Field Emission Model for PIC-DSMC Simulations Based on Nanoscale Surface Characterization

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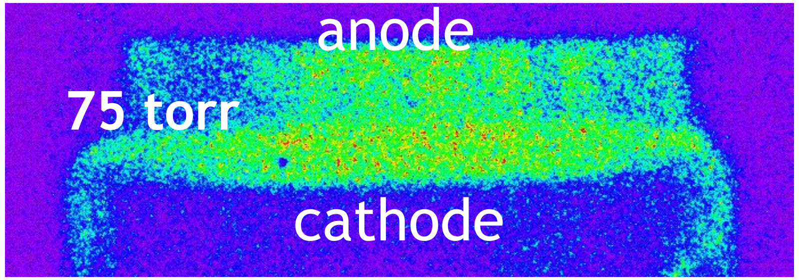
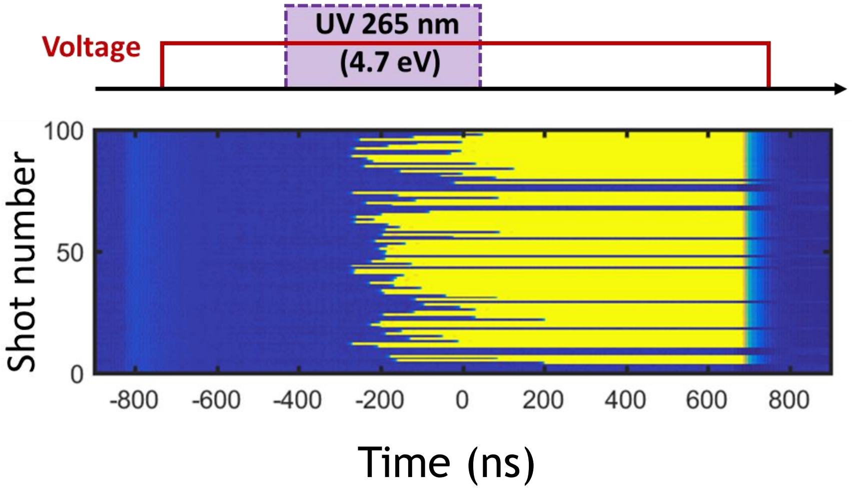
Introduction/Motivation

- We are interested in modeling a variety of discharge situations: from streamers at atmospheric pressure to vacuum arcs

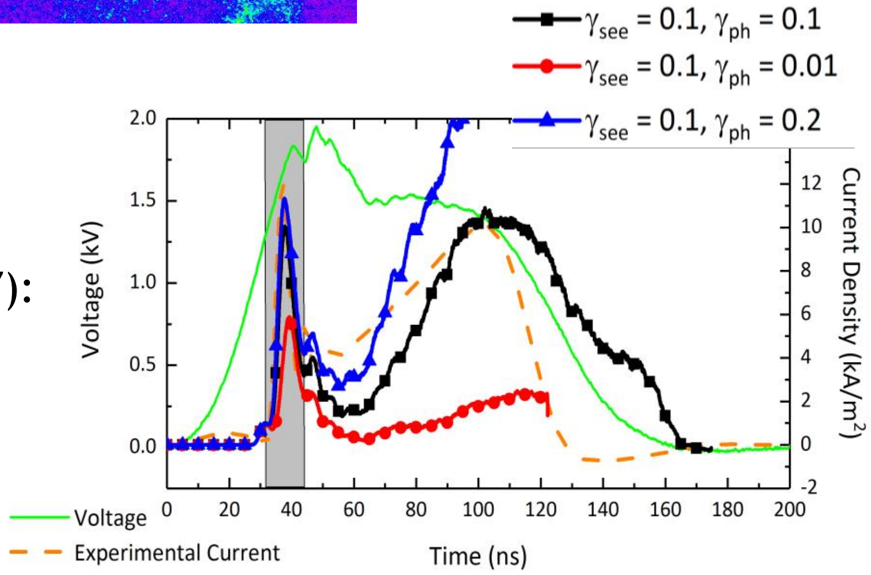
- We have multiple projects focused on how interactions with surfaces drive discharge
  - AMPPED is investigating photoemission and ion-induced SEE from surfaces:



Photon-assisted breakdown (E. Barnat, MeVArc 2018)



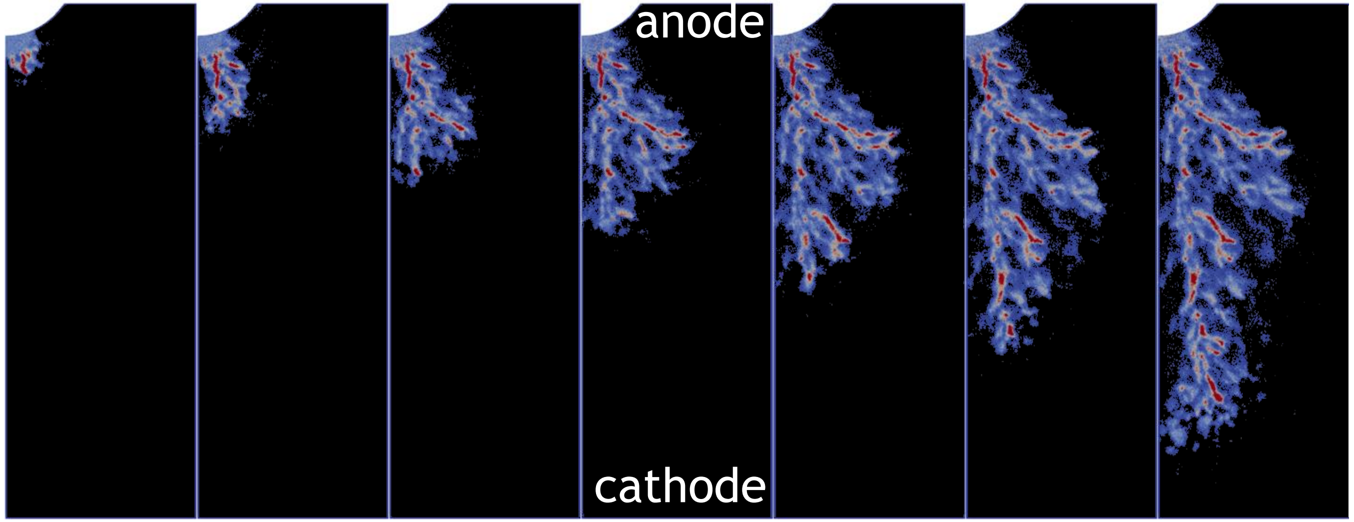
Dependence of low-pressure discharge on surface properties (A. Fierro, ICNSP 2017):



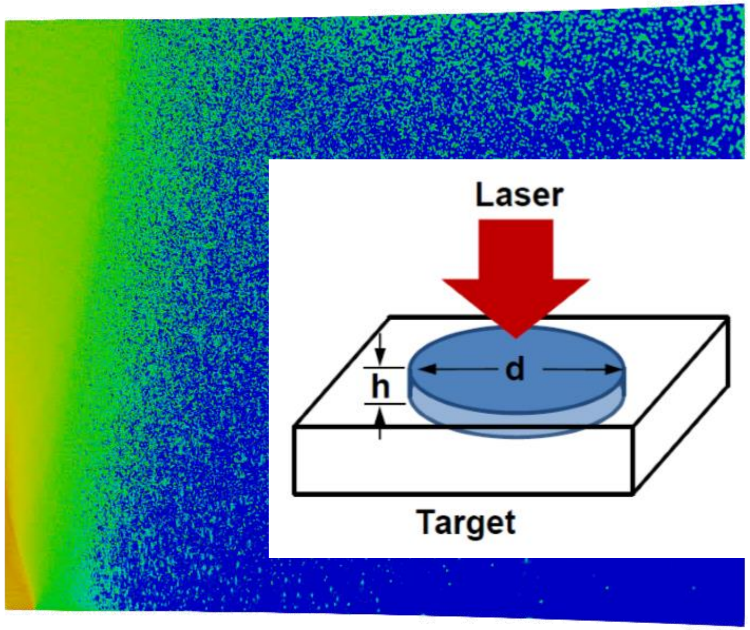
Introduction/Motivation

- We desire predictive PIC-DSMC breakdown simulations
  - Here predictive means capturing the bounds of discharge behavior due to stochastic variation of real surfaces (variation of contaminants, grain boundaries, dislocations, etc.) as built
  - It also means that we must perform rigorous Verification and Validation efforts before a model is considered useful

3D Streamer evolution (A. Jindal, ICOPS 2019):

