Nanophysics 15

Nanoelectronics (2) Tunnelling

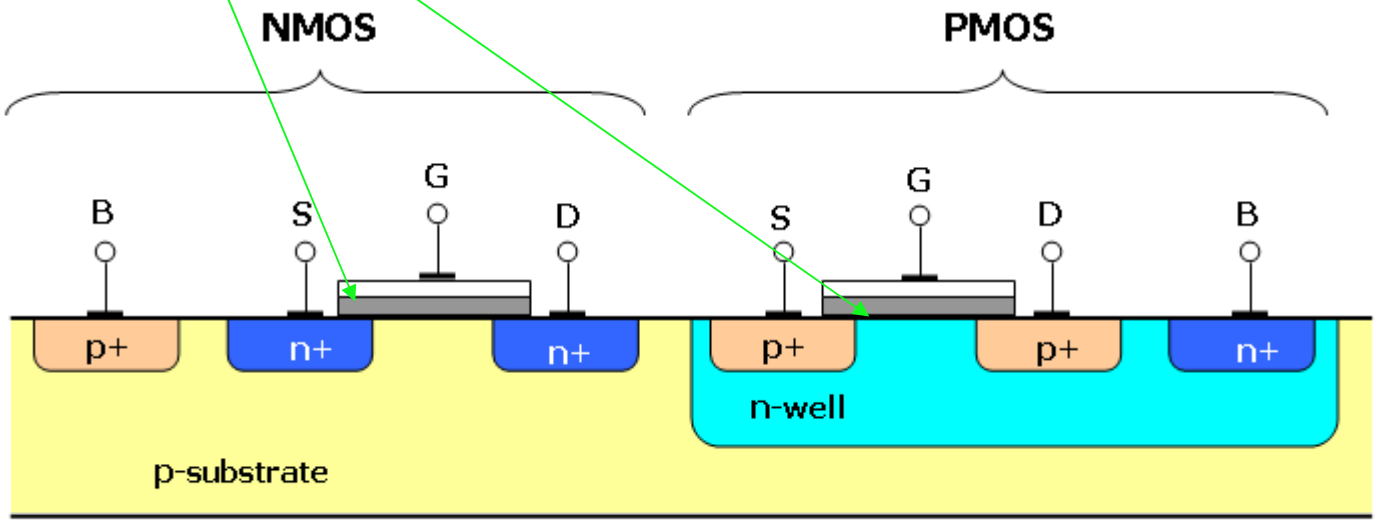
Supplementary materials

Outline

- Physics of Tunnelling (review)
  - Thin oxide layer can conduct through tunnelling
  - Implication for conventional field effect transistor technology
- Scanning Tunnelling Microscopy
  - Application of tunnelling physics
  - Imaging of spatially resolved wavefunctions
  - Observe local density of states by differential spectroscopy

CMOS, the workhorse of IC

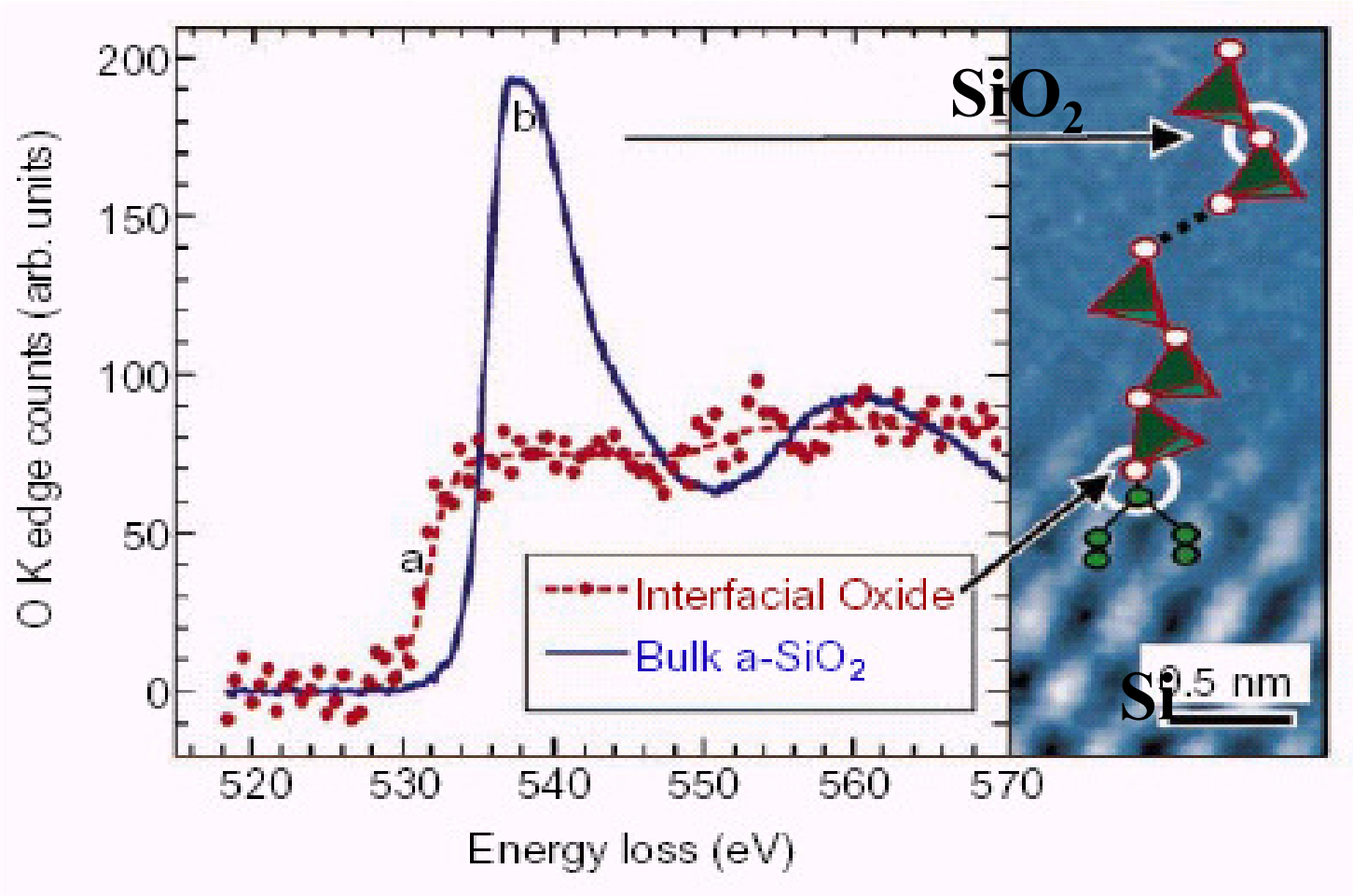
- Smallest dimension, the thickness of gate oxide layer



