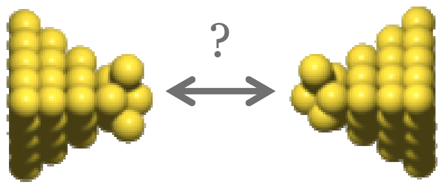
Absolute distances in nano-sized tunnel junctions

Group meeting

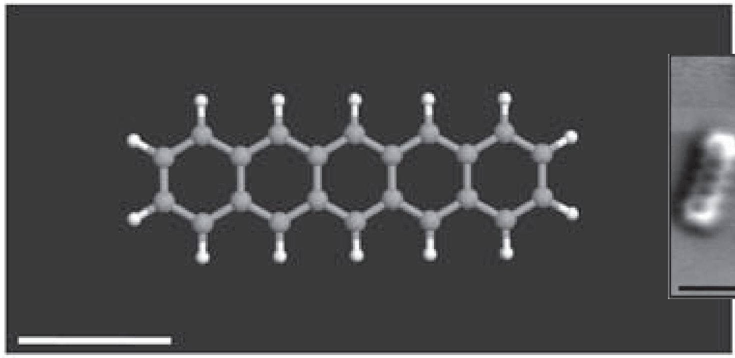
May 12, 2010

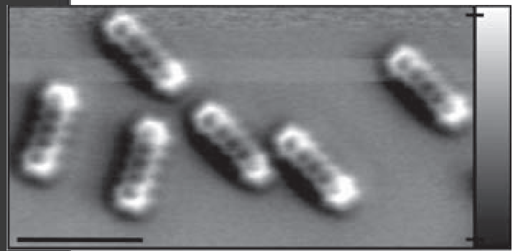
Marius Trouwborst

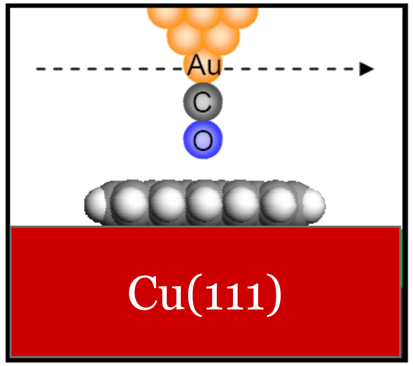


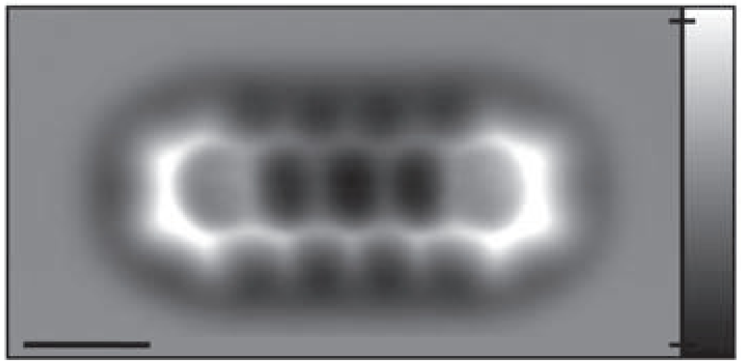
High resolution imaging

AFM image of Pentacene on Cu(111) at 5 K.









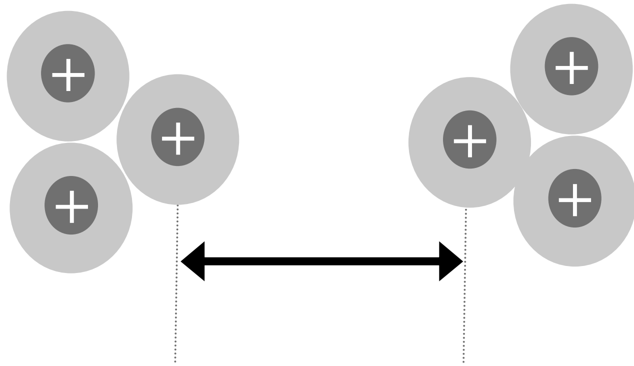
- Strong enhancement in resolution when tip is close to molecule (1Å < d<2 Å).
- Attributed to **Pauli Repulsive forces.**
- Information on absolute distance is crucial

Leo Gross *et al*, Science **325**, 1110 (2009)

Overview: effects on electrode separation

Various forces involved:

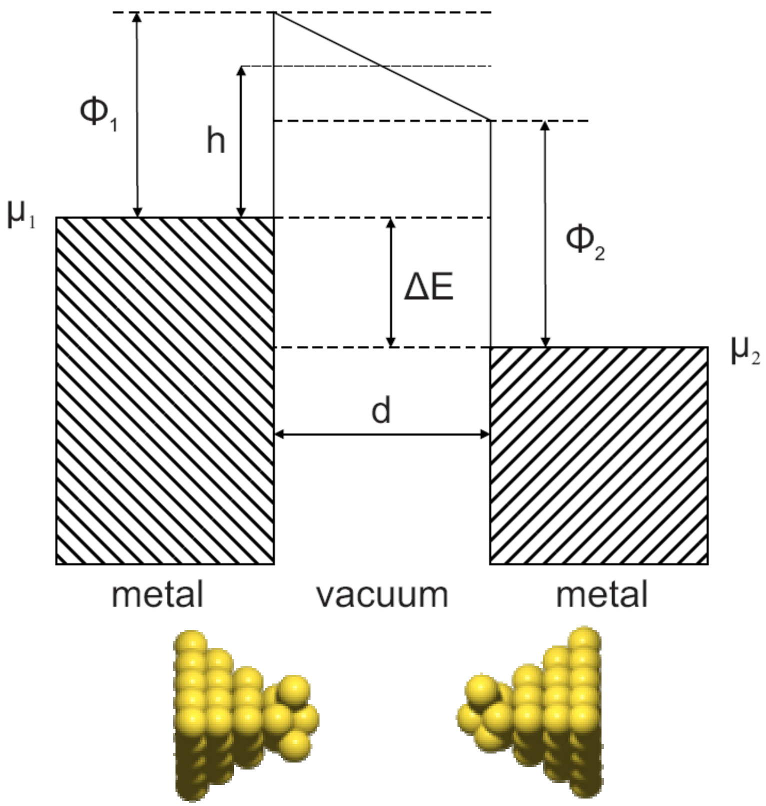
Electrostatic forces
Van der Waals forces
Metallic forces
Pauli Repulsive forces