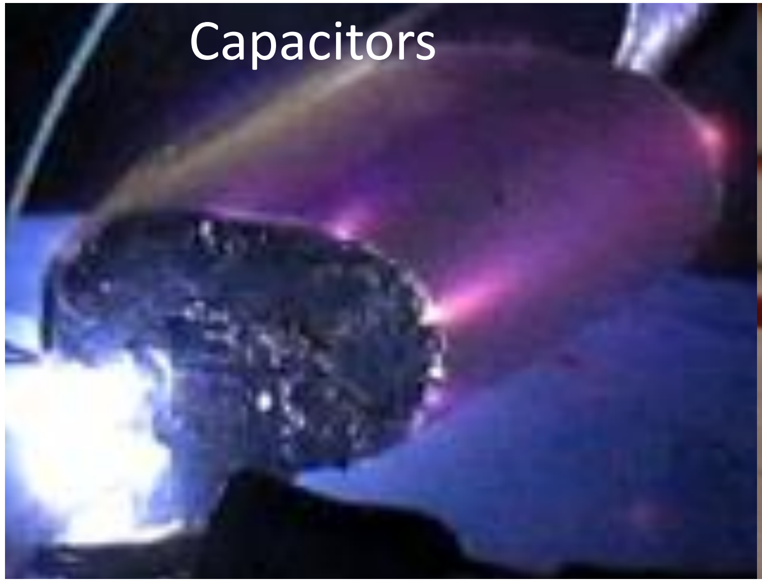


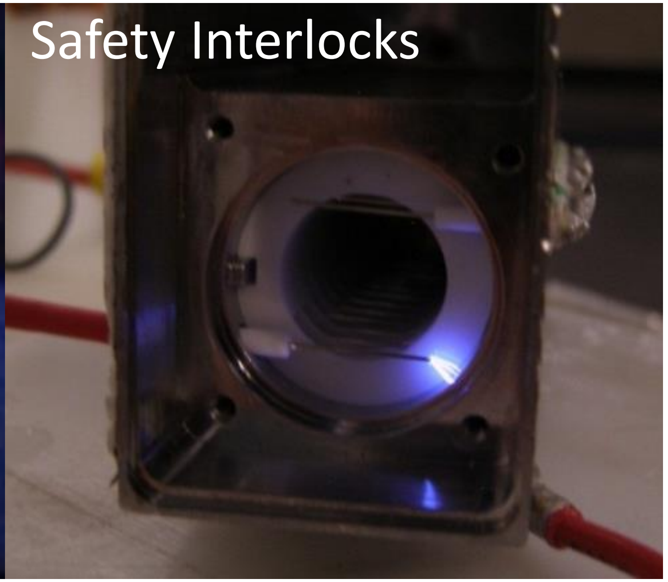
Laser-triggered switch
(A. Fierro, MeVArc 2018):



Vacuum Arc Initiation Project

- Vacuum discharge is critical to many modern devices.
  - Critical failure mechanism → Want to avoid
  - Mode of operation → Want to have predictable behavior





Vacuum Arc Initiation Project

- Vacuum discharge is critical to many modern devices.
  - Critical failure mechanism → Want to avoid
  - Mode of operation → Want to have predictable behavior

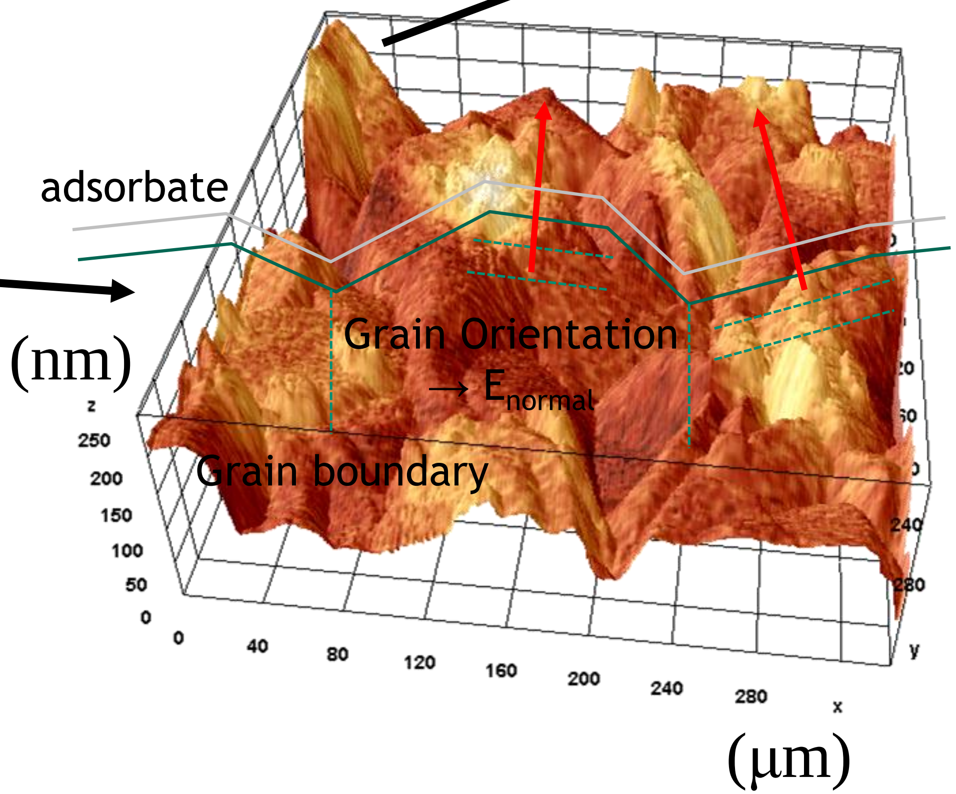
- We have a project to understand vacuum field emission from well-characterized surfaces to create physics-based models for use in large-scale PIC-DSMC breakdown simulations
  - Field emission is necessary precursor to a breakdown event. No field emission → no breakdown.
  - Employ Scanning Tunneling Microscopy and PhotoEmission Electron Microscopy to characterize surface very locally, and then apply high fields to initiate breakdown. Very locally = ~0.1-10 nm
  - Address the problem of not knowing the state prior to discharge at the location of discharge by characterizing and then discharging.
  - Apply known layers of dielectric (e.g.,TiO_2, MgO) to challenge models and begin investigation of role of surface contaminants.
  - Utilize a "meso-scale" (0.1-1.0 μm) model of the surface for PIC-DSMC simulation of breakdown

Why local characterization?

- Fowler-Nordheim field emission:
  - Typical use in macro-scale models is to curve-fit measured j(E) from the as-built electrode
  - Can result in β ~ 10-1000 !!!

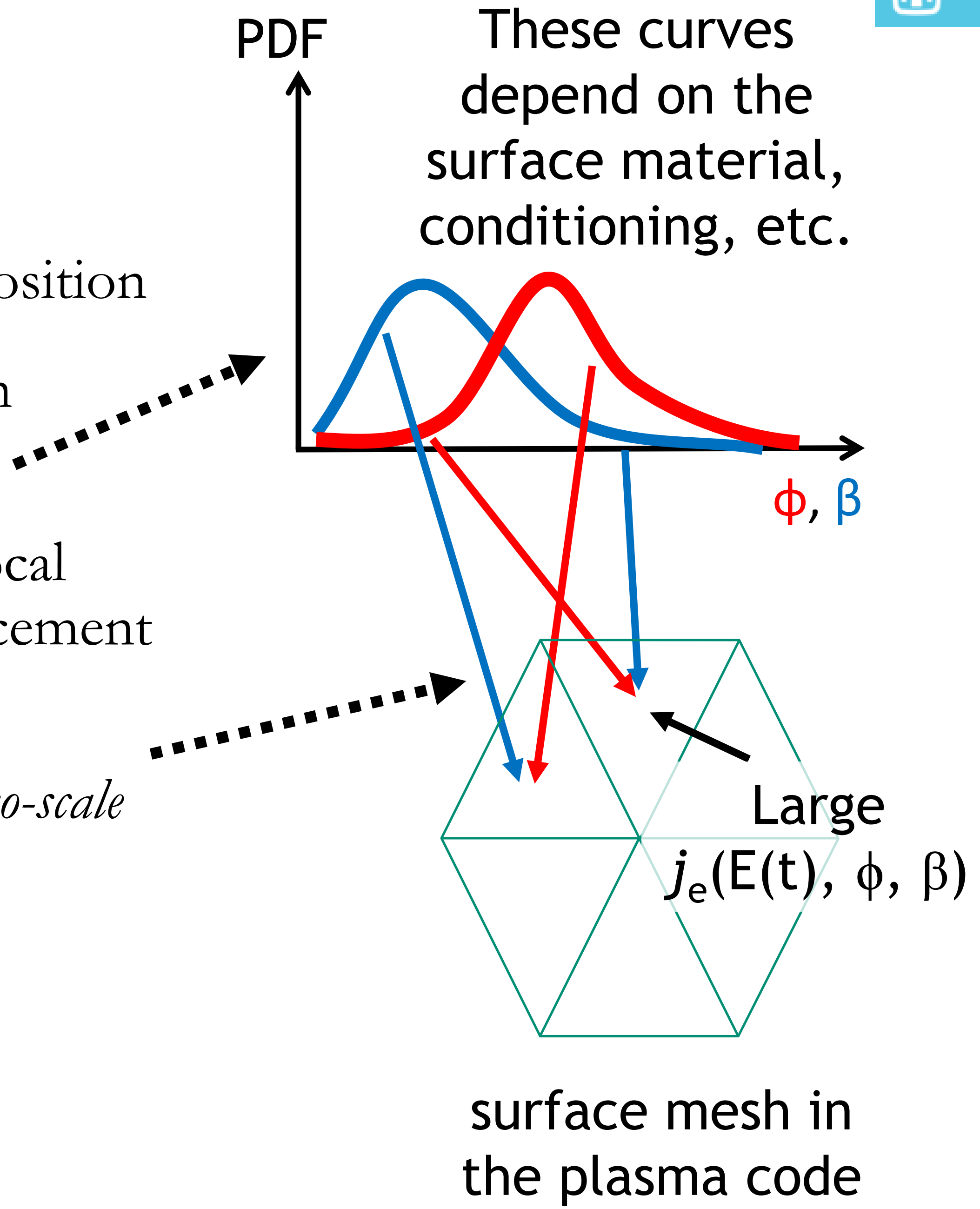
$$i = A_{eff} A_{FN} \frac{(\beta E)^2}{\phi t^2(y)} exp\left[-\frac{B_{FN} v(y) \phi^{3/2}}{\beta E}\right]$$

- We want to locally characterize the surface to eliminate β as a fit parameter
  - Use Scanning Tunneling Microscopy (STM) and Atomic Force Microscopy (AFM) to measure topology (β)
  - Use PhotoEmission Electron Microscopy (PEEM) to measure work function (ϕ)
  - Use measured distributions for ϕ and β to inform macro-scale model for discharge simulations



