What can STM/STS do?

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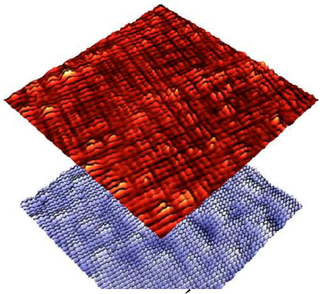

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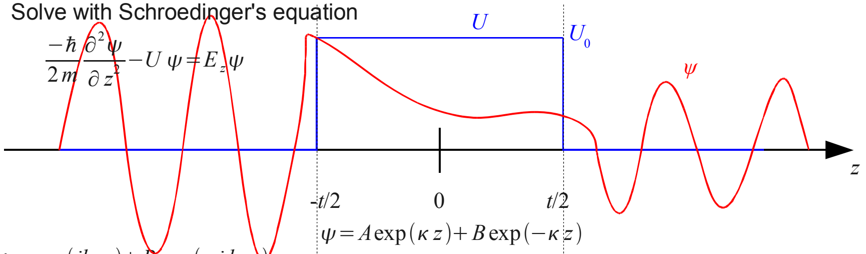
Plan

- Theory of STM/STS
  - 1D tunneling
  - Tunneling in STM/STS
- Possible measurements
  - Effect of tip
  - Atomic resolution
  - Atomic control
  - Spectroscopy
  - QPI

1D Tunneling: square potential barrier

Solve with Schroedinger's equation

$$\frac{-\hbar}{2m}\frac{\partial^2\psi}{\partial z^2}-U\psi=E_z\psi$$



$$\psi=\exp(ik_z z)+R\exp(-ik_z z)$$

$$k_z=\sqrt{\frac{2m}{\hbar^2}E_z}$$

$$\psi=A\exp(\kappa z)+B\exp(-\kappa z)$$

$$\kappa=\sqrt{\frac{2m}{\hbar^2}(U_0-E_z)}$$

$$\psi=T\exp(ik_z z)$$

R: The reflected wave
T: The transmitted wave

$$1+|R^2|=|T^2|$$

Solve by having continuous
$\psi, \frac{\partial\psi}{\partial z}$

$$|(T)^2|=\frac{1}{1+\frac{(k_z^2+\kappa^2)^2}{4k_z^2\kappa^2}\sinh^2(\kappa t)}$$

$$|(T)^2|\approx\frac{16k_z^2\kappa^2}{(k_z^2+\kappa^2)^2}\exp(-2\kappa t)$$

For $\kappa t \gg 1$

Higher D, STM

- Change ψ to $\Psi=\psi\exp(ik_x x+ik_y y)$
- Answer stays the same.
- k_x, and k_y are conserved.
- The energy E is also conserved (elastic tunneling).
- U depends on work function of both ends and the applied voltage (not a constant anymore)
- $E_z=E-\frac{\hbar^2}{2m}(k_x^2+k_y^2)$
- Stronger tunneling if k_x, & k_y *are* small (for E~U_0).

Important results for a single electron

$$|(T)^2| \approx \boxed{\frac{16k_z^2\kappa^2}{(k_z^2+\kappa^2)^2}} \exp(-2\kappa t)$$

Fast Exponential decay
1 Å → ×10
Depends on work function

Matrix element
Depends on matching boundary conditions

For a more general potential

$$|(T)^2| = g\exp\left(-2\int_{z_1}^{z_2} dz\sqrt{\frac{2\mathrm{m}}{\hbar^2}[U(z)-E_z]}\right)$$

Depending on approximations

$$g=\frac{16k_z^2\kappa^2}{(k_z^2+\kappa^2)^2}$$ or $$g=1$$ WKB approximation

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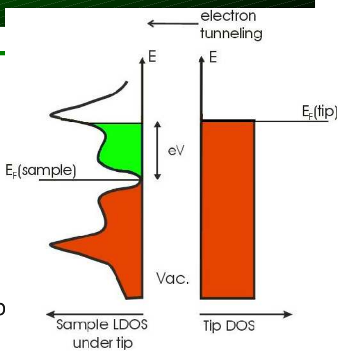
Multiple electrons

We need to insert the effect of the density of states and the temperature (Fermi function $f(E)$)

We assume small energy (vs work function) so κ is independent of energy.

Calculate the conventional current from sample to tip



$$I = M\exp(-2\kappa z)\int_{-\infty}^{+\infty} dE\, n_S(E+eV)\, n_T(E)[f(E)-f(E+eV)]$$

$$f(E)=\frac{1}{1+\exp\left(\frac{E-\mu}{k_B T}\right)}$$

n_S and n_T are the sample and tipdensity of states
M is a matrix element (could be inside the integral)
V is voltage applied on sample.

At T=0, the Fermi function disappear and leave the integral between -eV and 0

Spectra: conductance

The measured conductance G is given by:

$$G = \frac{dI}{dV} = M \exp(-2\kappa z) n_T(0) \int_{-\infty}^{+\infty} dE\, n_S(E+eV) \boxed{\frac{1}{4 k_B T \cosh^2\left(\frac{E}{2 k_B T}\right)}}$$

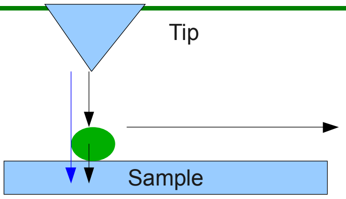
Where we assume n_T has a weak energy dependence (valid for small energies and a good tip

The smearing effect due to the temperature.
At $T=0 \rightarrow \delta(E)$
So $G \approx n_s(eV)$

G can be measured directly with a lock-i.n

Also from a I vs z curve, can extract κ hence the work function.

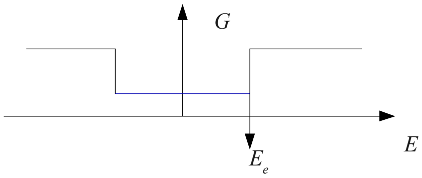
Inelastic tunneling



The electrons tunnel
But leave some energy in an excitation of energy E_e (molecular vibration, ...)

Only possible if $E>E_e$

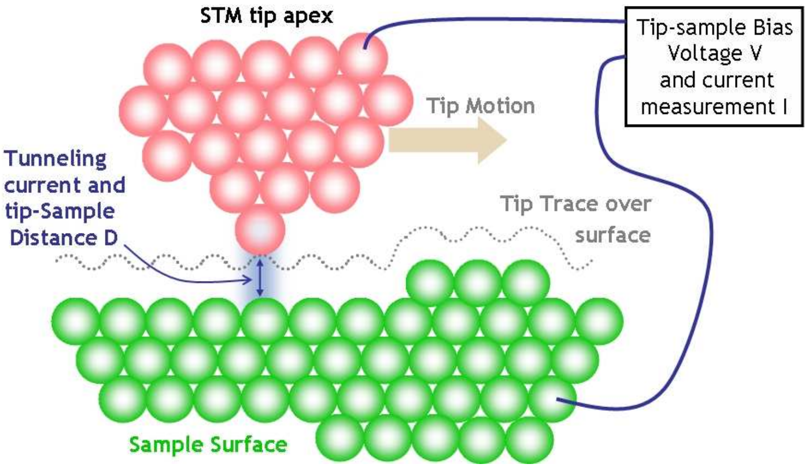
Conductance spectra:



Make the effect evident by taking derivative of conductance. So look at

$$\frac{d^2 I}{dV^2}$$

Basics of STM technique



Ref: Opensource Handbook of Nanoscience and Nanotechnology
http://en.wikibooks.org/wiki/Nanotechnology

Constant current feedback

When measurement are taken with a feedback current of I_0 under a voltage of V_0 the conductance is (T=0):

$$G(\vec{r},V)=I_0\frac{n_S(\vec{r},eV)}{\int_0^{eV_0} dE\, n_S(\vec{r},E)}$$

So
$$G(\vec{r},V)\propto n_S(\vec{r},eV) \leftarrow$$

GREAT tool
STS (scanning tunneling spectroscopy)
But there are some approximations

