MODELING THE ROLE OF β ON VACUUM FIELD EMISSION IN PIC DSMC SIMULATIONS: SCALING FROM NANO TO MESO SCALE

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Overview

- Here we discuss a physics-based "meso-scale" (0.1 - 1.0 μm) model of well-characterized "real" surfaces for use in large-scale PIC-DSMC vacuum breakdown simulations (Fig. 1).
- The meso-scale model is informed by locally characterizing sputter deposited Pt surfaces (0.1 – 10 nm) using Scanning Tunneling Microscopy (STM), Atomic Force Microscopy (AFM), and PhotoEmission Electron Microscopy (PEEM) before breakdown.
  - Field enhancement (β) factor probability density distribution (PDF) obtained from Poisson solve using Finite Element mesh created from STM and/or AFM measurements of the resolved real surface.
  - Work function (ϕ) PDF obtained directly from PEEM measurements of the resolved surface.

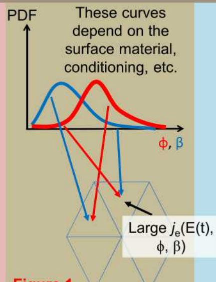

Figure 1

Surface Characterization

PEEM Measurement - ϕ Variation

- PhotoEmission Electron Microscopy was performed on sputter deposited Pt surfaces to obtain the spatial variation in the work function (ϕ)
- Although variation across the sample surface was only a few percent, ϕ is in the argument of the exponent in the Fowler-Nordheim equation, $j = \frac{q^3}{8\pi h}\frac{\beta E^2}{t^2(y)}e^{-6.83x10^7\frac{\phi^{3/2}v(y)}{\beta E}}$ and the tail of the distribution can initiate field emission and ultimately breakdown
- Significant decrease in ϕ of ~10% was observed due to surface contaminants from exposure to air (Fig. 2)
- Applied the ~10nm-scale PDF's in meso-scale model to set element ϕ's in PIC-DSMC simulation

AFM Measurement - β Variation

- Atomic Force Microscopy was performed on sputter deposited Pt surfaces
- Real AFM data point data interpolated and converted into model using SolidWorks, with surface relief scaled by 10x, otherwise variations observed in β deemed insignificant (Fig. 3)
- Generated topology meshed in Cubit, applying an unstructured tetrahedral FEM (Fig. 4)
  - Flat anode placed ~10 μm from as-measured surface
  - ~1 nm surface elements placed near cathode to resolve features
- β at nano scale based on ratio of E-field normal ($E_\perp$) to a "resolved" (0.1 – 10 nm) element face to that of applied E-field (E_{app}) seen by that element: $\beta = \frac{E_\perp}{E_{app}}$ (Fig. 5)