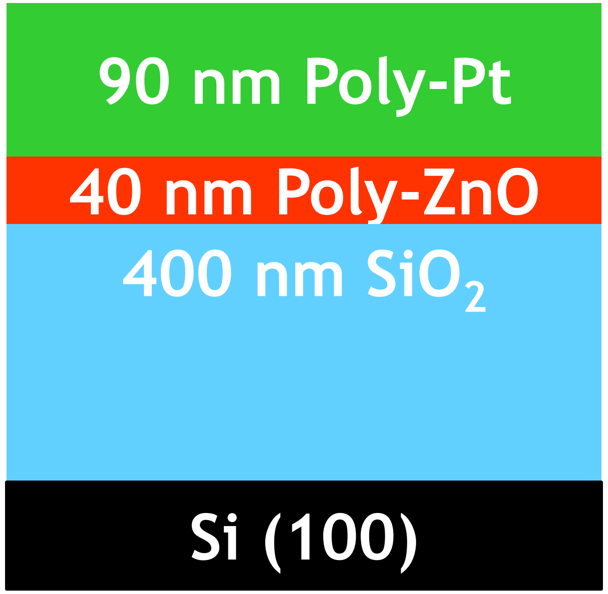
Overview

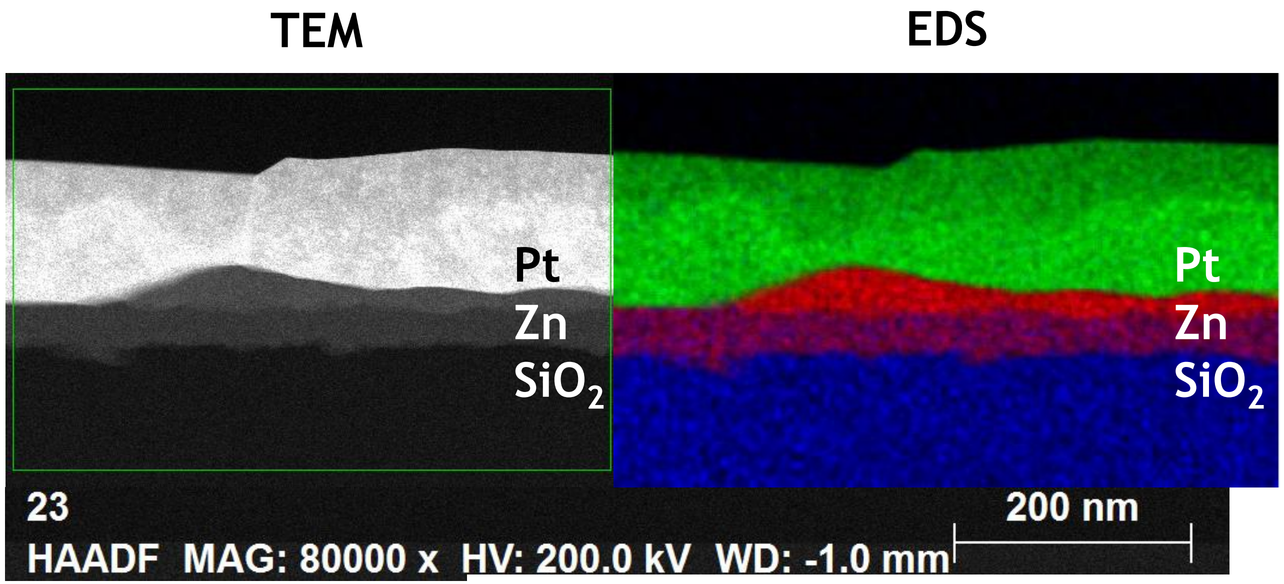
- Create Pt electrode via sputter deposition
- Controllably contaminate Pt via Atomic Layer Deposition
- Measure work function, local topology, and electron emission for sample
- Generate probability density functions (PDF) for local work functions and effective topological field enhancement
- Incorporate measured *atomic-scale* distributions into discharge simulations by populating time-varying *meso-scale* element-based data from the PDFs
- Compare family of plasma discharge simulations to measured breakdown behavior

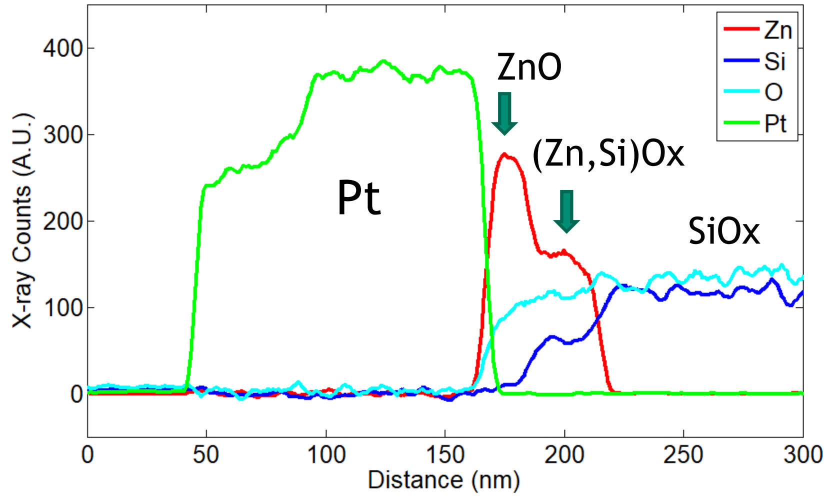


Characterization of the Electrode Stack

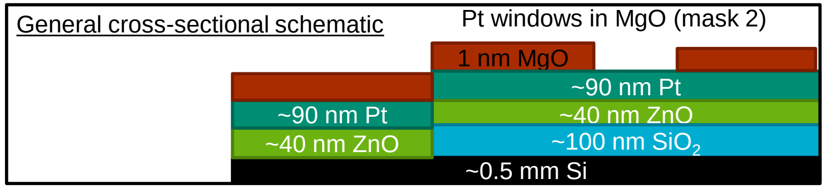
- Polycrystalline platinum electrode
  - Thermal SiO2-Si (100) substrate
  - RF sputtered Pt metal thin film & ZnO adhesion layer
  - Ambient anneal- 1 hr. at 900°C



