Advancing electrode models for PIC-DSMC simulation of vacuum discharge between real surfaces

Chris Moore, Morgann Berg, Ezra Bussman, Taisuke Ohta, David Scrymgeour, Sean Smith, Peter Schultz, Harold Hjalmarson, Paul Clem, Matthew Hopkins

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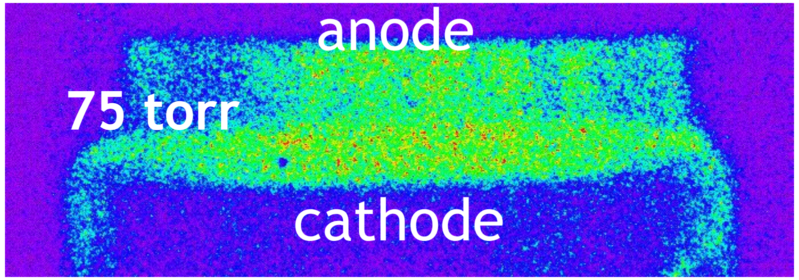
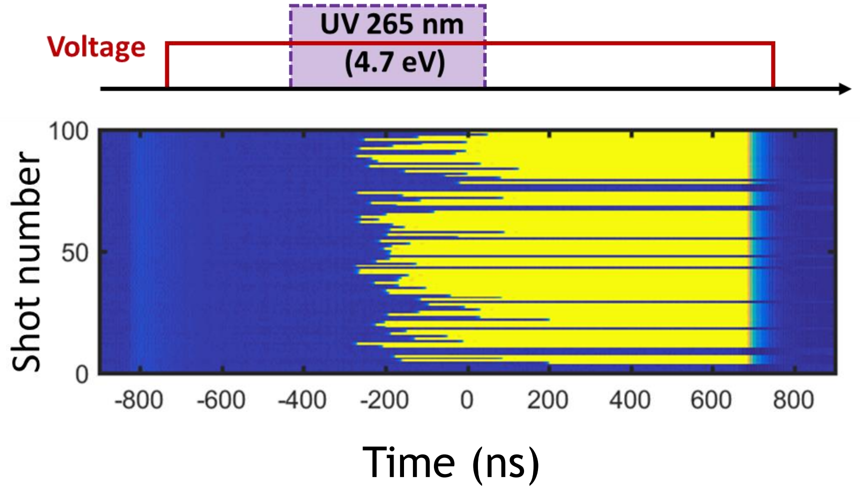
Introduction/Motivation

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

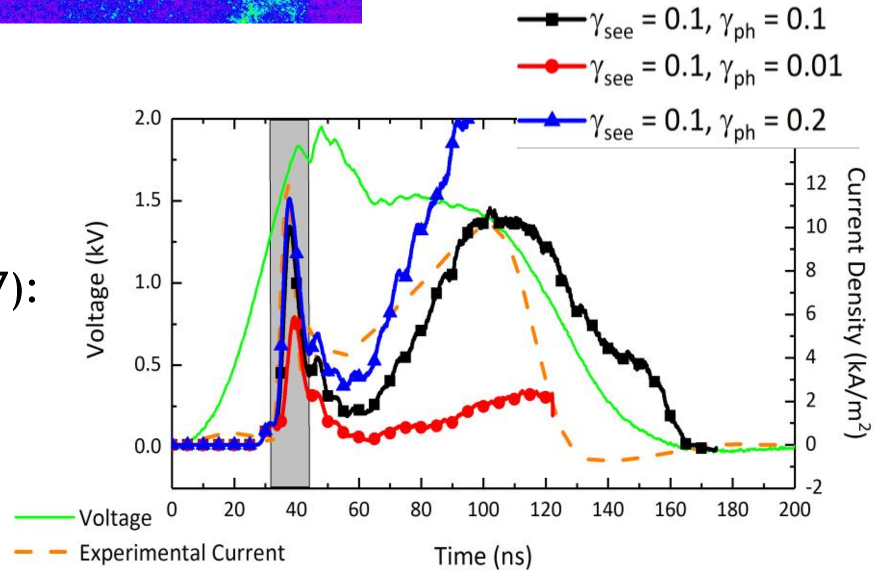
- We have multiple projects focused on how interactions with surfaces drive discharge
  - AMPPED is investigating photoemission and ion-induced SEE from surfaces:



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



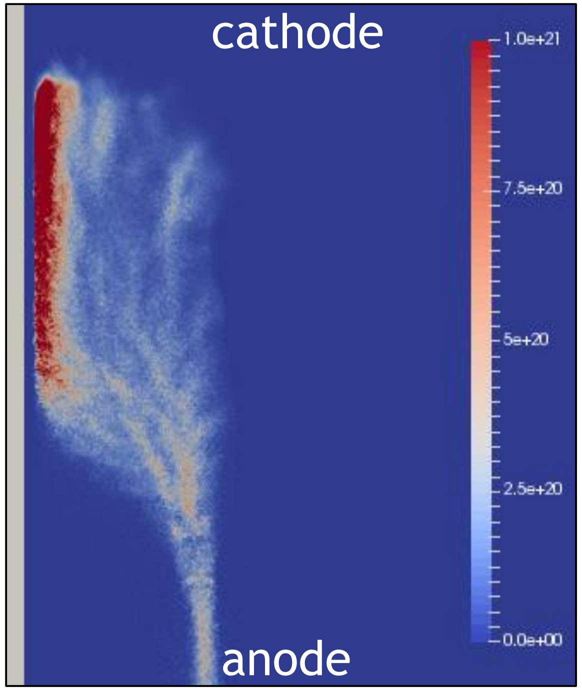
Dependence of low-pressure discharge on surface properties (A. Fierro, ICNSP 2017):



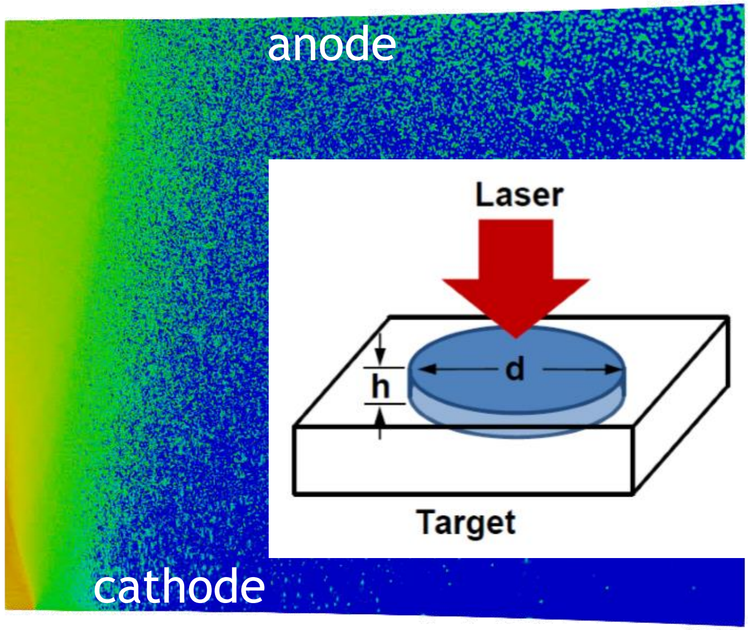
Introduction/Motivation

- 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
  - We must perform rigorous Verification and Validation efforts before a model is considered useful

Streamer evolution near dielectric surfaces (A. Jindal, ICOPS 2017):