http://upload.wikimedia.org/wikipedia/en/6/62/Cmos_impurity_profile.PNG

Limit to conventional FET

Electronic structure of ultrathin gate oxide

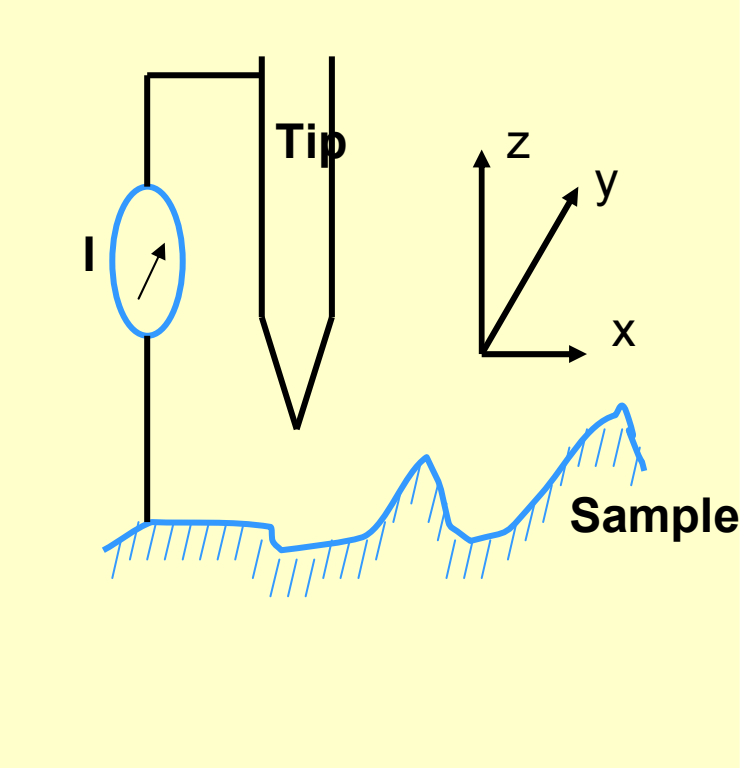


Nature， v399， p758 (1999)

Scanning tunnelling microscopy

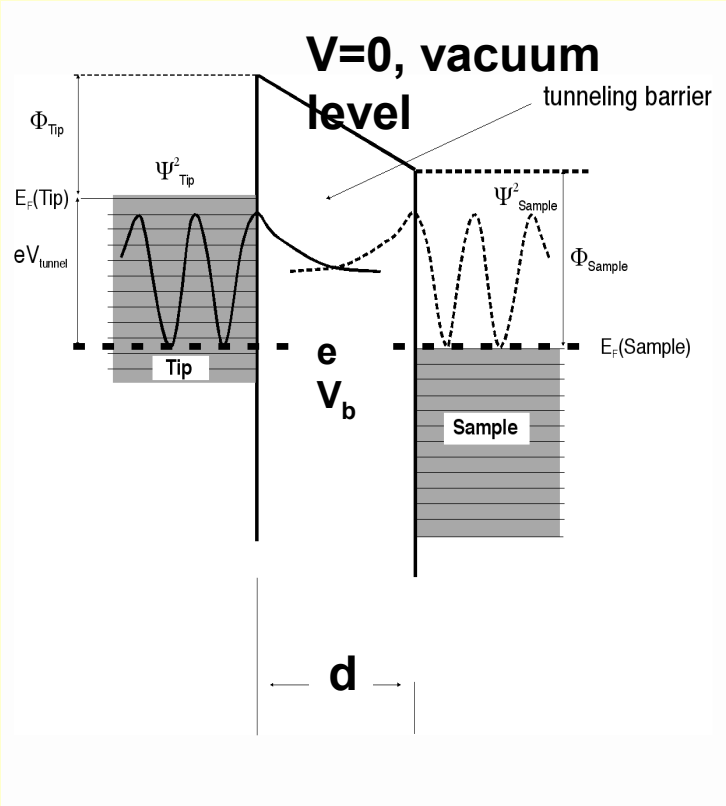
Operating principle

- A sharp tip is scanned over a surface
  - piezoelectric scanners allows control of x,y and z movement
- A bias voltage, V_b, is applied between tip and surface.
- The current, I, between tip and surface is measure



