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Sandia National Laboratories

Vacuum Field Emission
Models, Measurements, and Simulations

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[1]Applied Optical and Plasma Sciences
[2]Solid State Microsystems
[3]Electronic, Optical, and Nano Materials
[4]Physics Based Microsystems
[5]Materials Characterization and Performance
[6]Radiation Effects Theory
[7]Multiscale Science
[8]Electrical Science and Experiments
[9]Electromagnetic Theory

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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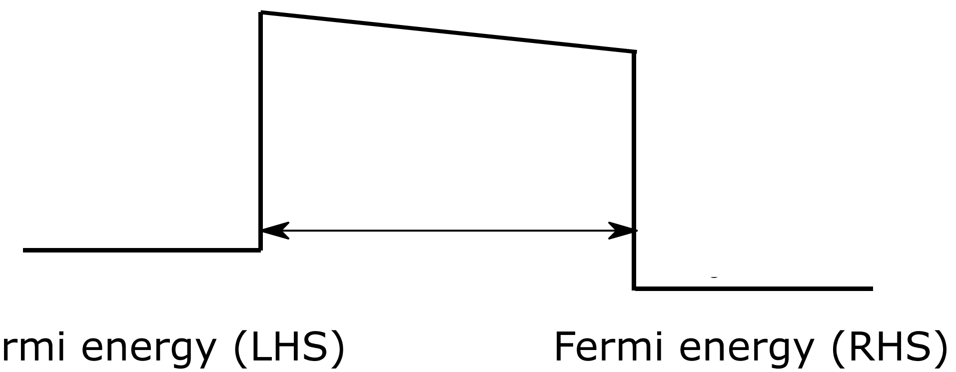
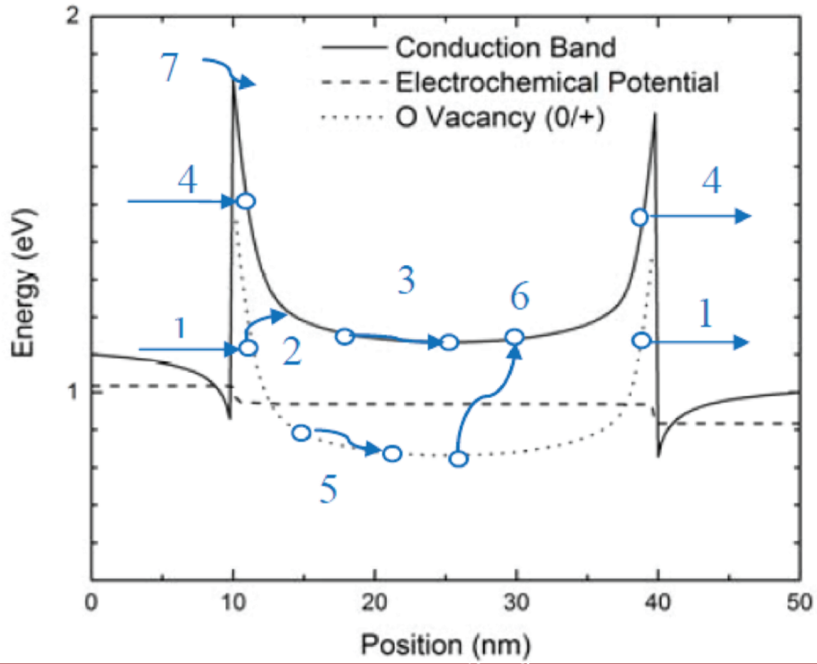
Introduction/Motivation

We have begun a new project to understand vacuum field emission from well-controlled surfaces to create physics-based models.

- Restricted to *vacuum* field emission to concentrate solely on field (and temperature) effects – no feedback from gas/plasma species.
- Field emission is viewed as the 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. Very locally → single metal grain and much smaller (down to atom).
- Address the problem of not knowing state prior to discharge at location of discharge by characterizing and then discharging.
- Apply known layers of dielectric (TiO_2) to challenge models and begin investigation of role of surface contaminants.
- Simulate electron transport resulting in field emission for some experimental situations. Extrapolate to uglier ones.

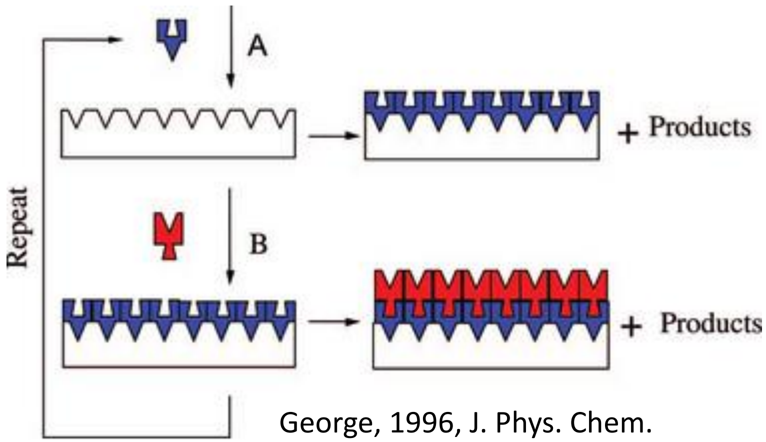
Band Structures





1: Free-to-defect tunneling
2: Defect-to-free tunneling
3: Free carrier transport
4: Free-to-free tunneling
5: Defect-to-defect hopping
5: Defect-to-defect Poole-Frenkel tunneling
6: Defect capture and emission
7: Thermionic emission

ALD (Atomic Layer Deposition)



George, 1996, J. Phys. Chem.

Kim, 2011, J. Electrochem Soc.

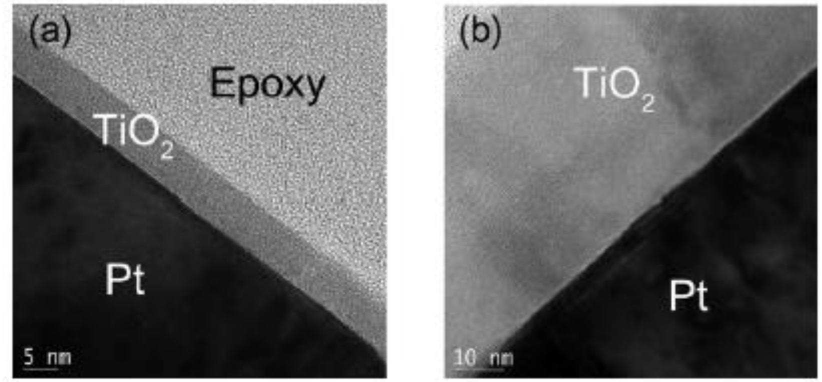
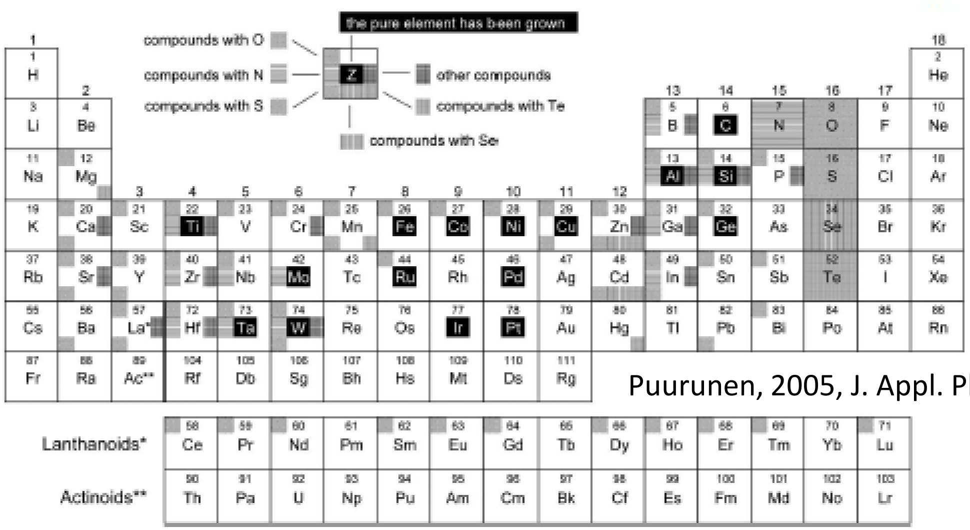
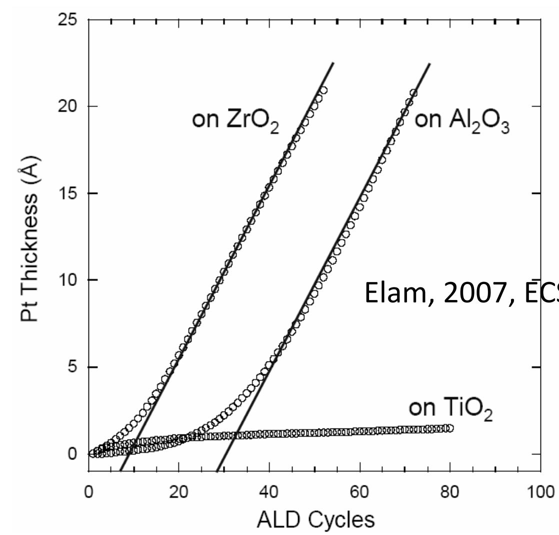