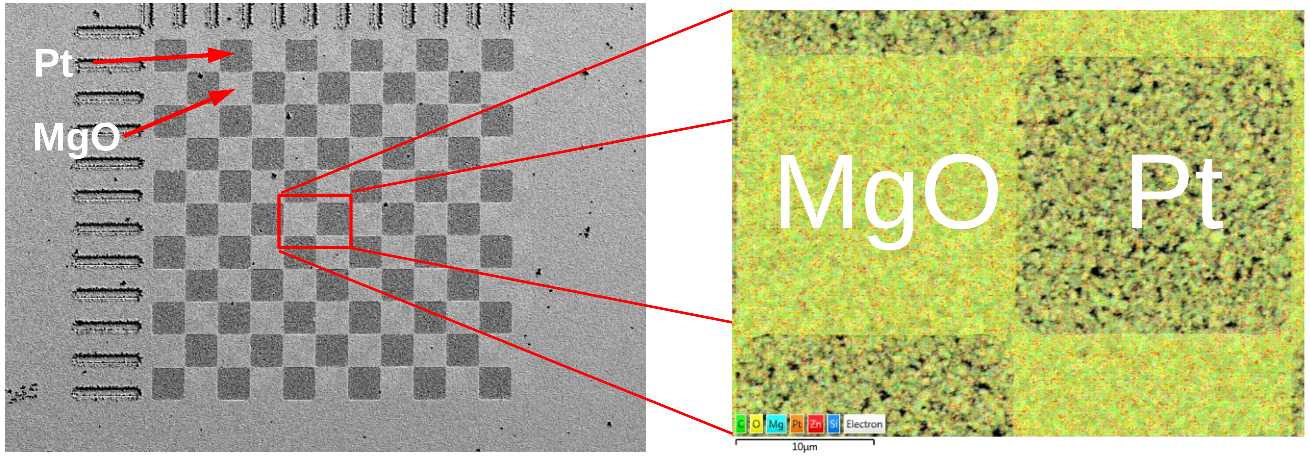


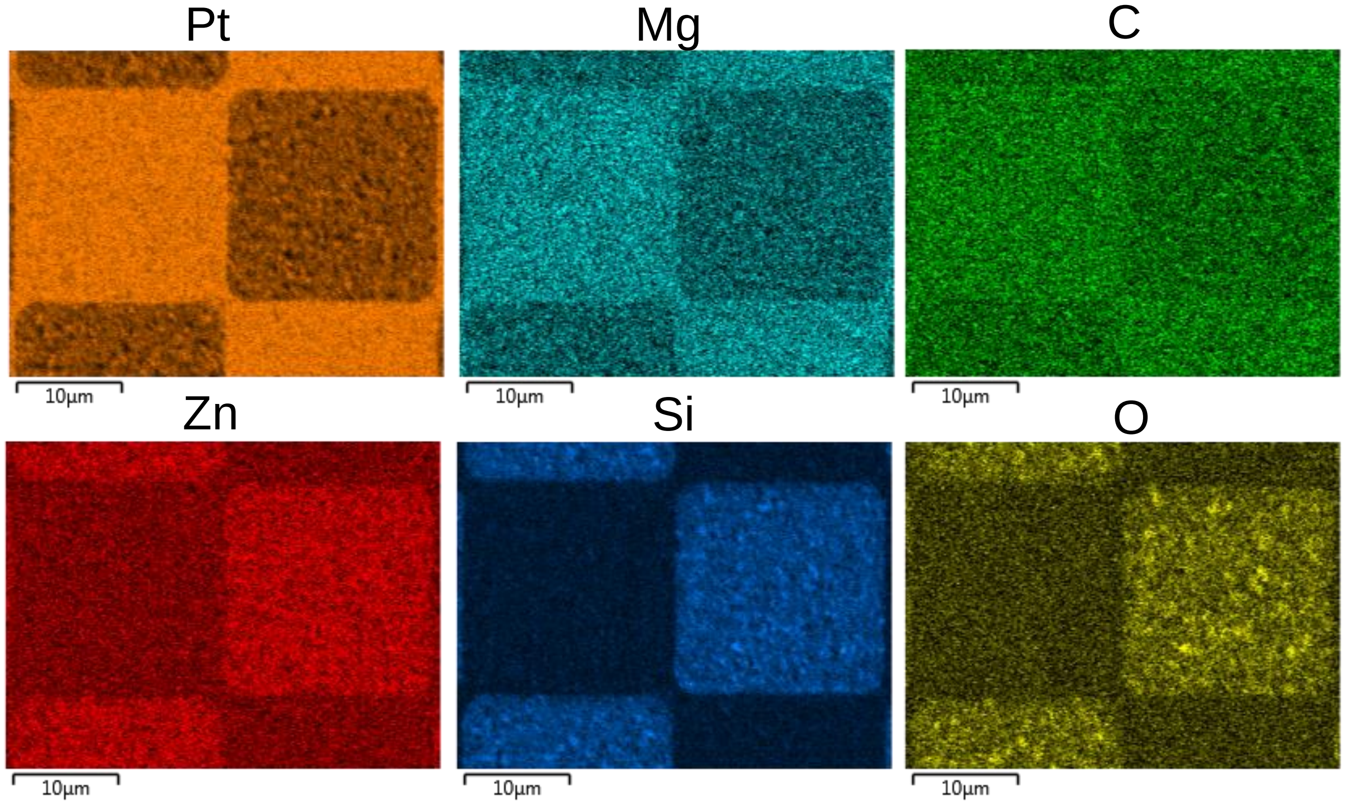


Characterization of the Electrode Stack



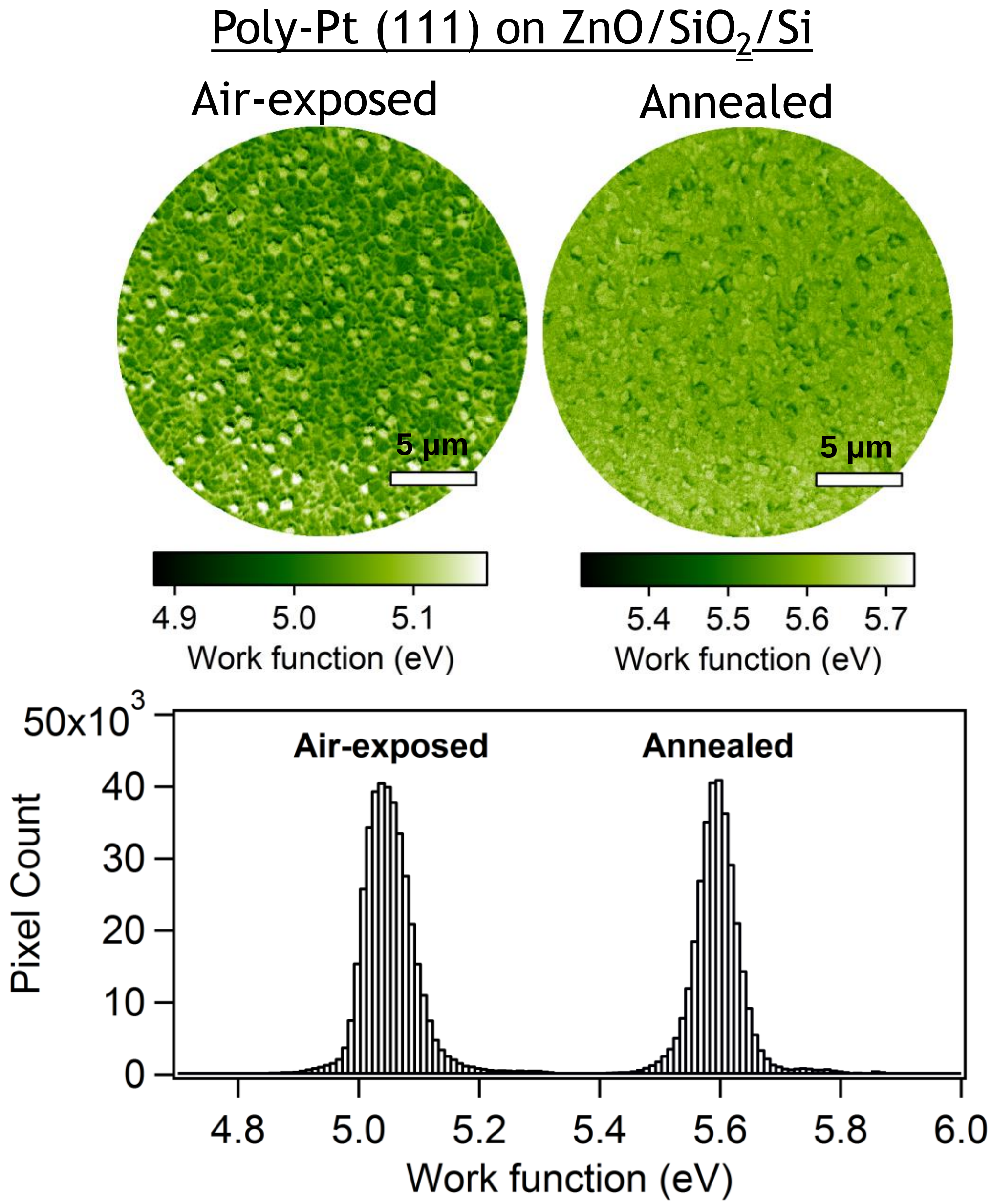
- To investigate surface contamination, put down a 1nm layer of MgO
  - Made "checkerboard" pattern via etch for direct comparison of Pt versus MgO/Pt emission and breakdown
- Use Scanning Electron Microscopy (SEM) and Energy Dispersive X-Ray Spectroscopy (EDS) to verify surface composition
  - Etch apparently went completely through the Pt, but also left patchy MgO
  - C contamination





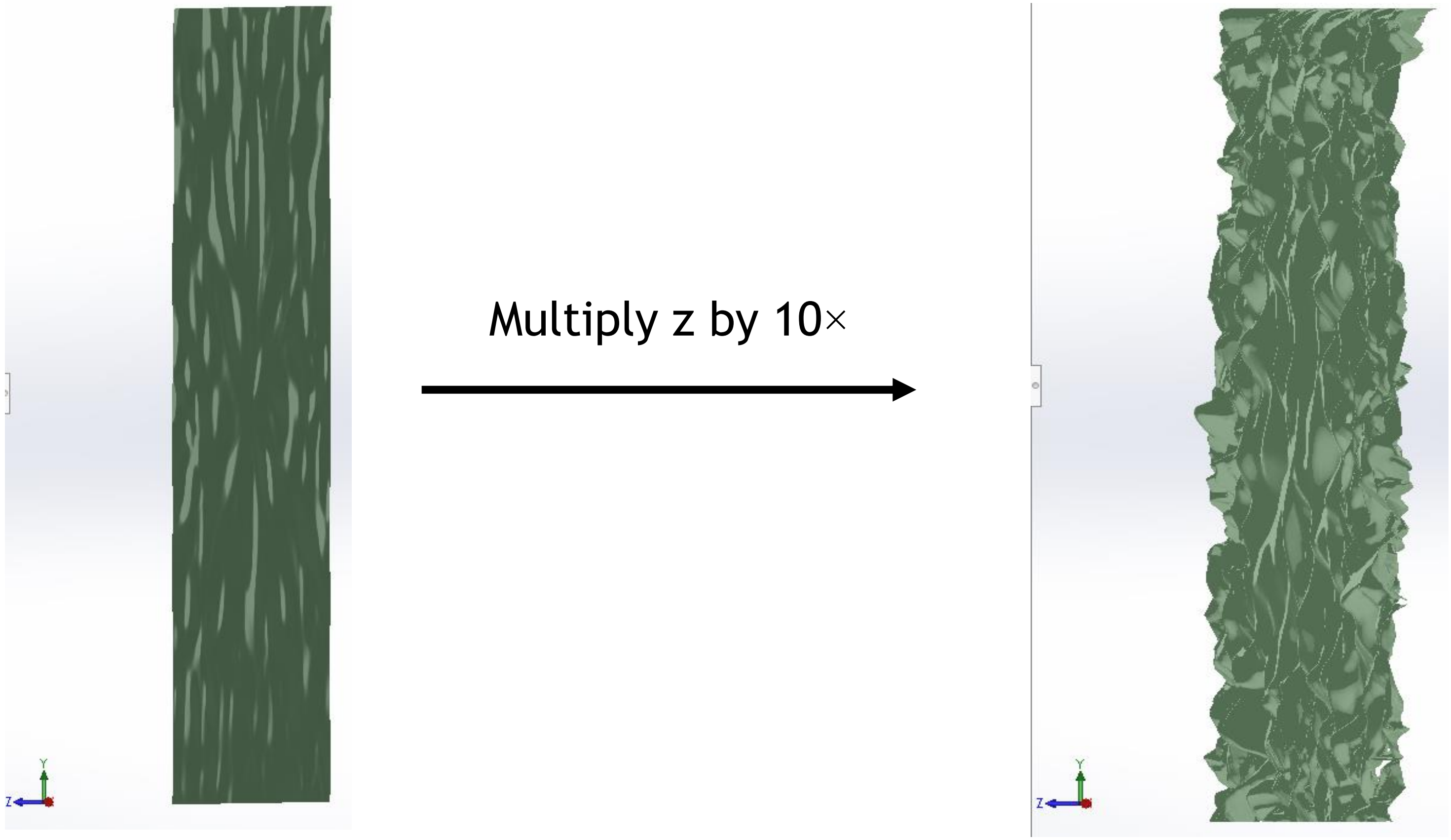
PEEM Measurement of Work Function Variation

- Measured spatial variation of local work function using PhotoEmission Electron Microscopy
  - Variation across given Pt surface relatively small – only a few percent
  - However, ϕ is in the exponential and the tail of the distribution can initiate field emission and eventually breakdown
- Significant (~10%) decrease in the work function due to surface contaminants picked up via exposure to air
- Use the ~10nm-scale PDF's in meso-scale model to set element work functions in PIC-DSMC simulations