The Basic Concept

Tunneling (1D model)



- Tunnelling can occur from all states between E_f and (E_f-eV_b) of the surface.
- Tunnelling current, I, depends
  - → on the tip-surface distance.
  - → on the density of states of both that of the sample and the tip.
- Tunnelling is a QM process can be described by Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dz^2}+V\psi=E\psi$$

Solving Schrodinger Equation

- Inside the tunnelling barrier, assume $eV_b << \phi$, then E-eV ~ - ϕ, Thus $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dz^2} = -\phi\psi$

  → This has the solution of the form

  $$\psi = Ae^{-\alpha z}$$

  → Substituting it back into SE, we get:

  $$\alpha = \sqrt{2m\phi/\hbar^2}$$

- Evaluate:

  → Probability e^- reaches z=d (tunnels through barrier)

  = exp(-2αd)

  $$\frac{\psi(z=d)}{\psi(z=0)} = \frac{Ae^{-\alpha d}}{A} = \exp(-\alpha d)$$

Vertical resolution of STM

- For typical tip materials (W), ϕ ~ 5 eV

  → We can calculate α:

$$\alpha = 1.2\text{Å}^{-1}$$

- Let d=1 Å, then we have

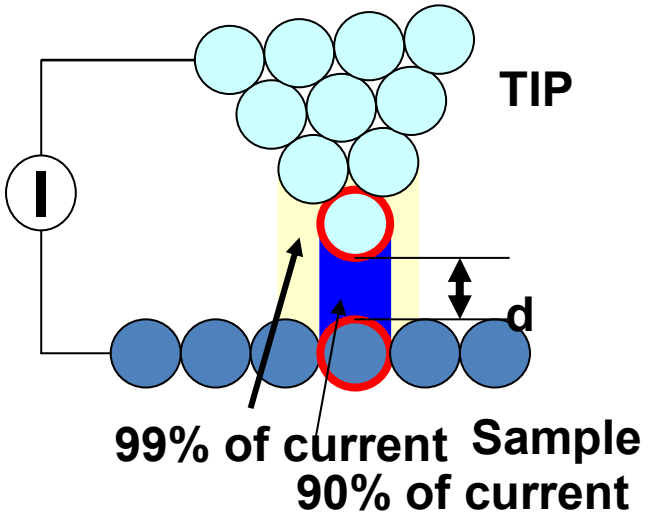
$$\frac{P(d=1?}{\mathrm{P(d=1.1?}} = \frac{e^{-2x1.2x1.0}}{e^{-2x1.2x1.1}} = 1.27$$

  → i.e. 27% increase in tunnel current for 0.1Å

- Vertical resolution is better than 0.1 Å

  → In practice, the vertical resolution can be routinely achieved to be better that 1 Å, i.e. individual atom layers can be seen easily

Lateral resolution



- Atomic resolution depends on localised tip and the nature of the tunnelling states on the sample surfaces
  - → Because of asperity, only a few atoms in the tip is involved in the tunnelling process
  - → Tip is capable of very high lateral resolution

Lateral resolution…

- Lateral atomic resolution depends on

  → the wavefunction (whether localized or delocalized), and

  → the amount of charge spill over into interstitial space.

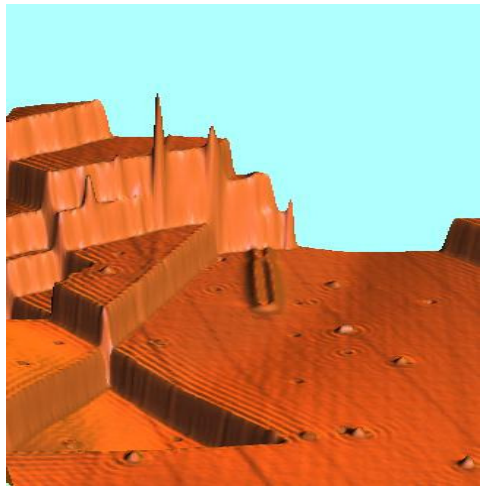
- Examples

  → Cu(111)

  → Si(100)