Figure 4. HRTEM images of TiO_2 films grown at 260°C: (a) 6 nm thick and (b) 50 nm thick.



Puurunen, 2005, J. Appl. Phys.

FIG. 3. Overview of the materials grown by ALD. Classification according to Reactant A, with details of the investigations in Table III. Growth of pure elements as well as compounds with oxygen, nitrogen, sulphur, selenium, tellurium, and other compounds grouped together are indicated through shadings of different types at different positions. The elements are named according to the recommendations of The International Union of Pure and Applied Chemistry (IUPAC, http://www.iupac.org/reports/periodic_table/, dated 1 November 2004).



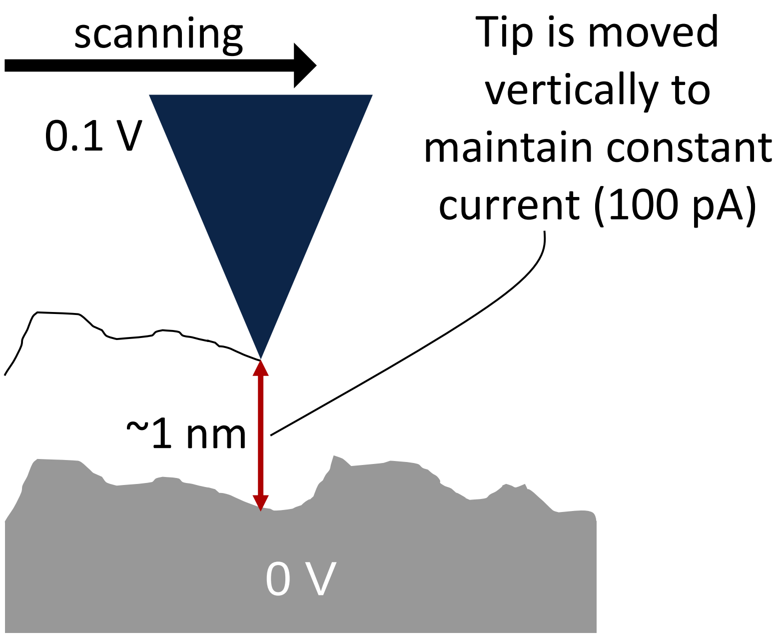
Elam, 2007, ECS Trans.

STM (Scanning Tunneling Microscopy)

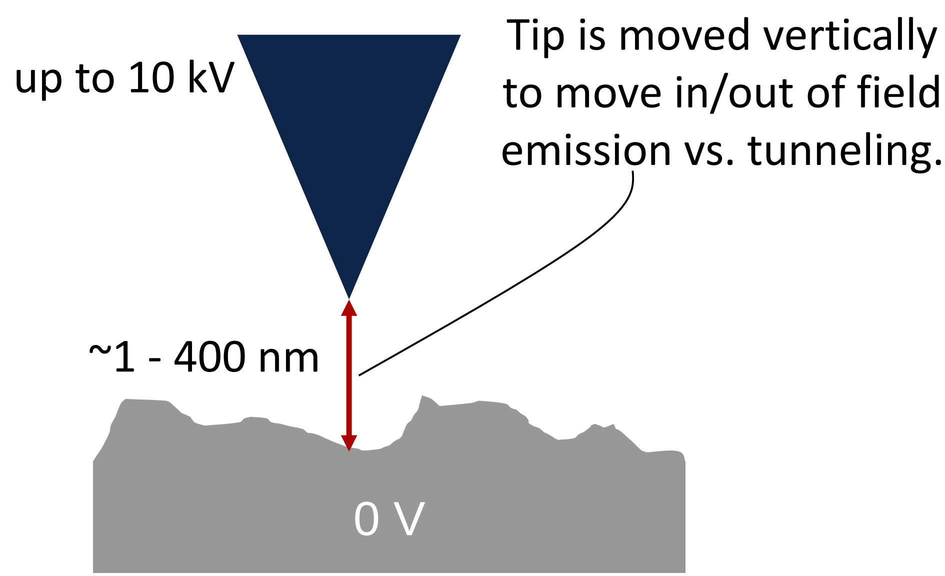
Expected to be a workhorse for field emission and breakdown studies.

- Can go down to sub-nm resolutions.
- Can measure topography in fixed current mode.
- Can measure field emission at applied E.

Typical “correct” usage.



Our planned special usage includes *performing discharge in the STM!*



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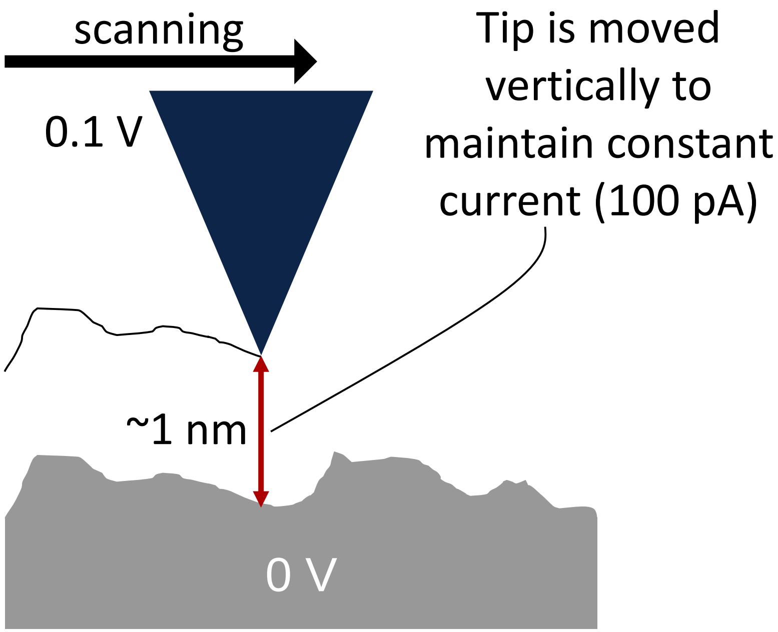