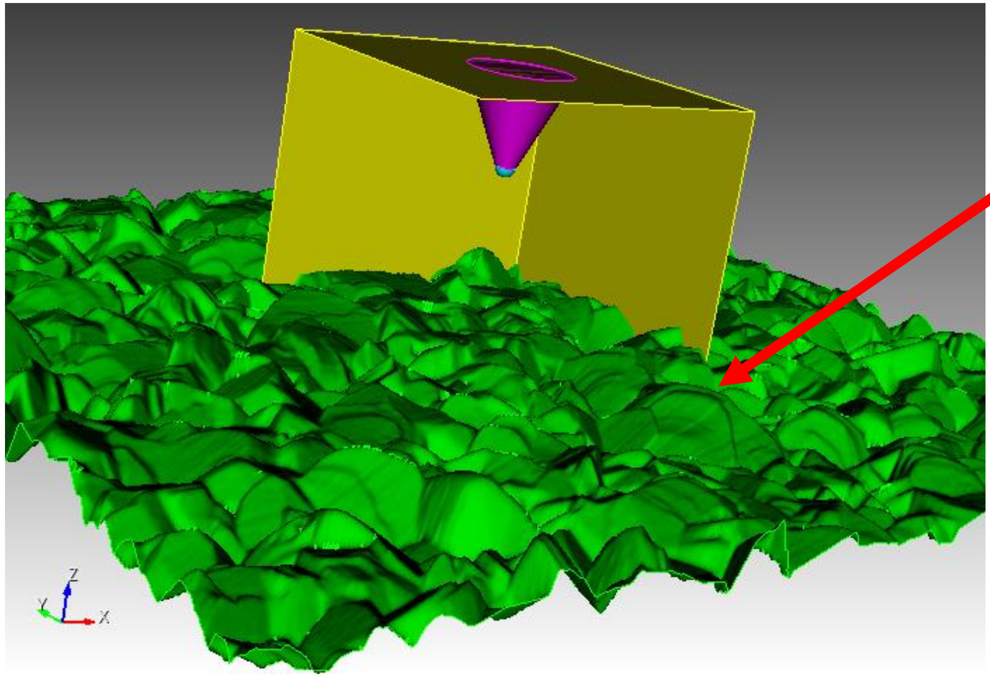
AFM Surface Characterization

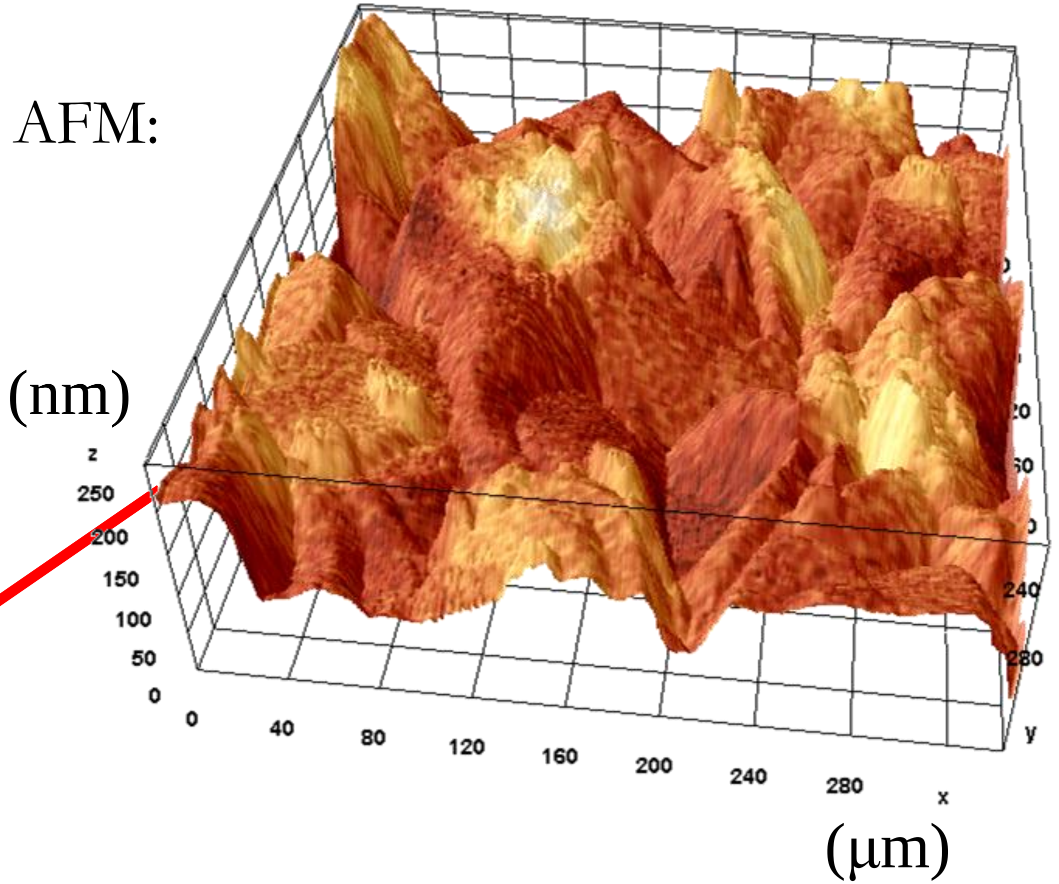
- Actual surface has virtually no significant topology and thus β ~ 1 everywhere.
- To demonstrate spatial variation of field emission across the surface we show results here based on multiplying the surface relief by 10×



AFM topology → topological atomic-scale β

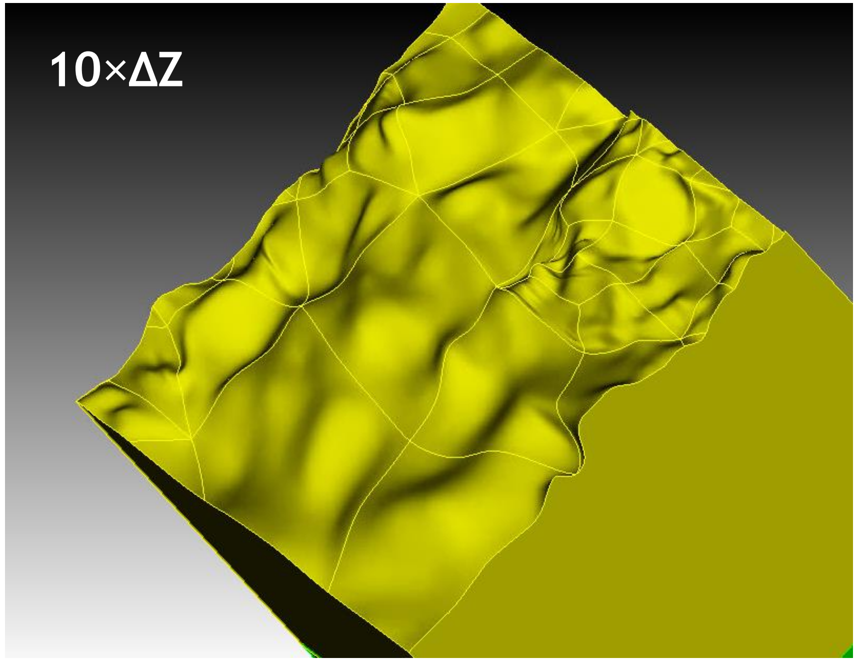
- Measure surface topology before breakdown using AFM:
- Load topology into Cubit and mesh the surface in order to use electrostatic solver
  - Place flat anode ~10μm from as-measured cathode
  - Use ~1 nm elements near cathode to resolve features



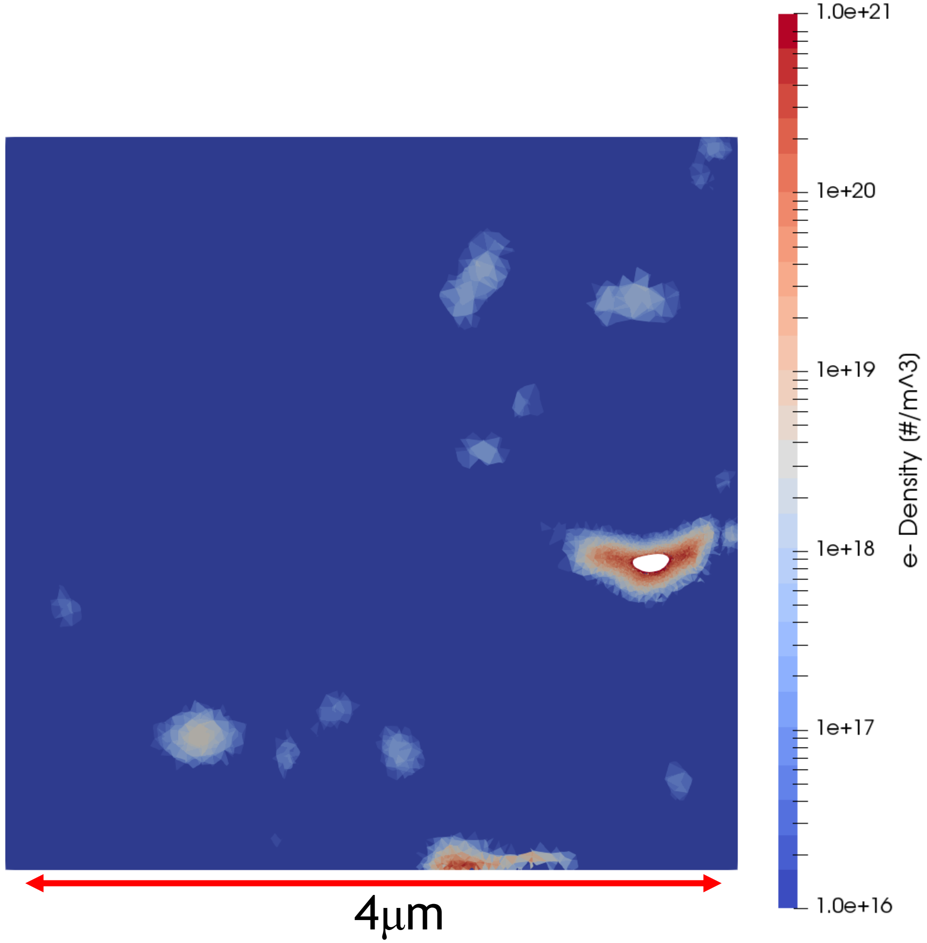


Simulation of Emission from AFM Surface

- With the resolved ($\Delta x < 10$nm) mesh, simulate the emission from the AFM surface
  - Show contours of e^- density just above the cathode surface
  - Some clipping of the topology is seen for the largest feature
- See several large-scale features that emit, otherwise very little emission

