SAND2019-10509C

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

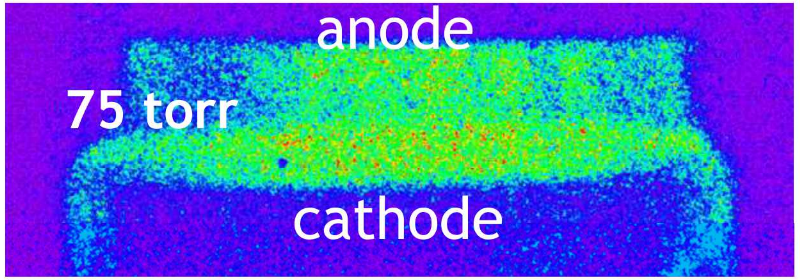
Chris Moore, Ashish Jindal, Ezra Bussmann, Taisuke Ohta, Morgann Berg, Cherrelle Thomas, David Scrymgeour, Paul Clem, Matthew Hopkins

Supported by the Laboratory Directed Research and Development program at Sandia National Laboratories, a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

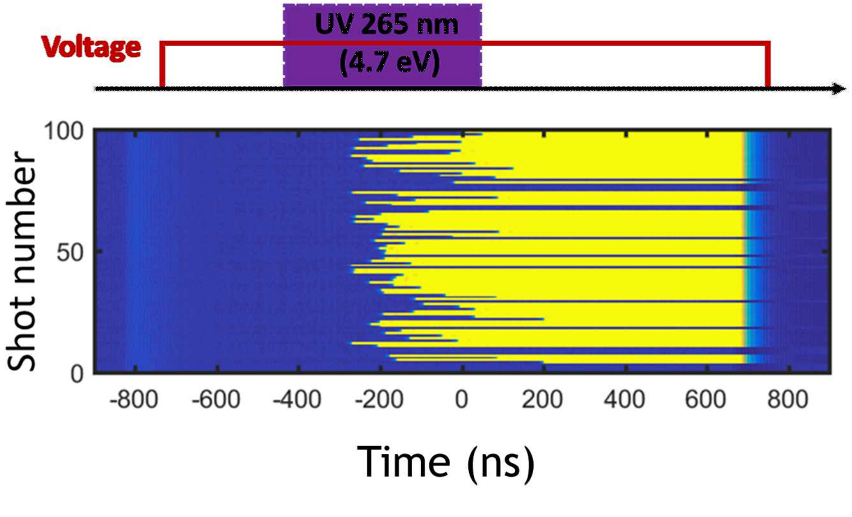
Additional Support: CINT User Facility (DE-AC04-94AL85000)

Introduction/Motivation

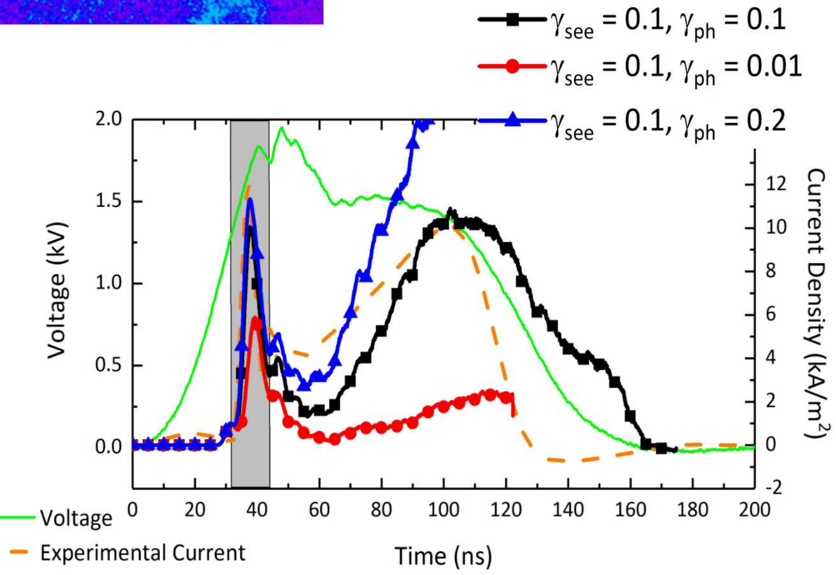
- We are interested in modeling a variety of discharge situations: from streamers at atmospheric pressure to vacuum arcs
- We have multiple projects focused on how interactions with surfaces drive discharge
  - AMPPED is investigating photoemission and ion-induced SEE from surfaces:



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



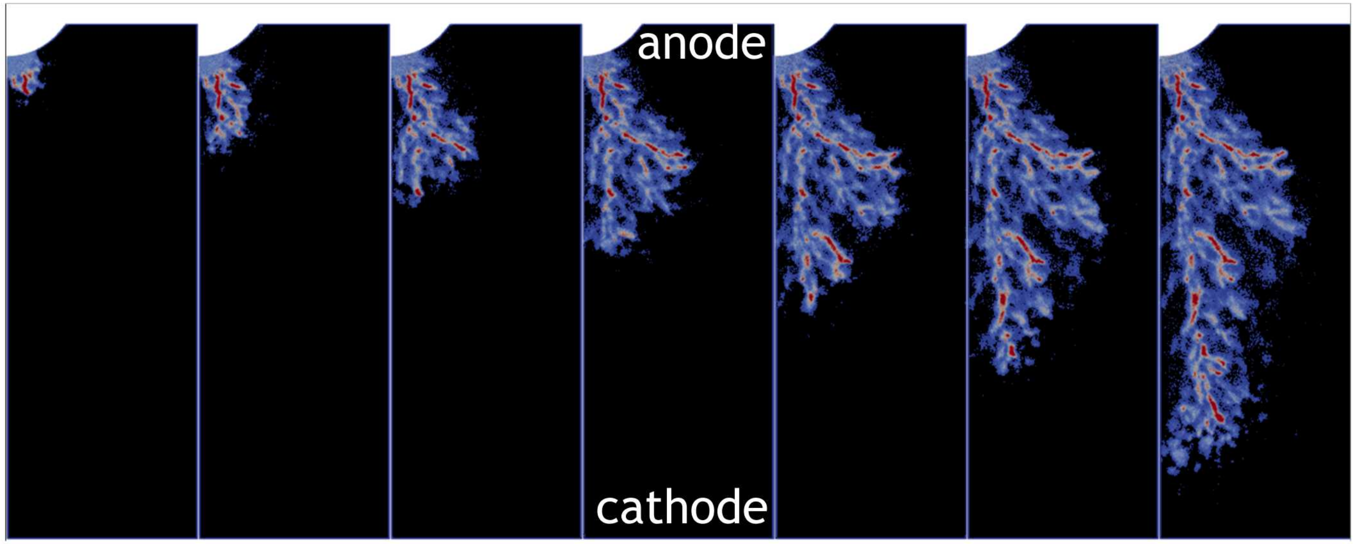
Dependence of low-pressure discharge on surface properties (A. Fierro, ICNSP 2017):



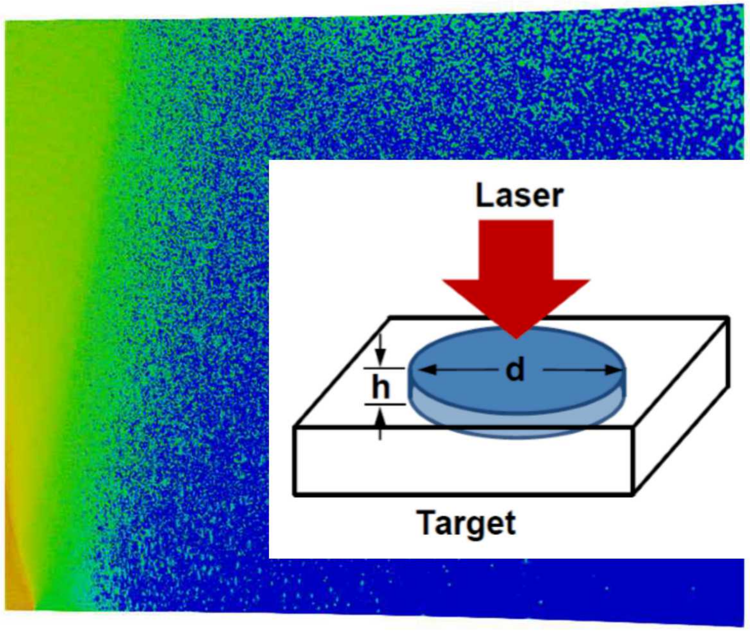
Introduction/Motivation

- 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):