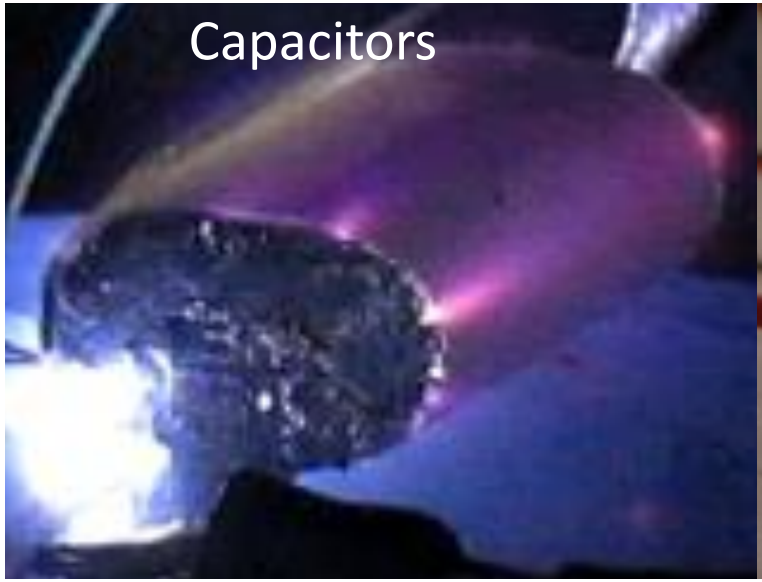


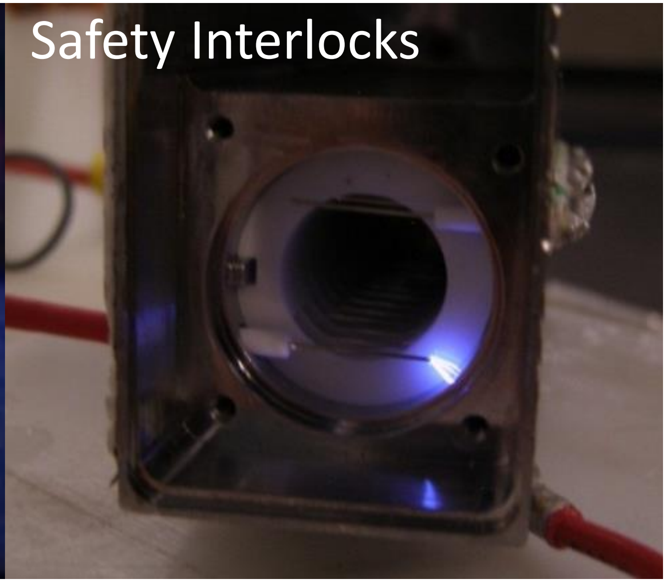
Laser-triggered switch (A. Fierro, MeVArc 2018):



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
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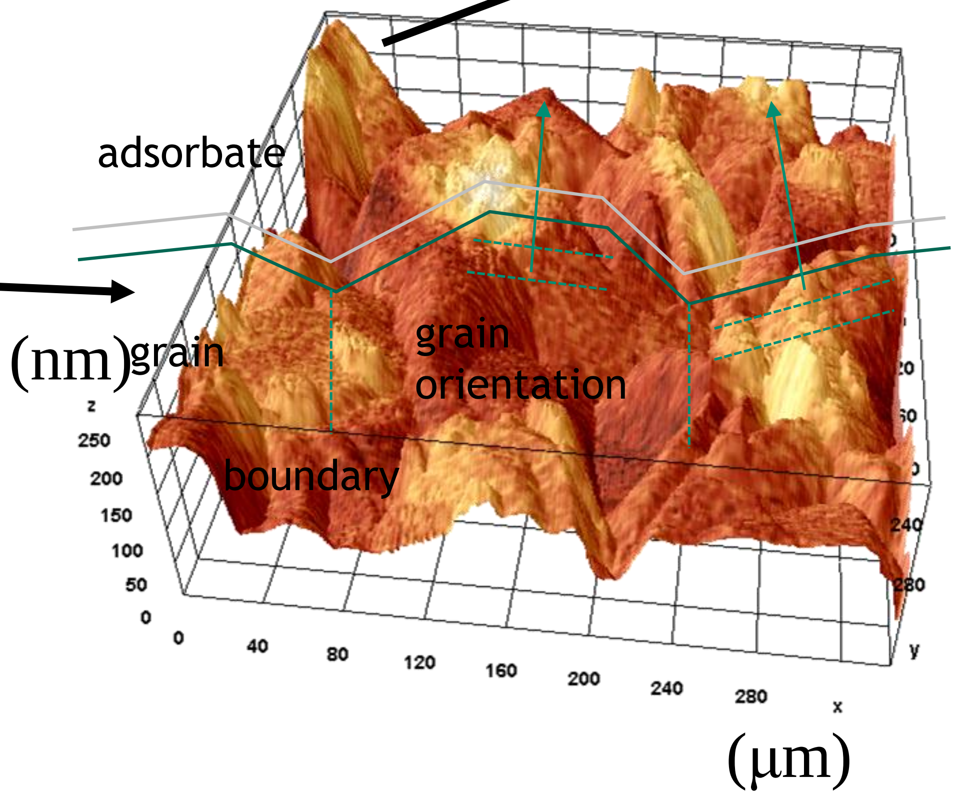
- We have a project to understand vacuum field emission from well-characterized surfaces to create physics-based models for use in large-scale PIC-DSMC breakdown simulations
  - Field emission is necessary precursor to a breakdown event. No field emission → no breakdown.
  - Employ state-of-the-art microscopy and other techniques 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 "macroscopic" (0.1 μm) model of the surface for PIC-DSMC simulation of breakdown

Why local characterization?

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

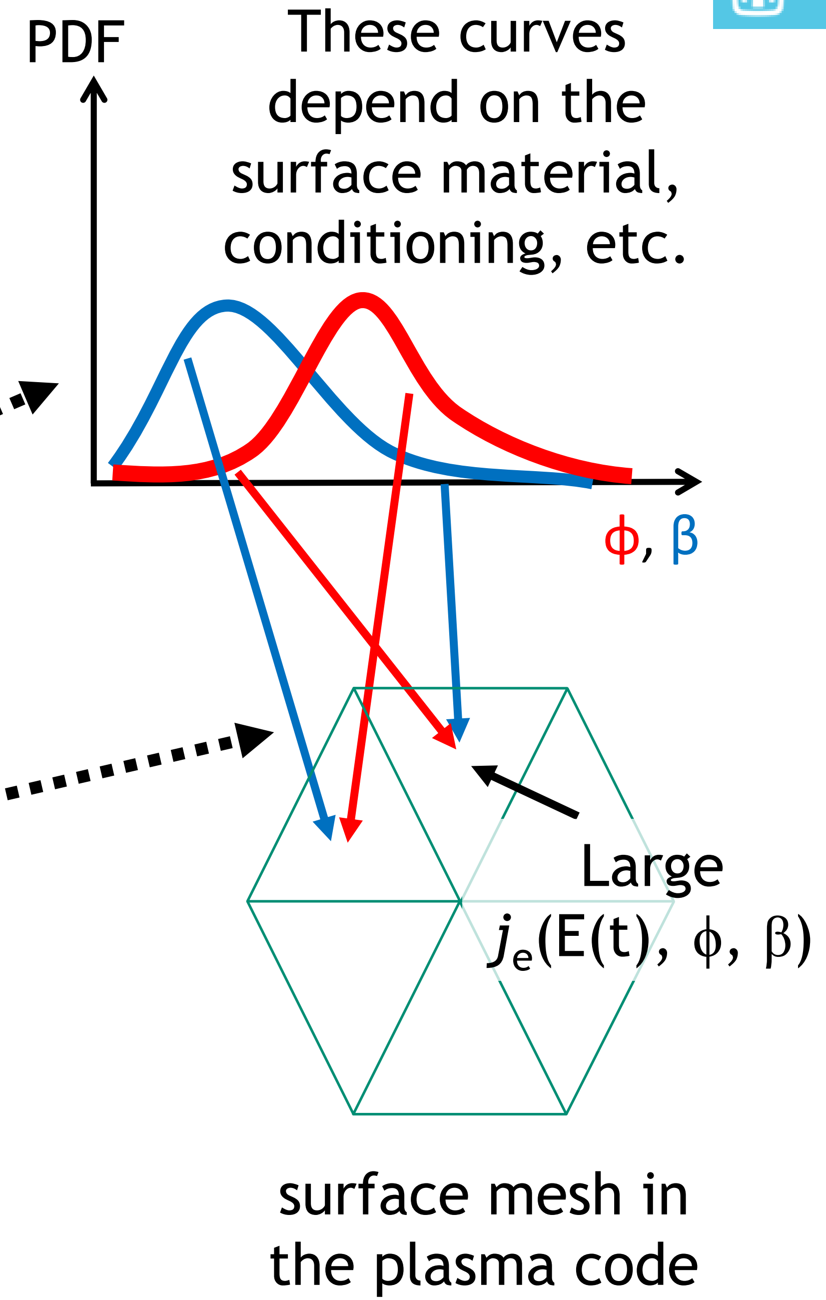
$$j = A_{eff} A_{FN} \frac{(\beta E)^2}{\phi} exp\left[-\frac{B_{FN}\phi^{3/2}}{\beta E}\right]$$

