Developing Field Emission Models Employing Nanoscale Surface Characterization

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Vacuum Arc Initiation

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

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

- We want 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 (STM) and Photoemission Electron Microscopy (PEEM) 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 and oxide layers.
  - Utilize a “meso-scale” (0.1-1.0 μm) model of the surface for PIC-DSMC simulation of breakdown.

RF vs. DC breakdown
“breakdown rate vs. conditioning” vs. “single shot probability vs. surface state”.
Then pulsed DC.
Vacuum Field Emission Measurements via STM

- A pin-to-plane configuration in a scanning-tunneling microscope (STM) is employed. We also incorporated atomic layer deposited (ALD) surface films.

**Usual scanning operation.**
Adjust $z$ to maintain constant current, e.g., 100 pA.

$$V_{tip} = 0.1 \text{ V}$$

$$z \sim 1 \text{ nm}$$

$$V_{sample} = 0 \text{ V}$$

**Field emission and discharge operation.** Set $z$ and apply “high” voltage.

$$V_{tip} = \text{up to 10 kV}$$

$$z \sim 1\text{–}400 \text{ nm}$$

$$V_{sample} = 0 \text{ V}$$

ALD is used to apply 1–10 nm layer of TiO$_2$

![Graphs showing Pt and Pt + 5 nm TiO$_x$ comparisons.](image)
Why Local Characterization?

- Fowler-Nordheim field emission:
  - Typical used in macroscale models to curve-fit measured $j(E)$ from the as-built electrode
  - Can result in $\beta \sim 10$-1000 !!!

- We want to locally characterize the surface to eliminate $\beta$ as a fit parameter:
  - Use scanning tunneling microscope (STM) and/or atomic force microscopy (AFM) to measure topology at $\leq 10$ nm resolution.
  - By meshing the microscopy surface and solving $E$-fields local to that surface, $\beta$ comes out naturally – no need to “fudge” it.

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

**PEY($h\nu$ sweep)**

- **Xe Lamp** (3.0-6.9 eV tunable)
- **He Lamp** He I (21.22 eV)
- **Hg Lamp Broadband** (3.4-4.9 eV)

**Beam Separator**

**Objective Lens**

**Detector**

**Hg Lamp** Broadband (3.4-4.9 eV)

**Electron Energy Analyzer (Filter)**

- **$\phi = E_{\text{vac}} - E_F$**

- 24 µm FOV, 40 nm pixel maps

**Photoemission yield curve**

**Sample**

- Photoemitted electrons
- Blank states
- Filled states
- Cores

**PEY Yield Intensity ($x10^3$)**

**Wavelength (nm)**

**Work function, $\phi$ (eV)**
PEEM Measurement of Work Function Variation

- Measured spatial variation of local work function using photoemission electron microscopy (PEEM)
  - Variation across given Pt surface relatively small – only a few percent
  - However, $\phi$ 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 ~10 nm-scale PDF’s in mesoscale model to set element work functions in PIC-DSMC simulations
Model Development

- 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

These curves depend on the surface material, conditioning, etc.

Large \( j_e(E(t), \phi, \beta) \)

surface mesh in the plasma code
AFM Surface Characterization

- Took the AFM \((x,y,z)\) spatial points (here \(\sim 20\) nm resolution) and map into Cubit meshing software.
- Actual surface has virtually no significant topology – we will see later that \(\beta \sim 1\) everywhere.
- To demonstrate significant spatial variation of field emission across the surface we also compute results with the surface relief multiplied by \(10\times\).

As-measured surface relief

Surface relief increased by \(10\times\)
AFM Topology → Topological Atomic-Scale $\beta$

- Planar anode ~10 um above surface (ignore tip in pic!)
- Compute $E_{\text{norm}}$ and $A_{\text{proj}}$ for every element face in the resolved STM mesh
  - < 10 nm elements; ~600K surface faces
- Get projection factor, $f_{\text{proj}} = \frac{\sum_{\text{faces}} A_{\text{face}}}{\sum_{\text{faces}} A_{\text{proj},\text{face}}}$
  - For present data $f_{\text{proj}} \sim 1.15$
- Create ~20 nm scale PDF of $\beta = \frac{E_{\text{norm}}}{E_{\text{applied}}}$
- Some elements will have $\beta < 1$
  - Globally the surface could be tilted
  - Sides of “sharp” atomic features

Electrostatic solve
Mesoscale Model for Surface Variations

- We have measured atomic-scale (1-10 nm) PDFs of the work function and topological field enhancement factor.