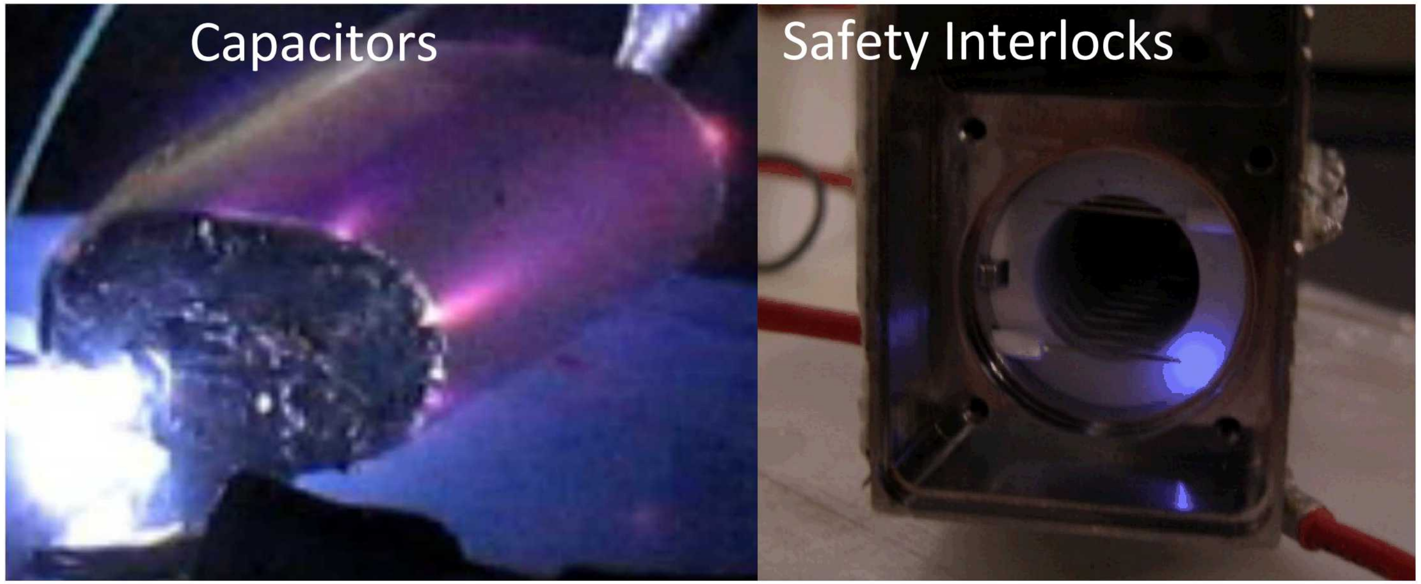


Laser-triggered switch
(A. Fierro, MeVArc 2018):



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

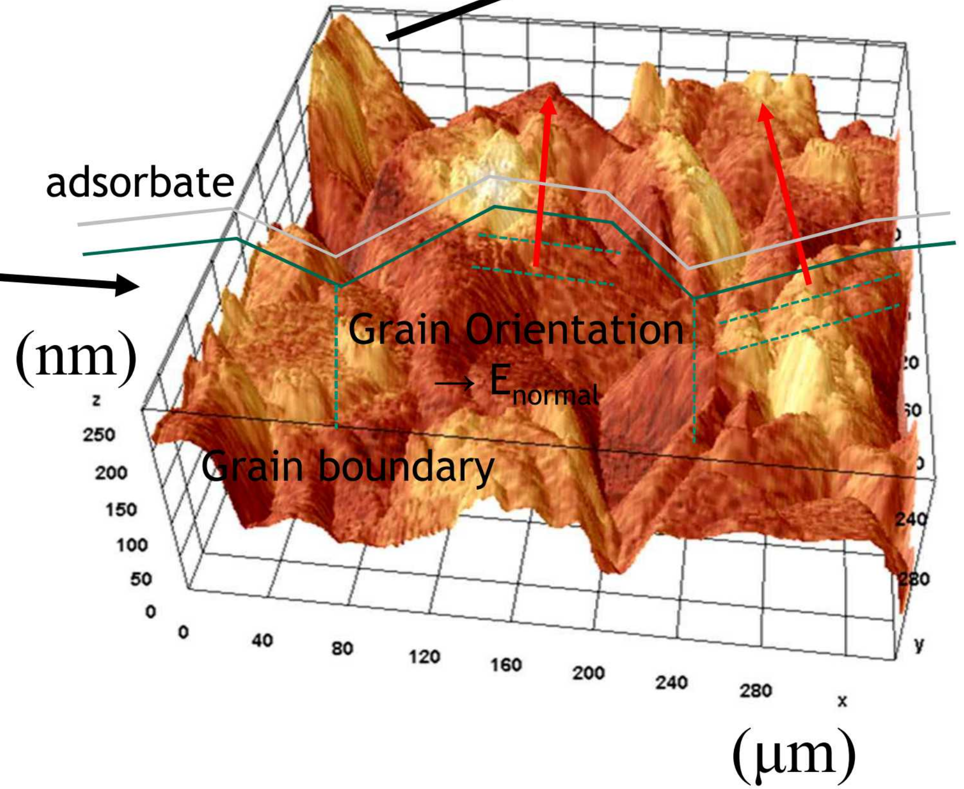
- We have a project to understand vacuum field emission from well-characterized surfaces to create physics-based models for use in large-scale PIC-DSMC breakdown simulations
  - Field emission is necessary precursor to a breakdown event. No field emission → no breakdown.
  - Employ Scanning Tunneling 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 !!!

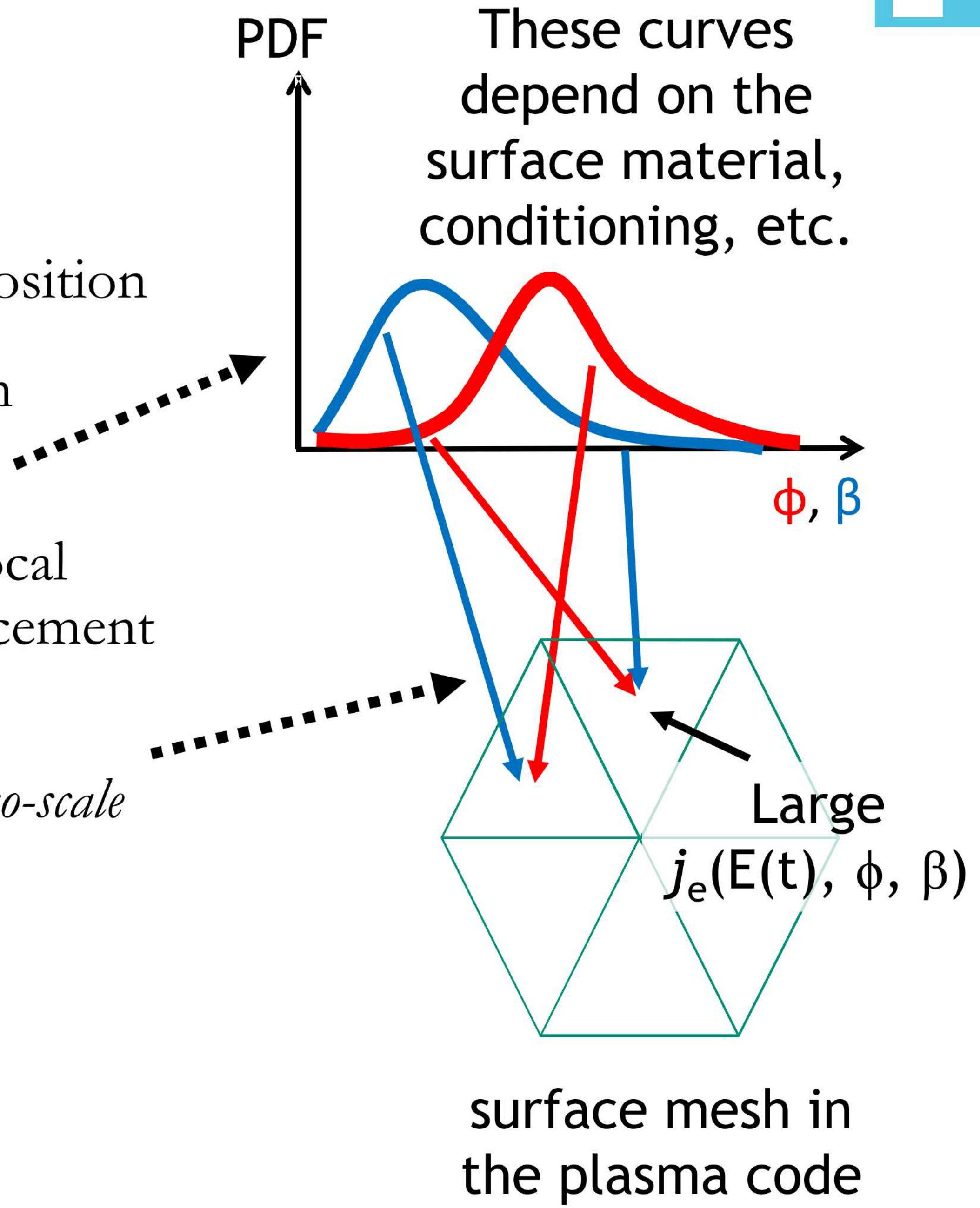
$$i = A_{eff} A_{FN} \frac{(\beta E)^2}{\phi t^2(y)} exp\left[-\frac{B_{FN} v(y) \phi^{3/2}}{\beta E}\right]$$