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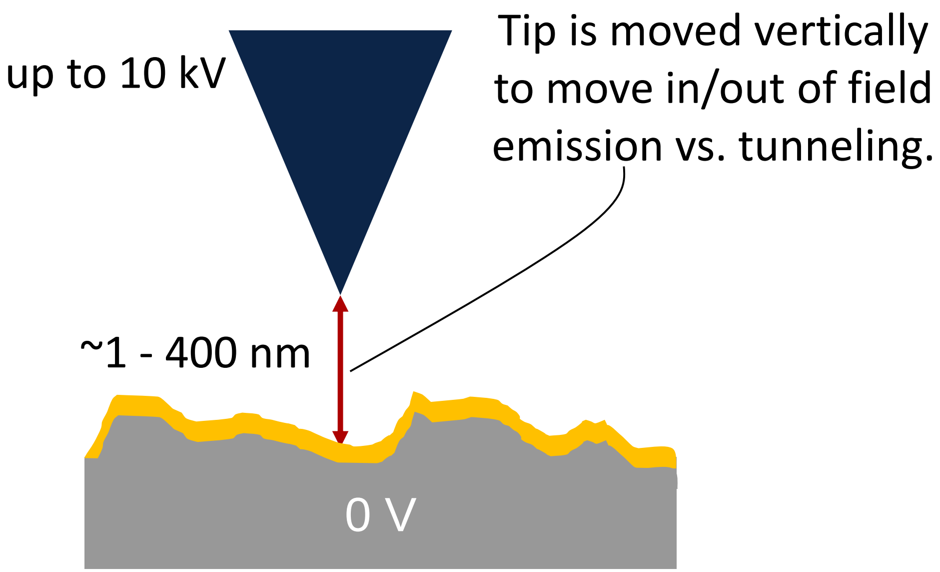
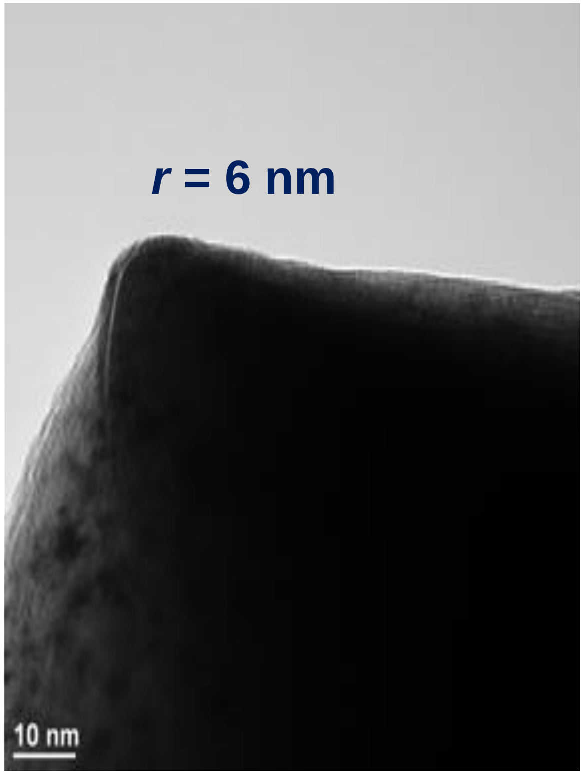


Locality, locality, locality...

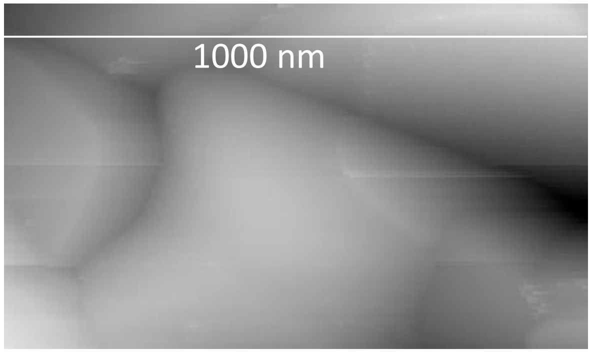
STM Results

TEMs of an STM tip.

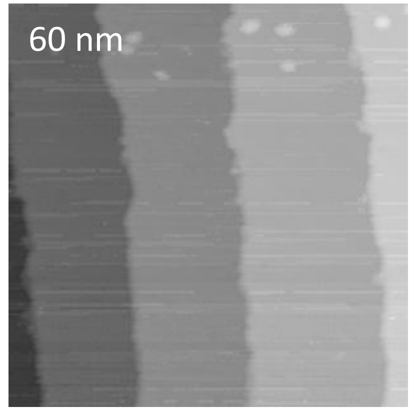


STM Results

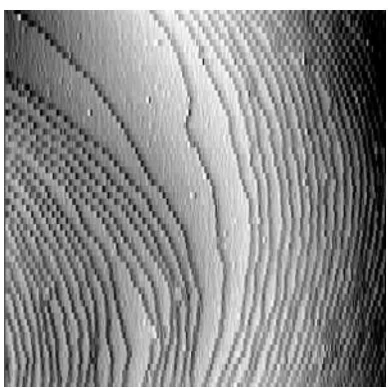
Sean sputtered Pt/ZnO/SiO_2/Si annealed to 900C
After heating to 640 C/5 mins in ultrahigh vacuum.

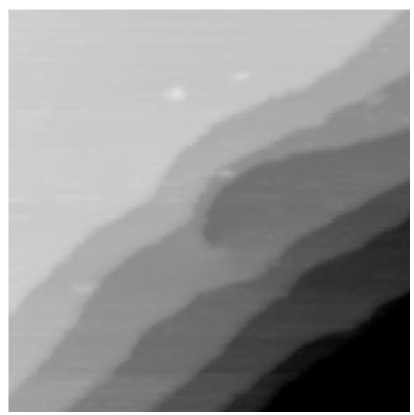


20150210_00x



200 nm



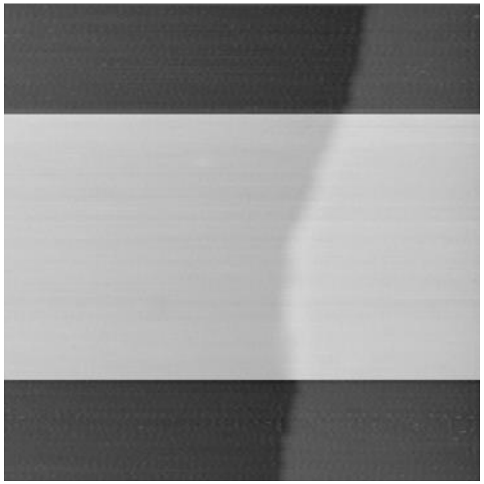


-0.1 V, 1 nA

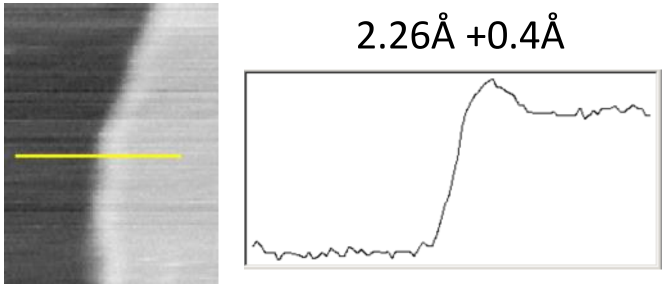
All atomic steps are 2.2-2.4 Å, consistent with 111. A 100 step is 1.9 Å.