But proportionality constant varies in space

In Fourier space:

$$\xcancel{G(\vec{k},V)\propto n_S(\vec{k},eV)}$$

Z ratio map

To avoid problem with feedback (integral) in

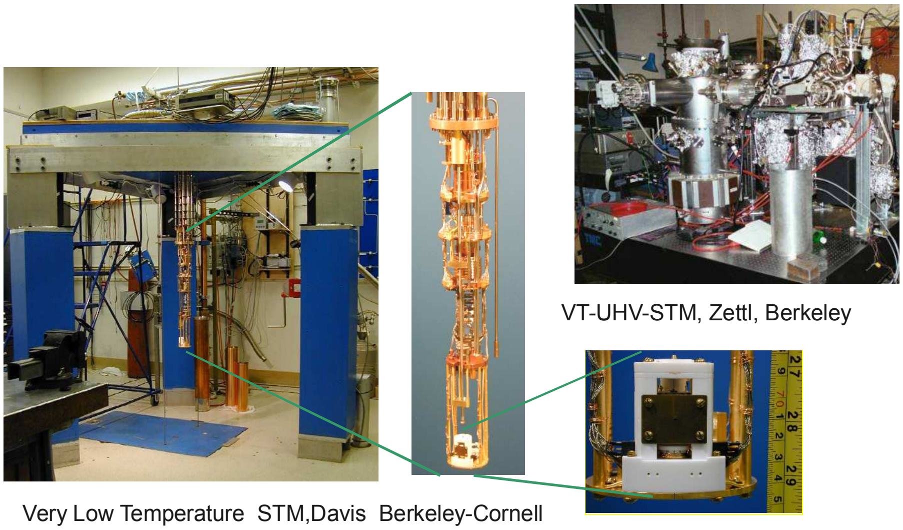
$$G(\vec{r},V)=I_0\frac{n_S(\vec{r},eV)}{\int_0^{eV_0}dE\,n_S(\vec{r},E)}$$

Then use Z ratio instead:

$$Z(\vec{r},V)=\frac{G(\vec{r},V)}{G(\vec{r},-V)}$$

This removes integral
- Better contrast (sometimes)
- Extract energy asymmetry
- Loose energy symmetric part

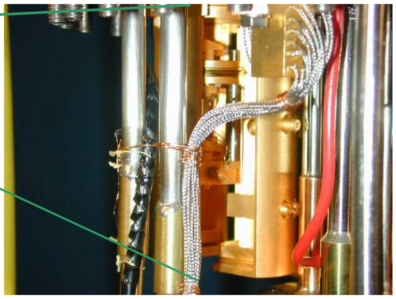
STM equipment

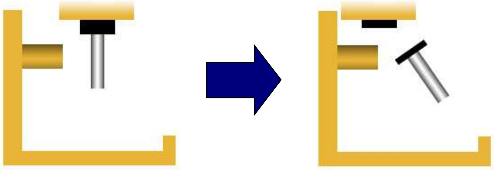


VT-UHV-STM, Zettl, Berkeley

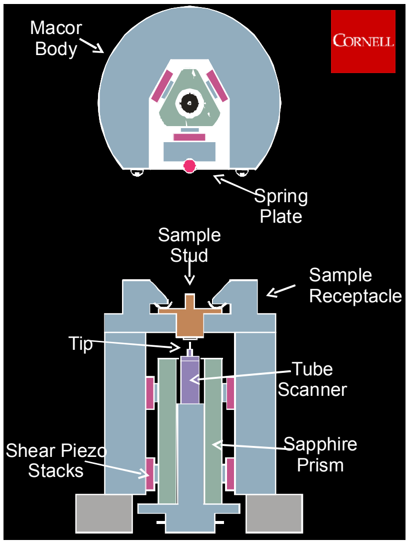
Very Low Temperature STM,Davis Berkeley-Cornell

Sample preparation (cleaving)





Instrument design for STM/STS

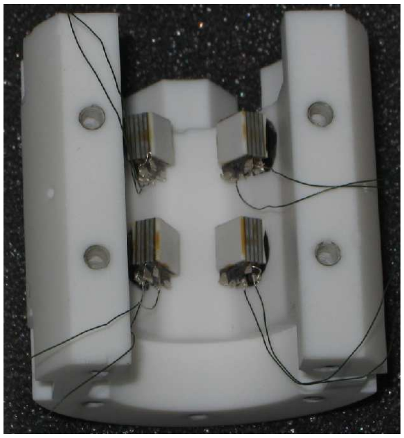


Rev. Sci. Inst. **70**, 1459 (1999).

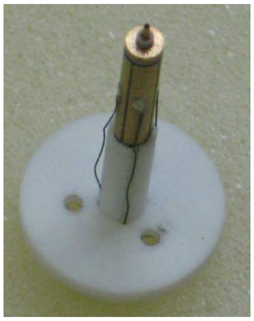
Microscope

A microscope in pieces

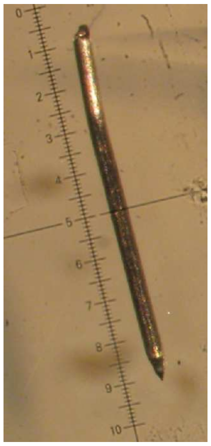
Microscope



Body of the walker



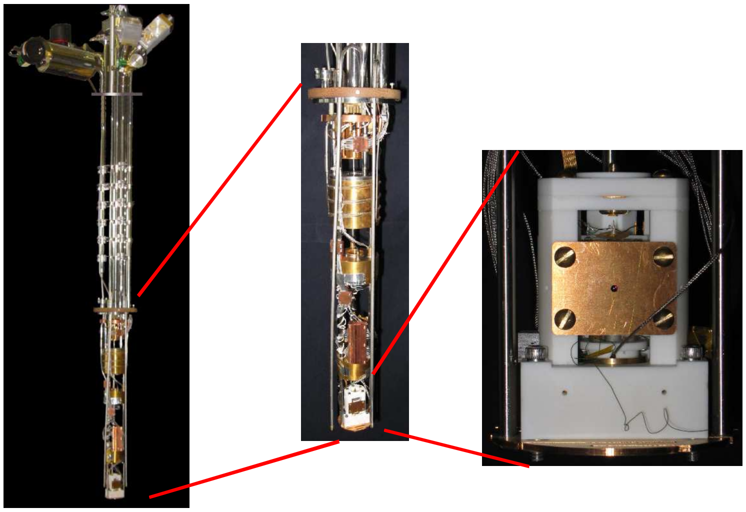
Heart of microscope
XYZ piezo tube and
Tip holder



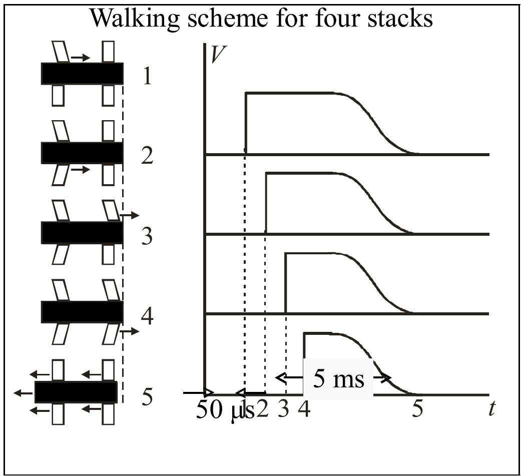
Tungsten tip
8mm

Assembled Microscope

Cryostat

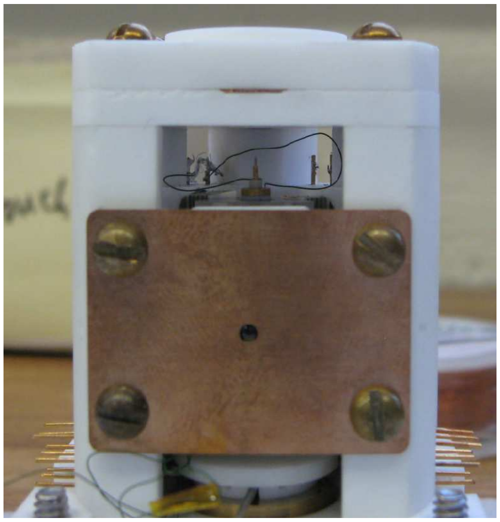


Coarse approach (walker)