Example 1: Cu(111) surface

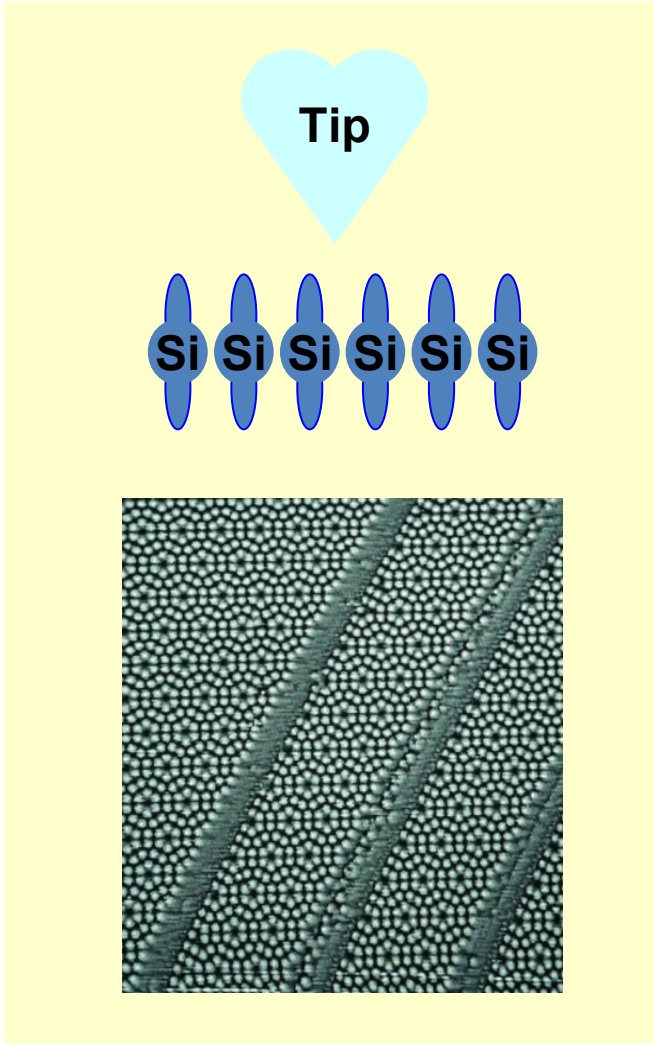
- **Surface states on Cu(111)**
  - → Delocalized on the surface (2D free-electron-like wave)
  - → Large charge spill-over into the inter-atomic region (This is the reason for the surface double layer)
  - → Minimal surface corrugation of the corresponding charge density.
- **Observations**
  - → No lateral atomic resolution feature
  - → Smallest features are ripple
    - ✓ Wavelength 15 Å >> atomic spacing
    - ✓ Height 0.04 Å << atom size
    - ➢ due to reflection of free electron-like waves from step edge or point defects



Example 2: Si(001) surface

- **Stepped Si(001) surface**
  (7x7) reconstruction
  - → Localized directional bonding (Si 2p states)
  - → High corrugation expected

- **Observations**
  - → Atomic feature is clearly resolved
  - → The complex pattern is due to (7x7) reconstruction of



Modes of imaging

- **Constant height mode**
  - less common
  - → Keep d constant, measure variation in the current I
  - → Need current feedback to avoid crashing
  - → Can scan fast, not limited by response time of vertical tip movement

- **Constant current mode**
  - Usual topographical mode
  - → Keep I constant by adjusting z (through feed back loop)
  - → No danger of crashing the tip

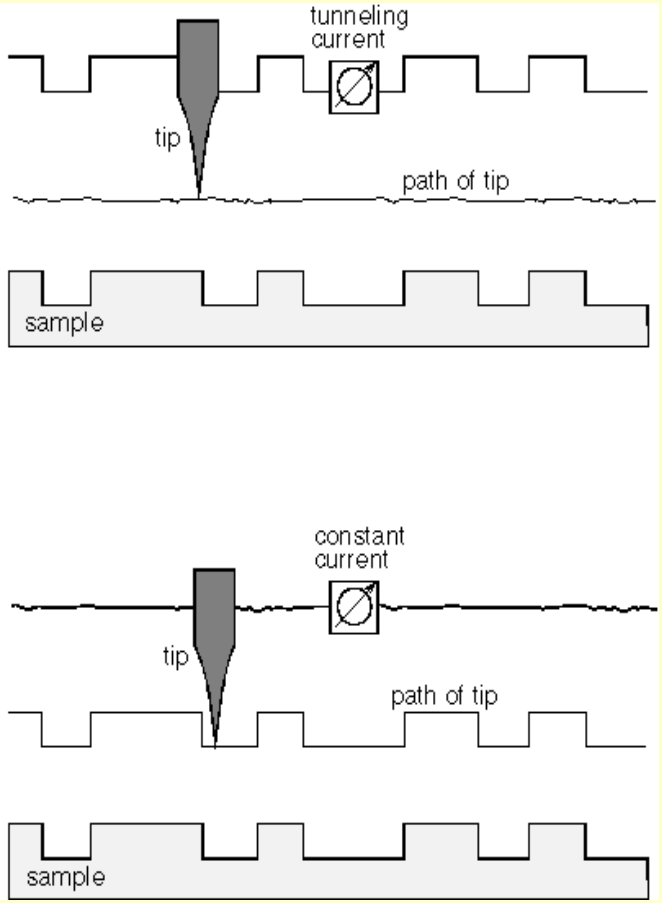
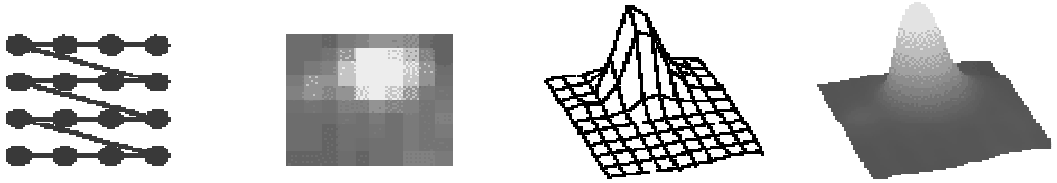
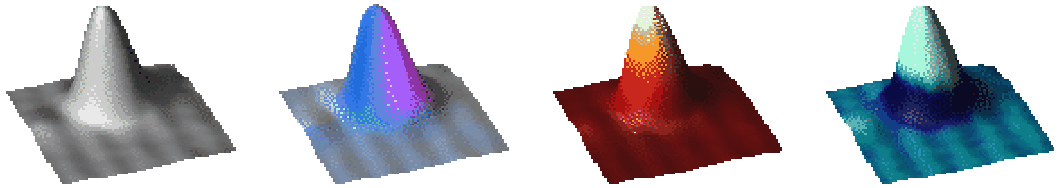