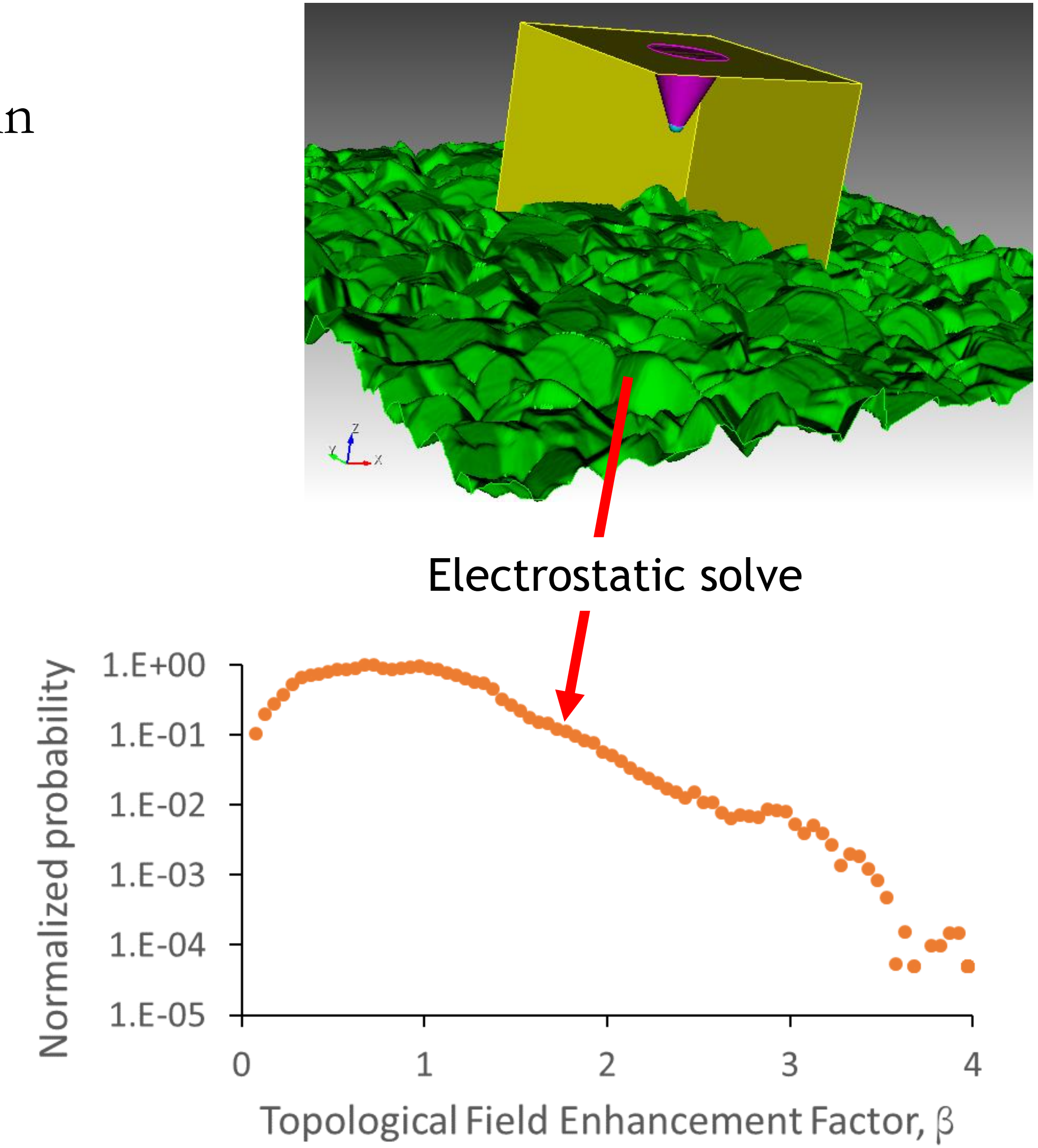


Simulate emission in PIC-code



AFM topology → topological atomic-scale β

- Compute E_{norm} and A_{proj} for every element face in the resolved STM mesh
  - <10nm elements; ~600K surface faces
- Get projection factor, $f_{proj} = \dfrac{\sum_{faces} A_{face}}{\sum_{faces} A_{proj,face}}$
  - For present data $f_{proj} \sim 1.15$
- Create ~10nm scale PDF of $\beta = \dfrac{E_{norm}}{E_{applied}}$
- Some elements will have β<1
  - Globally the surface could be tilted
  - Sides of "sharp" atomic features



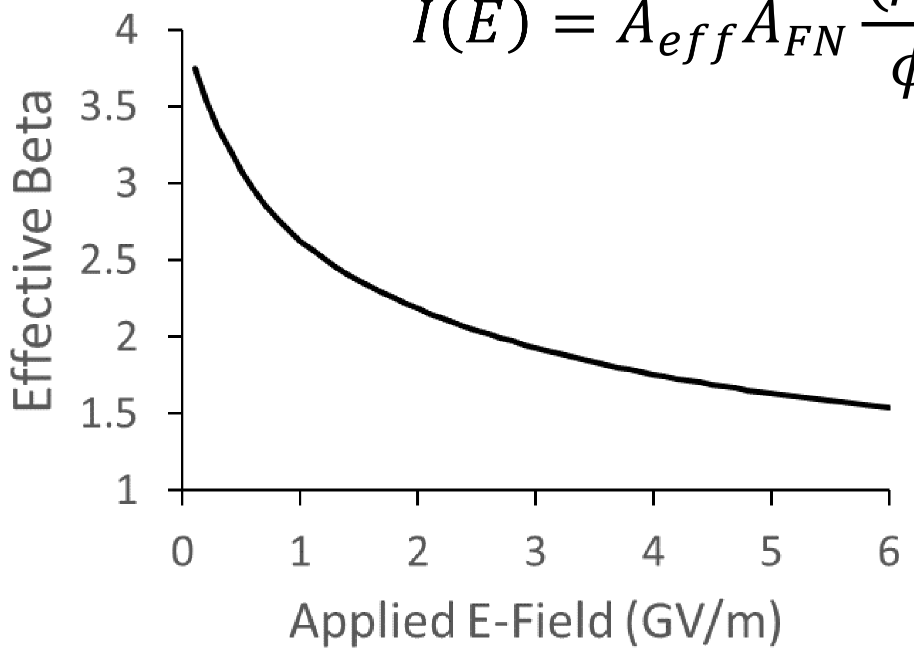
Meso-scale Model for Surface Variations

- We have measured atomic-scale (1-10nm) PDF's of the work function and topological field enhancement factor
- Must convert these to the meso-scale (0.1-10 μm). Some options:
  1. Just pick the meso-scale β and ϕ from the atomic-scale PDFs
  2. Make an effective β and ϕ to use at the meso-scale
  3. "Brute force" – for each meso-scale element face, pick N local emitters (unique β's and ϕ's)
- The first option obviously has artificially large variation for different surface realizations in simulations. We will not consider it further.
  - Sometimes get an extreme tail value and then field emit based on the meso-scale element's area
  - Other times there will be no tail values picked and no field emission until much higher fields

Meso-scale Model for Surface Variations

- Can we make an effective β (and ϕ) from the data and/or atomic-scale β PDFs?
- Measure/compute the total field emission current versus $E_{applied}$
- Non-linear solve for β_{eff}:

$$I(E) = A_{eff}A_{FN}\frac{(\beta_{eff}E)^2}{\phi t^2(y)}exp\left[-\frac{B_{FN}v(y)\phi^{3/2}}{\beta_{eff}E}\right]$$



→ **β_{eff} depends on $E_{applied}$!**

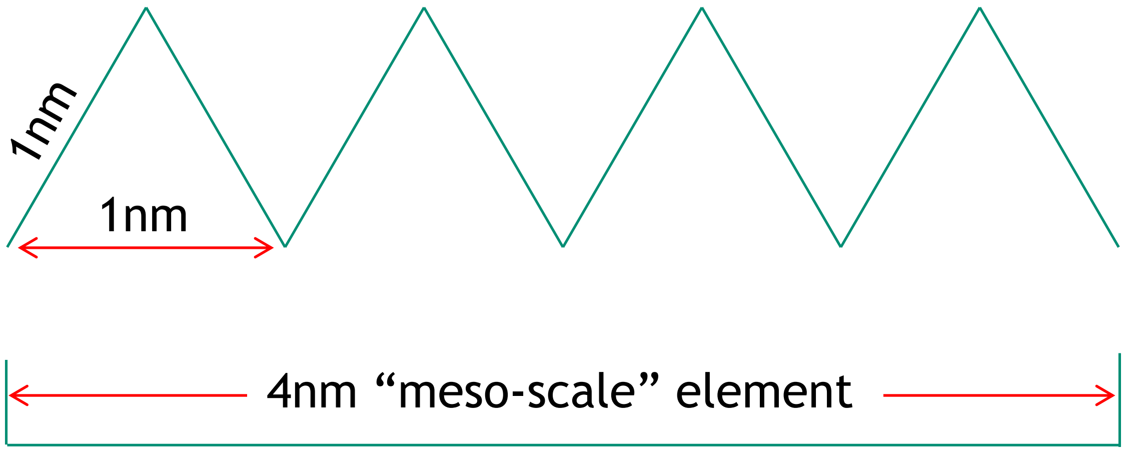
- This makes sense: small β regions "turn on" at higher fields and pulls the effective β lower
- The precise functional form depends on the atomic-scale β PDF