- 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



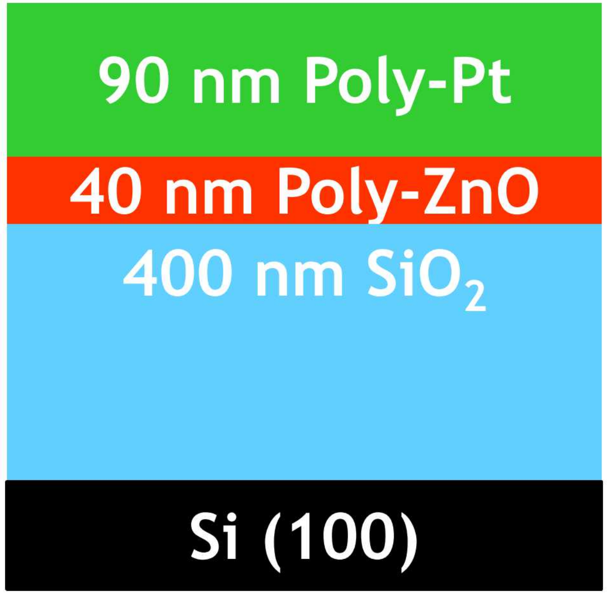
Overview

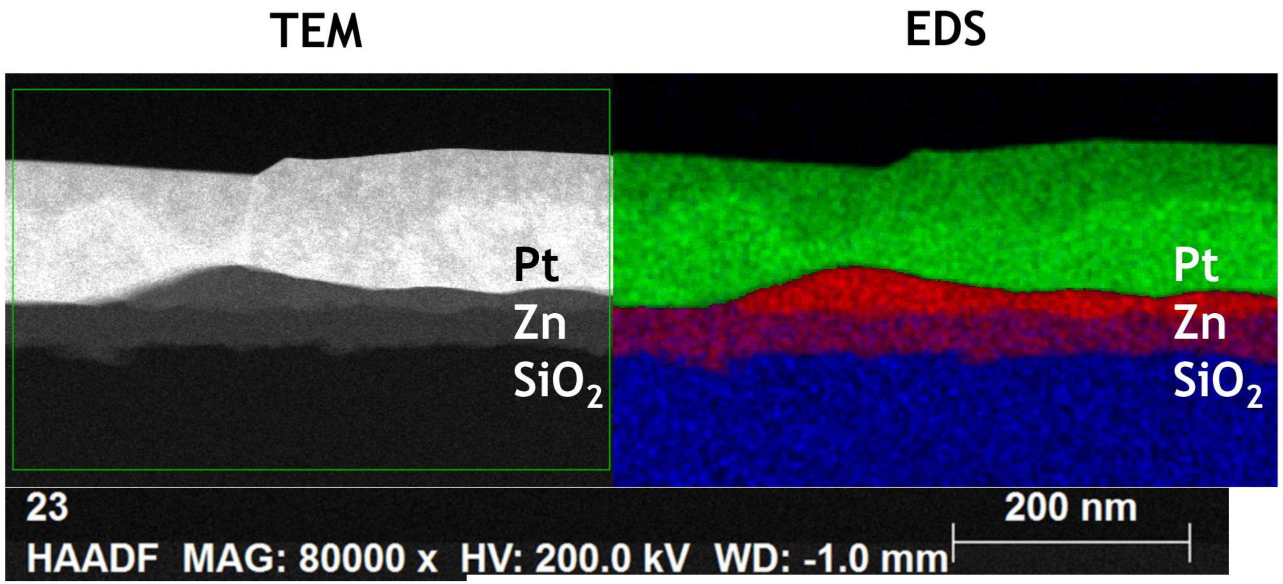
- Create Pt electrode via sputter deposition
- Controllably contaminate Pt via Atomic Layer Deposition
- Measure work function, local topology, and electron emission for sample
- Generate probability density functions (PDF) for local work functions and effective topological field enhancement
- Incorporate 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

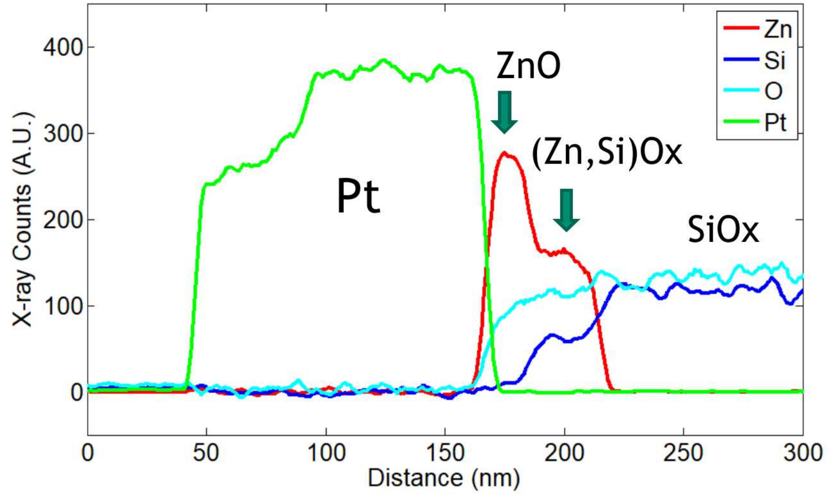


Characterization of the Electrode Stack

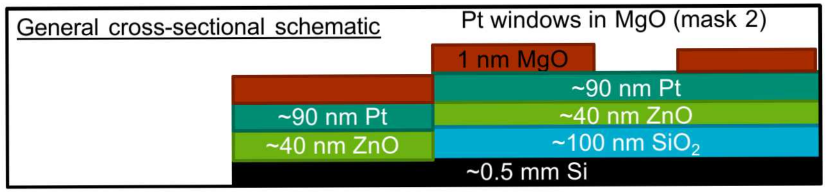
- Polycrystalline platinum electrode
  - Thermal SiO2-Si (100) substrate
  - RF sputtered Pt metal thin film & ZnO adhesion layer
  - Ambient anneal- 1 hr. at 900°C