ϕ, β Atomic Scale PDFs

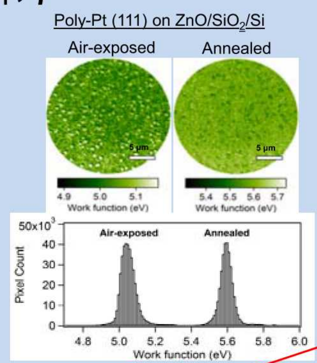

Figure 2

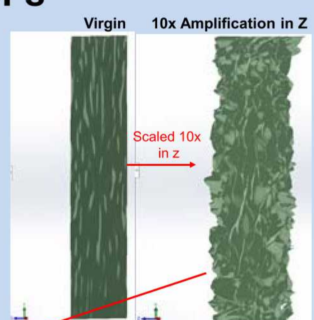

Figure 3

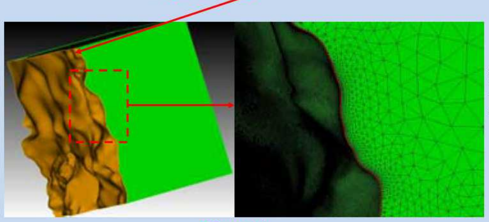

Figure 4

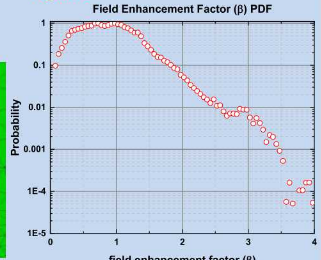

Figure 5

Meso-Scale Model

- To scale from nano to meso dimensions, we can employ the following approaches:
  - Generate an effective β and ϕ
    - Compute total field emission current vs. E_{app} for a resolved AFM area of 10x10 μm
    - n-linear solve for β_{eff} (Fig. 6): $i = A_{eff}\frac{q^3}{8\pi h}\frac{\beta_{eff}E^2}{t^2(y)}e^{-6.83x10^7\frac{\phi^{3/2}v(y)}{\beta_{eff}E}}$
    - β_{eff} decreasing with E_{app} expected since many small β regions "light up" at elevated E_{app}, collectively dragging down the effective β; exact behavior depends on atomic-scale β PDF
  - Apply "brute force"
    - A projection factor (f_{proj}) is calculated based on the projected (A_{proj}) and actual (A_{face}) areasa of every element from the resolved nano-scale mesh: $f_{proj} = \frac{\sum_{faces} A_{face}}{\sum_{faces} A_{proj}}$
    - N local emitters for each meso-scale element face are determined by sampling from the β and ϕ PDFs:

$$N = \frac{A_{meso}}{A_{nano}}f_{proj} = \frac{4nm}{1nm}(2) = 8$$

- Example: β and ϕ sampled from atomic-scale PDF's for 8 local faces, drawing 8 local emitters (Fig. 7)
- Since FE is very non-linear, threshold current contribution of 0.1% results in N = ~0.01% of total atomic-scale emitters, β, and ϕ being stored
- Example: 1 μm^2 element = 10^4-10^6 atomic-scale emitters, resulting in <1000 emitters stored

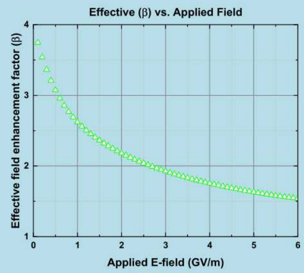

Figure 6

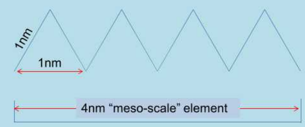

Figure 7

- At every Δt time step in PIC algorithm, compute $E_\perp$ on face of each surface element and loop over all ~100 atomic-scale local emitters, β_e, and ϕ_e: $i_{face} = A_{eff}\frac{q^3}{8\pi h}\frac{\beta_e E_\perp^2}{t^2(y)}e^{-6.83x10^7\frac{\phi_e^{3/2}v(y)}{\beta_e E_\perp}}$

Results

- Comparable behavior for current vs. E_{app} between meso-scale model and STM measurements (Fig. 8), with meso-model scaled by ~12 x i_{STM} for flat anode located 10.4 μm from mean cathode height. Difference probably from field variations due to changes in gap distance for STM surface.
- FE i-V curve for tip radius<100 nm placed ~200 nm away, with breakdown at ~ 4GV/m, suggesting that for smooth sputter deposited Pt, no small-β atomic-scale features grow into large-β features facilitating breakdown to occur at ~10 MV/m (Fig. 9).

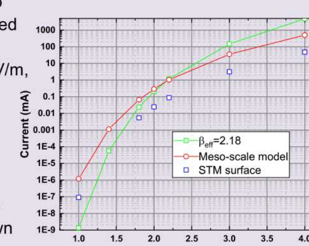

Figure 8

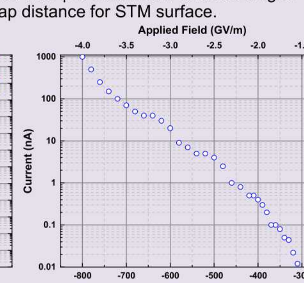

Figure 9

- Spatial electron density profiles just above cathode for meshed STM and flat meso-scaled surfaces are very dissimilar (Fig. 10), possibly due to atomic-scale emitter β_e's and ϕ_e's being picked independently of one another for every meso-scale surface element. Current model needs to be modified to take into account correlation between β and ϕ!

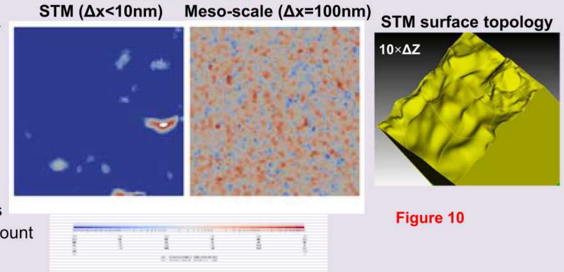

Figure 10

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