-0.1 V, 1 nA
tunnel

-10 V, 1 nA
FN tunnel

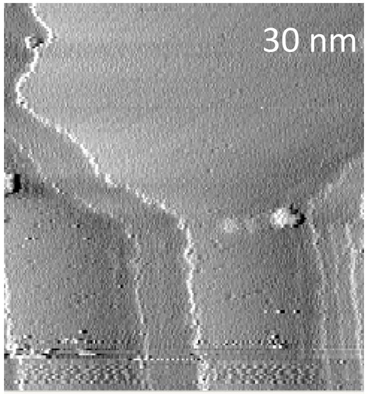


2.26Å +0.4Å



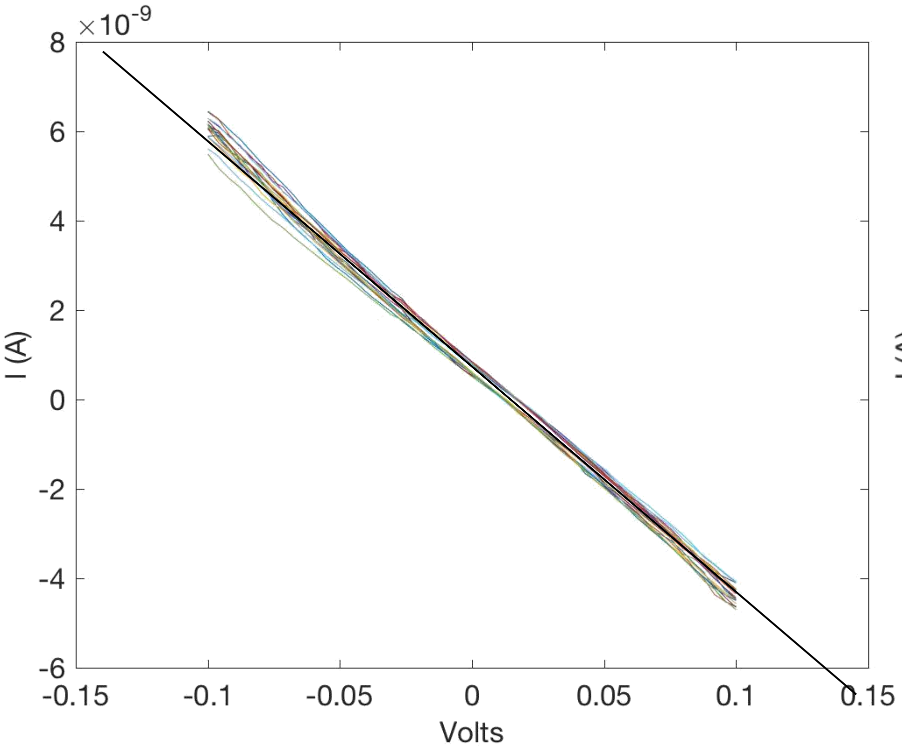
Step edge anomaly field enhancement

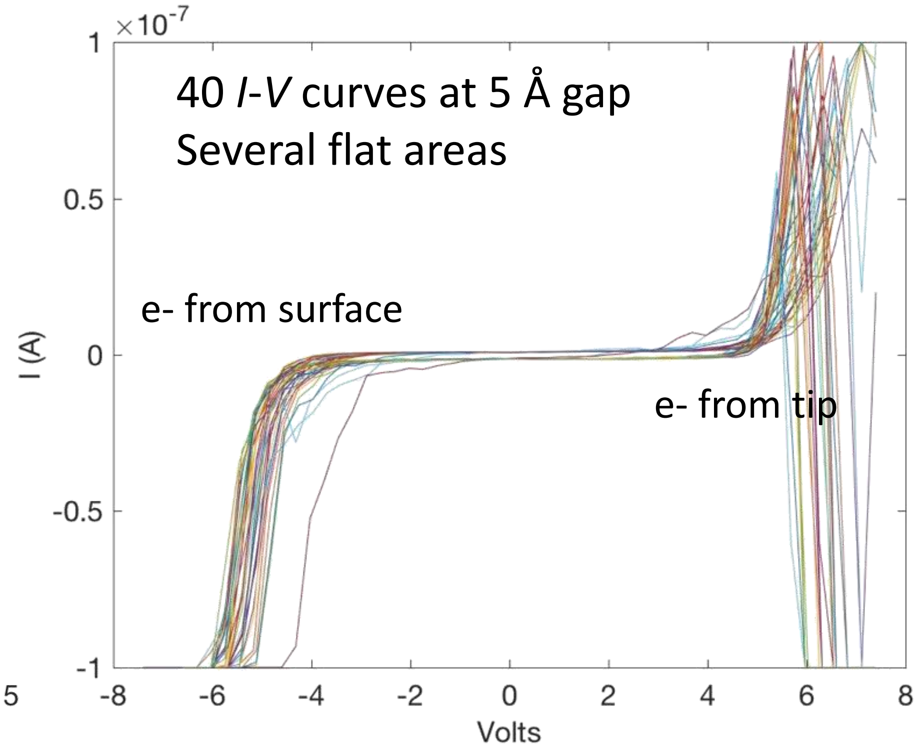
STM Results



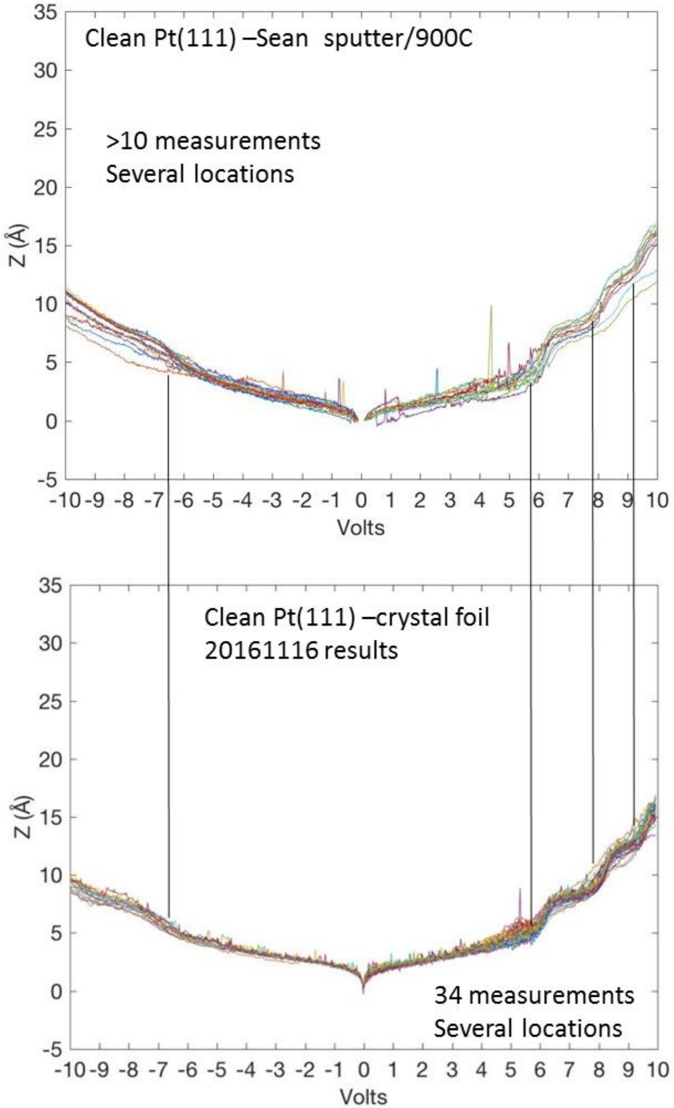
Surface is metallic → no bandgap.

1. Find a clean flat area.
2. Check tunnel gap is Ohmic around 0 V.
3. Establishes that tip is reasonably free of dielectric crud & surface is metallic.





STM Results



- FN resonances line up.
- Amazing that anything compares at all, these are from *different* tips with very different geometries.
- Prepared by different techniques and battered against surface in different ways.

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Electron Interferometry at Crystal Surfaces