Other effects influencing conductance and/or electrode separation:

Thermal effects (expansion)
Image potential

Simple square barrier model



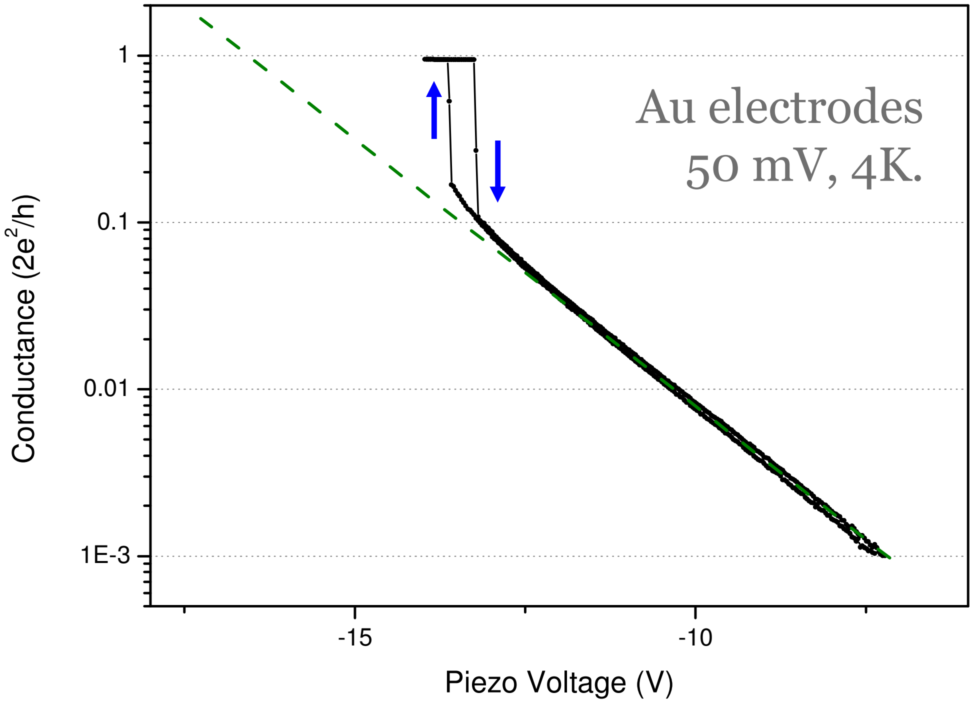
$$G = \frac{2e^2}{h} T = \frac{2e^2}{h} e^{-2\kappa d}$$

$$\kappa = \sqrt{2m\phi}/\hbar.$$

For gold (5.4 eV):

$\Delta \mathrm{Log}G/\Delta D \approx -1$ Å^{-1}

Conductance in tunneling regime



For $G<0.05\ G_0$, tunnel conductance decreases exponentially with distance

$$G = \frac{2e^2}{h}T = \frac{2e^2}{h}e^{-2\kappa d}$$

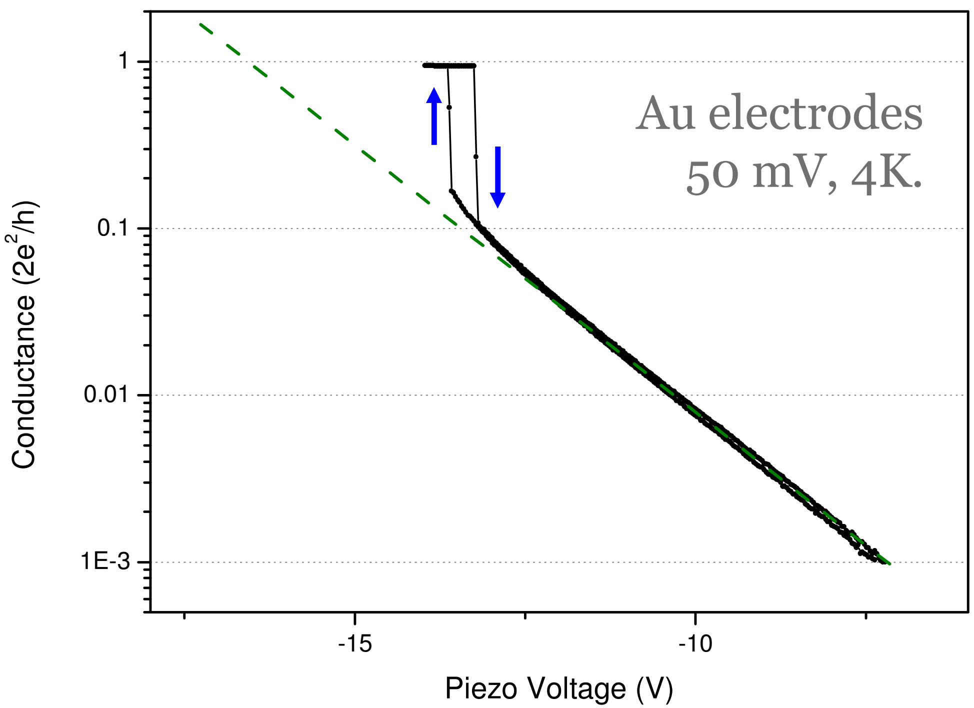
$$\kappa = \sqrt{2m\phi}/\hbar.$$

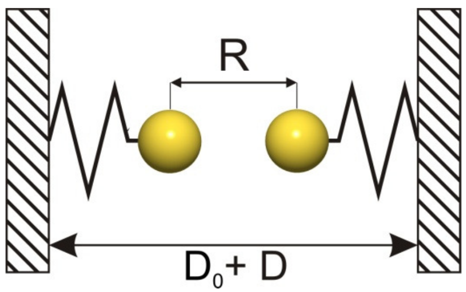
For gold (5.4 eV):