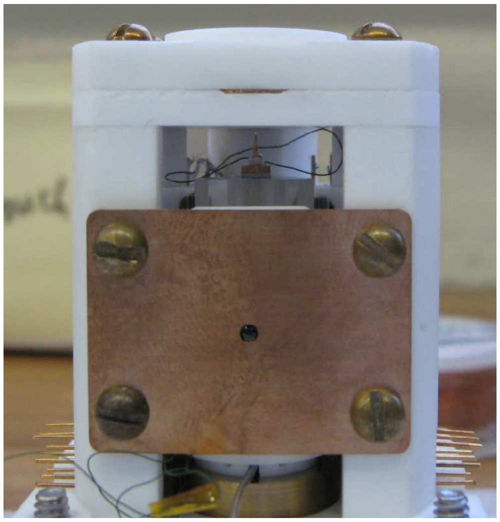


1 step = 250 Å at LT
Total displacement = 5 mm
horizontal reproducibility = 100 Å

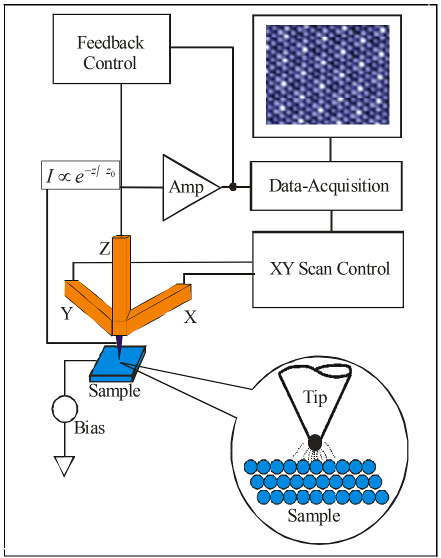
Walker motion (bottom)



Walker motion (top)

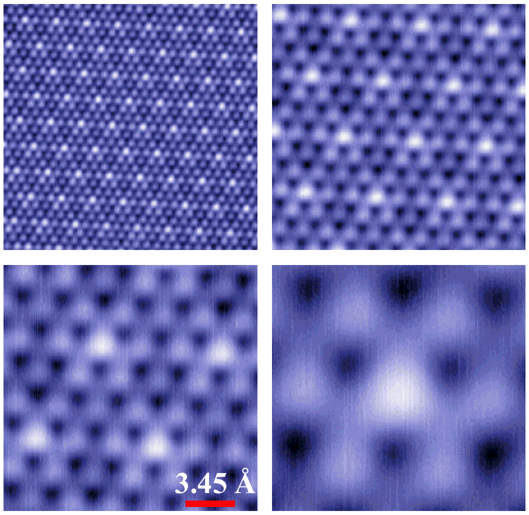


STM Technique



- In Vacuum (dirty)
- In air
  - UHV (variable T)
  - Cryogenic (great vacuum)
- Low T
  - Thermal stability
  - Surface stability

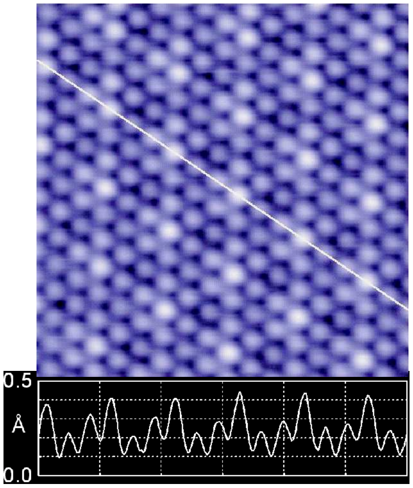
...Very High Resolution



Zoom on $NbSe_2$ (Charge density wave)

250 mK
50 pA, 50 mV

STM Images electron density – not the atoms

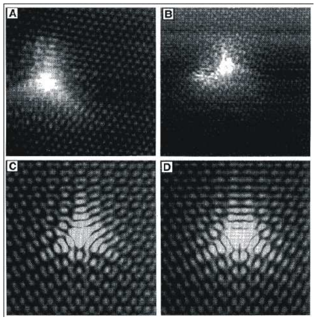


NbSe$_2$: Charge density wave

250 mK
50 pA, 50 mV

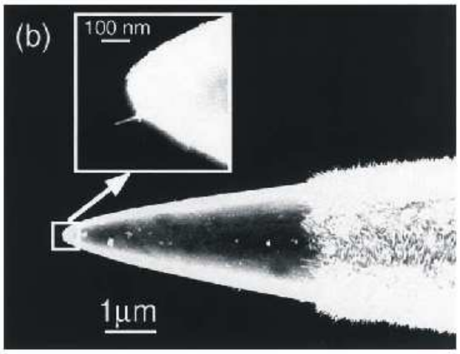
What's on the tip?

Tip with C$_{60}$ / defect on graphite



K.F. Kelly, Science: **273,** 1371 (1996)

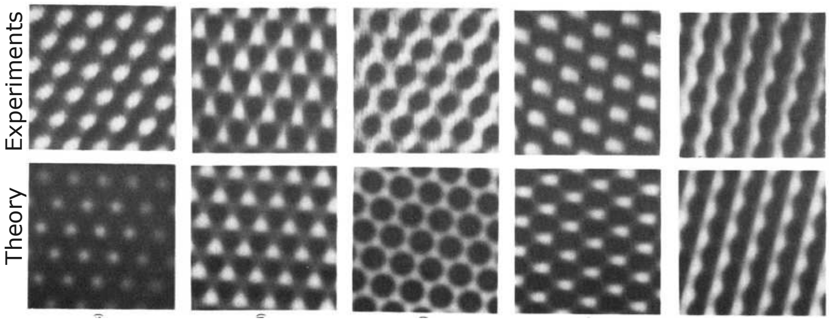
Nanotube grown on the tip



Y. Shingaya, Physica B **323**, 153 (2002)

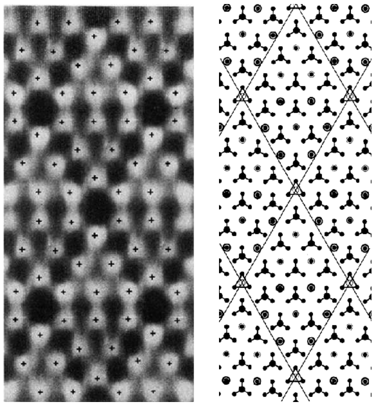
Standard tips:
- PtIr wire with angle cut (pliers)
- Tungsten tip shaped by electrochemical etching and field emission

Graphite (different tips)

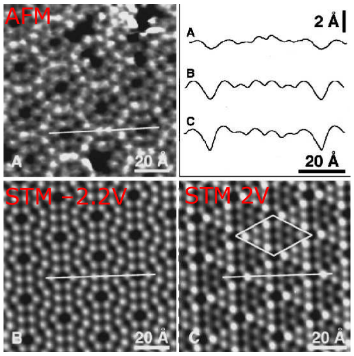


H.A. Mizes *et al.*, PRB **36**, 4491 (1987)

Surface reconstruction: Si(111) 7x7



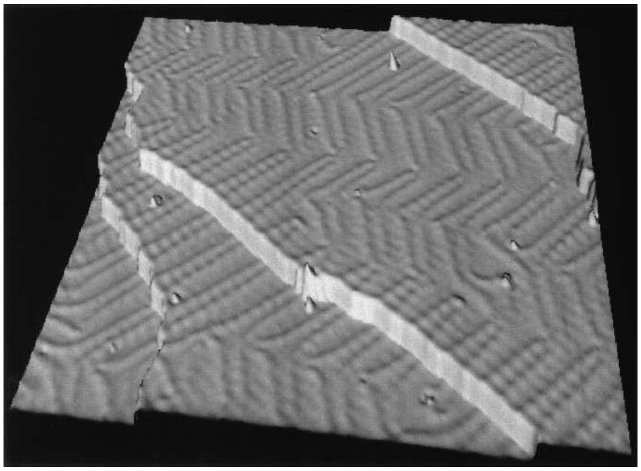
G. Binning *et al.*, PRL **50** ,120 (1983)



R. Erlandsson *et al.*, PRB **54**, R8309 (1996)

Reconstruction occurs at surfaces because of the broken bounds.
Another problem/advantage of surfaces is surface states.