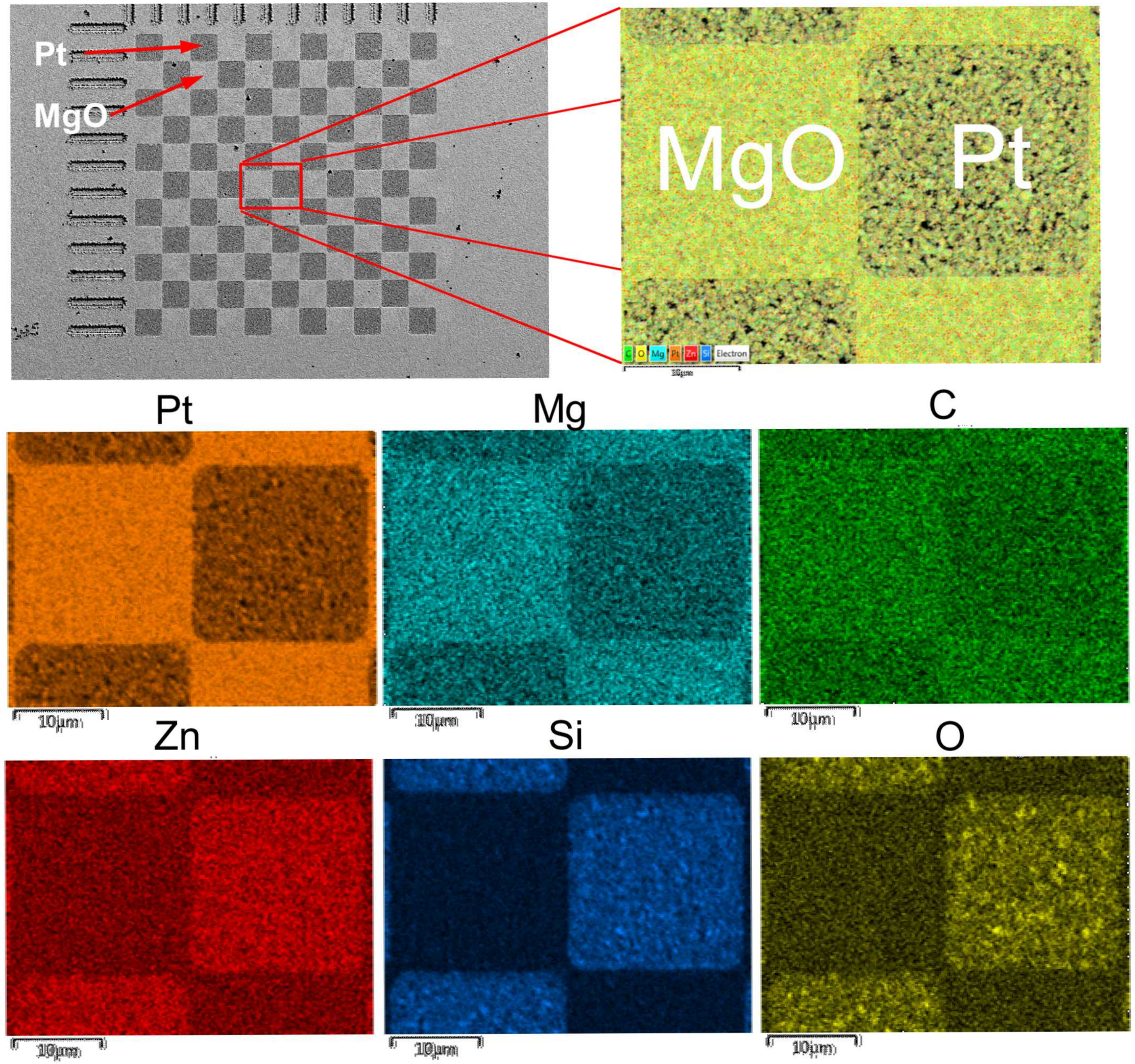




Characterization of the Electrode Stack



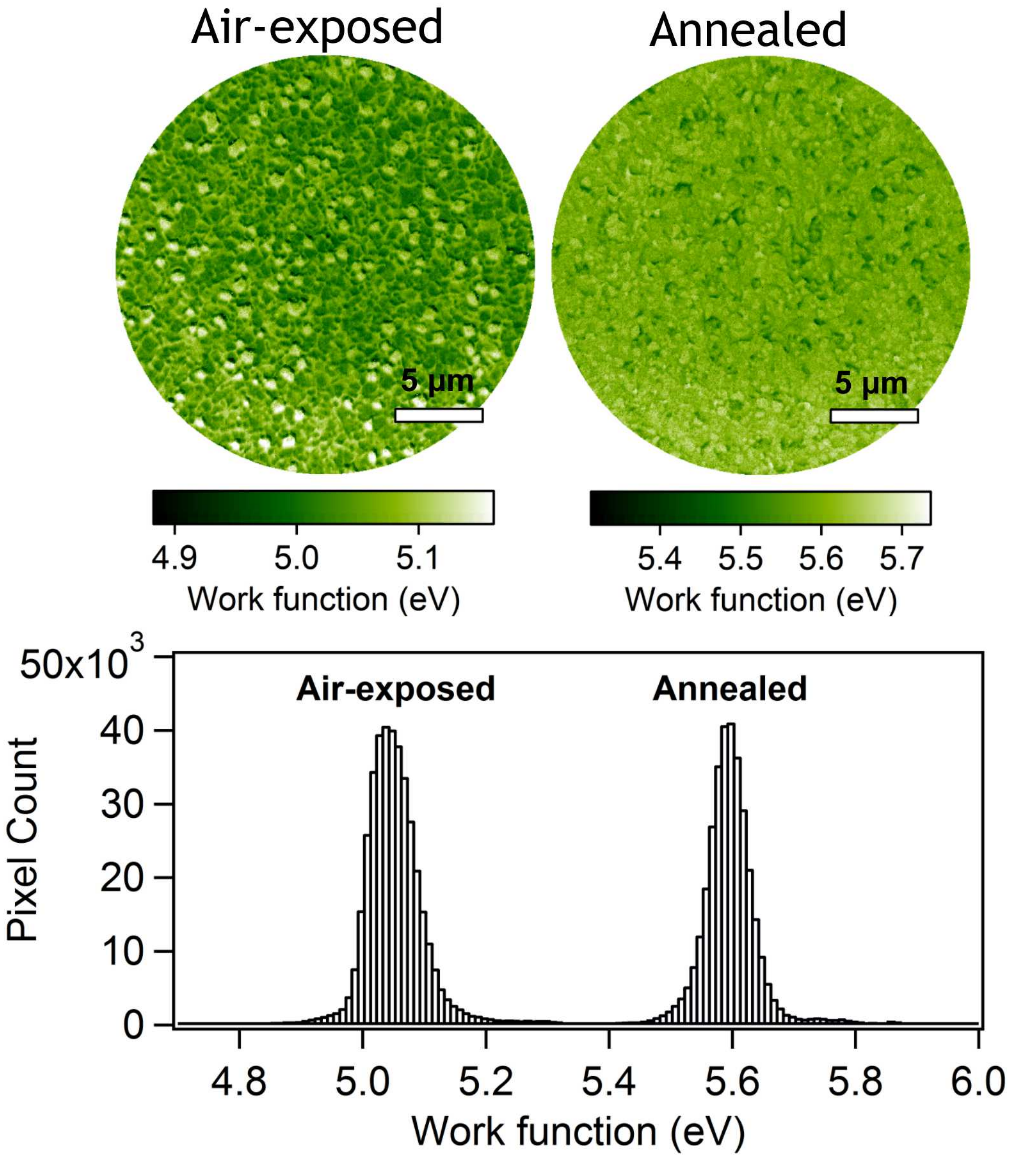
- To investigate surface contamination, put down a 1nm layer of MgO
  - Made "checkerboard" pattern via etch for direct comparison of Pt versus MgO/Pt emission and breakdown
- Use Scanning Electron Microscopy (SEM) and Energy Dispersive X-Ray Spectroscopy (EDS) to verify surface composition
  - Etch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



PEEM Measurement of Work Function Variation

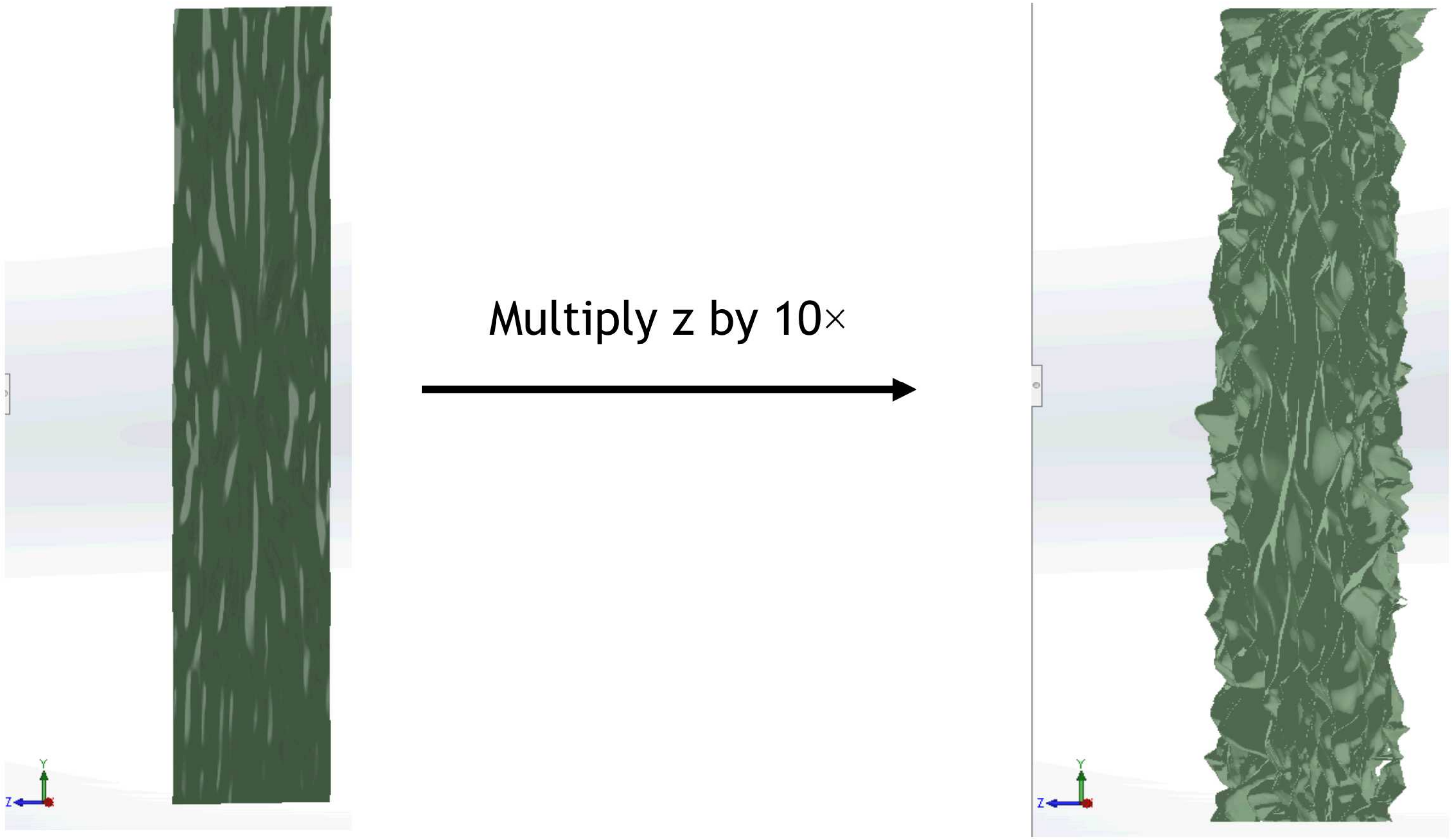
- Measured spatial variation of local work function using PhotoEmission Electron Microscopy
  - Variation across given Pt surface relatively small – only a few percent
  - However, ϕ is in the exponential and the tail of the distribution can initiate field emission and eventually breakdown
- Significant (~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