- We want to locally characterize the surface to eliminate β as a fit parameter
  - Use 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 in discharge simulations



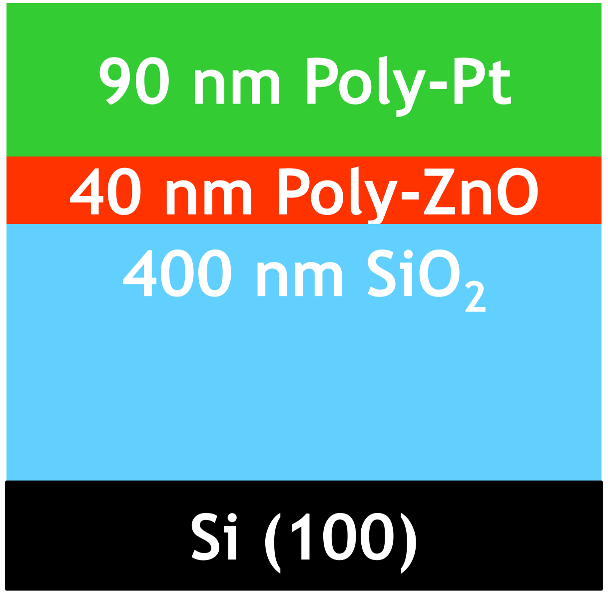
Overview

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

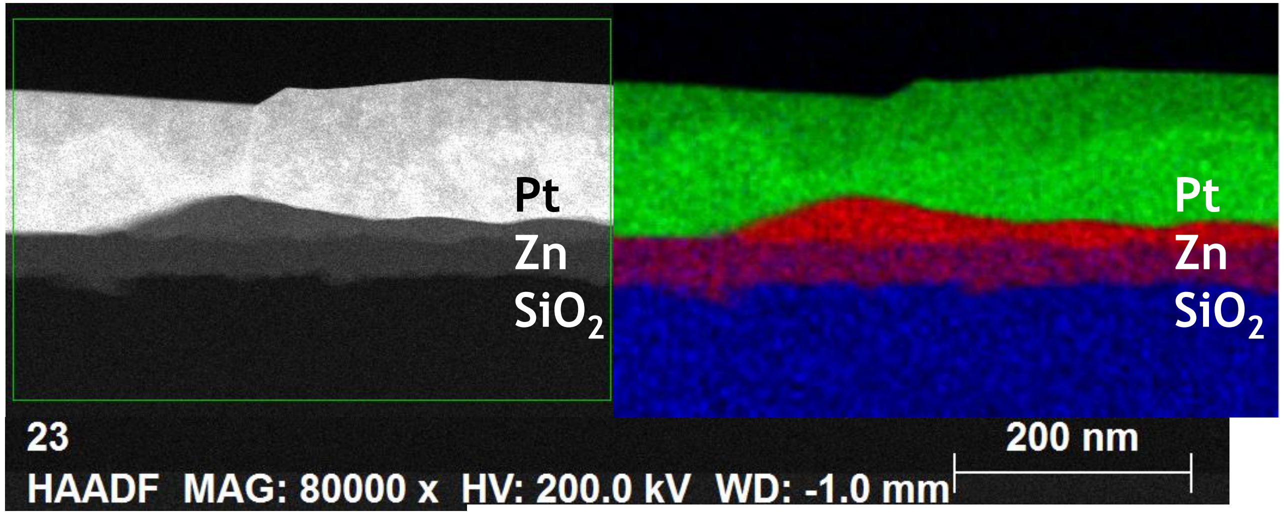


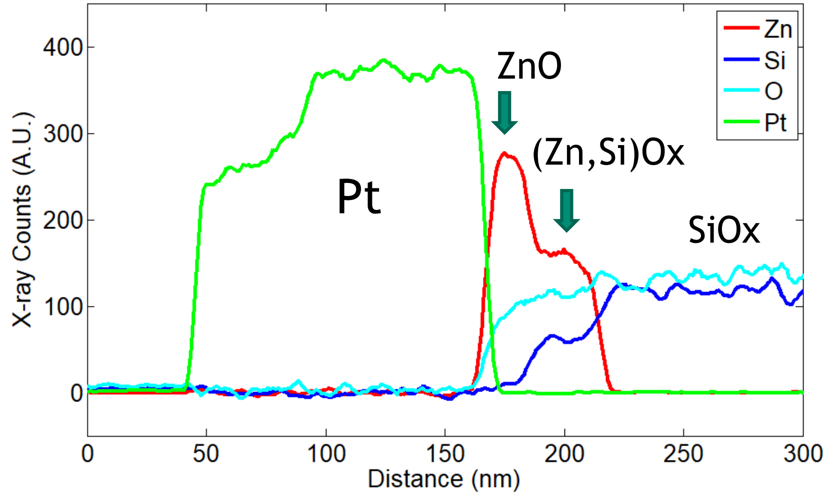
Characterization of the Electrode Stack

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



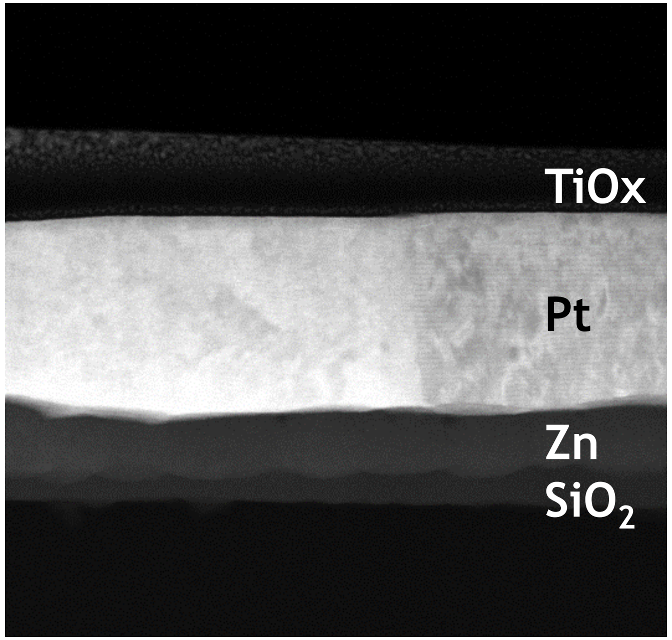
TEM **EDS**



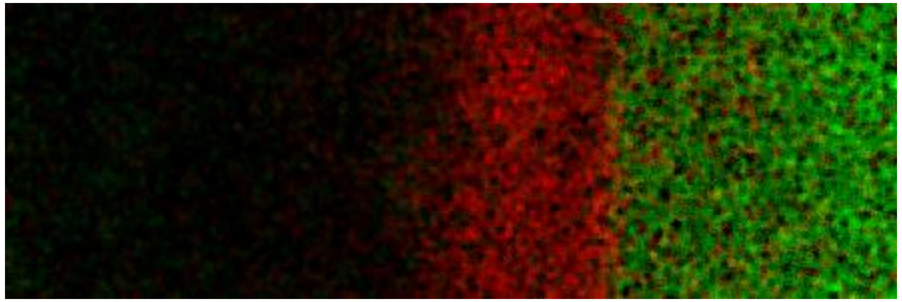


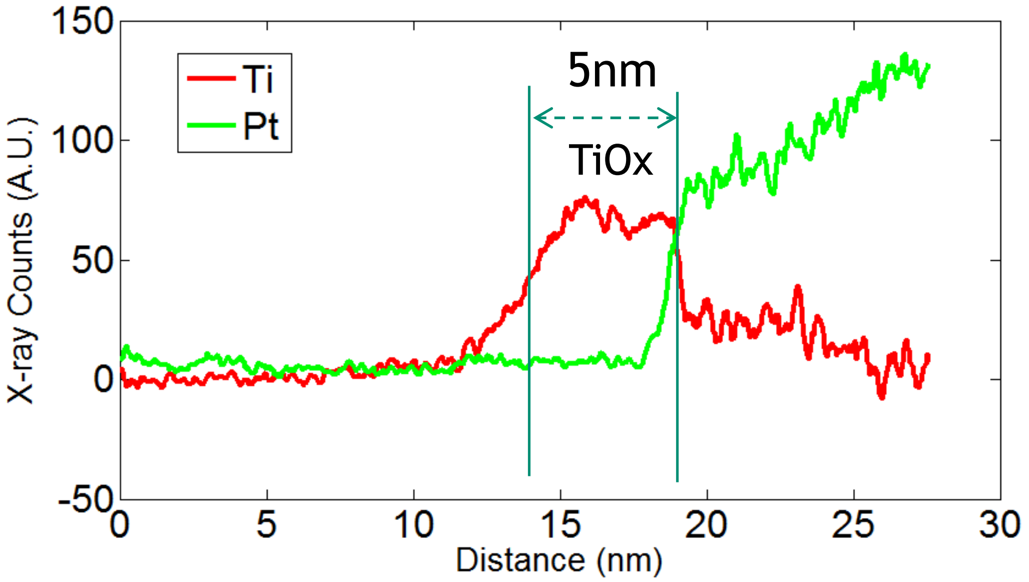
Characterization of the Electrode Stack

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