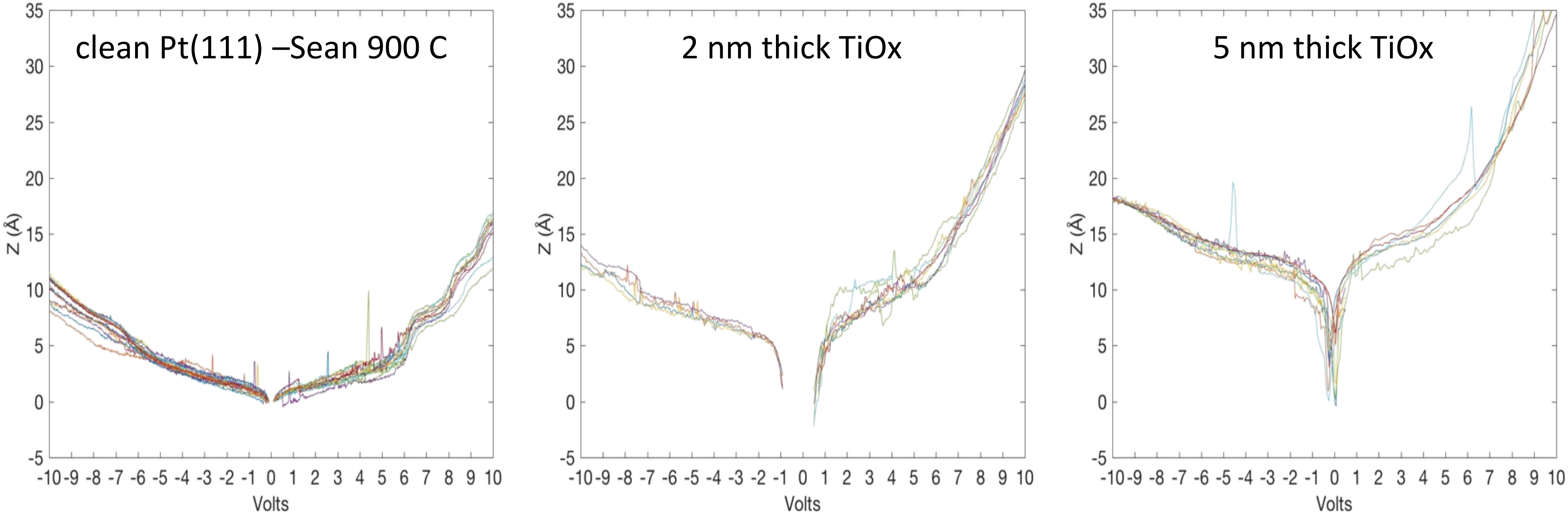
R. S. Becker, J. A. Golovchenko, and B. S. Swartzentruber
AT&T Bell Laboratories, Murray Hill, New Jersey 07974
(Received 10 April 1985)

Electron standing waves formed in the vacuum gap between the probe and the sample of the tunneling microscope are observed. The sensitivity of the standing-wave positions and frequencies to the surface potential are demonstrated. Further effects possibly due to Bragg backscattering from the surface atomic planes of the sample are discussed.

PACS numbers: 73.20.Cw, 73.40.Gk

STM Results

Characterize variability by looking at a few locations for each type of sample.



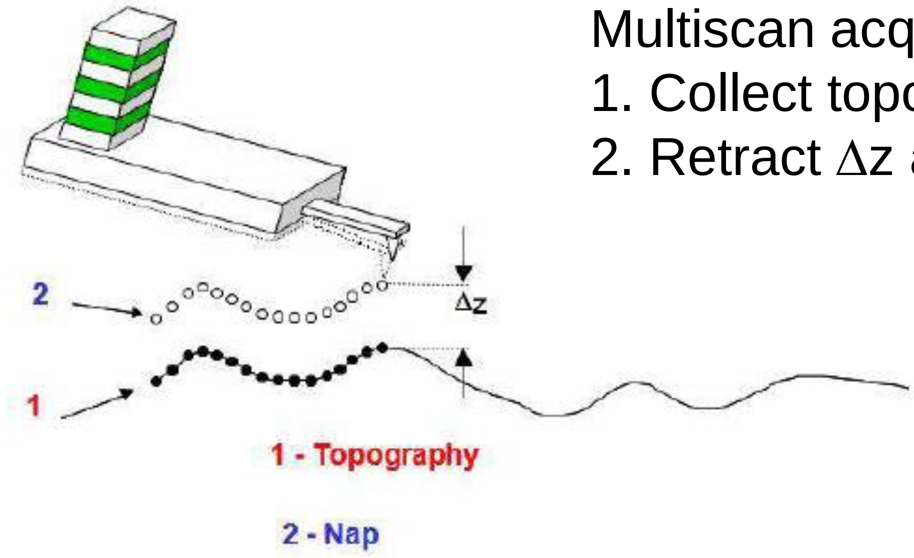
Note that at fixed voltage a larger gap in the 5 nm layer can achieve the same current as a smaller gap for 2 nm layer, and even smaller gap for clean Pt.

→ The oxide layer *increased* field emission!

AFM (Atomic Force Microscopy)

Scanning Surface Potential Microscopy (SSPM) aka
Kelvin Probe Microscopy (KPM) aka
Scanning Kelvin Probe Microscopy (SKPM)

Method to detect potential difference between probe tip and sample

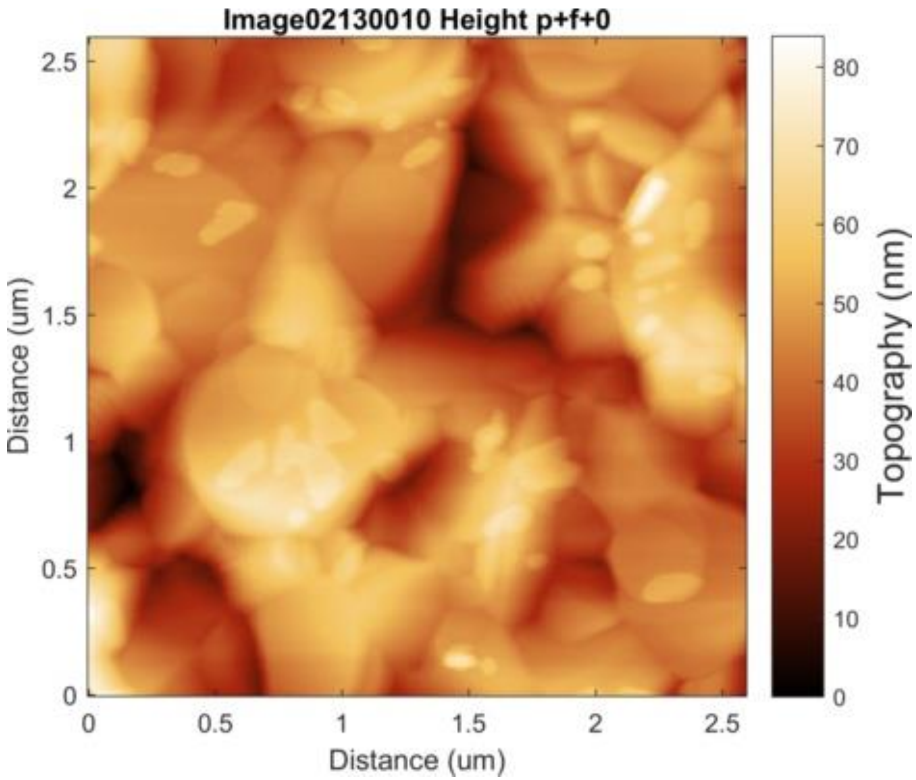


Multiscan acquisition
1. Collect topography
2. Retract Δz and collect electrical image