Poly-Pt (111) on $ZnO/SiO_2/Si$



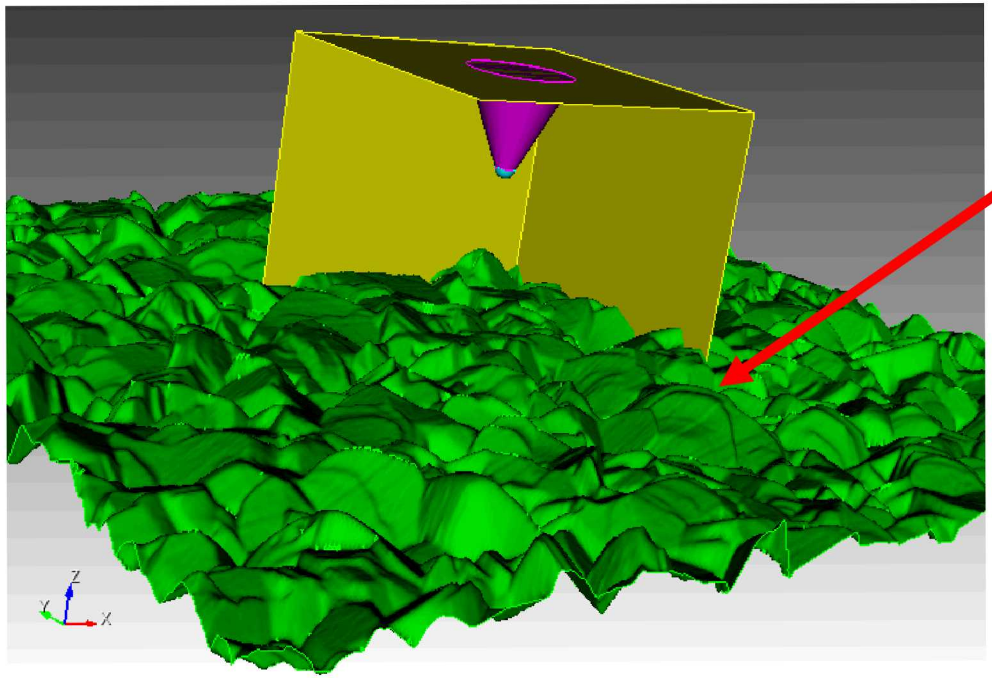
AFM Surface Characterization

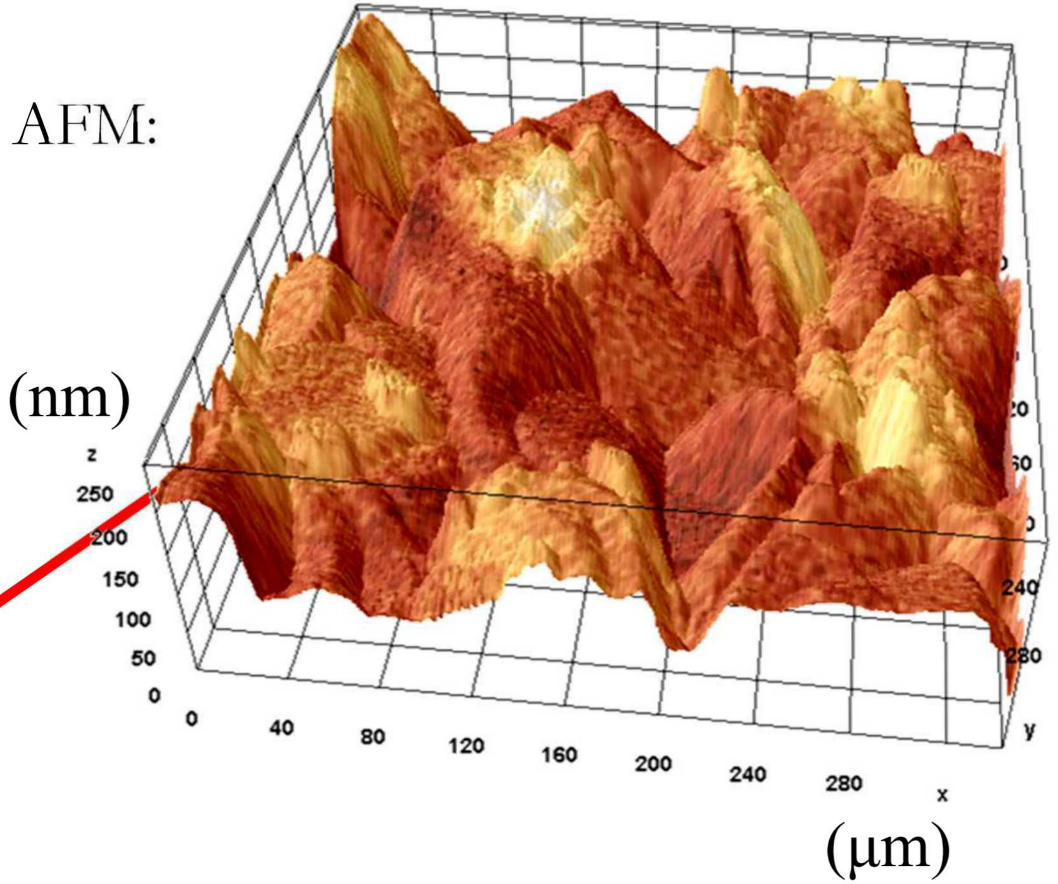
- Actual surface has virtually no significant topology and thus β ~ 1 everywhere.
- To demonstrate spatial variation of field emission across the surface we show results here based on multiplying the surface relief by 10×



AFM topology → topological atomic-scale β

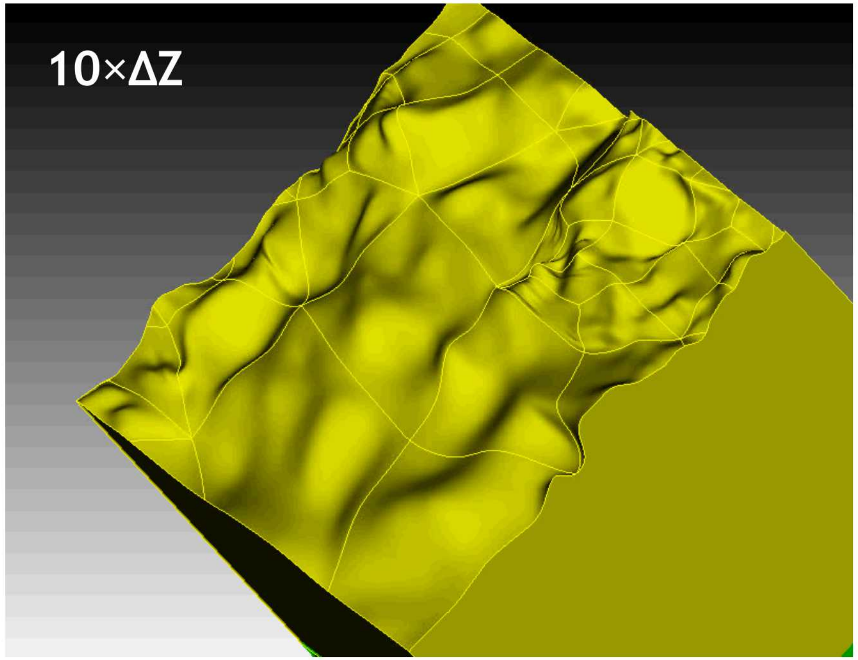
- Measure surface topology before breakdown using AFM:
- Load topology into Cubit and mesh the surface in order to use electrostatic solver
  - Place flat anode ~10μm from as-measured cathode
  - Use ~1 nm elements near cathode to resolve features