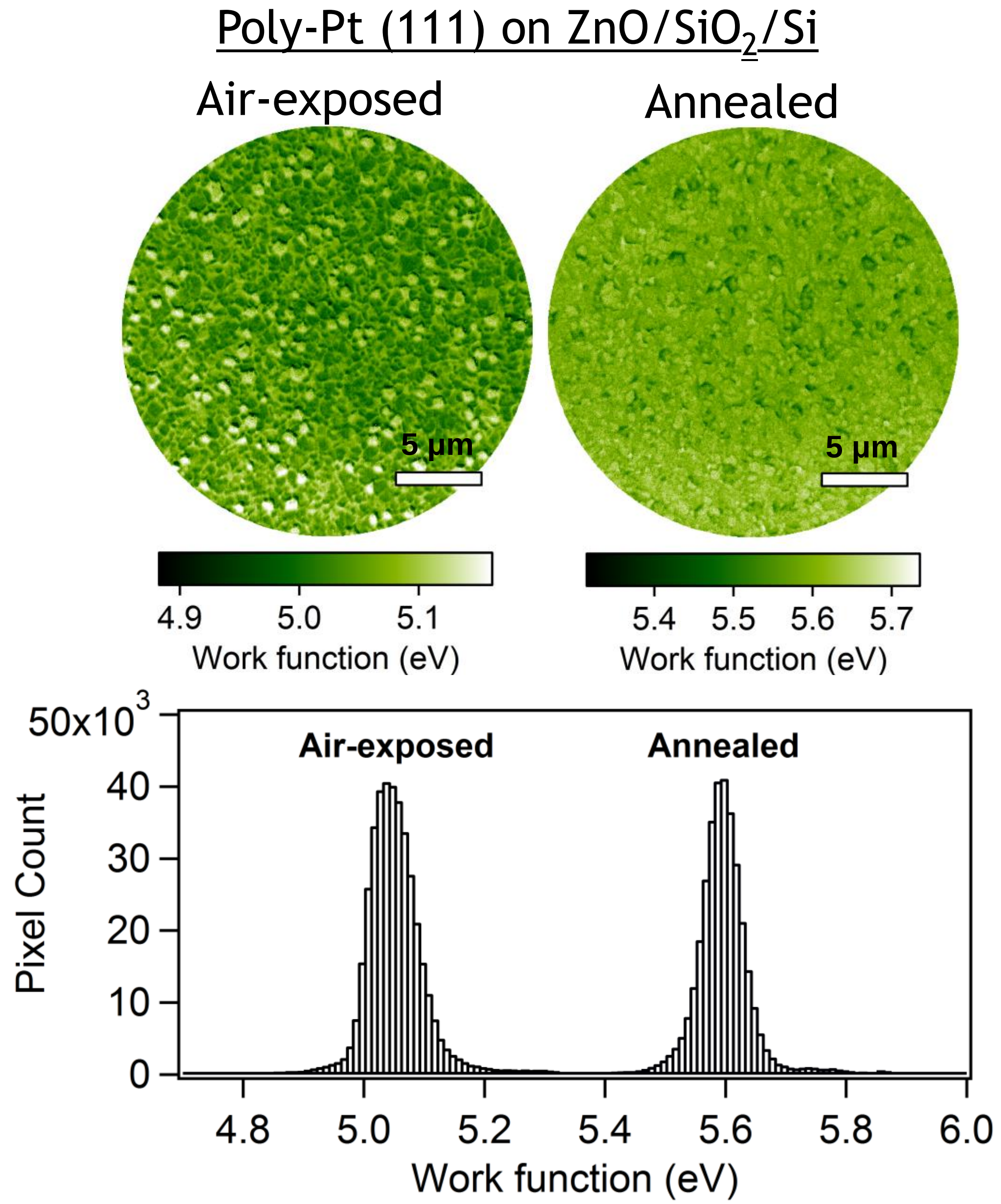
EDS maps (Ti-red; Pt-green)





PEEM Measurement of Work Function Variation

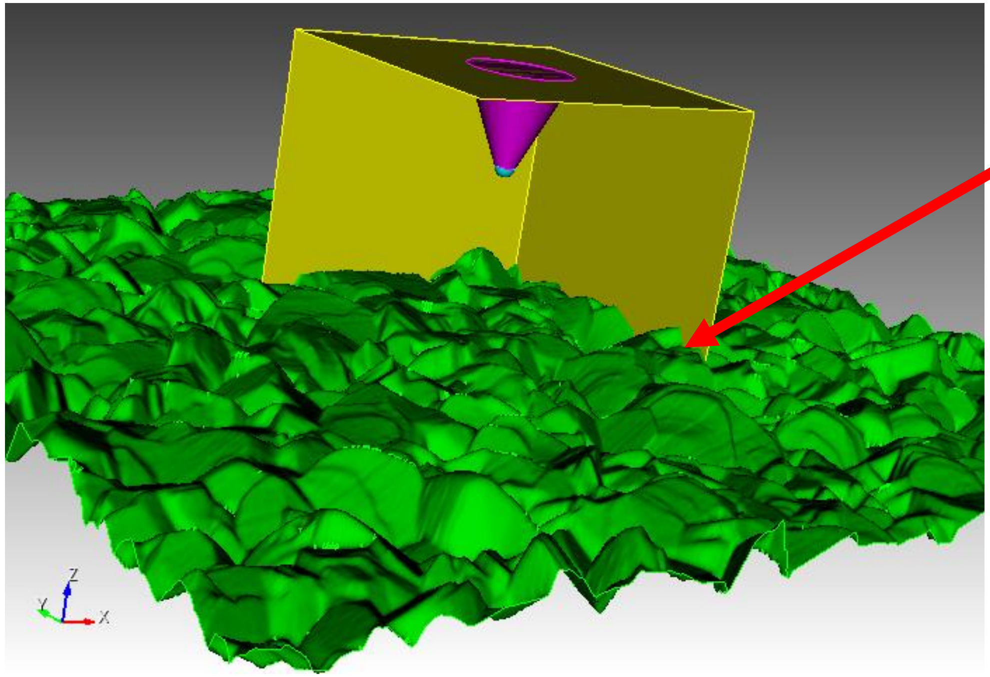
- Measured spatial variation of local apparent work function using PhotoEmission Electron Microscopy
  - Variation across given Pt surface relatively small – only a few percent
  - However, ϕ is in the exponential and the tail of the distribution can initiate field emission and eventually breakdown
- Significant (~10%) decrease in the work function due to surface contaminants picked up via exposure to air
- The air-exposed and annealed PDF's can be loaded into PIC-DSMC simulation and used to set initial condition of the electrode properties