Meso-scale Model for Surface Variations

- We are left with "brute force" -- for each meso-scale element face, pick N local emitters (randomly pick unique β's and ϕ's) from the atomic-scale measured distributions:

$$N = \frac{A_{element}}{A_{resolved}} f_{proj}$$

- Must scale the number of local emitters to draw:



8 local faces that the β and ϕ PDF created from

$$f_{proj} = \frac{\sum_{faces} A_{face}}{\sum_{faces} A_{proj,face}} = 2$$

Draw 8 local emitters

Meso-scale Model for Surface Variations

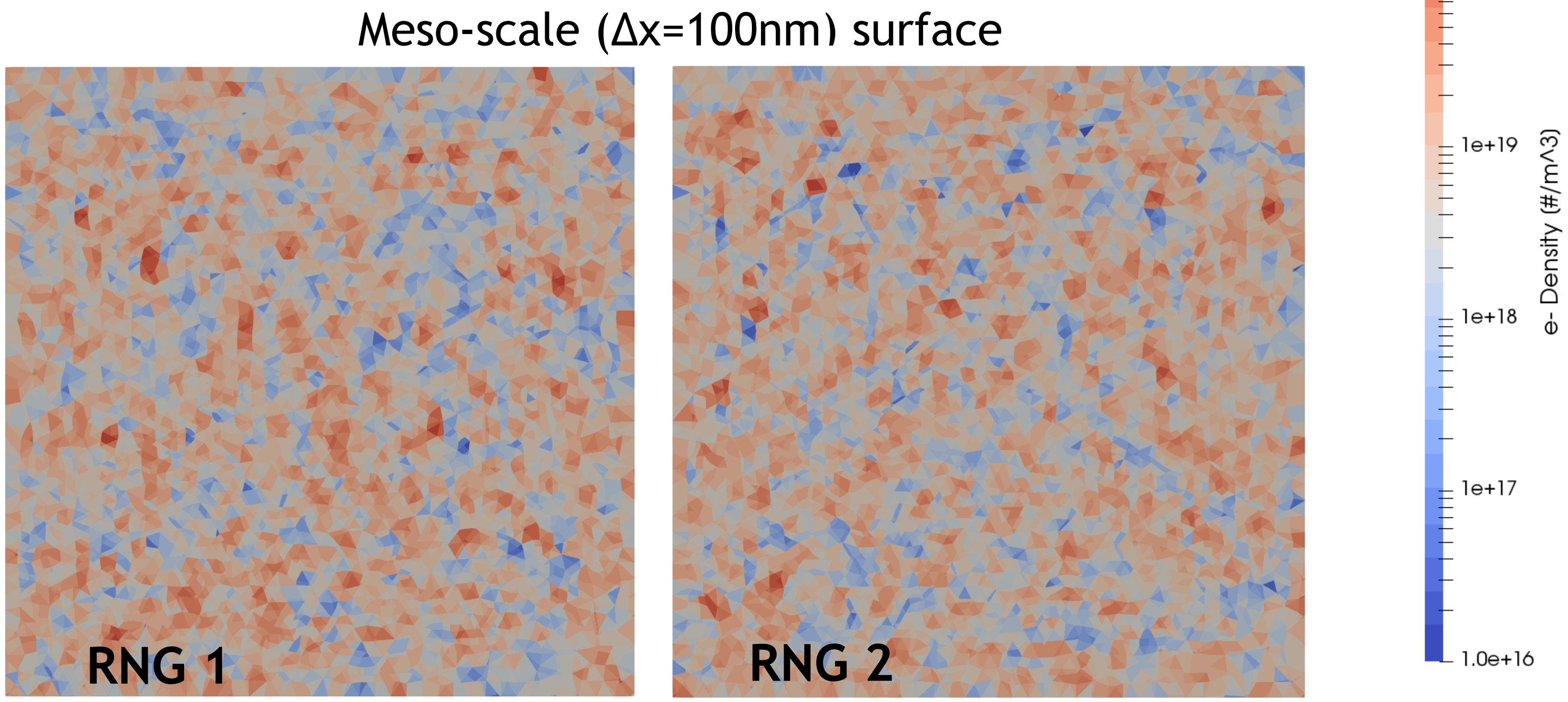
- However, we don't have to store all N local emitters for each surface element face
  - Field emission is highly non-linear and the majority of emitters (β and ϕ) can be neglected
- Store every atomic-scale emitter (β and ϕ) that appreciably contributes to the current
  - A threshold current contribution of 0.1% results in storing ~0.01% of the atomic-scale emitters
  - 1 μm^2 element has 10^4–10^6 atomic-scale emitters → store <1000 emitters.

- PIC field emission algorithm each Δt:
  - Compute E_{norm} on each surface element face
  - Loop over all ~100 atomic-scale emitters:

$$I_{face} = \sum_{emitters} A_e A_{FN} \frac{(\beta_e E_{norm})^2}{\phi_e t^2(y)} exp\left[-\frac{B_{FN} v(y) \phi_e^{1.5}}{\beta_e E_{norm}}\right]$$

Meso-scale Field Emission Simulations

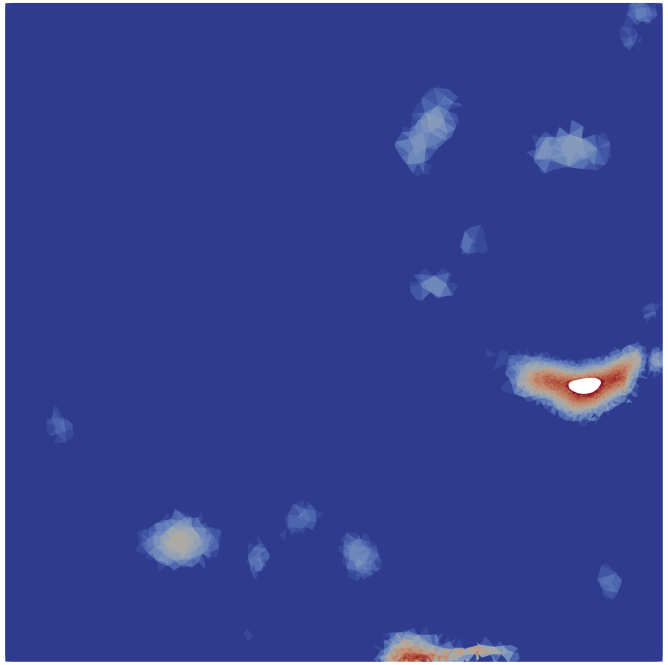
- Meso-scale model does show stochastic variation in the e- density just above the surface based on the random seed
- Goal is to be able to sample many possible surfaces (e.g. different β's and ϕ's) and compute breakdown probabilities for as-built surfaces



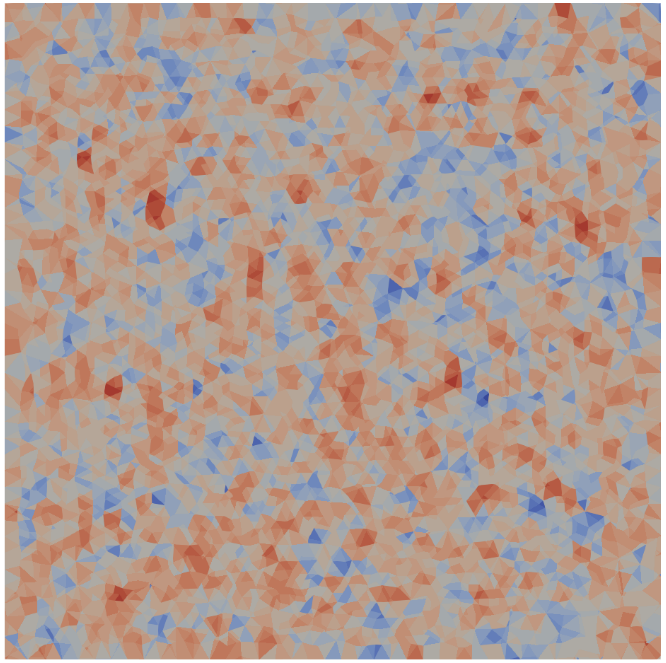
Meso-scale Field Emission Simulations

- Contours of electron density just above the cathode show very different spatial variation between the meshed STM surface and the flat, meso-scale surfaces
  - The STM surface was sputtered deposited Pt → large, ~micron-scale features are apparent
  - The current model picks atomic-scale emitter properties (β's and ϕ's) independently for every "meso-scale" surface elements. Clearly not independent for sputtered deposited Pt