$\Delta \mathrm{Log}G/\Delta D \approx -1$ Å^{-1}

At $\sim 0.1\ G_0$, deviation from exponential tunneling due to metallic interaction

Metallic binding forces





For G<0.1 G_0, jump to contact due to atomic binding forces

Reduced electrode distance due to attractive forces

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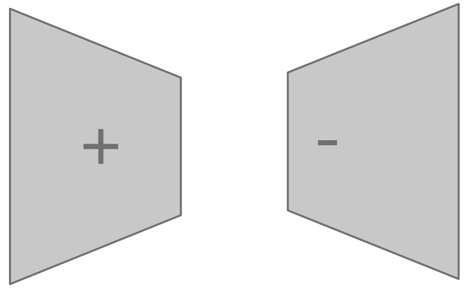
Electrostatic interactions



$C = \varepsilon A/d$

$U = C V^2/A$

Area≈1*1 nm

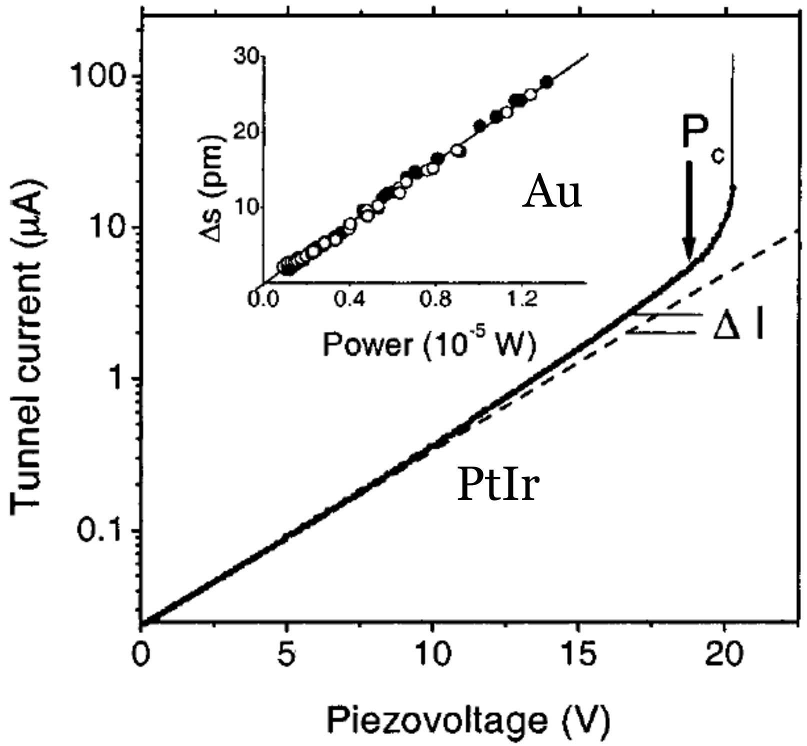
$$F_{electrostatic} = \varepsilon A V^2/d \approx 0.05 \text{ nN}$$

Bias voltage ≈ 1 V

Distance ≈ 2 Ångstrom

Rough estimation: junction with spring constant ≈ 1 N/m could result in 0.5 Ångstrom smaller electrode gap (at 1V, 2 Ångstrom).

Heating / Thermal expansion

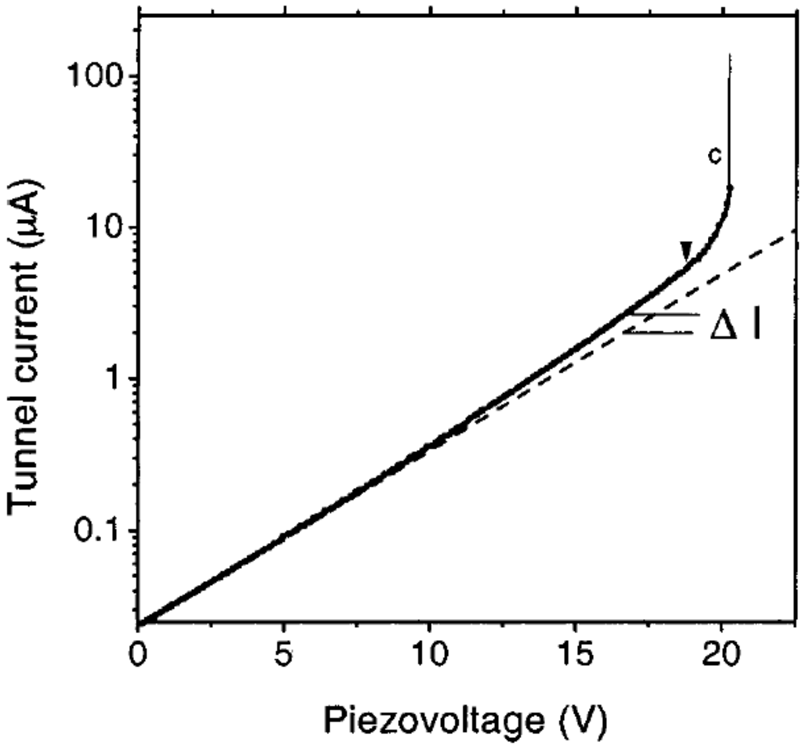


P = V²/R
2V, 1 MOhm = 4 μ W

Power dissipation of 4 μ W could result in ~0.1 Ångstrom smaller electrode gap

O.Yu. Kolesnychenko, Appl. Phys. Lett. 79, 2707 (2001)