Image formation and processing

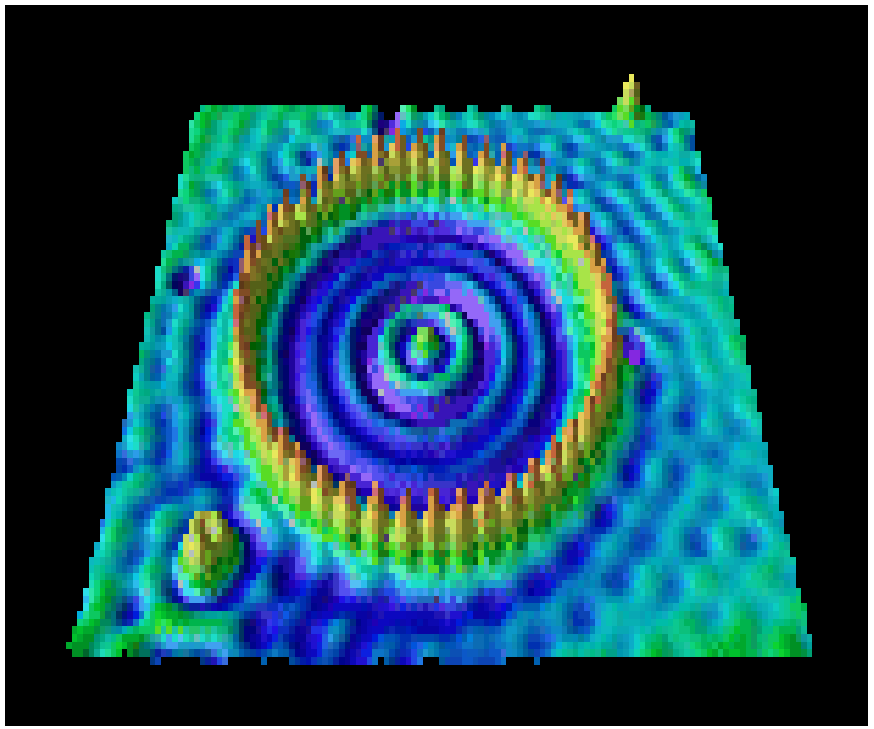
- Image scanning and display



- False colour display



Quantum corral



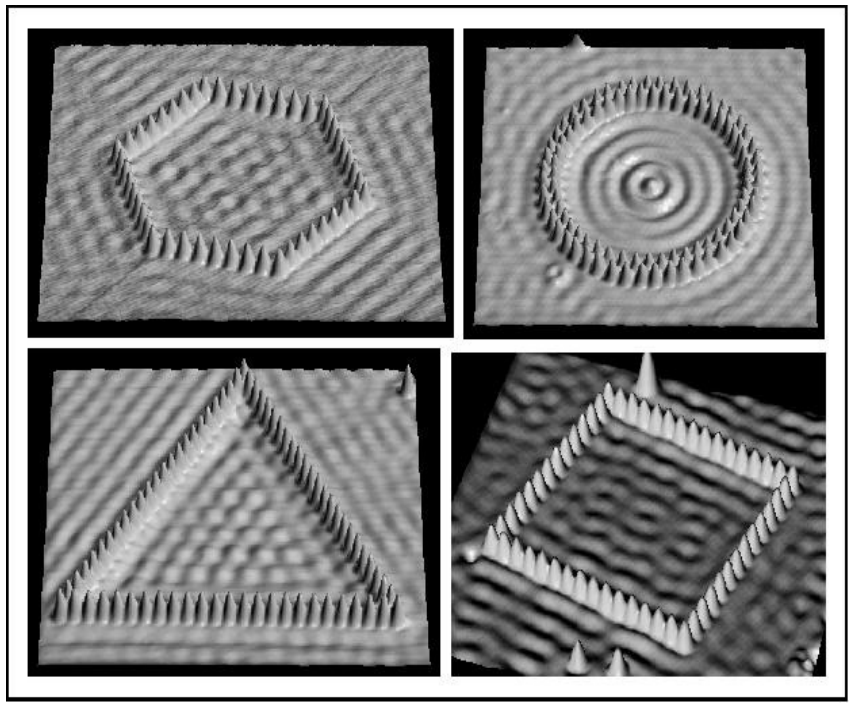
M.F. Crommie, C.P. Lutz, D.M. Eigler, *Science 262 (1993) 218*

A circular ring of 48 Fe atoms assembled on the Cu(111) surface at 4K, mean radius 71.3 Å

Atomic landscape ⮌ Electronic landscape ⮌ Quantum Corral

Variation on corrals

- One can construct walls of Fe atoms of different shapes, hence different standing wave pattern of surface states.



Quantum Corral

- The artificial corral structure results in space confinement of surface state wavefunction.
- The wave nature of the surface electron is demonstrated by the formation of ripples within the quantum corral.