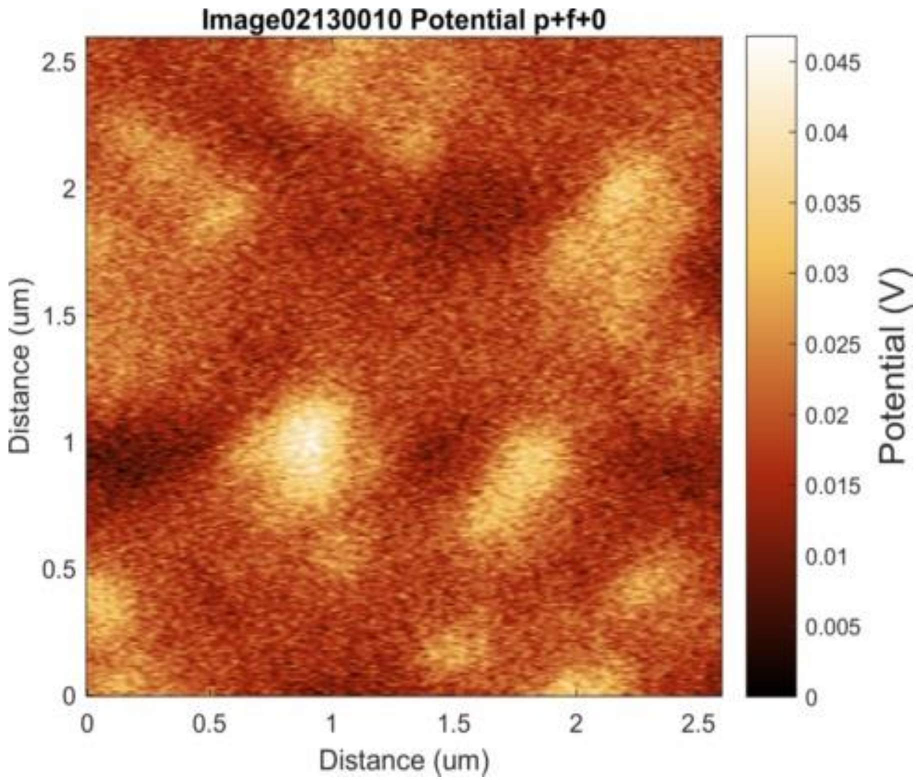
Resolution < contact mode measurements

AFM Comparison

5 nm TiO_2 on 900ºC Pt/ZnO/SiO_2/Si



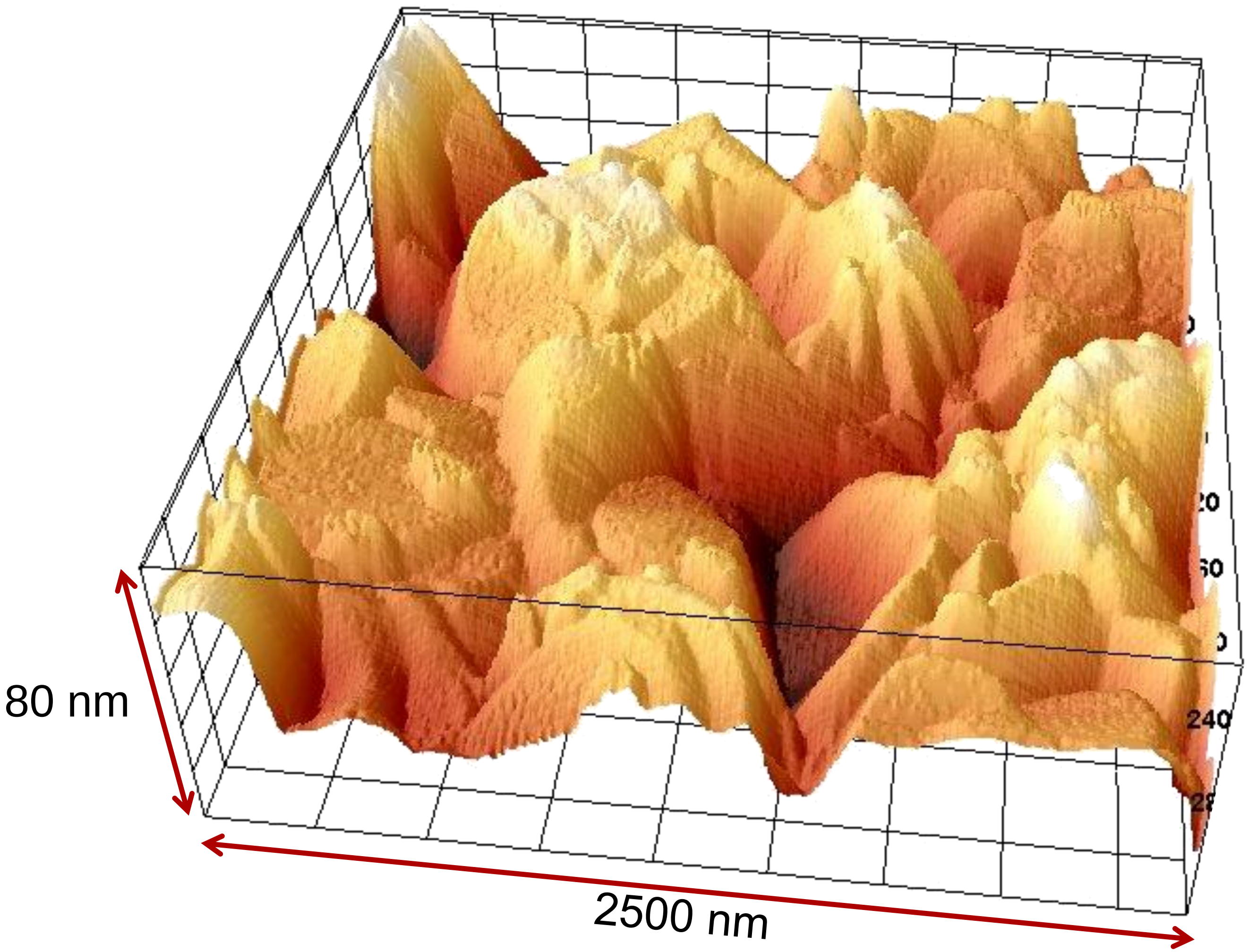
Topography



Potential

AFM Comparison

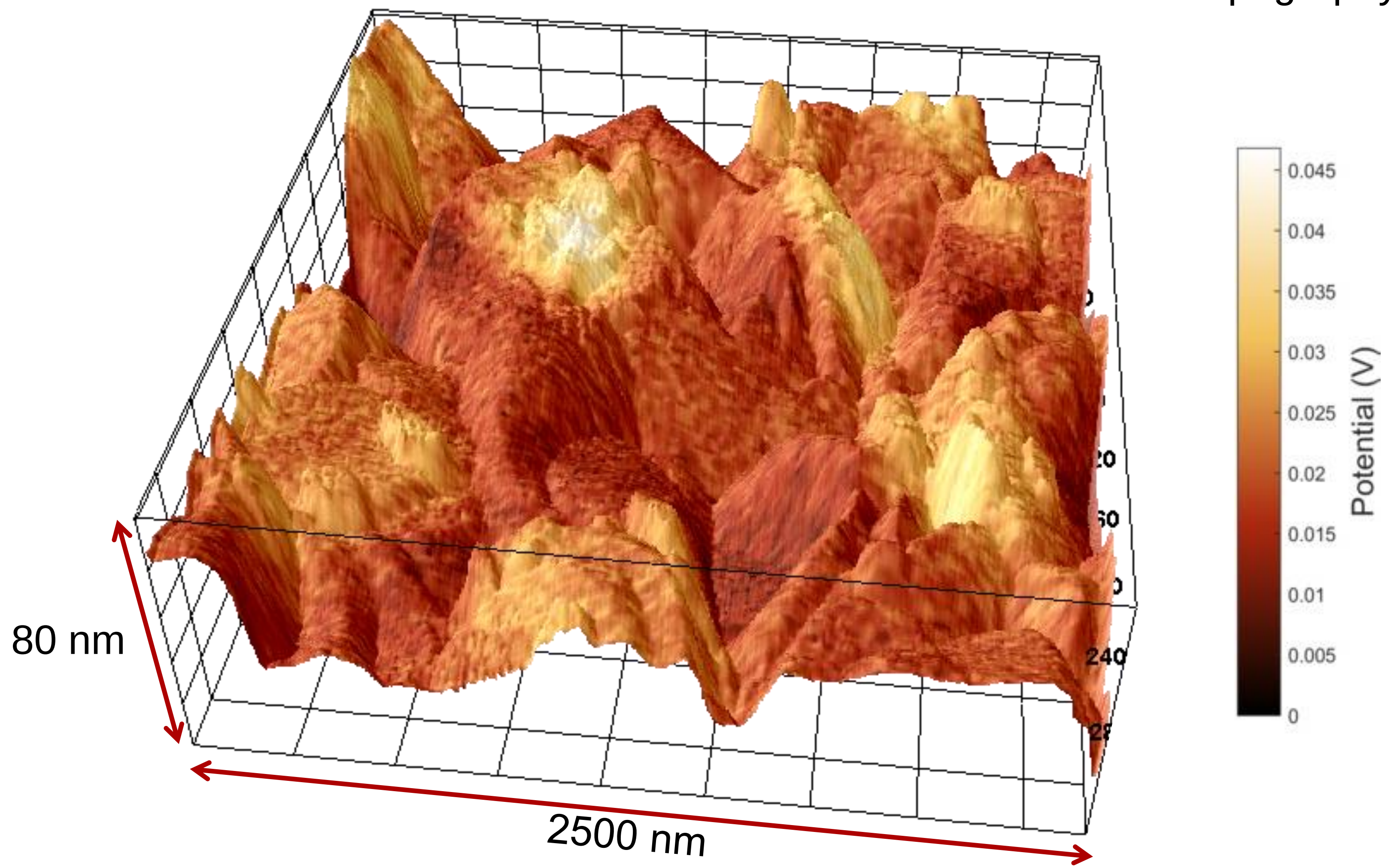
5 nm TiO_2 on 900ºC $Pt/ZnO/SiO_2/Si$



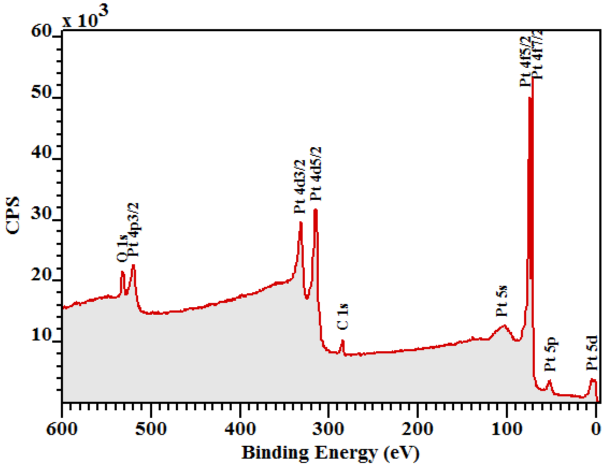
AFM Comparison

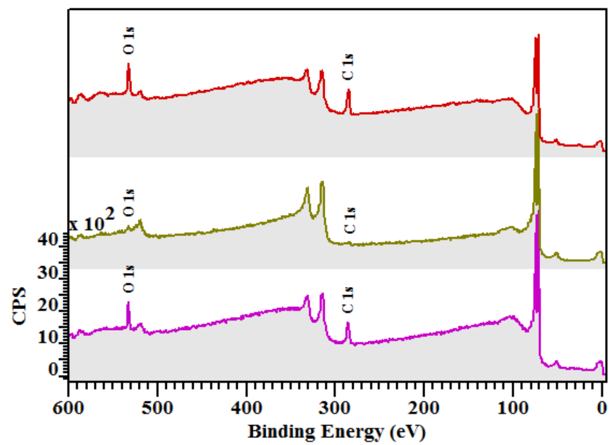
5 nm TiO_2 on 900ºC $Pt/ZnO/SiO_2/Si$

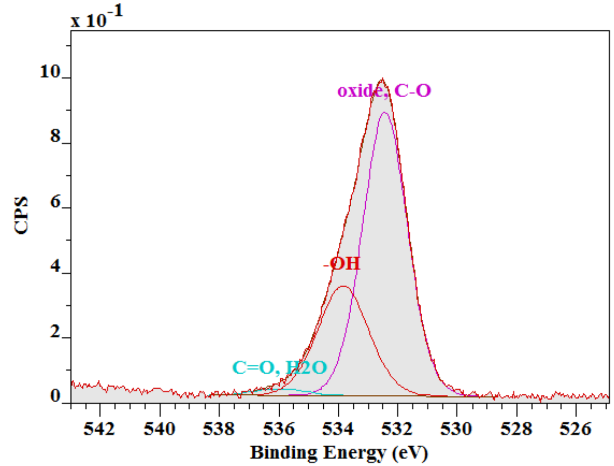
Potential is not always correlated to topography!

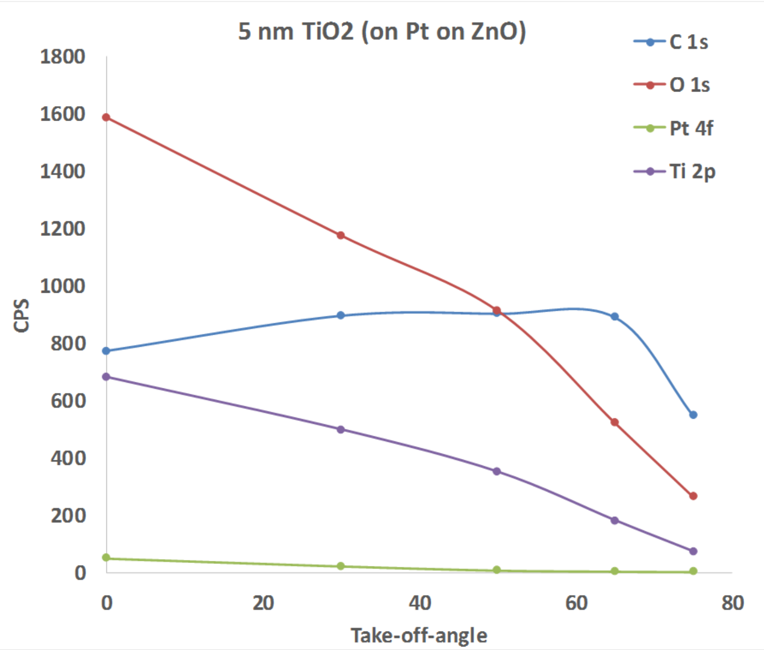


XPS (X-Ray Photoelectron Spectroscopy)









Substrate Designator:	5 nm TiO2 on Pt on ZnO_00			
	Intensity			
Emission Angle (degrees)	C 1s	O 1s	Pt 4f	Ti 2p
0	772	1585.85	48.1921	680.766
30	894.801	1174.42	20.9266	497.498
50	901.677	912.071	6.13556	349.818
65	888.825	520.7	2.35738	180.272
75	544.989	262.51	0.893102	71.4935
		Hydrocarbon Thickness (Å):	**15.93**	
		Uncertainty (Å):		
		RMSE of Fit:	0.9255	
		Oxide Thickness (Å):	**69.28**	
		Uncertainty (Å):		
		RMSE of Fit:	0.007656	

Electron Transport

A continuum approach, REOS (Radiation Effects in Oxides and Semiconductors), models the reactive transport of electrons, holes and other species such as vacancies. Energy transport in terms of the heat equation as well as electron, hole and lattice temperatures.

Continuity Equations

$$\frac{\partial c_i}{\partial t} = -\nabla \bullet \mathbf{J}_{si} + \sum_j \nu_{ij} R_{ij} + G_i$$