Thermal expansion & electrostatic forces

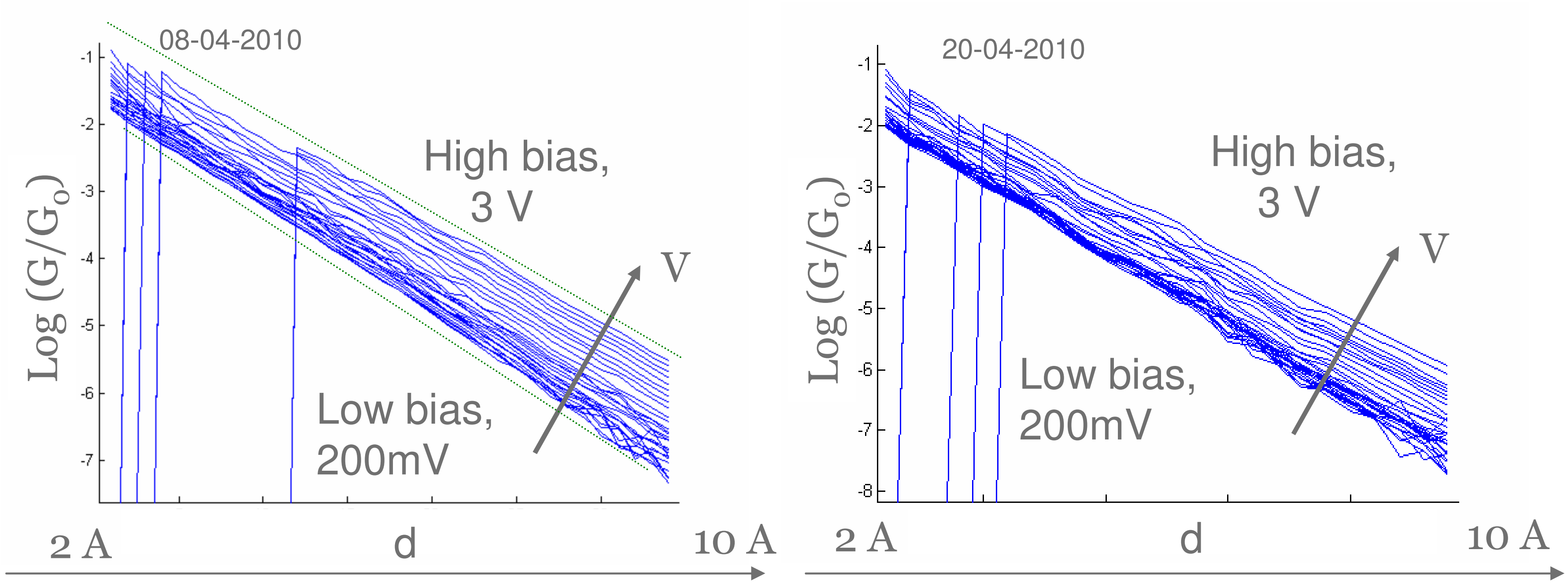


Both effects would decrease the electrode separation.

This would result in deviation in dI/dV from exponential behavior.

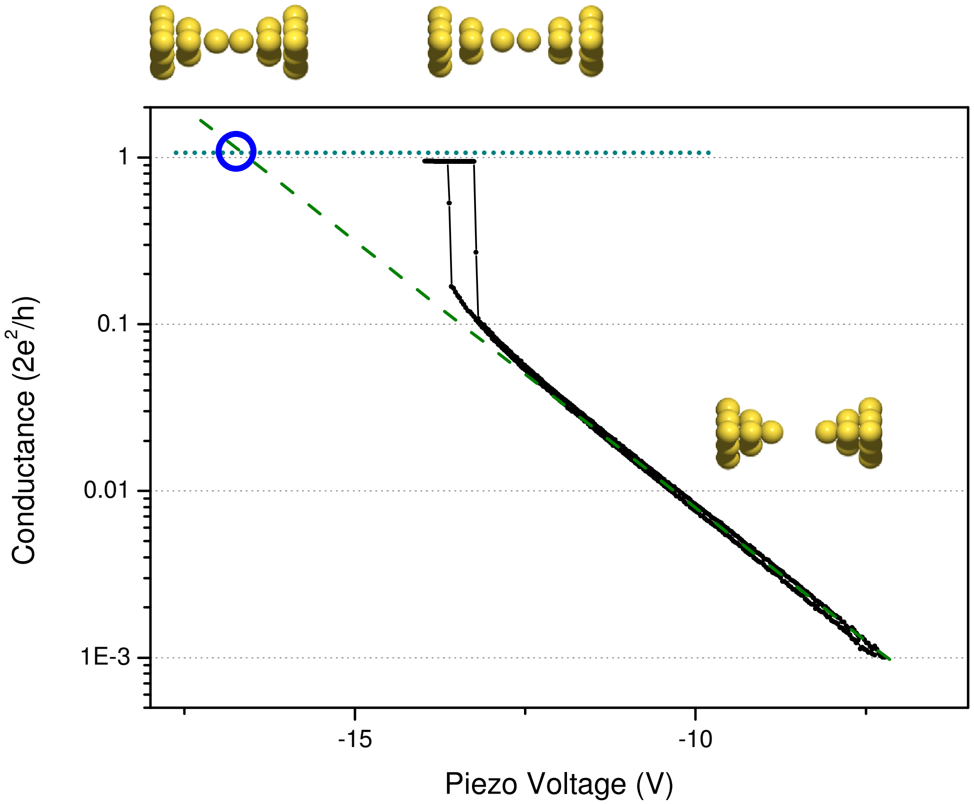
Repeat measurements at higher bias voltages.

dI/dV as a function of d



- dI/dV measurements for different bias voltages (steps of 200 mV).
- The overall slope of dI/dV(d) decreases with increasing bias voltage $\bar{\varphi} = (\varphi - eV/2).$
- **No systematic deviations from exponential behavior for larger biases (up to ~2 V, 0.01 G_0).**

Absolute electrode separation



Zero electrode separation by extrapolating to 1 Go ?

Take into account barrier lowering by ***image charges***!