- Must convert these to the mesoscale (0.1-10 μm). Some options:
  1. Just pick the meso-scale $\beta$ and $\phi$ from the atomic-scale PDFs.
  2. Make an effective $\beta$ and $\phi$ to use at the meso-scale.
  3. “Brute force” – for each meso-scale element face, pick N local emitters (unique $\beta$’s and $\phi$’s).

- Option #1 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 mesoscale element’s area.
  - Other times there will be no tail values picked and no field emission until much higher fields.

- We will proceed to do #2 and #3 and compare to resolved $\beta = 1$ everywhere.
Mesoscale Model for Surface Variations

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

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

\[
\rightarrow \beta_{\text{eff}} \text{ depends on } E_{\text{applied}}!
\]
  - This makes sense: small $\beta$ regions “turn on” at higher fields and pulls the effective $\beta$ lower
  - The precise functional form depends on the atomic-scale $\beta$ PDF

\[
\text{e.g. see: } \quad \text{Feng and Verboncoeur, PoP 13, 073105 (2006)} \quad \text{Jinpu Lin et al., J. Appl. Phys. 121, 244301 (2017)}
\]
Mesoscale Model for Surface Variations

- We are left with “brute force” -- for each mesoscale element face, pick N local emitters (randomly pick unique $\beta$’s and $\phi$’s) from the atomic-scale measured distributions:

\[
N = \frac{A_{\text{element}}}{A_{\text{resolved}}} f_{\text{proj}}
\]

- Must scale the number of local emitters to draw:

8 local faces that the $\beta$ and $\phi$ PDF created from

\[
f_{\text{proj}} = \frac{\sum_{\text{faces}} A_{\text{face}}}{\sum_{\text{faces}} A_{\text{proj,face}}} = 2
\]

Draw 8 local emitters
Mesoscale Model for Surface Variations

- However, we don’t have to store all N local emitters for each surface element face
  - Field emission is highly nonlinear, and most emitters ($\beta$ and $\phi$) can be neglected

- Store every atomic-scale emitter ($\beta$ and $\phi$) that appreciably contributes to the current
  - A threshold current contribution of 0.1% results in storing ~0.01% of the atomic-scale emitters
  - 1 $\mu$m$^2$ element has $10^4$–$10^6$ atomic-scale emitters → store < 1000 emitters.

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

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

- With the resolved (Δx < 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

10×ΔZ

4 μm
Mesoscale 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 $\beta$’s and $\phi$’s) and compute breakdown probabilities for as-built surfaces.
- 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 ($\beta$’s and $\phi$’s) independently for every “meso-scale” surface elements. Clearly not independent for sputtered deposited Pt.
Mesoscale Field Emission Simulations

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

- Took local field emission i-V curves with tip radius < 100 nm at a distance of ~200 nm
- Relatively feature-less surface with small-\(\beta\) 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-\(\beta\) atomic-scale features that grow into large-\(\beta\) 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 \(\beta\) to get breakdown at ~10 MV/m that was not present on our ~10^{-6} \text{cm}^2 sampled area.
Conclusions

• Investigating surfaces at the atomic scale to characterize features relevant to vacuum field emission.
  • Surfaces that we characterized are extremely flat: $\beta \sim 1$ over 100’s of $\mu$m$^2$
  • Want to clarify $\beta$-based field emission so $\beta$ really is only geometry induced field enhancement.

• By examining field emission at the nanoscale, we have attempted to create a mesoscale physics-based model suitable for predictive (and stochastic) PIC simulation of emission
  • Still have a long way to go – working on how to handle the correlation between beta and work function.

• Characterized region, then performed local discharge in STM (spatially constrained surface participation) → Breakdown occurred at $\sim 4$ GV/m!
  • Region was flat and uninteresting – the breakdown field is consistent with breakdown from region with a small $\beta$

We have a Low Temperature Plasma Research Facility to collaborate with external partners. Please see www.sandia.gov/prf.