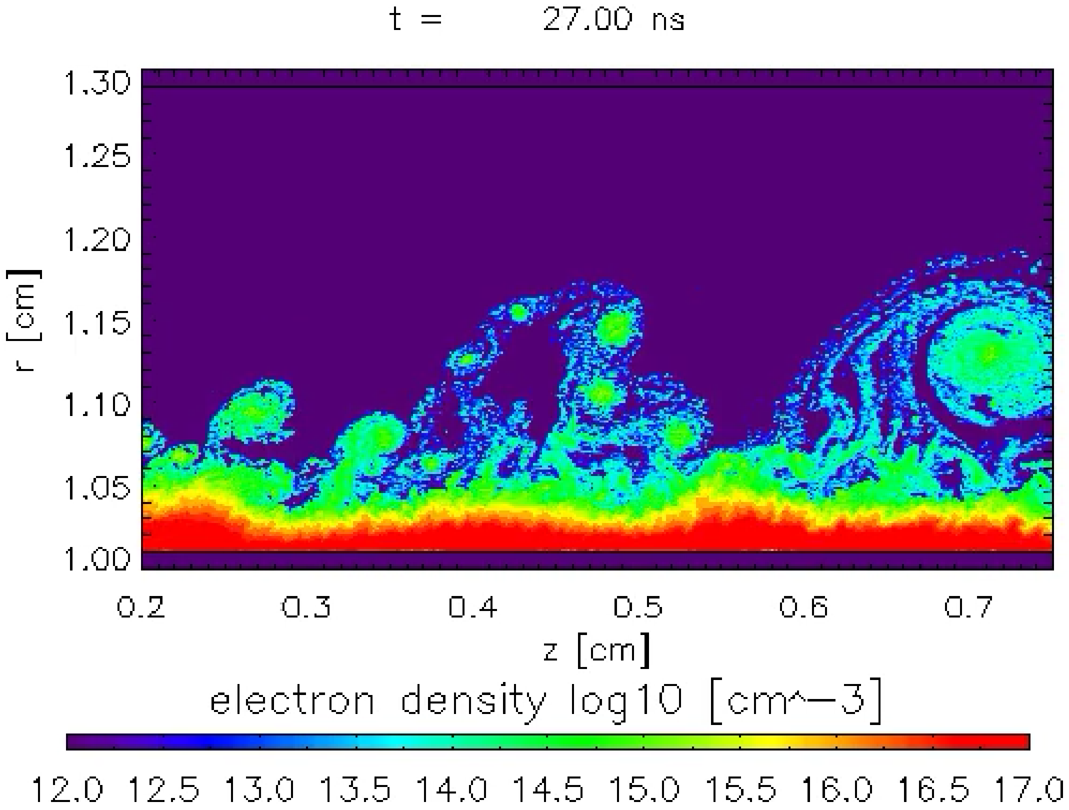
Magnetized diffusion is slower at 20 MA than 10 MA.

This is consistent with data taken on Z. See presention by C. Myers.

With a linear rise to 20 MA, v_{plasma} ~ 1.6 cm/μs.



With a linear rise to 10 MA, v_{plasma} ~ 4.3 cm/μs.



- v_{plasma} is estimated from extent of H^+ 10^{16} cm^{-3} density.
- Slower joule heating results in later emission.
- Higher B-field inhibits diffusion for similar surface T_{ion}.*

$$D_B = \frac{\omega_c}{\nu_c} D_\perp \simeq \frac{k_B T}{m\omega_c} = \frac{k_B T}{eB}$$

* Bennett, et al. Phys. Rev AB **24**, 060401 (2021).

Conclusions and Outlook

- Based on the high temperatures and ionization cross sections, simulations of the Z Accelerator assume desorbed molecules are fully dissociated and ionized.
- High resolution simulations tested this assumption in kinetic simulations incorporating 10 ionization, 5 charge exchange and 10 elastic scattering interactions.
- The density distributions when full ionization is assumed lead the distributions from breakdown by 3 ns.
- Plasmas expand at rate of ~ 1.6 cm/μs at 20 MA.
- The impact of reducing the current drive (B-field) is consistent with Bohm diffusion. This is promising for higher-current systems.
- Under investigation:
    - electrode melt
    - behavior of the later-forming anode plasma
    - scaling with energy density
    - instabilities driven by interactions with currents entering from the adder region
    - the impact of ion mass or *q*/*m*

Fig. 12 from Phys. Rev AB **24**, 060401 (2021).