$$\left\{ \begin{aligned} c_i &= \text{Density of species i} \\ J_{si} &= \text{Current density of species i} \\ \nu_{\text{ij}} &= \text{Reaction coefficient for species i in reaction j} \\ R_{\text{ij}} &= \text{Reaction rate for species i in reaction j} \\ \text{G}_{\text{i}} &= \text{Generation rate for species i} \end{aligned} \right.$$

Drift-Diffusion Species Current

$$\mathbf{J}_{si} = z_i c_i \overline{\mu}_i \mathbf{E} - D_i \nabla c_i$$

$$\left\{ \begin{aligned} \overline{\mu}_i &= \text{mobility} \\ \mathbf{E} &= \text{electric field} \\ \text{z}_{\text{i}} &= \text{species charge sign} \end{aligned} \right.$$

Electron Transport

A stochastic approach, EMC (Ensemble Monte Carlo), explicitly models electron scattering events, vacancy generation, etc.

The Boltzmann equation that describes transport in solids can be written as

$$\frac{\partial f(\boldsymbol{r},\boldsymbol{p},t)}{\partial t} = -\frac{1}{2\pi\hbar}\sum_{\boldsymbol{r}',\boldsymbol{p}'} |V_{\boldsymbol{rp},\boldsymbol{r}'\boldsymbol{p}'}|^2 f(\boldsymbol{r},\boldsymbol{p},t)\{1-f(\boldsymbol{r}',\boldsymbol{p}',t)\} - f(\boldsymbol{r}',\boldsymbol{p}',t)\{1-f(\boldsymbol{r},\boldsymbol{p},t)\}\delta(E_i - E_f)$$

in which $f(\boldsymbol{r},\boldsymbol{p},t)$ is the particle distribution function for position $\boldsymbol{r}$, momentum $\boldsymbol{p}$ and time t. The effects of scattering are contained in the interaction potential V.