- The ripple here and those found on stepped Cu(111) surface are of the same origin.
- In the case of quantum corral, the ripple pattern can be calculated using ‘particle in a box (ring)’ model

To understand the quantum quarrel

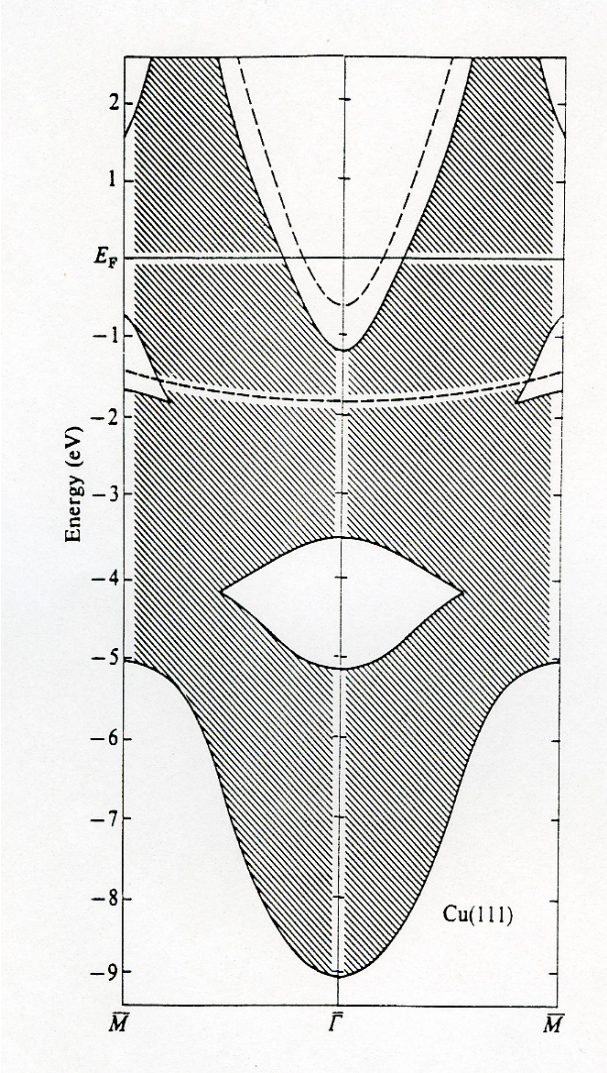
- Understand the concept of surface states (revision)
  - Free electron nature of surface states
- Understanding the interaction of impurity, steps with surface states
  - Reflection at steps and standing wave formation
    - Experimental measurement of dispersion relationship (energy vs. wavevector) of the wavefunction
- Constructing quantum corrals to confine the wavefunction of the electrons in the surface state
- Understading of the electronic structure of the quantum corral
  - Solving two dimensional Schrodinger equation., solution for wavefunction is based ob Bessel equations, energy level quantized. (explore the Bessel function, the zeros corresponds to the nodal positions)
  - STM image of the charge density (wavefunction squared)

Review: Surface State Wavefunction

- **What is an electronic surface state ?**
  - ➔ An electron state whose wavefunctions is spatially localized on crystal surface.

- **Properties of surface states in Cu(111) surfaces.**
  - ➔ Close-packing of atoms gives a small atomic potential corrugation
  - ➔ Valence electrons are delocalized, so it can move freely within the surface plane, so it behaves like a 2D free electron gas with a dispersion relation:

$$E - E_0 = \frac{\hbar^2 k^2}{2m}$$



k is the component of electron wavevector in the surface.

Scattering off the surface step

- The surface step is assumed to form impenetrable barrier to the surface state electron.

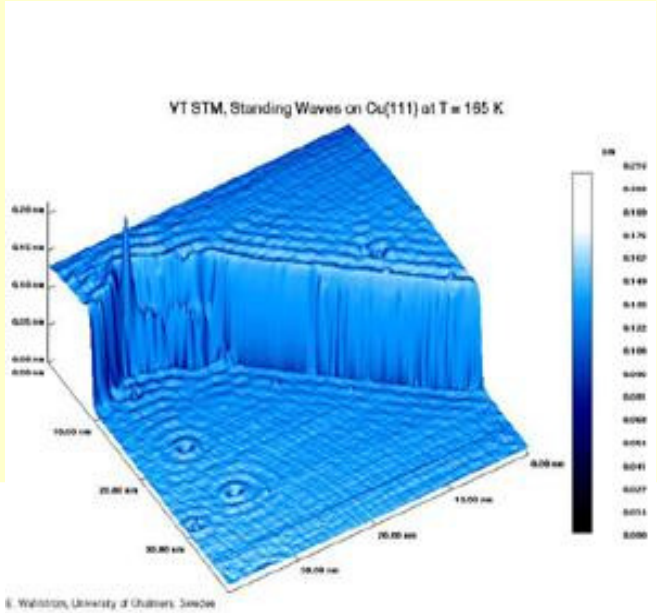
- Near the step, the incoming wave and the reflected wave form a stationary wave

- STM can measure a stationary wave pattern such as standing wave

$$\psi(k,x) \propto e^{ikx} + e^{-i(kx+\xi)}$$

$$|\psi(k,x)|^2 \propto \left|e^{ikx} + e^{-i(kx+\xi)}\right|^2 = \left|e^{i\frac{kx-\delta}{2}}\right|^2 \cos^2\left(kx + \frac{\delta}{2}\right)$$