Au(111) Herringbone reconstruction



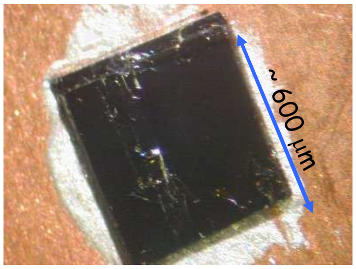
W. Chen *et al.*, PRL **80**, 1469 (1998)

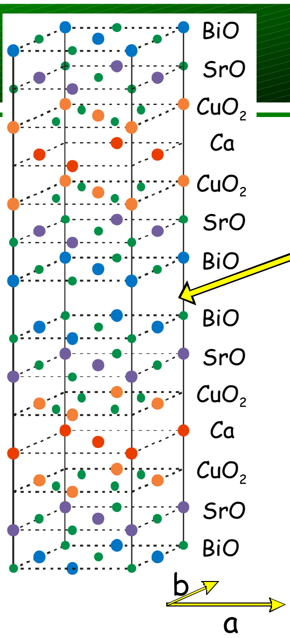
Structure of $Bi_2Sr2CaCu_2O_{8+\delta}$

$a \approx b = 5.4$ Å

$c = 30.7$ Å

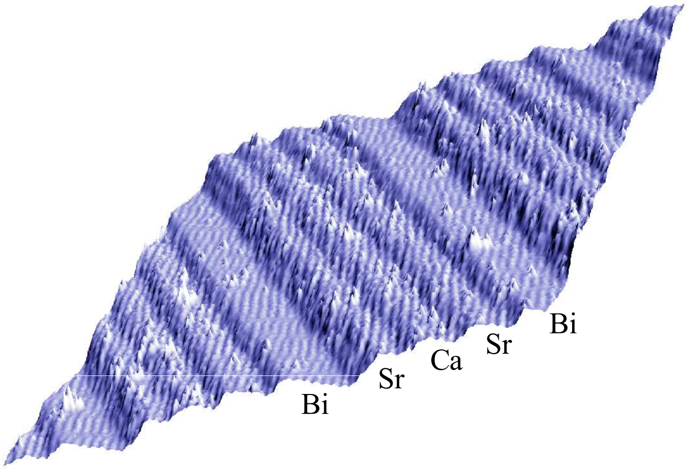
$T_c \sim 90$ K





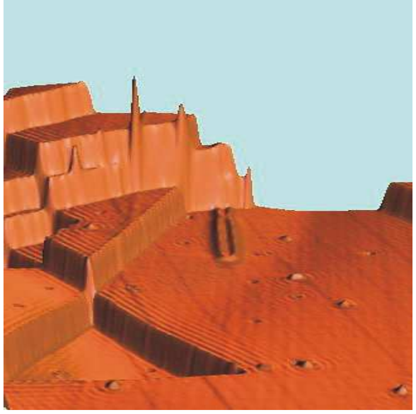
Cleave Here
Reveals
BiO Surface

Terraces on a Cleaved BSCCO Surface



Applied Physics Letters **73** (1), 58-60 (1998).

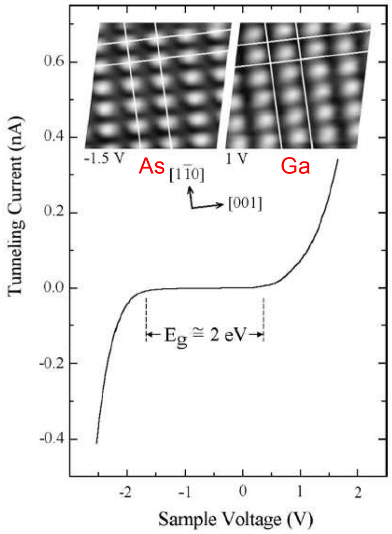
Copper (111)



- Terraces
- Friedel oscillations:
  - Step edge
  - Impurities
- Electron interference

M.F. Crommie , CP Lutz DM Eigler, Nature **363,** 524-527 (1993)

Doped GaAs 110 (semiconductor)



Large Voltages

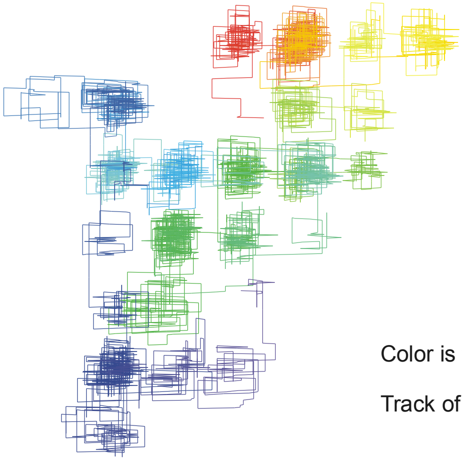
- Tip effect, electric field ("band bending")
- Measurement NOT DOS

Ga and As atoms seen separately

A. Depuydt *et al.*, PRB **60**, 2619 (1999)

Atomic motion tracking

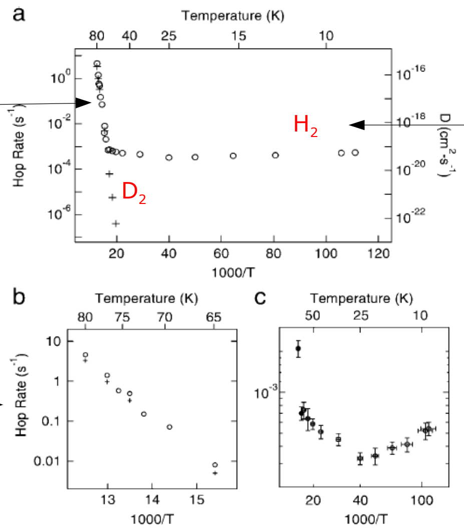
Hydrogen atom tracking



Color is time

Track of one hydrogen atom

Hydrogen diffusion on Cu(001)



High T
Thermal activation

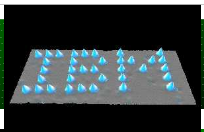
Tunneling process

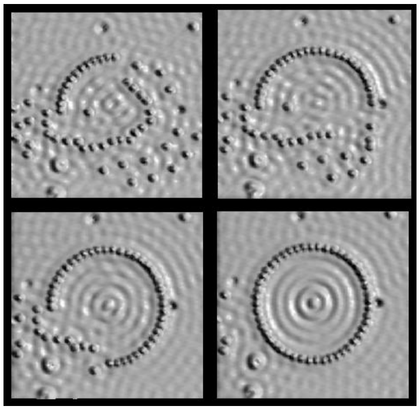
Zoom Low T

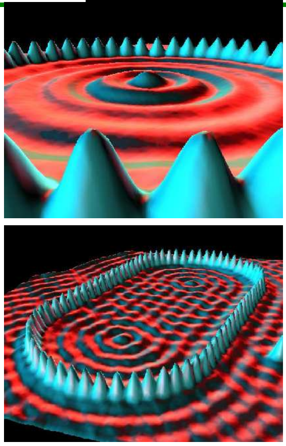
L. J. Lauhon and W. Ho, PRL **85**, 4566 (2000)

Atomic manipulations

Atomic manipulations
Building a quantum corral





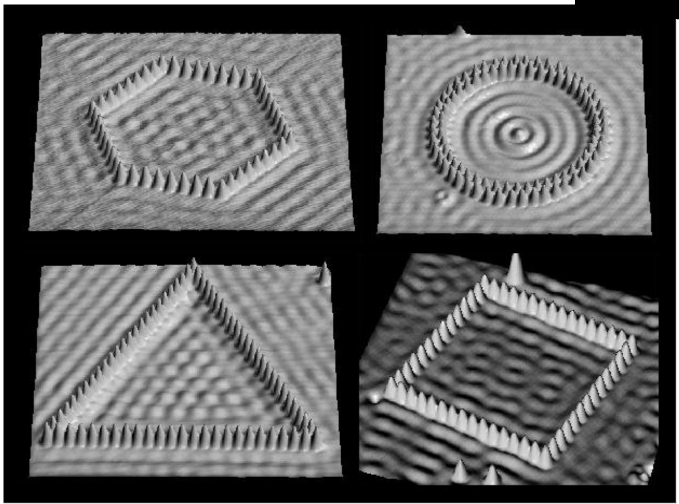


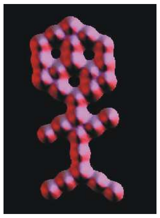
Fe on Cu(111)

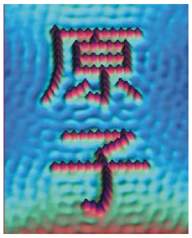
M.F. Crommie, C.P. Lutz, D.M. Eigler

Confinement of electrons to quantum corrals on a metal surface.
Science 262, 218-220 (1993).