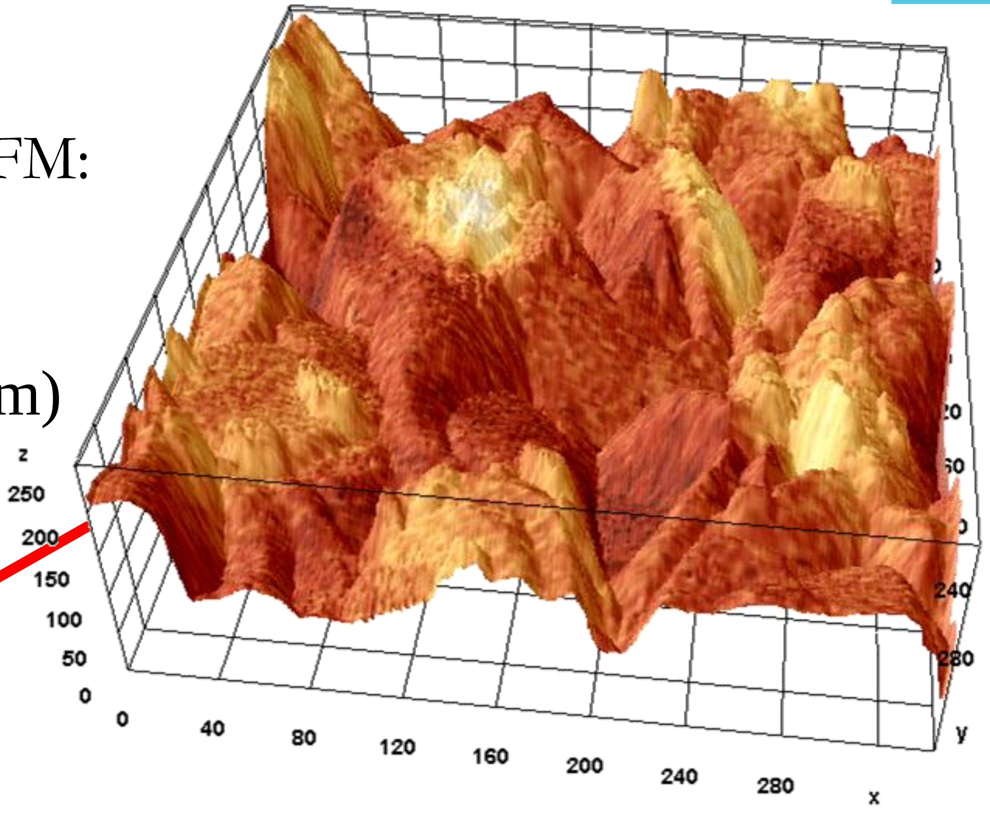


AFM topology → topological β

- Measure surface topology before breakdown using AFM:

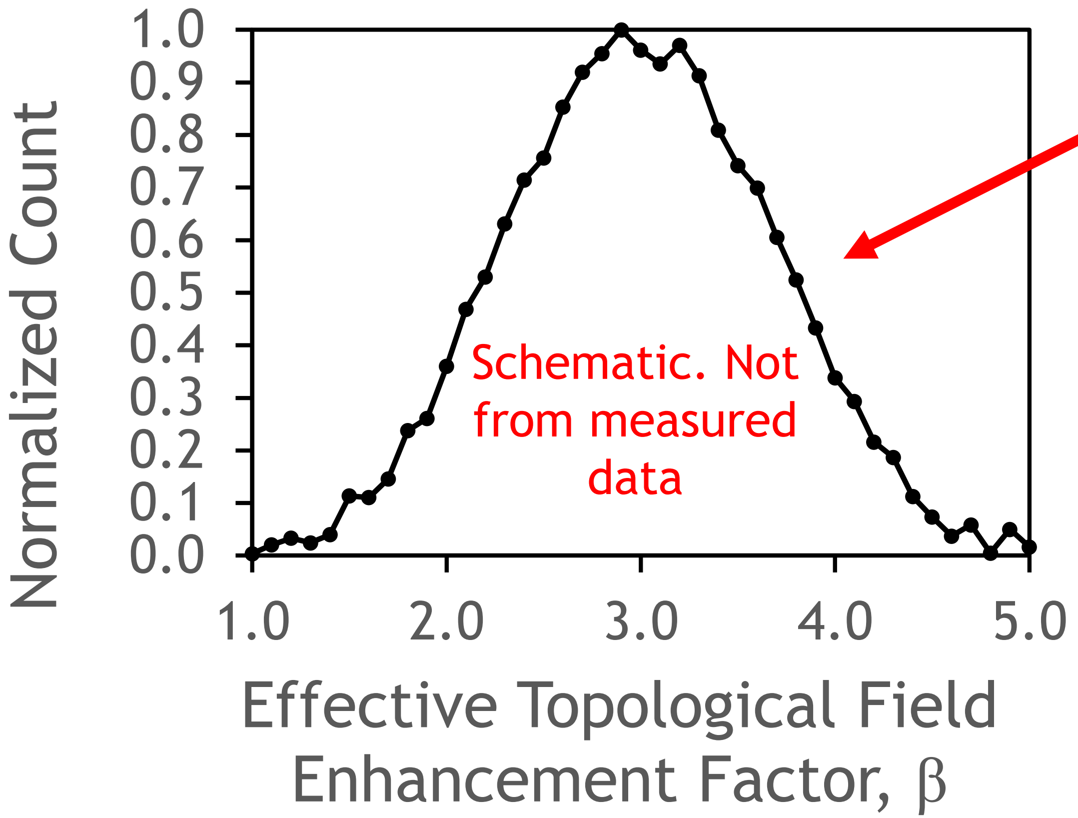
- Load topology into Cubit and mesh the surface in order to use electrostatic solver for E:

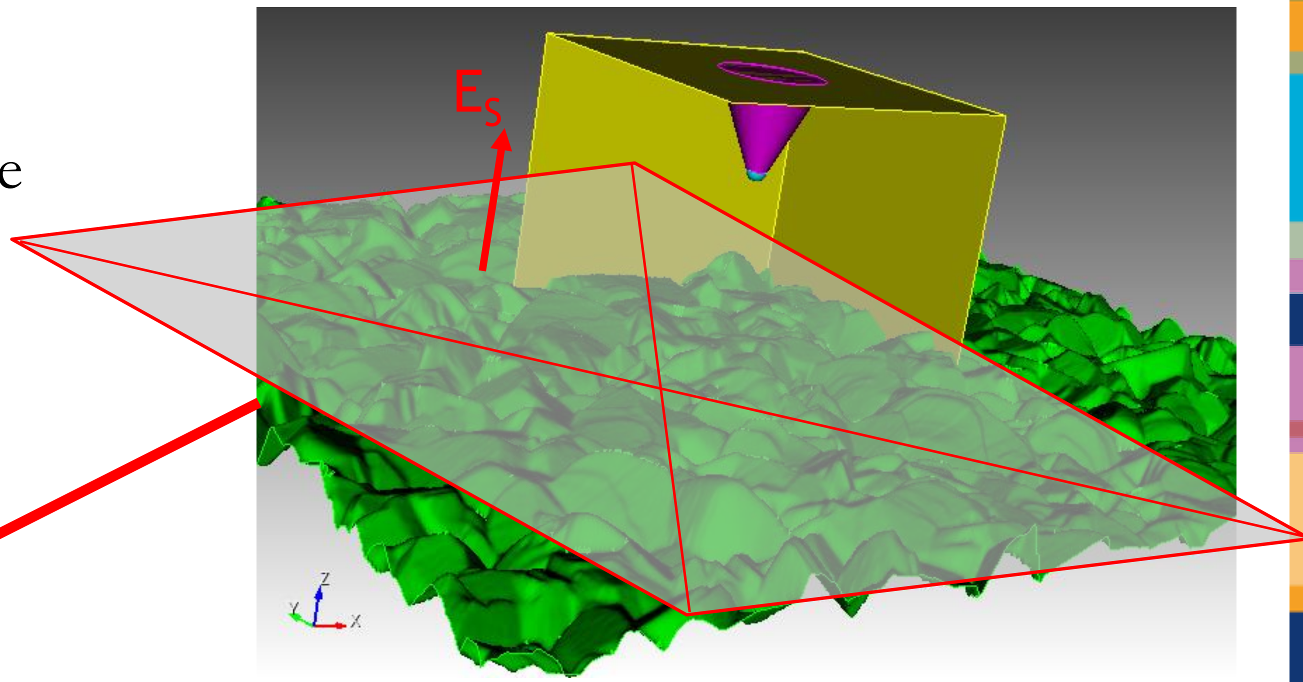




AFM topology → topological β

- Determine E_S just off the surface for the simulation mesh size (0.1–1 μm) → generate distribution for $\beta_{effective} = E_S/E_{applied}$