Setting $\delta = \pi$ $\quad |\psi(k,x)|^2 \propto \sin^2(kx)$



Dispersion Relationship of electrons in surface state

Summing over all surface state electrons

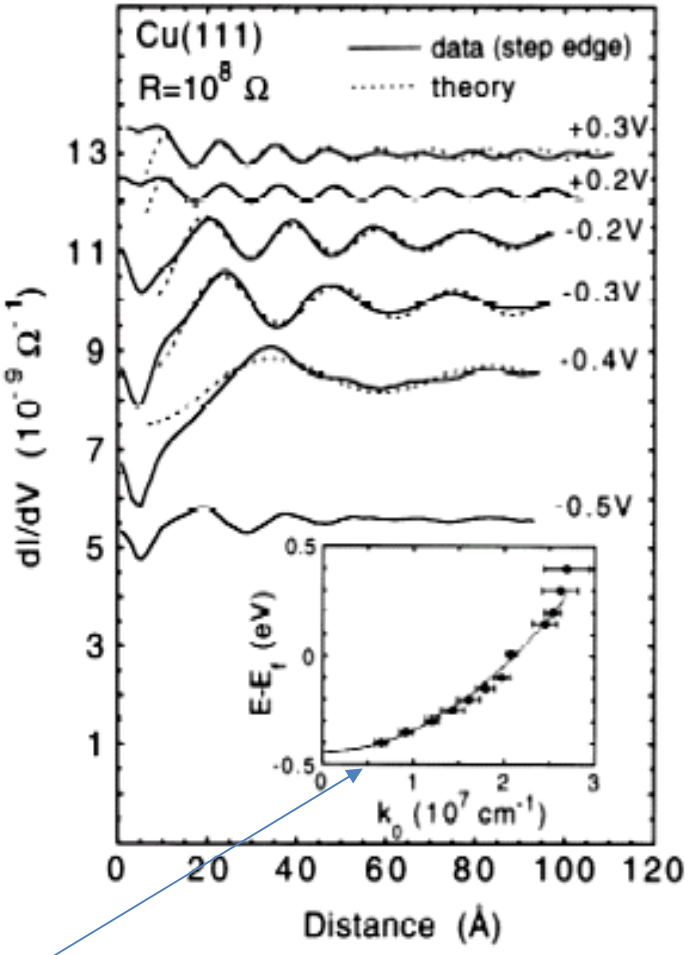
$$I(V,r) \propto \sum_k |\psi_k(r)|^2 \delta(\varepsilon_k(V) - \varepsilon_f)$$

$$= \sum_k^{k_0} \sin^2(kx)\delta(\varepsilon_k(V) - \varepsilon_f)$$

$$\propto (1 - J_0(2k_0 x))LDOS_{without\_step}$$

- **The energy dependence allows us to map out the *dispersion relationship* for the surface states, ε(k).**
- **It is free-electron like**

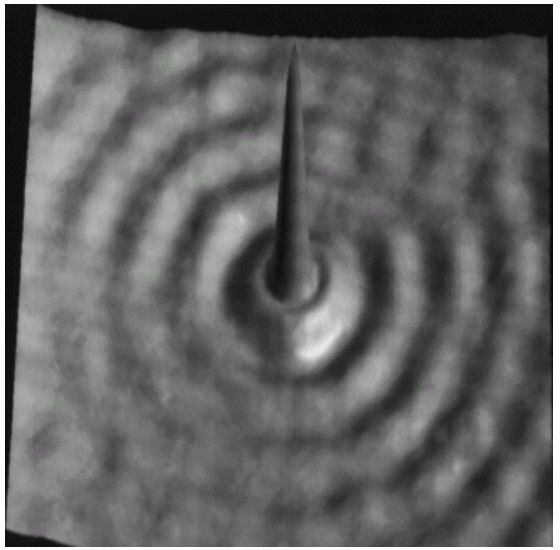
$$\varepsilon_k - \varepsilon_0 = \frac{\hbar^2 k^2}{2m^*}$$



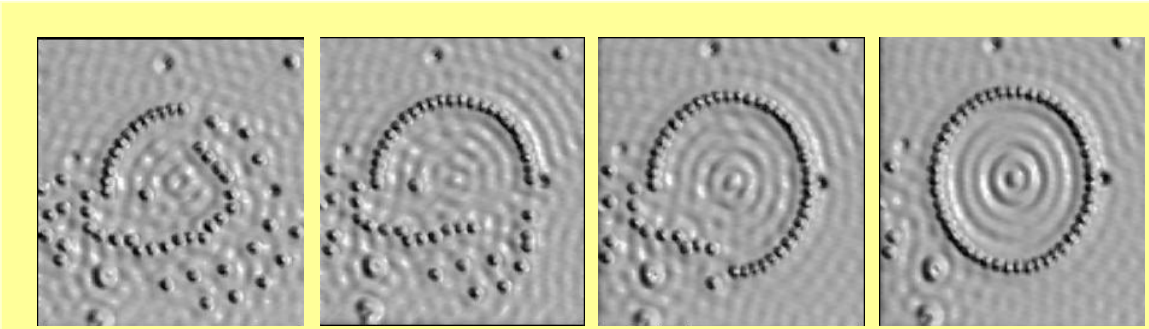
ε_0= - 440meV
m^*=0.40m_e

Surface scattering off Fe atoms on Cu

- Again, standing wave pattern is observed from an impurity Fe atom. However, the mathematical description is more complicated because of the spherical symmetry.
- We can use the scattering property of Fe atoms to construct artificial walls to confine surface electrons.