Atomic manipulations







M.F. Crommie, C.P. Lutz, D.M. Eigler, E.J. Heller

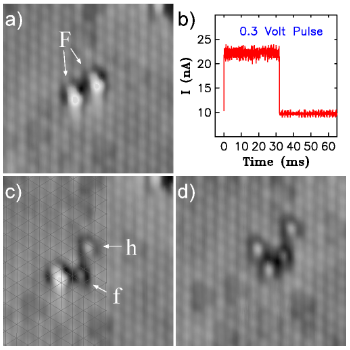
Waves on a metal surface and quantum corrals.
Surface Review and Letters 2 (1), 127-137 (1995).

Other Manipulations / tip techniques

Chemistry with STM

O_2 on Pt(111)

Dissociation by Tunneling Electrons

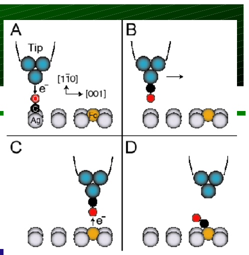


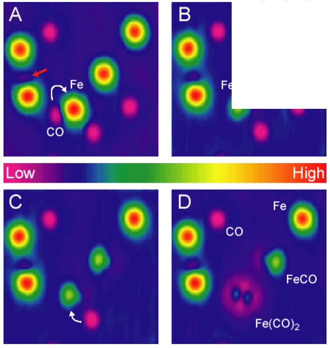
B. C. Stipe *et al.*, PRL **78**, 4410(1997)

On Ag(111)

$Fe+CO \Rightarrow FeCO$

$Fe(CO)_2$



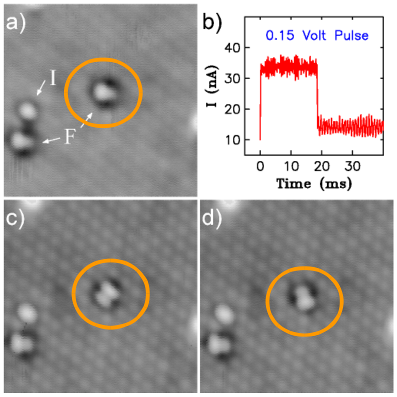


H. J. Lee and W. Ho, Science **286**, 1719 (1999)

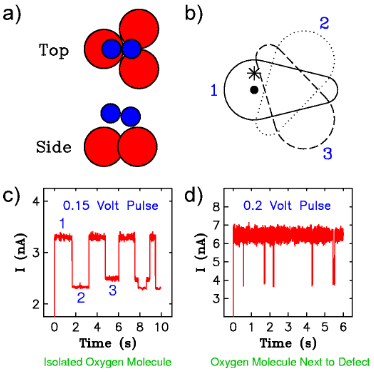
STM and molecular rotation

O_2 on Pt(111)

Reversible Rotation by Tunneling Electrons

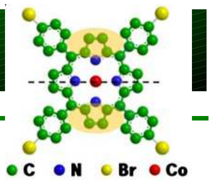


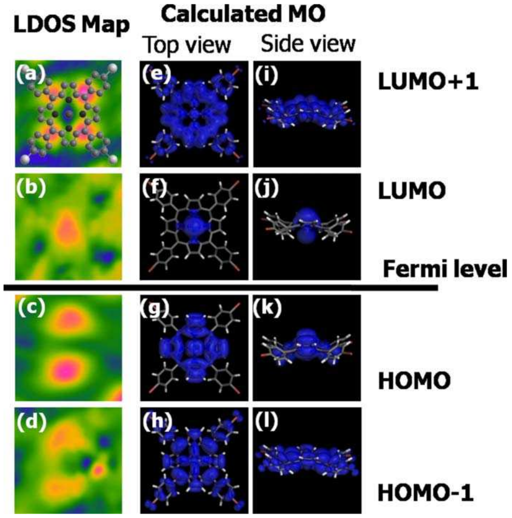
Single Molecule Reversible Rotation



B. C. Stipe, M. A. Rezaei, W. Ho, Science **279**, 1907 (1998)

Surface chemistry

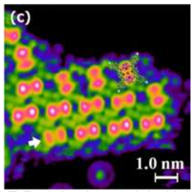




LUMO=Lowest unoccupied molecular orbital

HOMO=Highest occupied molecular orbital

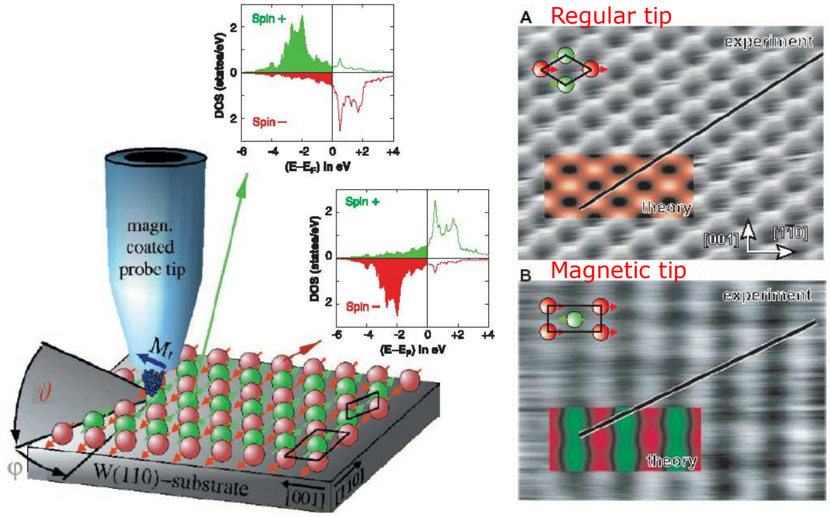
Metalloporphyrin on gold (111)



Kim et al., PRB 80, 245402 (2009)

Magnetic imaging

STM polarized STM (Mn on W)



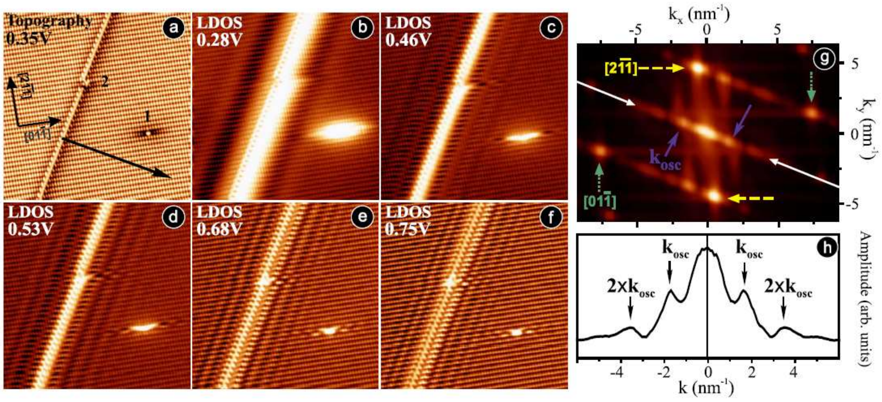
A Regular tip

B Magnetic tip

S. Heinze *et al.*, science **288**, 1805 (2000)

Conductance maps

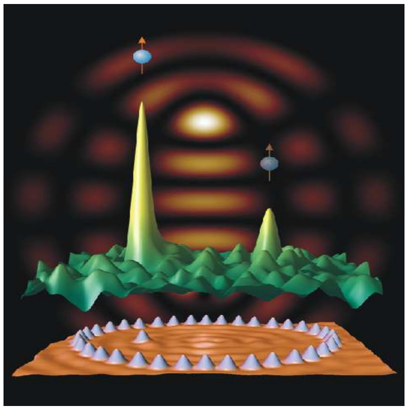
Surface waves (Ge 111 surface states)