The software EMC obtains a steady-state solution to this equation by using an iterative method that uses a Monte Carlo technique.

An important feature of this software is the use of a distribution function that includes Fermi statistics. This feature is necessary for the inclusion of carrier-carrier scattering effects that control fully developed electrical breakdown effects.

Electronic Structure – Density Functional Theory

To inform continuum models of electron transport, we need detailed information of the electronic structure of bulk materials, interfaces and surfaces, and defects that comprise the physical system.

A first principle approach, SeqQuest models the electronic structure using a pseudopotential approach and local orbitals, used to model large computational models with accurate treatment of defects. We will also use VASP when a plane wave approach is more appropriate.

- Band structure – transport of electrons through surface oxides
- Electronic levels of bulk defects – defect-mediated transport
- Φ – work functions – transport between the surface material and vacuum
- Surface structure and defects – modifies transport to vacuum
- First principles treatment of charge and fields

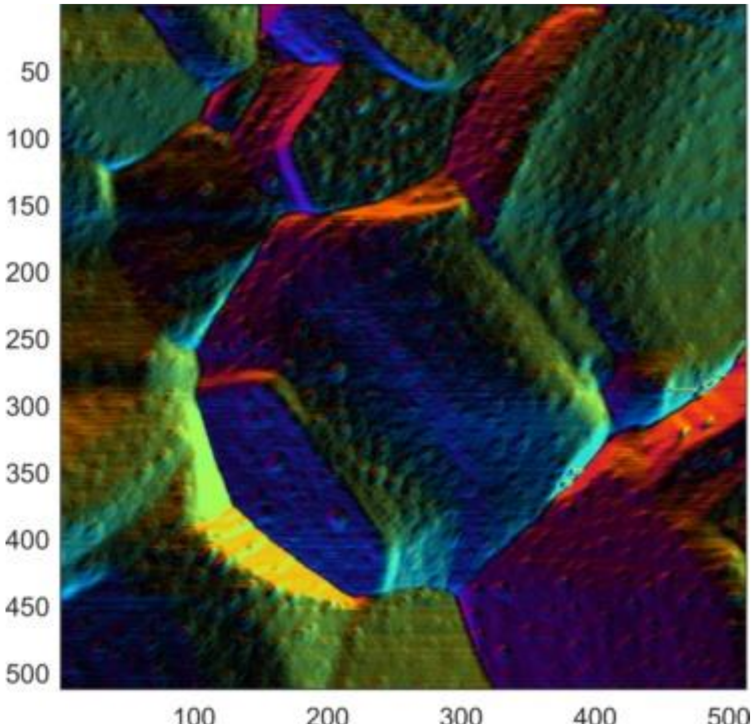
Conclusions

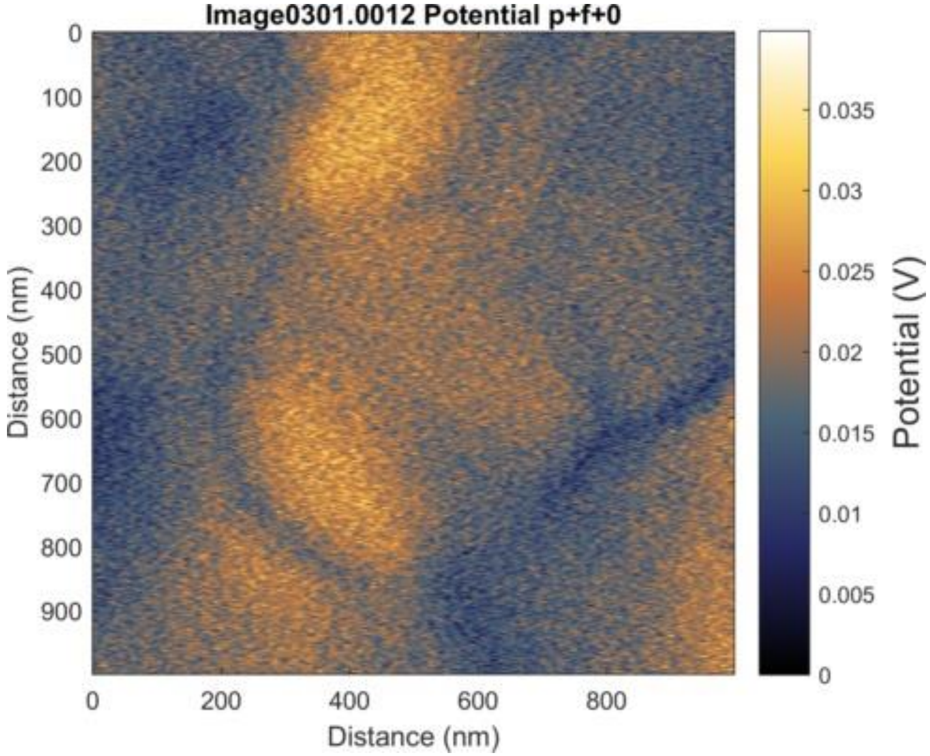
- Investigating surfaces at the atomic scale to characterize features relevant to vacuum field emission.
- By examining field emission at the nanoscale, we expect to build global models for physics-based and experimentally corroborated local models.
- Want to clarify β-based field emission so β really is only geometry induced field concentration.
- "Work function" + (purely geometric) β is not the whole story in practice.
- Will characterize region, then perform discharge by strongly spatially constraining surface participation.
- Surprising to some of us, adding a thin dielectric layer made it *easier* to extract current.

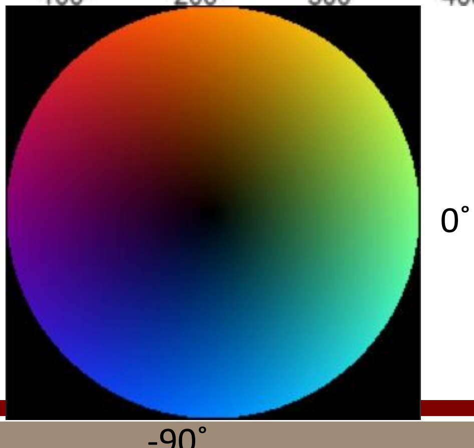
THANK YOU!

BACKUP SLIDES FOLLOW

Combined, where angle ϕ is indicated by color radially, and magnitude of slope (ϑ) represented by magnitude from middle where edge is 15˚







Not obvious there is a relation between emission and slope.

Ensemble Monte Carlo (EMC)

1. Injection of particles, photons or energetic electrons, at a constant rate
2. Electron-hole creation by the absorbed particle
   1. Determined by the collision process or the absorption spectrum
3. “Free flight” of electrons and holes in momentum space
   1. Solve the equations of motion for momentum and position
4. Scattering (changes in momentum and energy)
   1. Plasmon emission
   2. Impact ionization
   3. Phonon emission
   4. Radiative recombination
   5. Emission from the sample (with no return)
5. Collection or emission

AFM

Force between tip and surface $$F = \frac{1}{2}\frac{\partial C}{\partial z}V^2$$

Apply bias to tip and scan a sample $$V = (V_{DC} - V_{sp}) + V_{ac}\sin(\omega t)$$

V_{DC} = applied DC bias
V_{AC} = applied AC bias
V_{sp} = surface potential

$$V^2 = (V_{DC} - V_{sp})^2 + 2(V_{DC} - V_{sp})V_{ac}\sin(\omega t) + V_{ac}^2\sin^2(\omega t)$$

Combine

$$F = \frac{1}{2}\frac{\partial C}{\partial z}\left(\left[(V_{DC} - V_{sp})^2 + \frac{1}{2}V_{ac}^2\right] + 2[(V_{DC} - V_{sp})V_{ac}\sin(\omega t)] - \left[\frac{1}{2}V_{ac}^2\cos(2\omega t)\right]\right)$$

Signal at 1st harmonic
Apply V_{DC} to nullify this signal

Contributors to the DC potential difference:

- Difference in work function between the tip and surface
- Trapped charge
- Any permanent or applied voltage between the tip and the sample