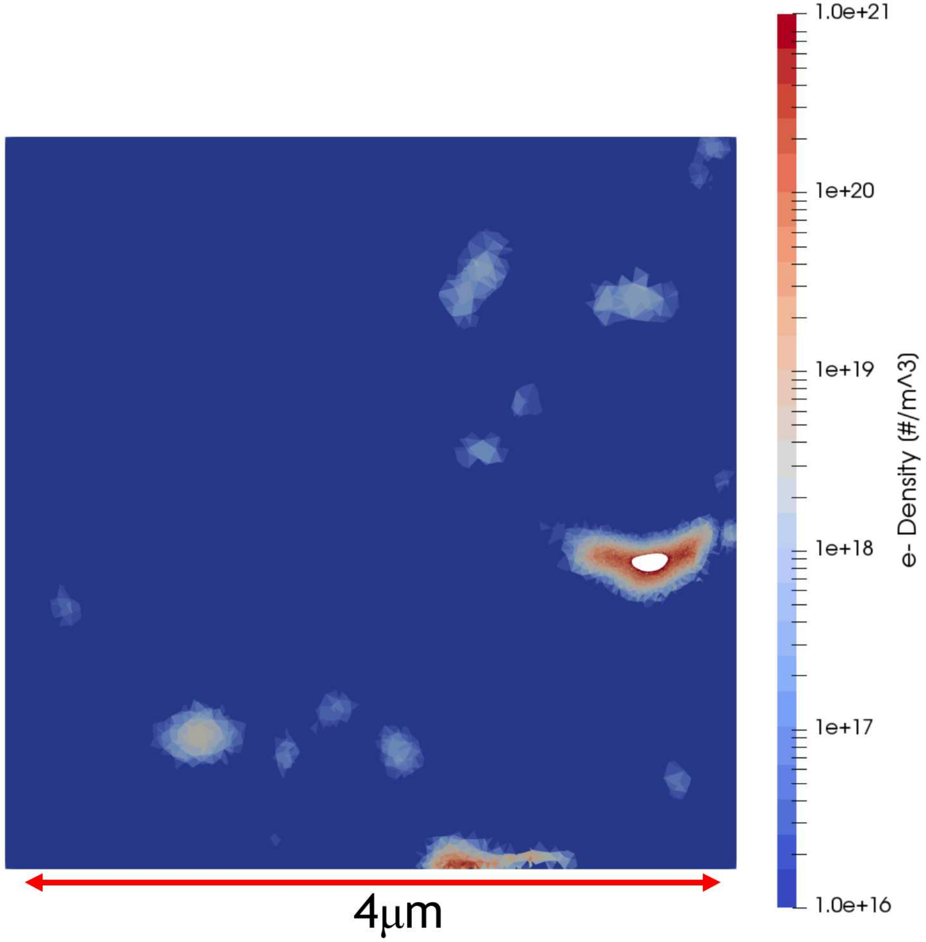


Simulation of Emission from AFM Surface

- With the resolved (Δx<10nm) 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

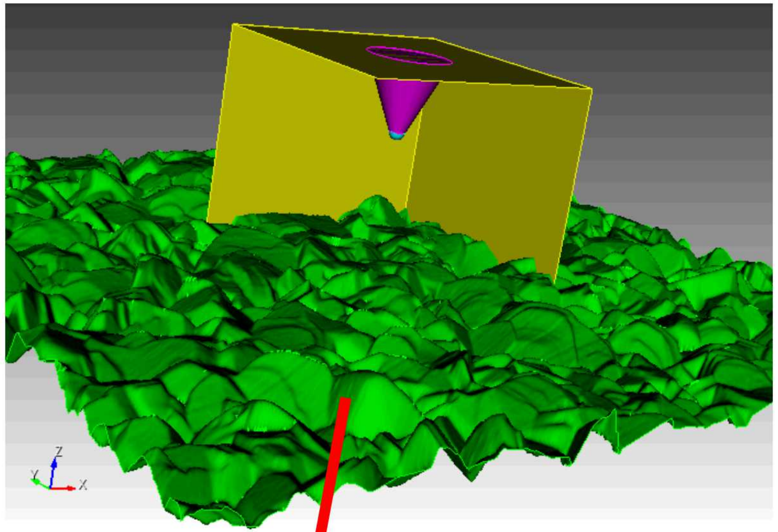


Simulate emission in PIC-code

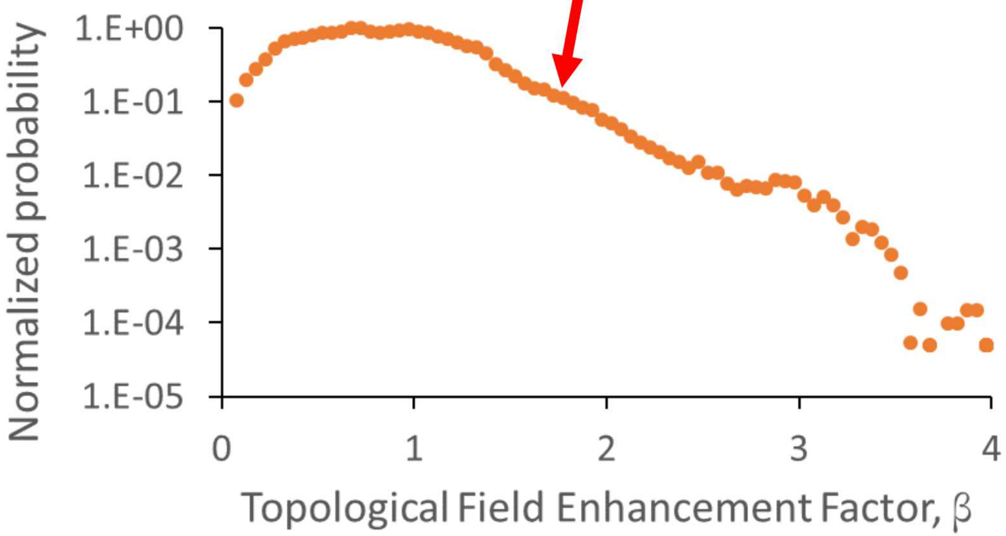


AFM topology → topological atomic-scale β

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



Electrostatic solve



Meso-scale Model for Surface Variations

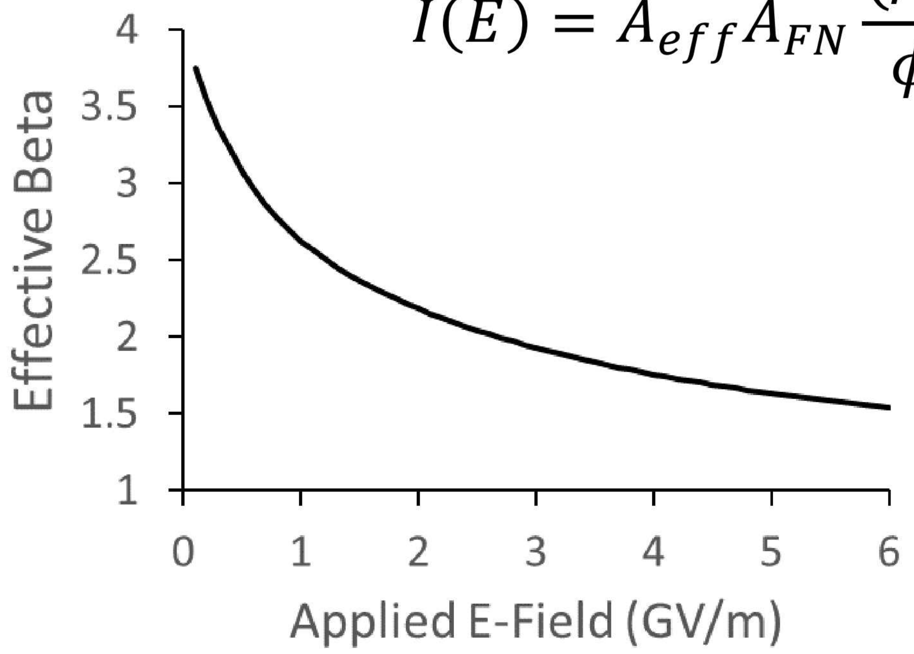
- We have measured atomic-scale (1-10nm) PDF's of the work function and topological field enhancement factor
- Must convert these to the meso-scale (0.1-10 μm). Some options:
  1. Just pick the meso-scale β and ϕ from the atomic-scale PDFs
  2. Make an effective β and ϕ to use at the meso-scale
  3. "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}:

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



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

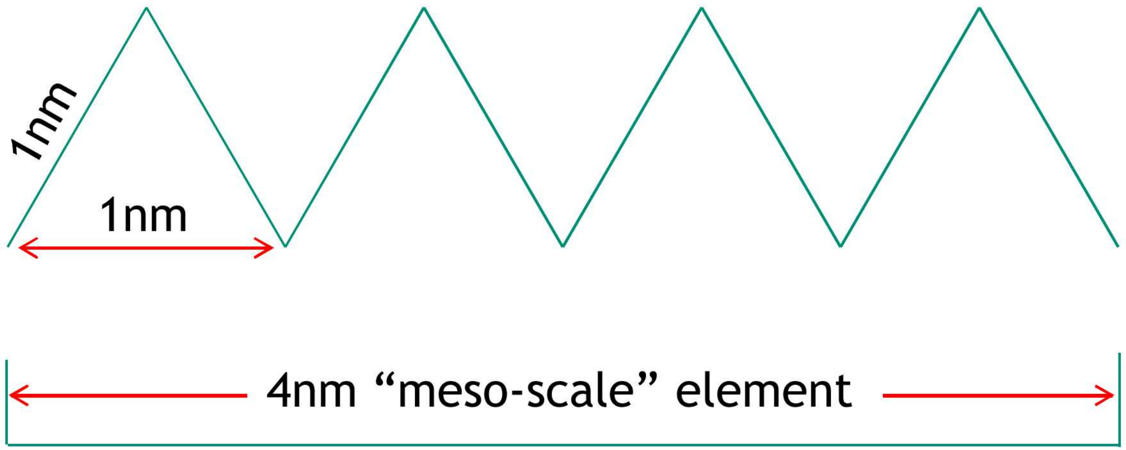
- This makes sense: small β regions "turn on" at higher fields and pulls the effective β lower
- The precise functional form depends on the atomic-scale β PDF