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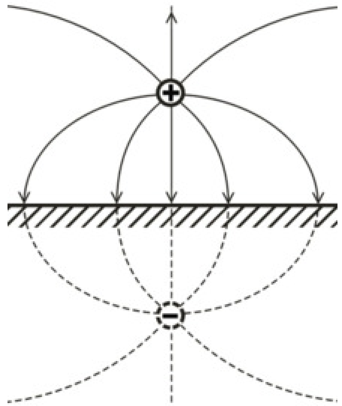
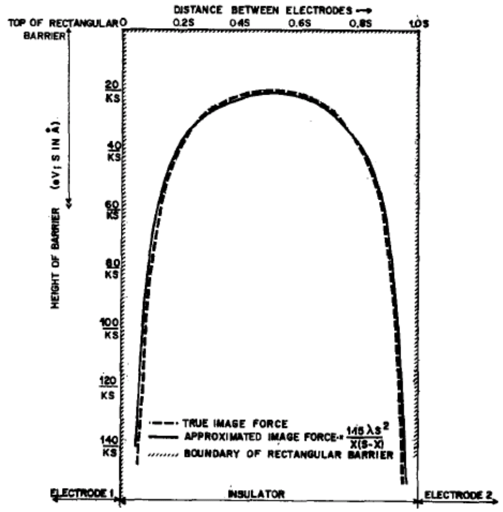
Image charges & real barrier





- Image charges strongly reduce potential barrier.

- **The reduced barrier, however, has never been directly observed in tunnel junctions:**

1) **Only second order effect on tunnel slope.**
2) **Effect cancels out by metallic adhesion.**

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Image charges & real barrier

Image charges strongly reduce potential barrier.

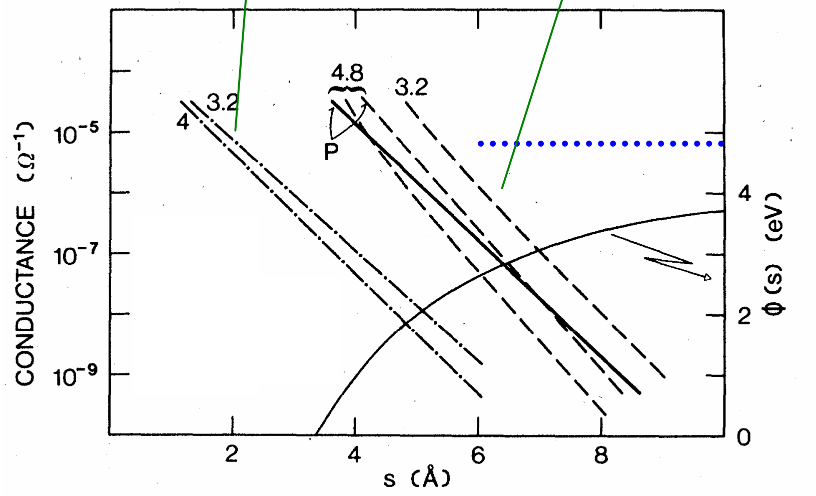
Assume: $\phi(d) = \phi_0 - \frac{\alpha}{d}$ 10 eVÅ

$$I \propto \exp[-2d\sqrt{\phi(d)}]$$

$$\frac{d(\ln I)}{ds} = 2\phi_0^{1/2}\left[1 + \frac{\alpha^2}{8\phi_0^2 d^2} + O\left(\frac{1}{d^3}\right)\right](1+\beta) \quad .$$

Without Image forces

With Image forces

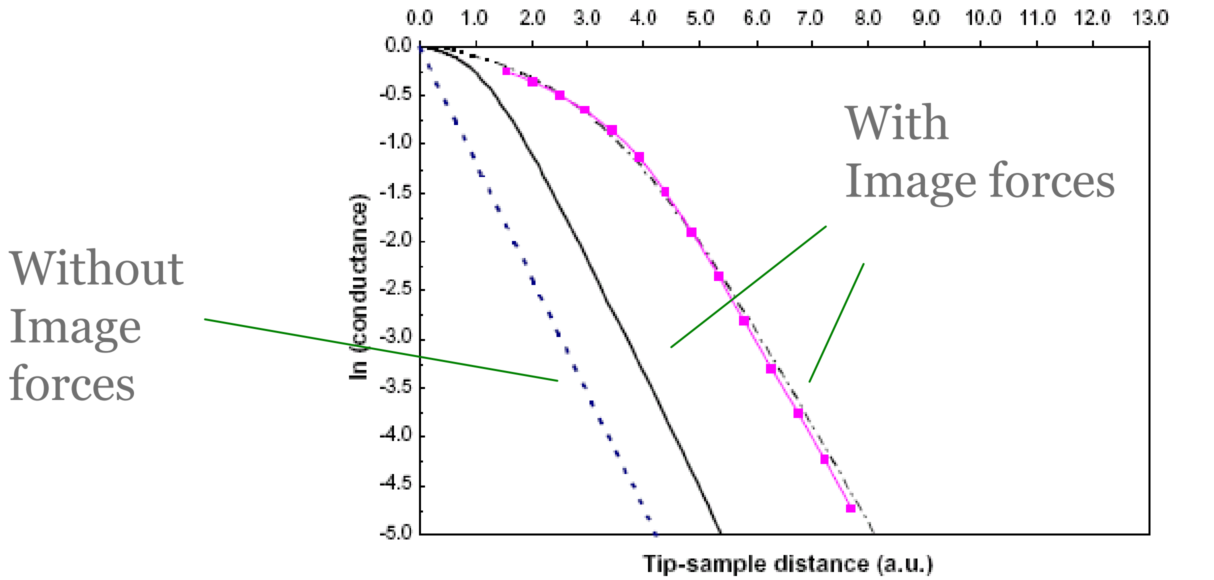


The tunnel slope (dI/dV(d)) hardly effected due to **second order** correction.

The absolute conductance, however, increases dramatically.