DOS wave caused by domain boundary (crystal defect)

Muzychenko, PRB 81, 035313 (2010)

Quantum Mirage: combining atomic control and dI/dV maps



H. C. Manoharan, C. P. Lutz & D. M. Eigler, Nature 403, 512 (2000).

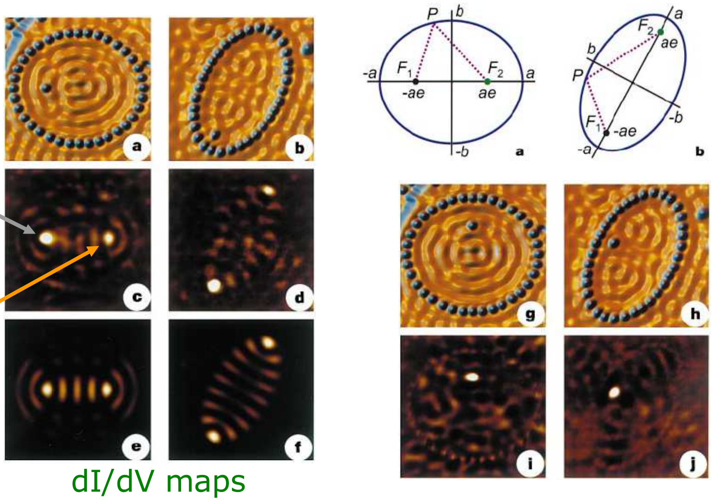
Mirage Quantique

Cu(111)/Co

Topo

Co : kondo state

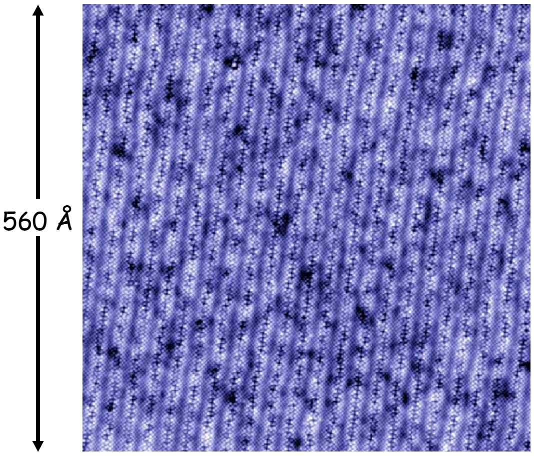
Mirage



dI/dV maps

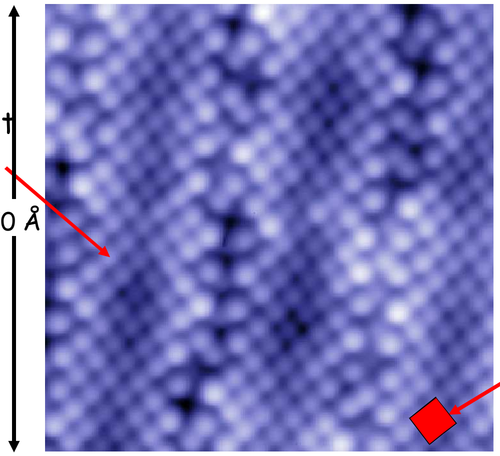
H. C. Manoharan, C. P. Lutz & D. M. Eigler, Nature 403, 512 (2000).

$Bi_2Sr_2CaCu_2O_{8+\delta}$



T= 4.2K, B = 0T
100pA, -100mV

$Bi_2Sr_2CaCu_2O_{8+\delta}$



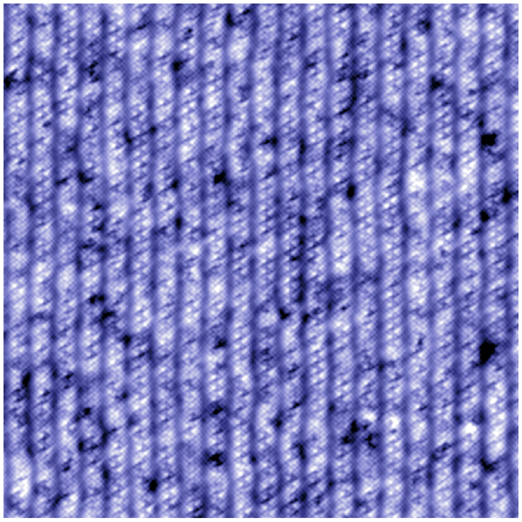
Each bright spot is a Bi atom.

Size & orientation of CuO_2 unit cell (~ 5Å below surface).

T= 4.2K, B = 0T
100pA, -100mV

$Bi_2Sr_2Ca(Cu_{1-x}Zn_x)_2O_{8-\delta}$: $x \approx 0.6\%$

Can you find the defects (Zn)?

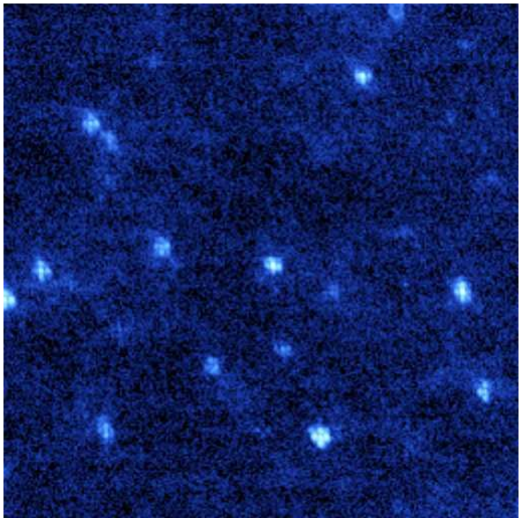


500 Å, 4.2 K
200 pA, -200 mV

Sample: H. Eisaki, S. Uchida

$Bi_2Sr_2Ca(Cu_{1-x}Zn_x)_2O_{8-\delta}$: $x \approx 0.6\%$

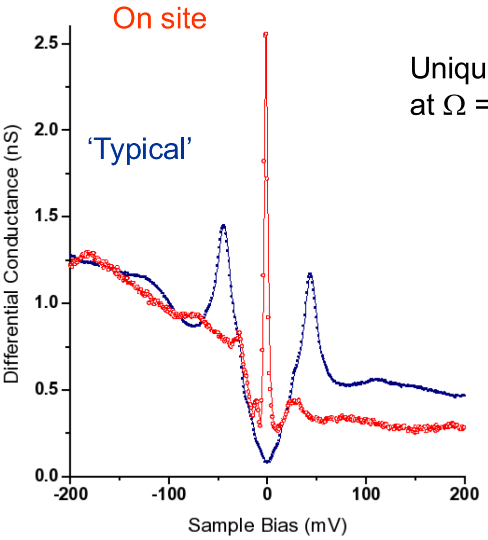
LDOS Map at
–1.5 meV



S.H. Pan, *et al.* *Nature* **403,** 746 (2000).