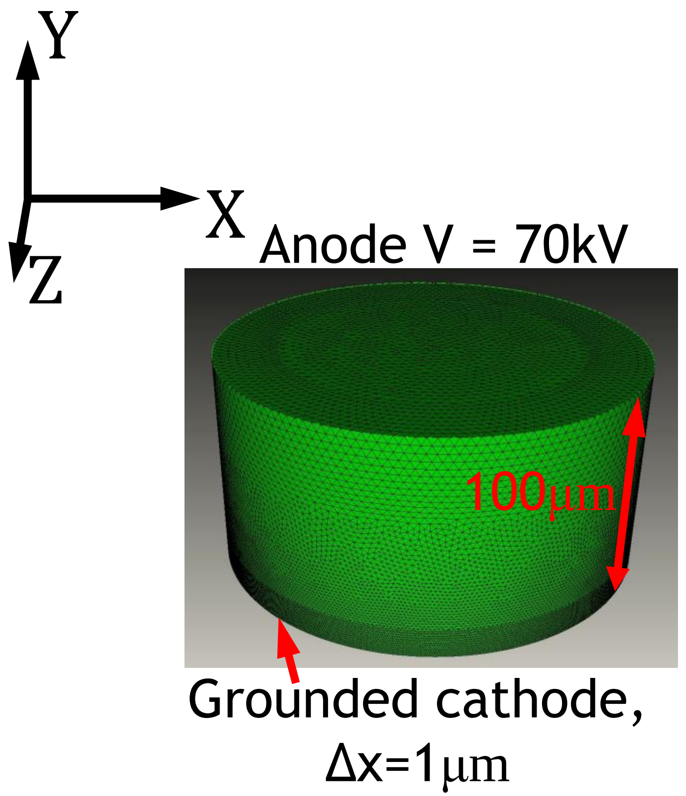




- This PDF for $\beta_{effective}$ loaded into PIC-DSMC simulation and used to set initial condition of the electrode properties

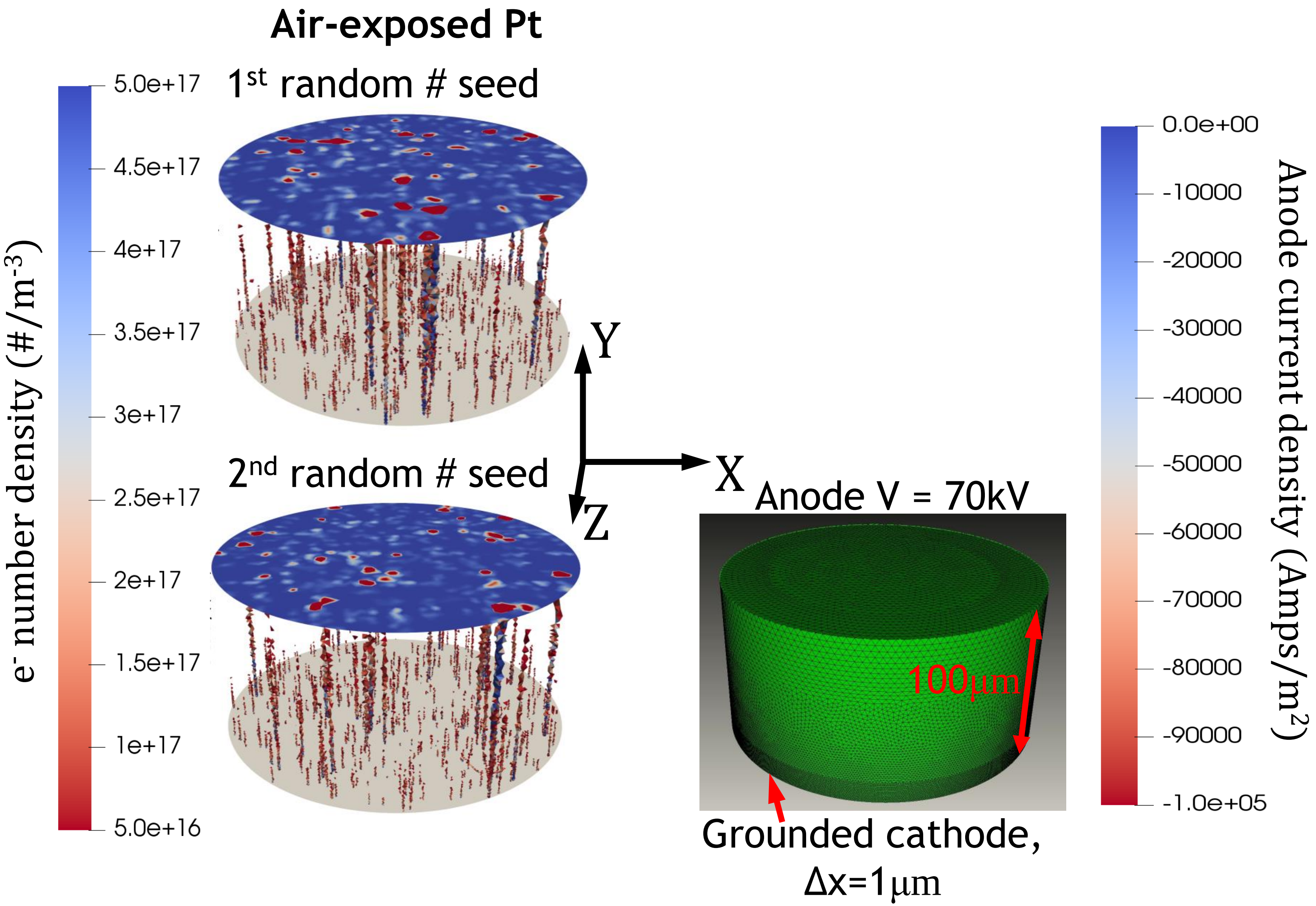
Macroscopic Emission from Real Surface

- Surface element properties (β and ϕ) in the PIC-DSMC simulation initialized using experimentally measured PDF's.
- Local E, β and ϕ used to compute field emission current density for each element
- Emission between planar electrodes shown for simplicity, can be applied to complex geometries