Binnig et al, Phys. Rev. B. 30, 4816 (1984)

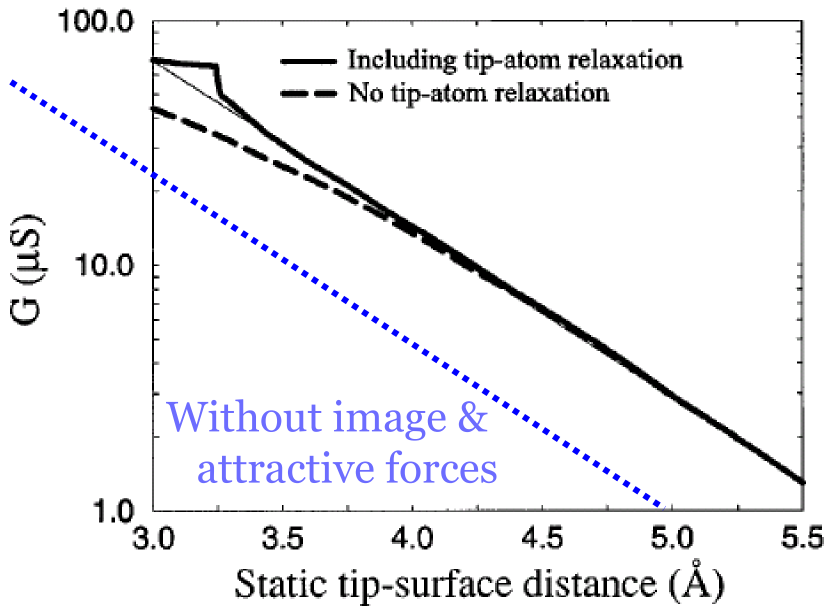
Image charges & real barrier



Change in tunnel slope only at small electrode gaps.
The absolute conductance increases dramatically (>10*).
Strongly depends on exact model.

Blanco *et al*, Progress in surf. Sc. 81, 403 (1996)

Image charges & real barrier



Change in tunnel slope cancels out by attractive metallic forces

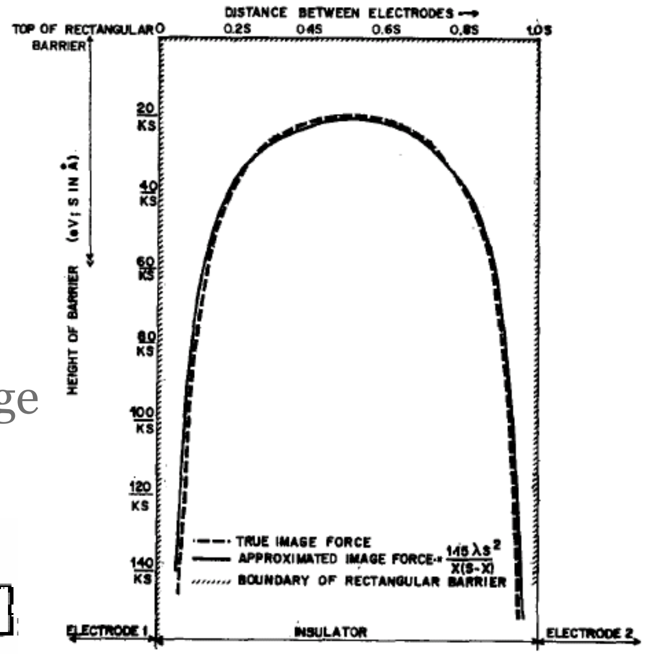
Olesen et al, Phys. Rev. Lett. 76, 1485 (1996)

Image charges & real barrier

More complete description of image barrier
includes influence of bias voltage

Square barrier height | High bias voltage correction | zero bias voltage correction

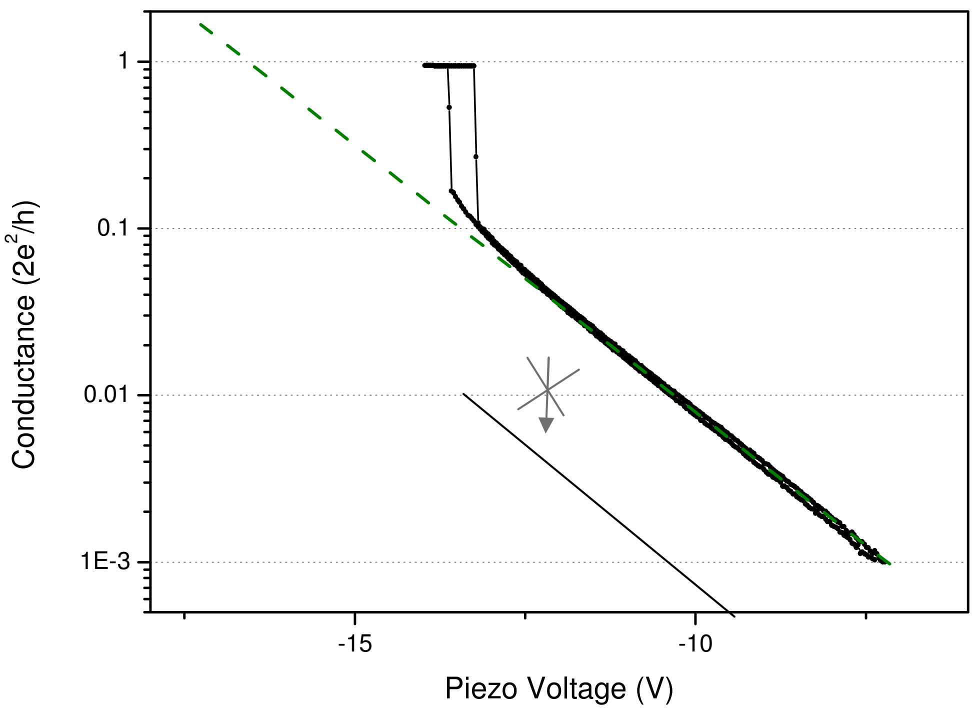
$$\varphi_I = \varphi_0 - (V/2s)(s_1+s_2) - [5.75/K(s_2-s_1)] \ln[s_2(s-s_1)/s_1(s-s_2)]$$



For a more accurate description, the shape of the electrodes should be included

J.G. Simmons, Journal of Appl. Phys. 34, 1793 (1963)

Image charges & real barrier



Note: the jump to contact can not occur at much larger electrode Separations.