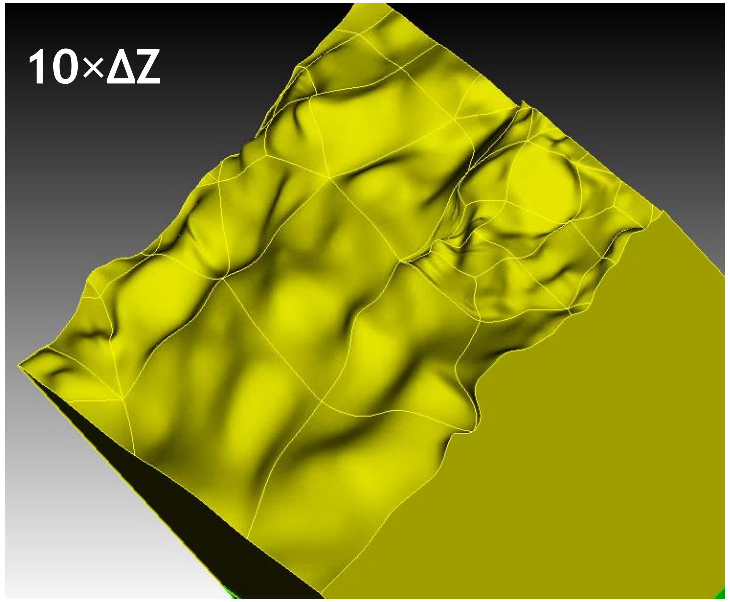
STM (Δx<10nm) surface

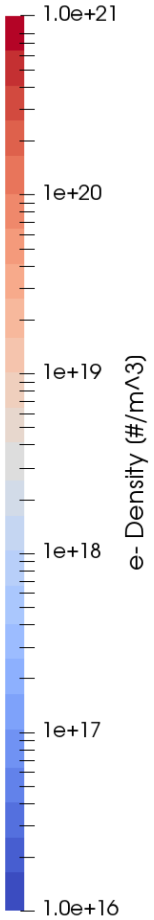


Meso-scale (Δx=100nm) surface



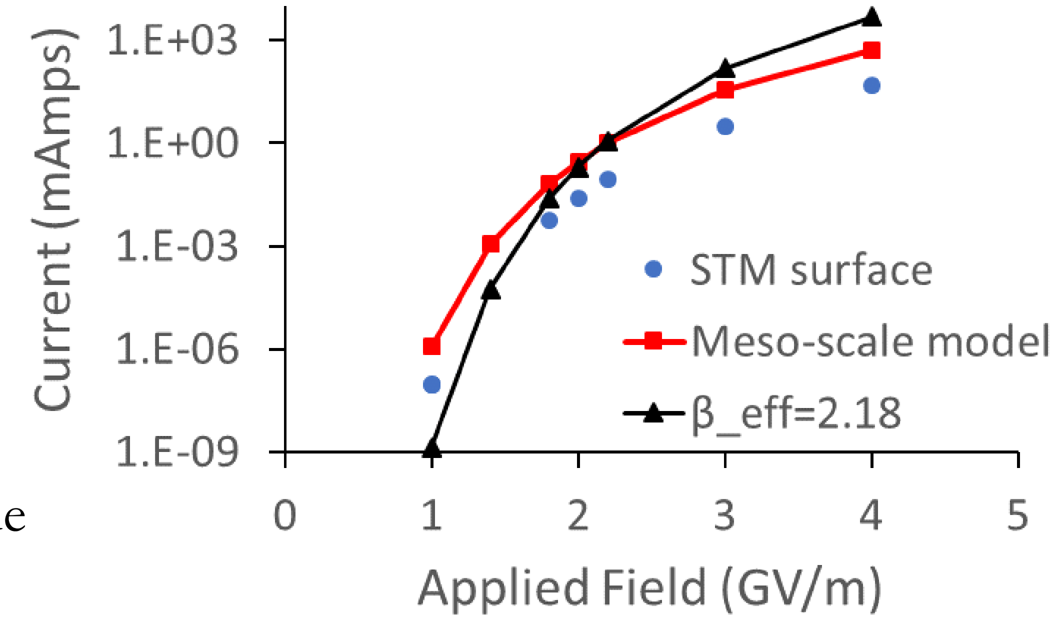
STM surface topology

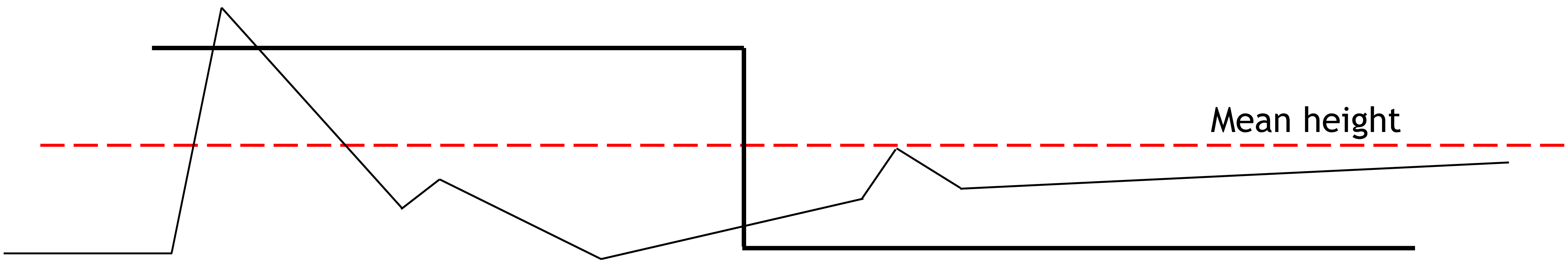




Meso-scale Field Emission Simulations

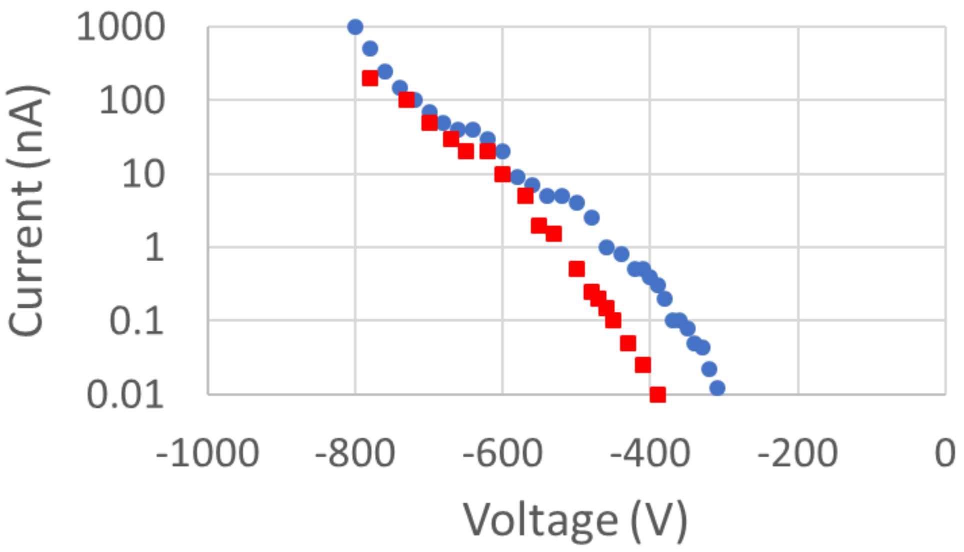
- Compare computed global current versus applied field for the resolved STM surface and meso-scale model surface
  - Stochastic variation in the meso-scale currents small
- The meso-scale model currents have the same trend as the STM surface, but ~$12 \times i_{STM}$
  - Difference partially (mostly?) from variation in fields due to changes in gap distance for the STM surface
  - Flat anode placed 10.4μm from the mean STM cathode height





Initial Local STM Breakdown Results

- Took local field emission i-V curves with tip radius < 100nm at a distance of ~200nm

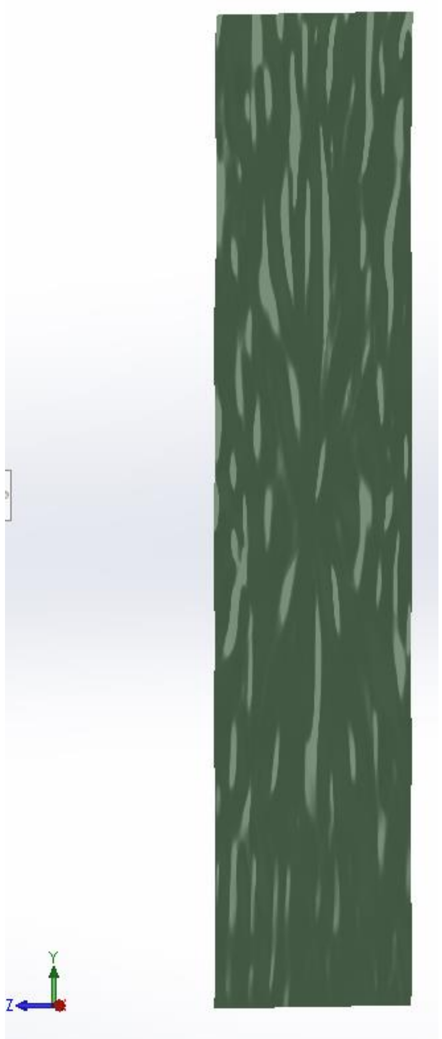


- Relatively feature-less surface with small-β within the region of the tip field footprint

- Breakdown at ~4 GV/m!

- This seems to be evidence that, at least for relatively smooth sputter deposited Pt, we do not have small-β atomic-scale features that grow into large-β features which then allow breakdown to occur at ~10 MV/m.

- Perhaps there is a special feature somewhere on a ~1 cm^2 electrode that results in (or can grow to) a large enough β to get breakdown at ~10 MV/m that was not present on our ~10^{-6} cm^2 sampled area.



Δz<0.1 μm over 10μm

Conclusions

- Investigating surfaces at the atomic scale to characterize features relevant to vacuum field emission.
  - Want to clarify β-based field emission so β really is only geometry induced field enhancement.
- By examining field emission at the nanoscale, we have attempted to create a meso-scale physics-based model suitable for predictive (and stochastic) PIC simulation of emission
  - Still have a long way to go – any ideas/suggestions??
- Characterized region, then performed local discharge in STM (spatially constrained surface participation) → Breakdown occurred at ~4 GV/m!
  - Region was flat and uninteresting – the breakdown field is consistent with breakdown from region with a small β

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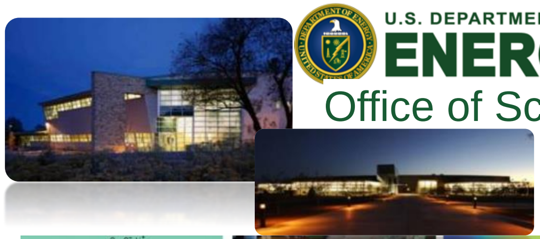

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