500 Å, 4.2 K
200 pA, -200 mV

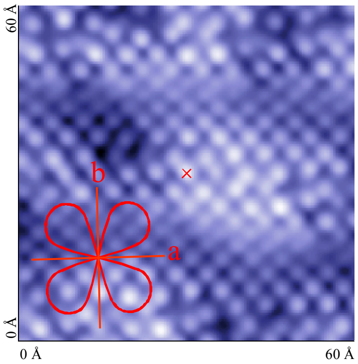
$Bi_2Sr_2Ca(Cu_{1-x}Zn_x)_2O_{8-\delta}$ spectra



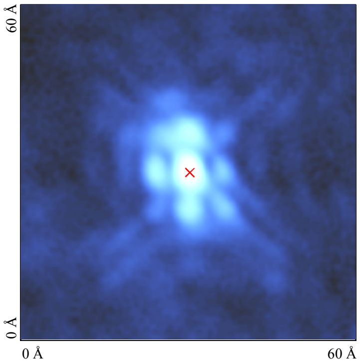
Unique resonance
at Ω = -1.5 meV

Nature **403,** 746
(2000).

Zn Impurity State Location and Orientation



Topography (BiO Plane)

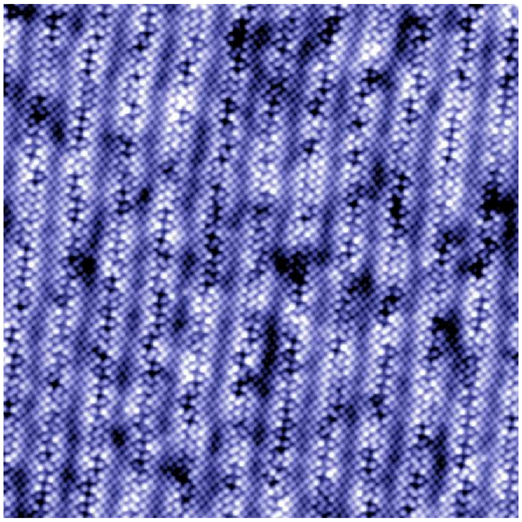


LDOS Map, V = -1 mV

Nature **403,** 746 (2000).

60 Å, 4.2 K
200 pA, -200 mV

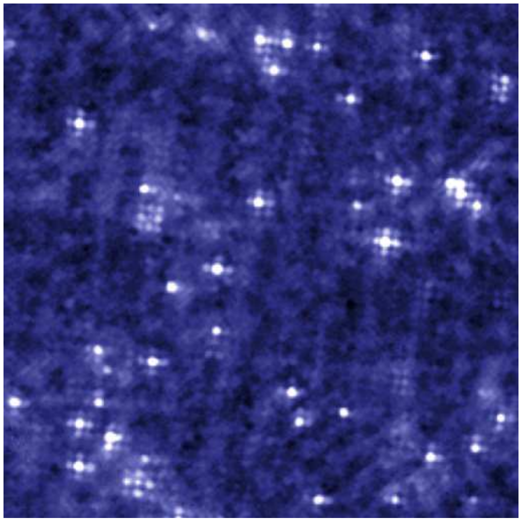
$Bi_2Sr_2Ca(Cu_{1-x}Ni_x)_2O_{8+\delta}$ Topo, $x \approx 0.5\%$



256 Å, 4.2 K
100 pA, -100 mV

Sample: H. Eisaki, S. Uchida

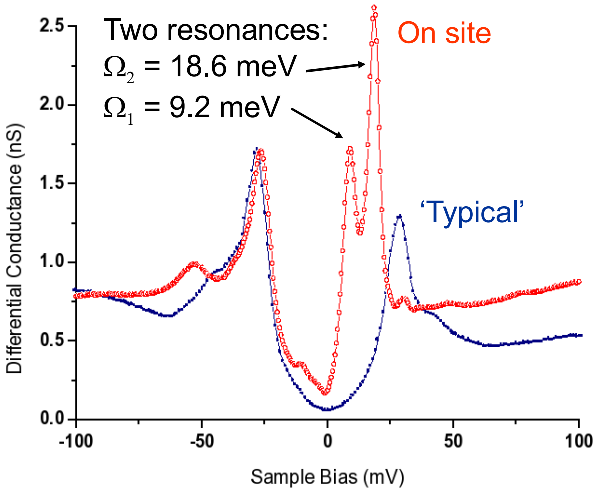
$Bi_2Sr_2Ca(Cu_{1-x}Ni_x)_2O_{8+\delta}$, $x \approx 0.5\%$ conductance map at +10 meV



256 Å, 4.2 K
100 pA, -100 mV

E.W. Hudson. *et al.*, *Nature* **411**, 920 (2001).

$Bi_2Sr_2Ca(Cu_{1-x}Ni_x)_2O_{8+\delta}$ Spectra



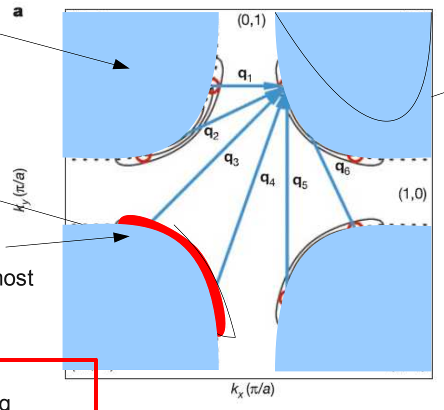
Two resonances:
$\Omega_2 = 18.6$ meV
$\Omega_1 = 9.2$ meV

On site

'Typical'

QPI

Quasi-Particle Interference (QPI)



First Normal metal
Fermi Surface

Add superconductivity
Gap with nodes

Banana like dispersion

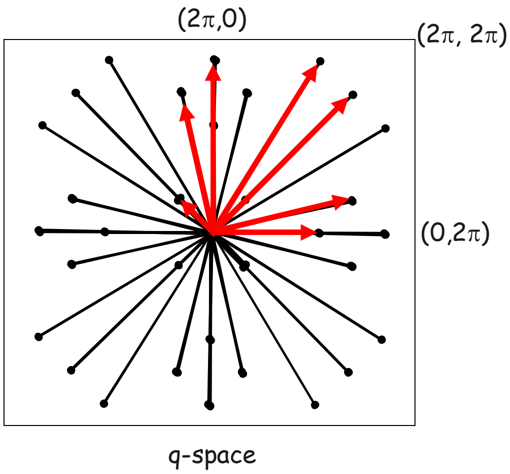
Points with the largest
Density produce the most
Scattering (q vectors)

Node

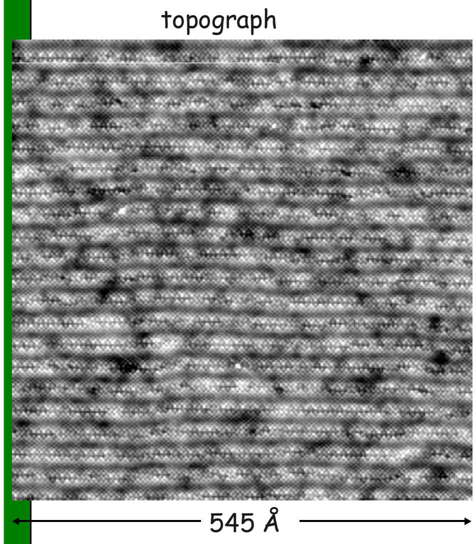
Needed:
- Source of scattering
- Large joint density of states

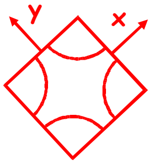
K. McElroy *et al.*, Nature **422**, 592 (2003)

Expected structure of FFT of LDOS(r,E) (for a fixed E)



Finally, some data...