Conclusions

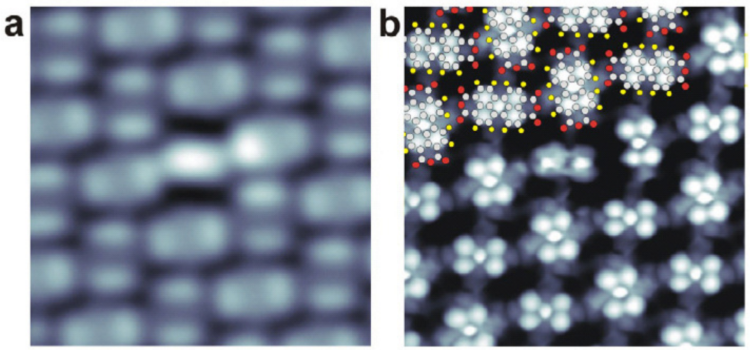
- For our junction geometry, heating or electric field does not change the electrode separation for voltages up to 2 V over 1 MOhm tunnel barrier.

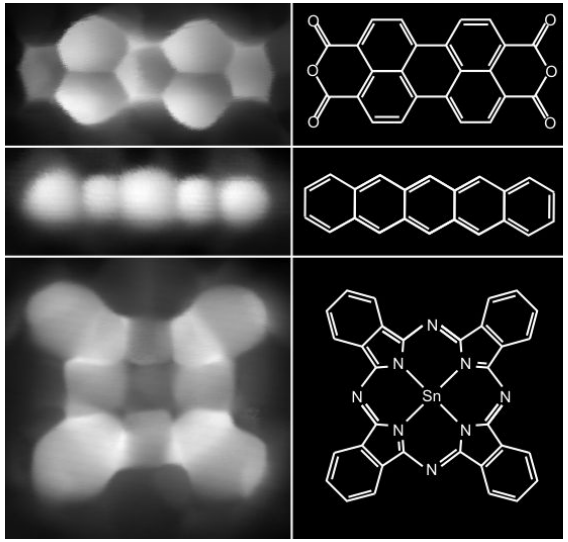
- The image potential is expected to have a large influence on the conductance (increase up to 3 orders of magnitude). Hence, there is a large uncertainty about the absolute electrode separation.

Appendix

Present work: Enhanced STM resolution with H_2

Without H_2 **With H_2**

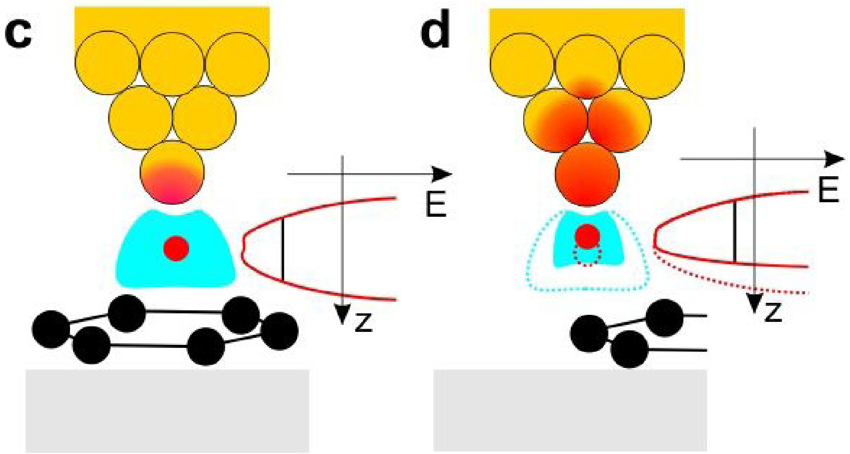


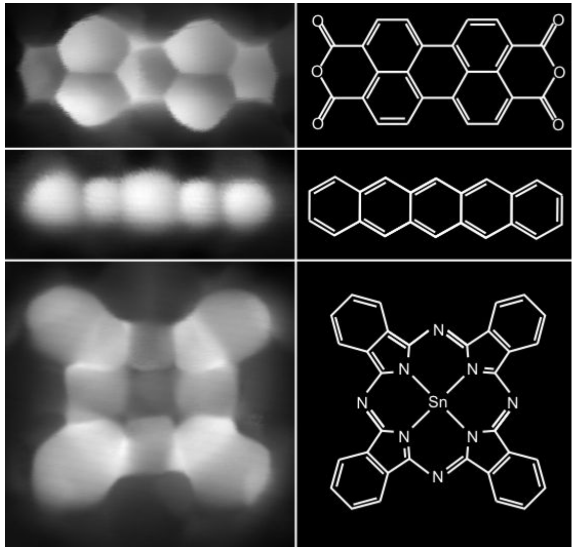


- STM resolution highly enhanced in hydrogen atmosphere.
- Chemical structure resolved.

Ruslan Temirov, Stefan Tautz *et al*, New Journal of Physics **10** (2008) 053012
arXiv:0910.5825