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

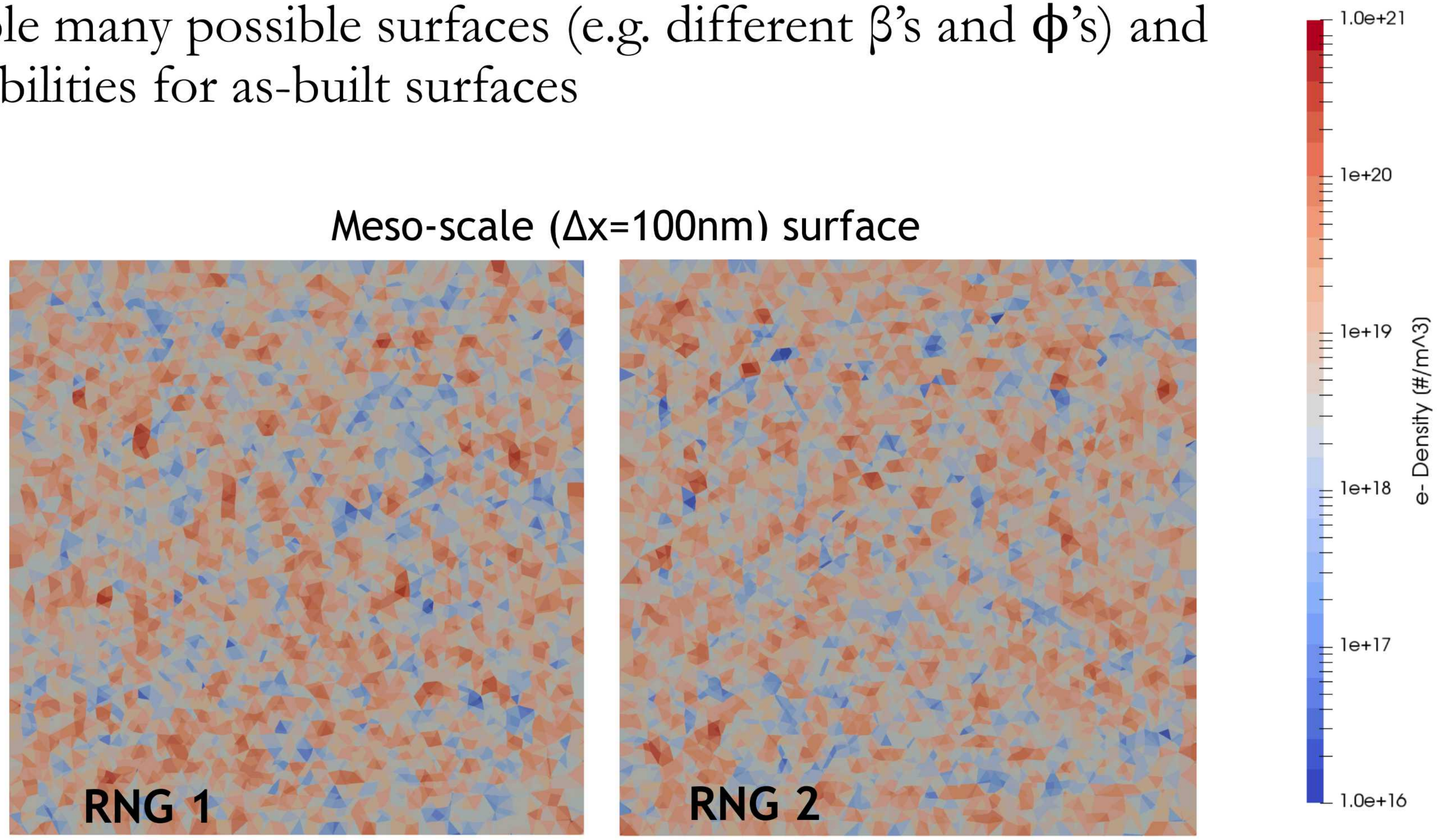
Meso-scale Model for Surface Variations

- 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

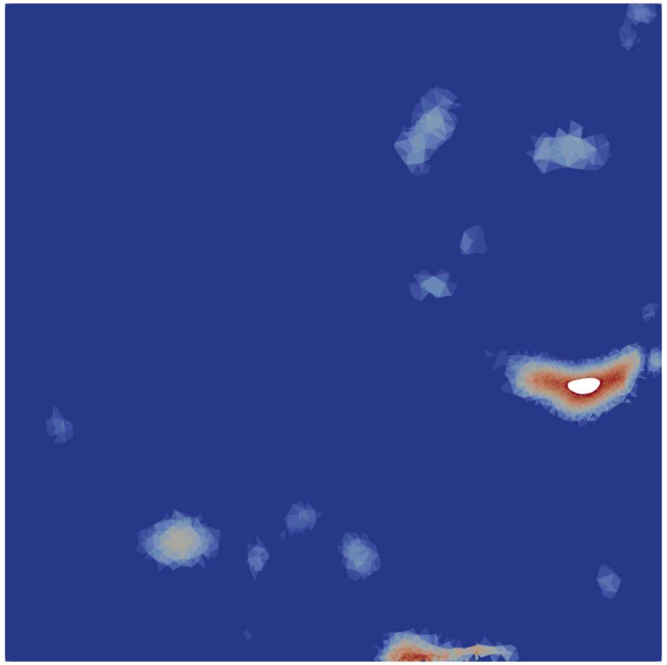
- Meso-scale model does show stochastic variation in the e- density just above the surface based on the random seed
- Goal is to be able to sample many possible surfaces (e.g. different β's and ϕ's) and compute breakdown probabilities for as-built surfaces