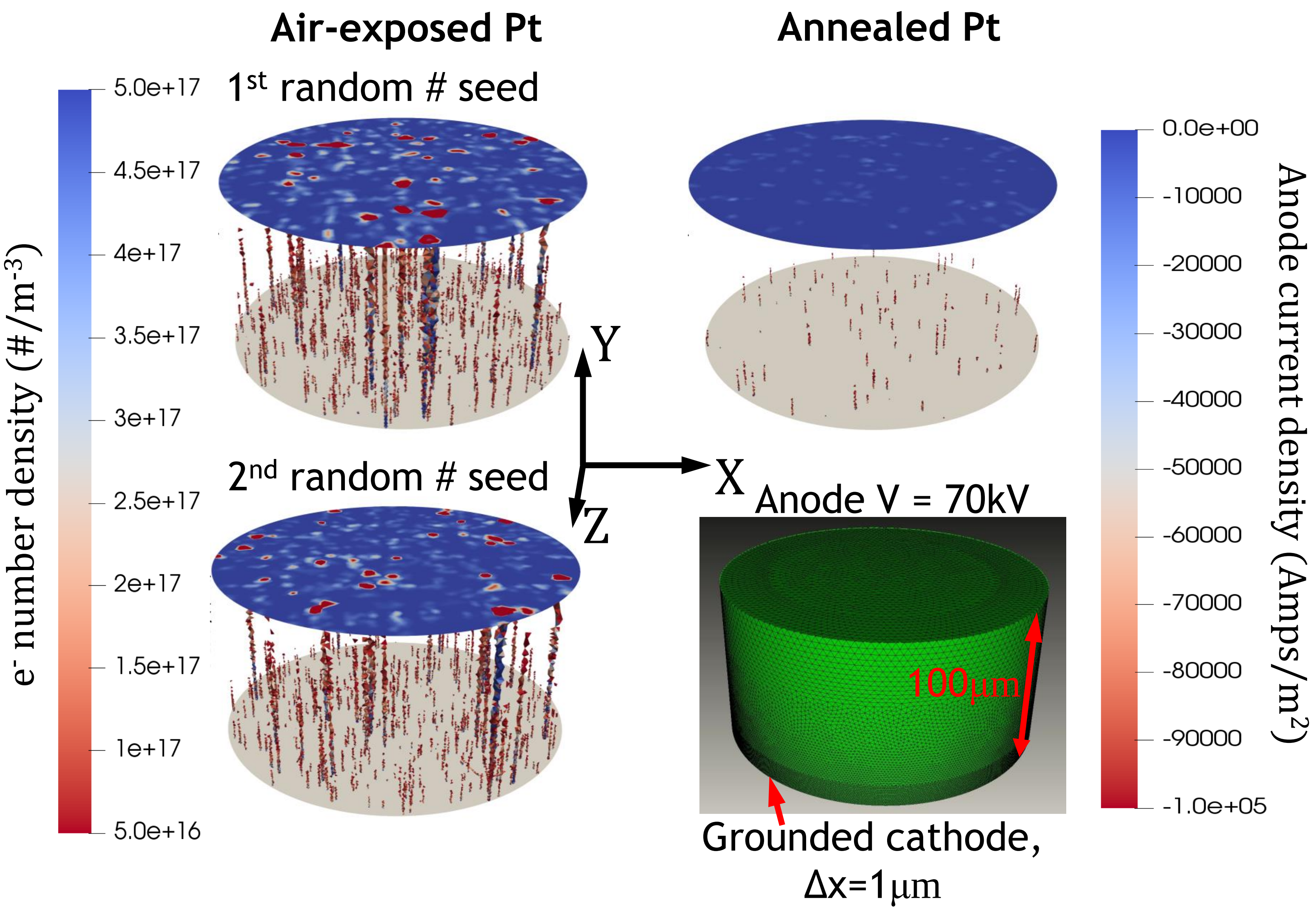
Macroscopic Emission from Real Surface

- Air-exposed Pt has significant variation in the initial field emission across the electrode due to variation in β and ϕ
- Changing the random seed results in different distribution of initial emission sites. Important for understanding why some parts fail



Macroscopic Emission from Real Surface

- Air-exposed Pt has significant variation in the initial field emission across the electrode due to variation in β and ϕ
- Changing the random seed results in different distribution of initial emission sites. Important for understanding why some parts fail
- Higher ϕ for annealed Pt results in ~10x less emission



Great but…

- We assumed that β and ϕ were independent… however they appear to be correlated
- Why? Short answer: step density where each atomic step acts like a small dipole

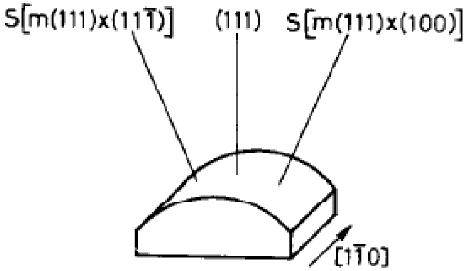
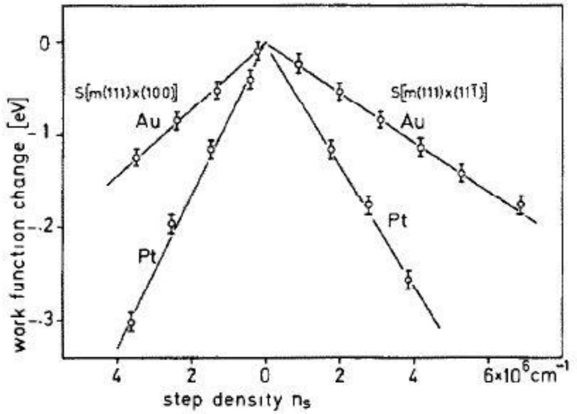
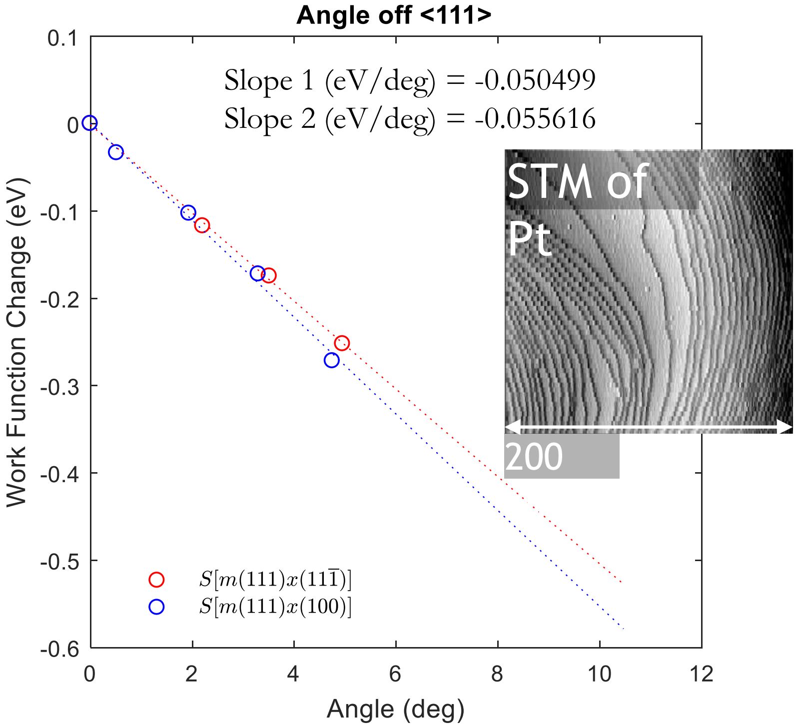


Fig. 1. Schematic representation of curved Pt and Au sample.



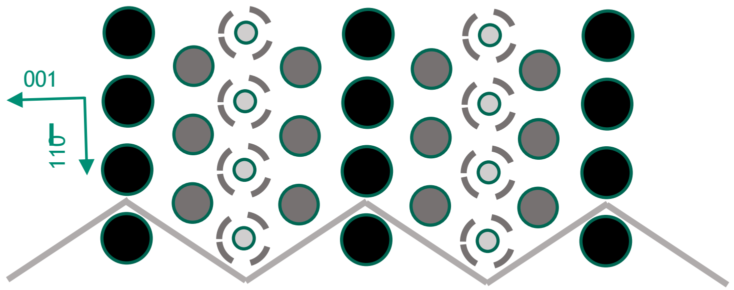
K. Besocke, B. Krahlurban, and H. Wagner, *Surf. Sci.* **68, 39 (1977).