Present work: Enhanced STM resolution with H_2

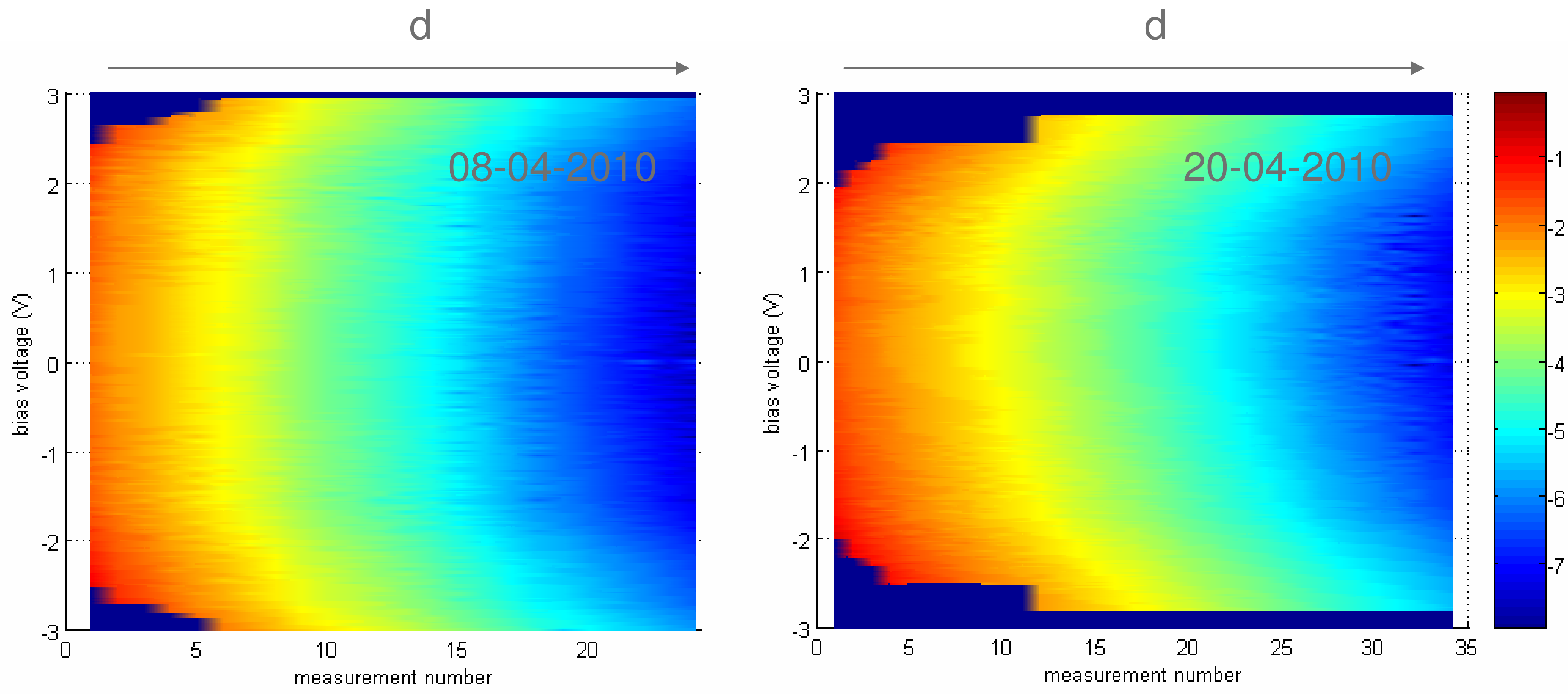




- Chemical structure resolved
- Possibly due to "Pauli repulsion"

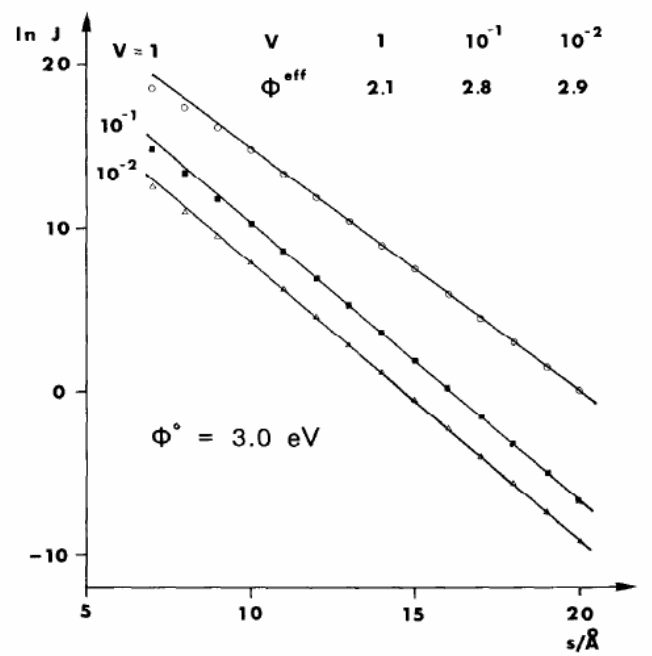
Similar effect in ^{4}He environment?

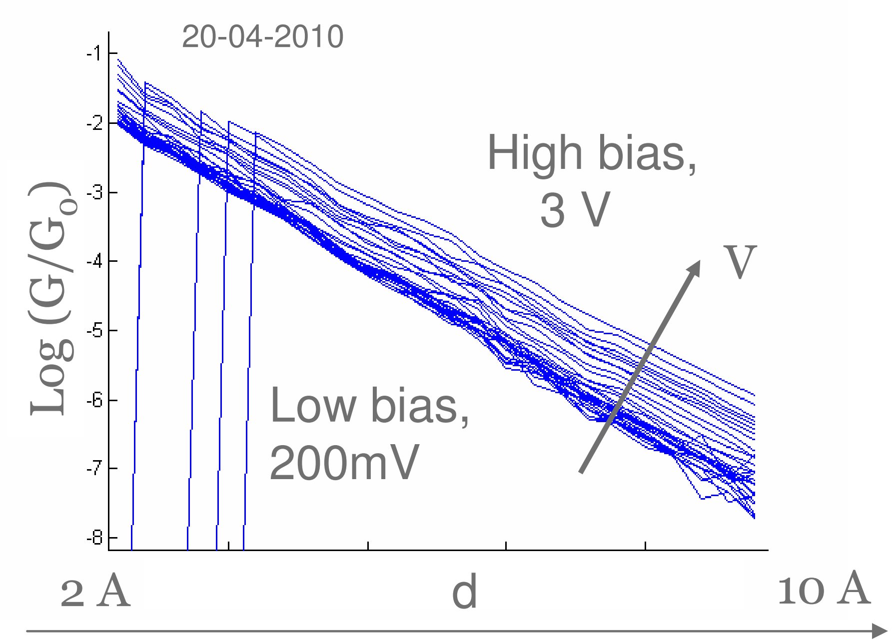
Ruslan Temirov, Stefan Tautz *et al*, New Journal of Physics **10** (2008) 053012
arXiv:0910.5825



- Numerical derivative from a fit within 50 mV, average of bwd/fwd sweep
- logarithmic color scale of dI/dV in G0 (-1=0.1 etc.)
- General trend: dI/dV increases at given d with V (as expected from tunneling)
- So far no apparent anomalies in the color pattern.

dI/dV as a function of d





- The overall slope of dI/dV(d) decreases with increasing bias voltage.
- Simmons: $\bar{\varphi} = (\varphi - eV/2).$

J. Payne, Surf. Science 159, 485 (1985)