IBM web-image



a circular ring of 48 Fe atoms assembled on the Cu(111) surface at 4K, mean radius 71.3 Å

Local density of states
(particle in a circular box …)

- **Solving the azimuth equation first by setting**

$$\Phi = Ae^{im\phi}$$

→ substituting this back into azimuth equation gives

$$e^{im\phi} = e^{im(\phi+2\pi)}$$

$$\text{m is an interger}$$

→ cyclic boundary conditions:

$$C = -m^2$$

- **Solving the radial equation**

$$r\frac{d}{dr}\left(r\frac{dR(r)}{dr}\right)+\frac{R(r)Er^2}{\hbar^2/2m_e^*}-m^2R(r)=0$$

➔ Rearranging

$$r\frac{d}{dr}\left(r\frac{dR(r)}{dr}\right)+(k^2r^2-m^2)R(r)=0$$

➔ This is an example of Bessel's equation

Bessel Functions

- Let $x = kr,\ y = R(x)$

$$x^2 \frac{d^2 y}{dx^2} + (x^2 - m^2)y = 0$$

- The Bessel function has two kinds of solutions $J_m(x)$ and $Y_m(x)$ [also called $N_m(x)$]. The $Y_m(x)$ is considered non-physical for our case because it has infinite value at r=0.

→ Solution $R=J_m(kr)$

with boundary condition: $R(r=a)=0$

so $J_m(ka)=0$

→ Obtain k from the boundary condition:

$$\Phi = Ae^{im\phi} \qquad k^2 = \frac{2m_e^* E}{\hbar^2}$$

Thus, possible values of ka are the 'zero' of J_m i.e. where J_m cuts the x-axis.

Bessel Functions

- **Note:**

  → Radial solution depends on the value m in $\Phi = Ae^{im\phi}$

  → For simplicity,
  consider only the cylindrical symmetric solutions, i.e. m=0

  so $R(r) = J_0(kr)$

  with $J_0(ka) = 0$

  We need to find values of x=ka where zero of J_0(ka) occurs (from math book)

Bessel Functions ...

- From tables (Abramwitz & Stegun)

S ***(S^{th} zero)***	***Value of x Where zero occurs***
1	2.40
2	5.52
3	8.65
4	11.79
5	14.93
6	18.07

This gives us the allowed values of k.

$$k = \frac{x_S}{a}$$

From this, we can get allowed energy values.

Results ...

$$E = \frac{\hbar^2 k^2}{2m_e^*}$$

- To calculate the energy, we need to know

  → Effective mass of the electrons

  $m_e^* = 0.38\ m_e$ (for surface state at Cu(111) surface)

  → Radius of the box

  a = 7.13 nm

  → Value of s: no. of nodes = 5, assuming a node at the Fe atoms

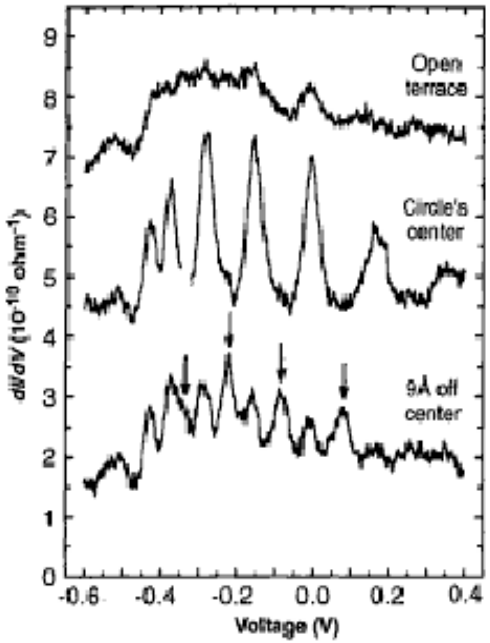
  s = 5

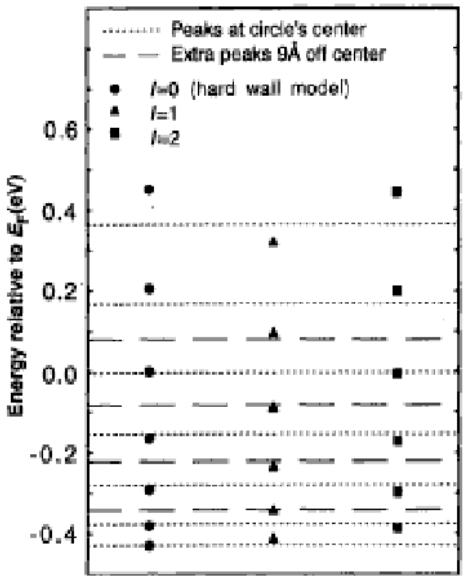
  → Thus

  ka = 14.93, i.e. k = 14.93 /a

  $E = 7.1 \times 10^{-20}$ J = 443 meV

Local spectroscopy of electrons within a Quantum Corral





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Atomic landscape ➲ Electronic landscape ➲ Quantum Corral

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Comments ...

- What is the reference point for V = 0 (bottom of the well) in the real surface system ?
  - → Calculation: - 0.443eV
  - → Experiment: - 0.450 eV below F_F

    The s = 5 state lies at E_f,

    The V_b used by Eigler was + 10 meV (on the sample)

    ✓ a remarkable match !!!

- If moving the tip out of the centre, pick up cylindrical unsymmetric, see additional peaks. Match well with m=1, 2, etc.
- The peak height (vs. r) do not quite match, so other waves are also present
- The peaks (vs. V) have a width (not δ function)
  - → leakage out of the box or inelastic scattering

Summary

- **Tunnelling is detrimental to FET**
- **Tunnelling is very useful in STM**
- **STM**
  - **Applications to imaging of surface electronic state wavefunction**
    - ➔Surface state and its dispersion relationship.
    - ➔The scattering property of atomic states and impurity Fe atoms on Cu(111)
    - ➔Confinement of surface electron states and standing wave pattern.
  - **Spectroscopy measurements using STM**
    - ➔STM current measures the sum of local density of states, confirmation of the quantum mechanical calculation of a particle in a box