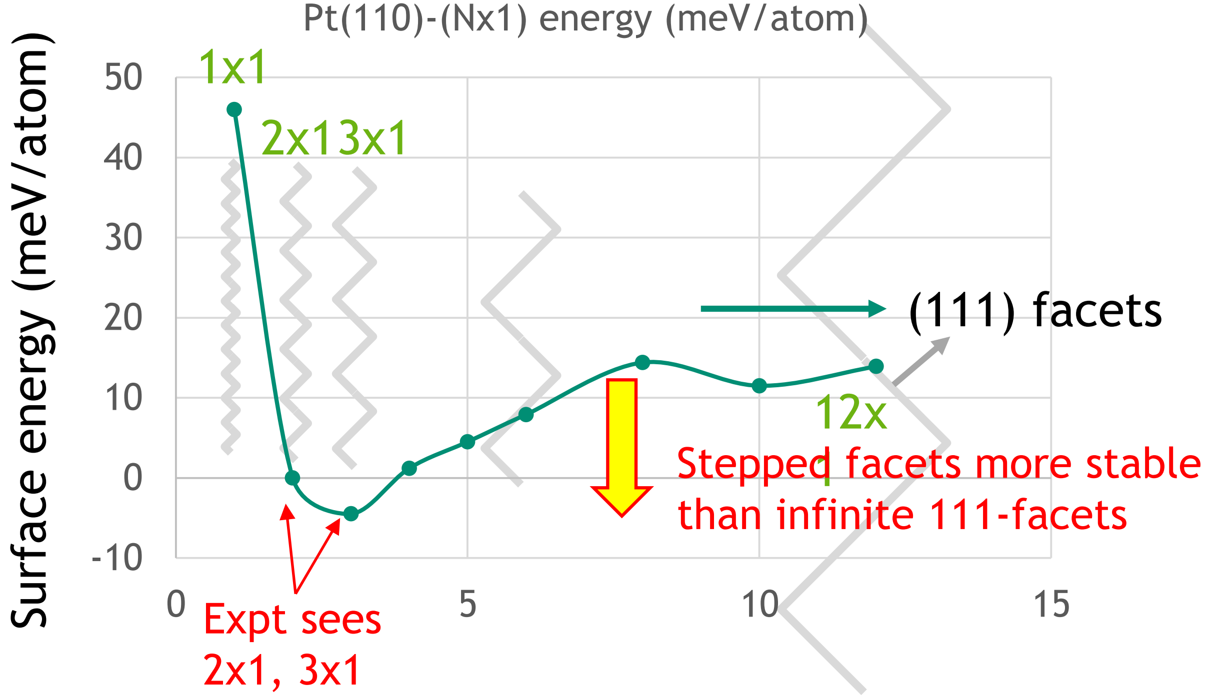


Characterizing the surface with DFT

- Characterize surface structure of clean Pt
- Correlate local structure with local apparent work function (β and ϕ correlation)
- Establish baseline understanding between theory and STM/PEEM
- How do structure and features (e.g. steps, dislocations) affect field emission? What about adsorbates/contaminants?
  - Compute band structure

Pt(110) 2x1 missing row





Thermodynamics/kinetics vs. internal energy
There is a step-creation cost on the flat (111)

Ensemble Monte Carlo Model

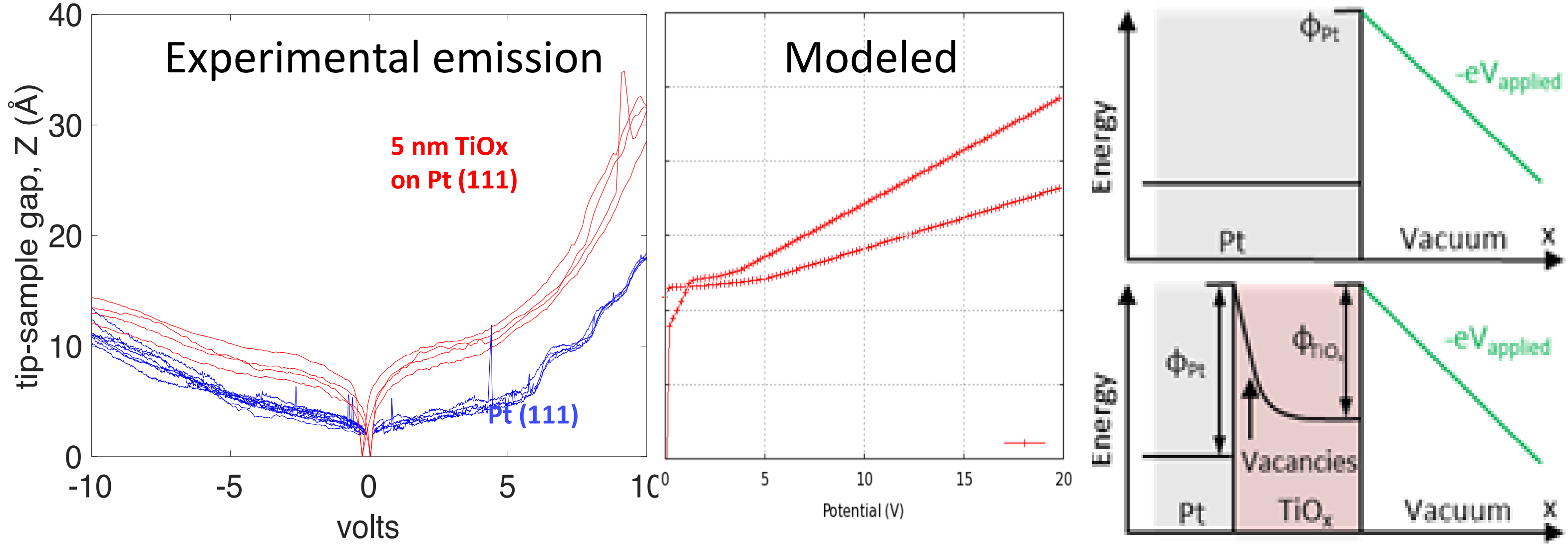
$$J(\mathbf{r}_A,\mathbf{r}_B)=\frac{2}{(2\pi)^3}\int \mathbf{v}(\mathbf{k})T(\mathbf{k},\mathbf{r}_A,\mathbf{r}_B)\{f_A(1-f_B)-f_B(1-f_A)\}d^3\mathbf{k}$$

1. Injection of particles, photons or energetic electrons, at a constant rate
2. "Free flight" of electrons and holes in momentum space (dictated by band structure)
   1. Solve the equations of motion for momentum and position
   2. Quantum treatment of surface boundary → e^- can tunnel through barrier given applied field
3. Scattering (changes in momentum and energy)
   1. Carrier-carrier scattering
   2. Phonon scattering
   3. Impact ionization
   4. Auger recombination
   5. Photon absorption

Ensemble Monte Carlo Model

$$J(\mathbf{r}_A, \mathbf{r}_B) = \frac{2}{(2\pi)^3} \int \mathbf{v}(\mathbf{k}) T(\mathbf{k}, \mathbf{r}_A, \mathbf{r}_B) \{ f_A (1 - f_B) - f_B (1 - f_A) \} d^3\mathbf{k}$$

- Inflection point at the transition from barrier tunneling to field emission tunneling
  - Occurs at effective work function
- Key insight: Band bending occurs even in thin layers of TiOx
  - "Thick" layer limit: Emission dictated by TiOx work function



Future work

- Perform breakdown on measured Pt sample
- Compute effective β based on measured topology
- Appropriately account for correlation between β & ϕ in macroscale model
- Characterize MgO/Pt surfaces
- Time-dependent β based on material properties and current density

Conclusions

- Investigating surfaces at the atomic scale to characterize features relevant to vacuum field emission.
  - Will characterize surface, then perform discharge, and finally re-characterize the surface
- By examining field emission at the nanoscale, we expect to create a macroscopic physics-based model for emission
  - Implemented initial macroscopic model into PIC-DSMC simulation that utilizes measured PDF's to give spatially variable β and ϕ
- Want to clarify β-based field emission so β really is only geometry induced field enhancement.
- "Work function" + (purely geometric) β is not the whole story in practice.

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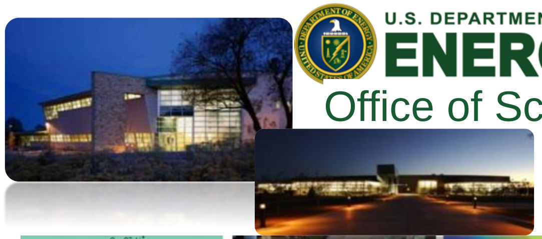

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