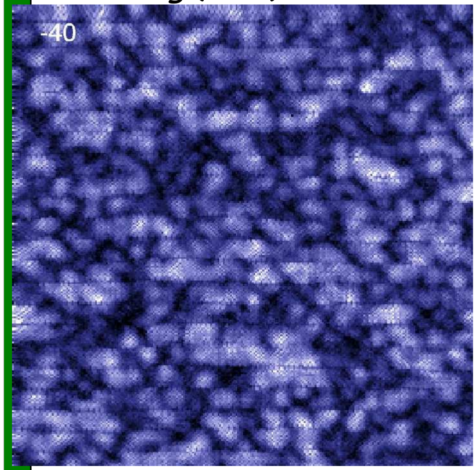
Bi-2212
T_c=76 K
Δ~51meV

energy
(meV)

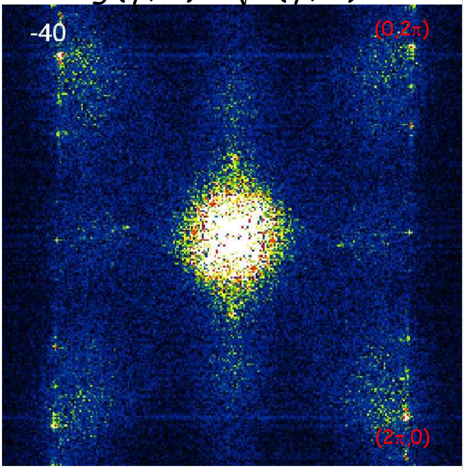
Imaging quasiparticle wavefunctions

$g(\vec{r},E)$

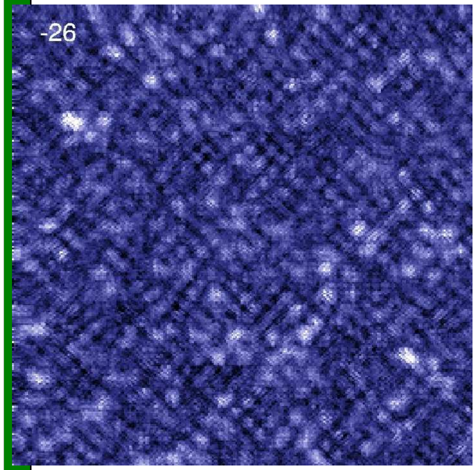
$g(\vec{q},E)=\sqrt{P(\vec{q},E)}$

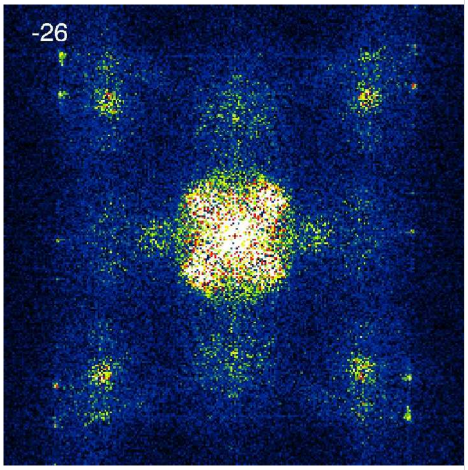


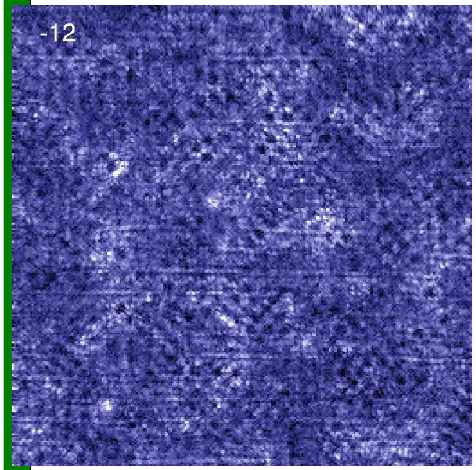
FFT



545 Å



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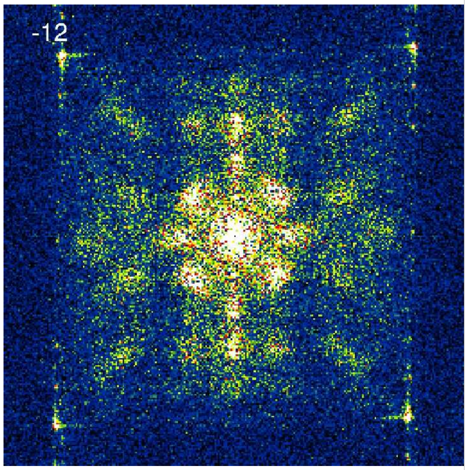
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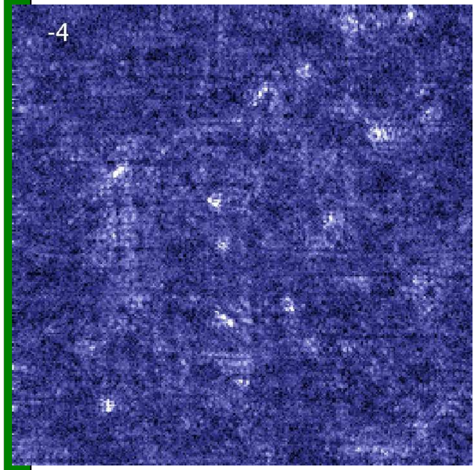
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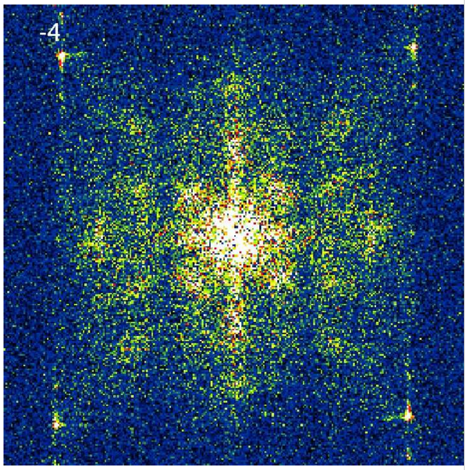
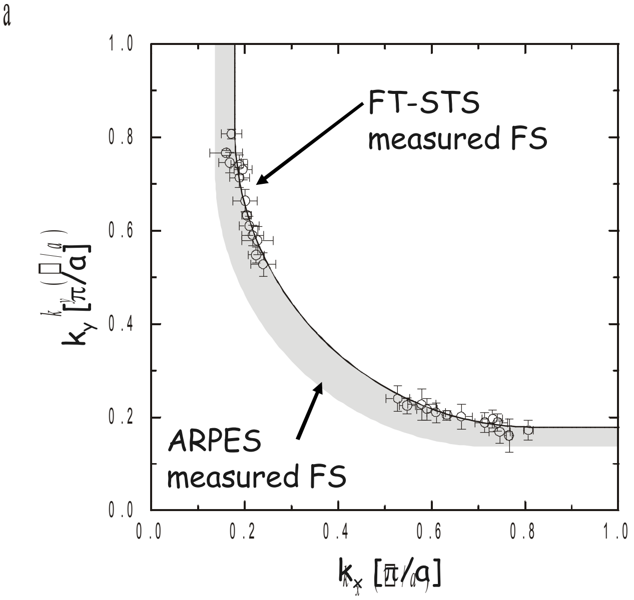

-4

ARPES & STM: Fermi surface comparison



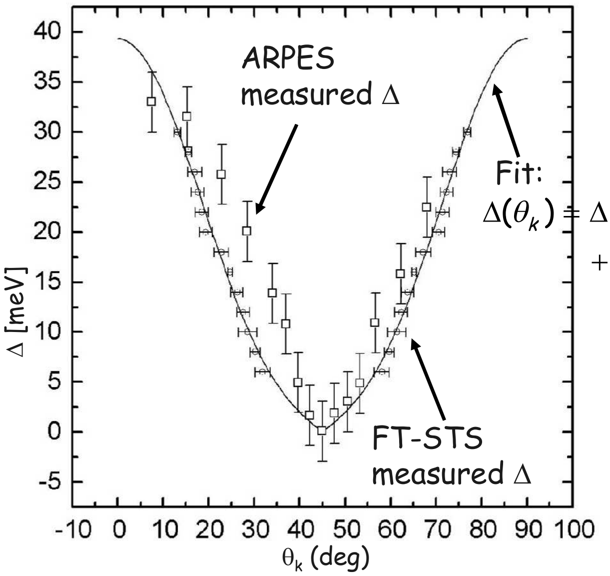
FT-STS measured FS

ARPES measured FS

Works because
- Quasiparticle scattering
- Angular dependence of gap

Nature, April 10, 2003

FT-STS |Δ(k)| : Reasonable agreement with ARPES



ARPES measured Δ

FT-STS measured Δ

Fit:

$$\Delta(\theta_k) = \Delta_0[A\cos(2\theta_k) + B\cos(6\theta_k)]$$

Nature, April 10, 2003

Conclusion

- From simple tunneling theory
- To complex density of states structures (or even quantum mirages)