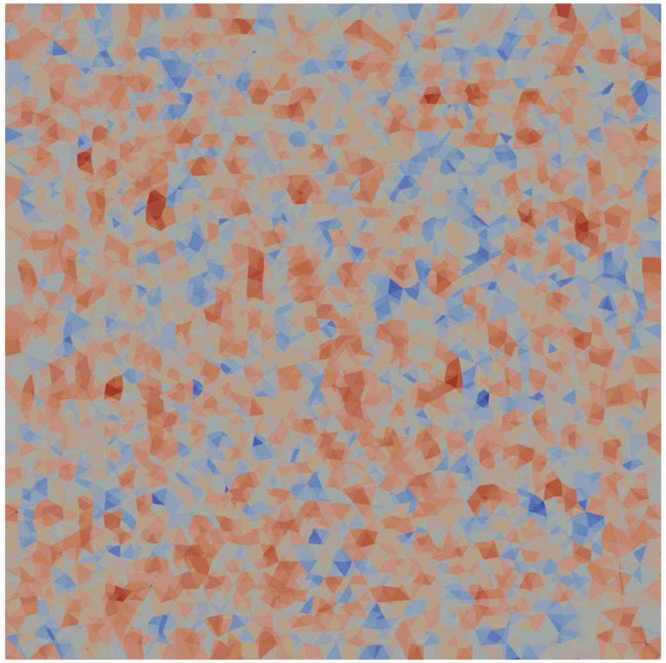
Meso-scale Field Emission Simulations

- 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

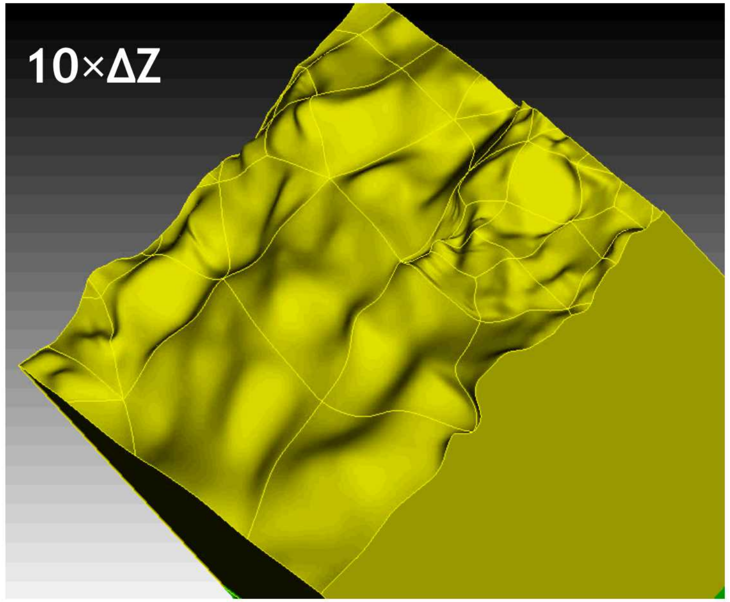
STM (Δx<10nm) surface

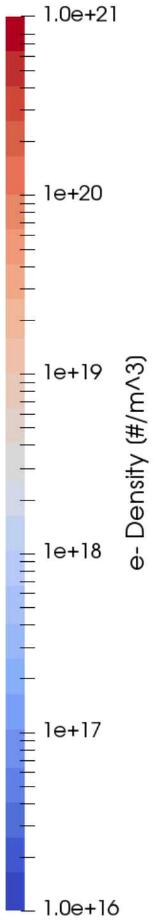


Meso-scale (Δx=100nm) surface



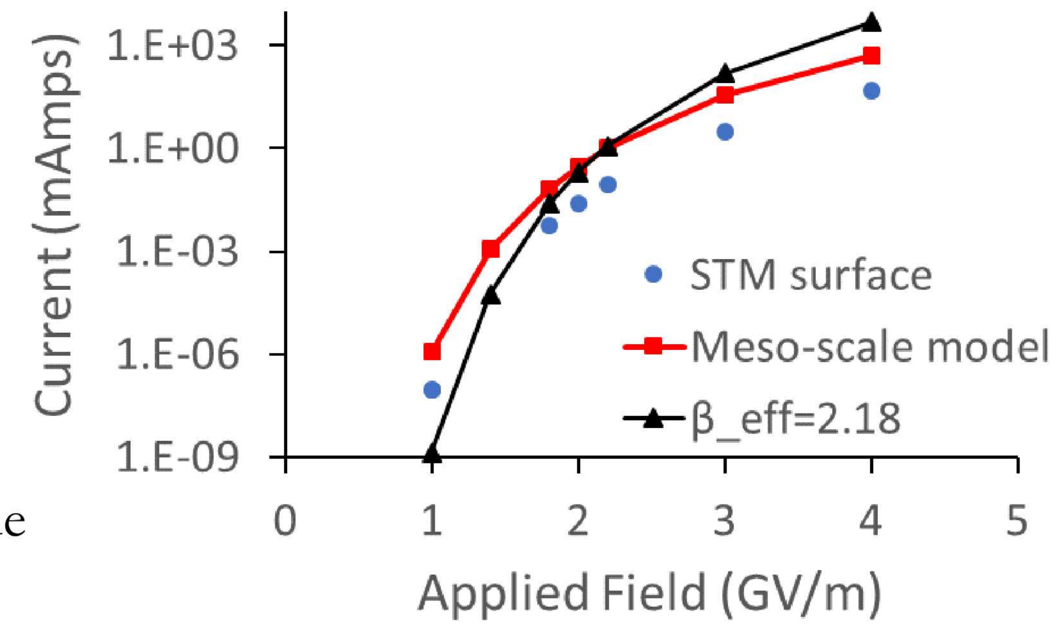
STM surface topology

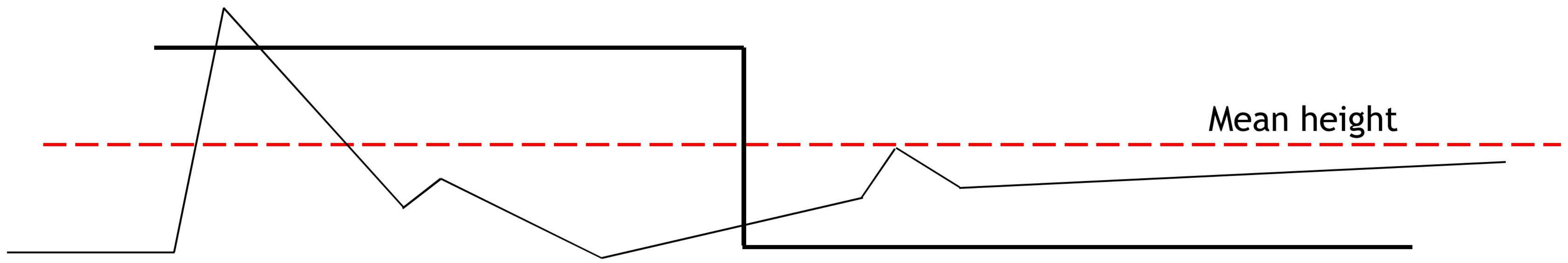




Meso-scale Field Emission Simulations

- 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×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



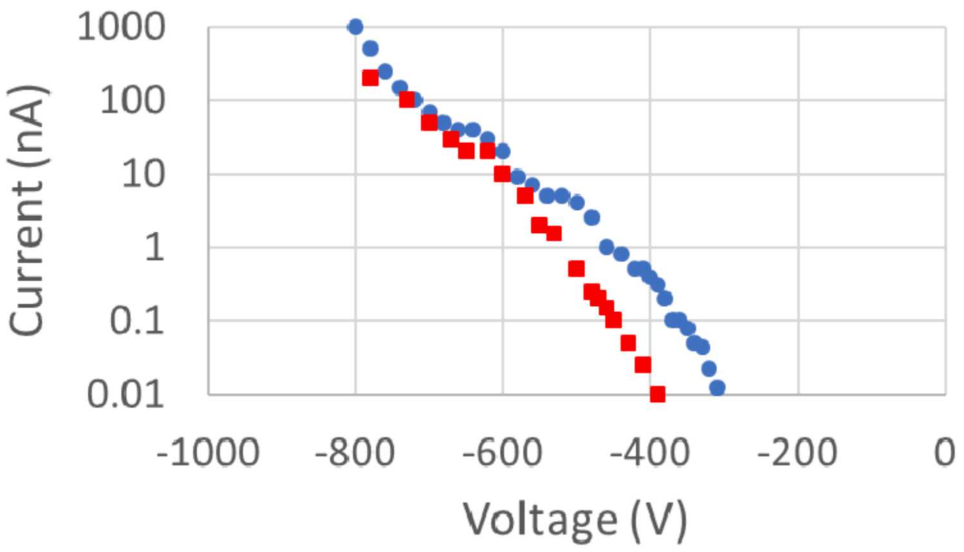


Initial Local STM Breakdown Results

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

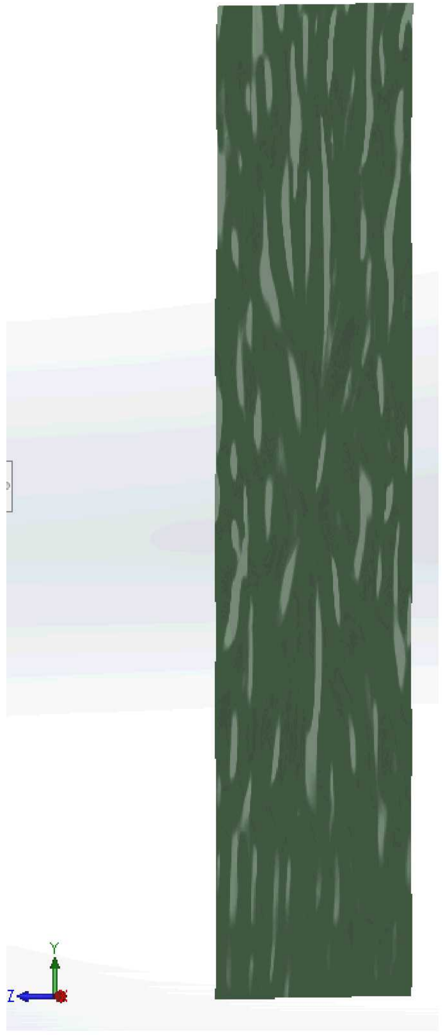
- Relatively feature-less surface with small-β within the region of the tip field footprint

- 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

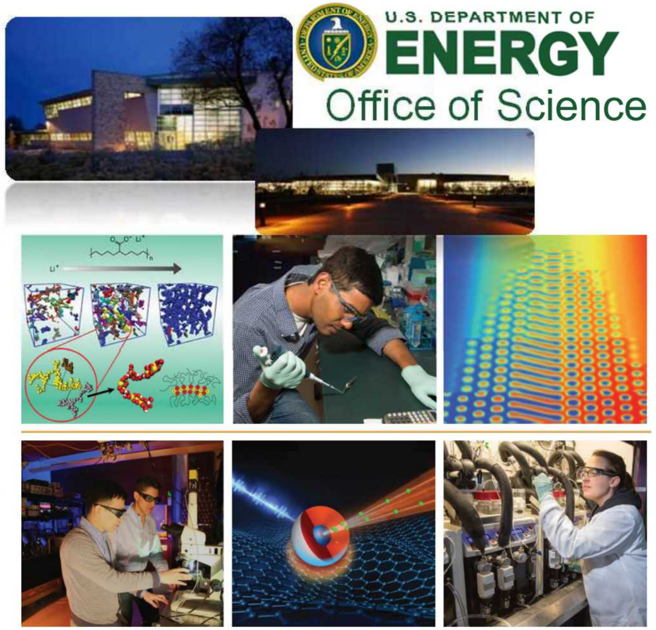
- Investigating surfaces at the atomic scale to characterize features relevant to vacuum field emission.
  - Want to clarify β-based field emission so β really is only geometry induced field enhancement.
- By examining field emission at the nanoscale, we have attempted to create a meso-scale physics-based 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

Sandia National Laboratories

Center for Integrated Nanotechnologies

U.S. DEPARTMENT OF ENERGY

Office of Science



http://cint.lanl.gov