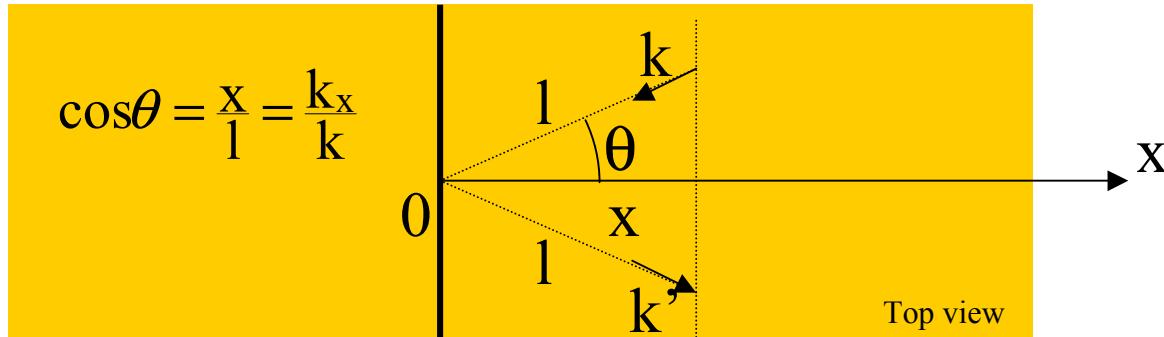


3.8 Quantum interferences - finite lifetime model

Inelastic processes on the terrace

e-e scattering
e-ph scattering



$$\psi_k(x, y) = (e^{ik_x x} + e^{\frac{-2x}{L_\varphi} \frac{k}{k_x}} r(k_x) e^{i\varphi(k_x)} e^{-ik_x x}) e^{ik_y y} \text{ where } L_\varphi \text{ is the phase relaxation length.}$$

Numerical integration of the LDOS expression (*) (see. Transp. 3.5) gives (with $\varphi = -\pi$ and previous remarks) :

$$\rho(E, x) = L_0 (1 - r(k) e^{-2 \frac{x}{L_\varphi}} J_0(2 k x))$$

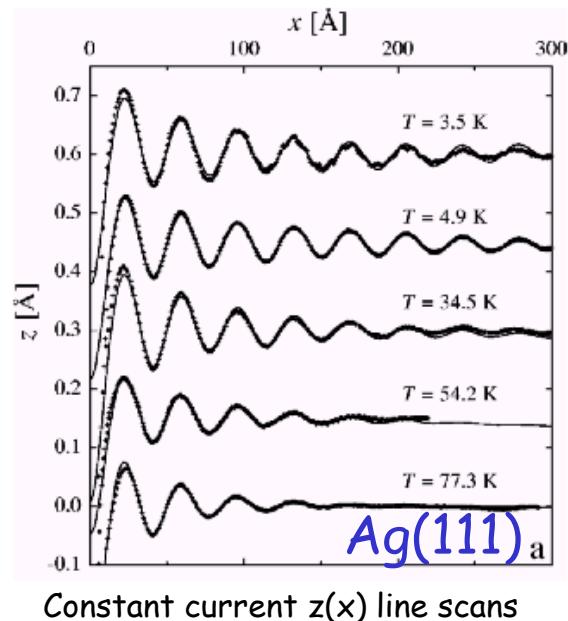
Inelastic processes on the terrace lead to an additional decay of the LDOS modulation !!!

3.9 Quantum interferences - phonons

From dI/dV images, $L_\phi(E)$ and $k(E)$ are extracted.
It is thus possible to get the lifetime of a quasiparticle (hole or electron),
using the relation :

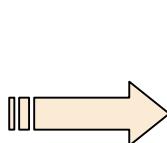
$$\tau(E) = \frac{L_\phi}{v} = \frac{L_\phi m^*}{k}$$

Electron - phonon interaction



Damping of the standing waves with increasing T

2. Main effect : Fermi Dirac broadening at high T



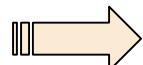
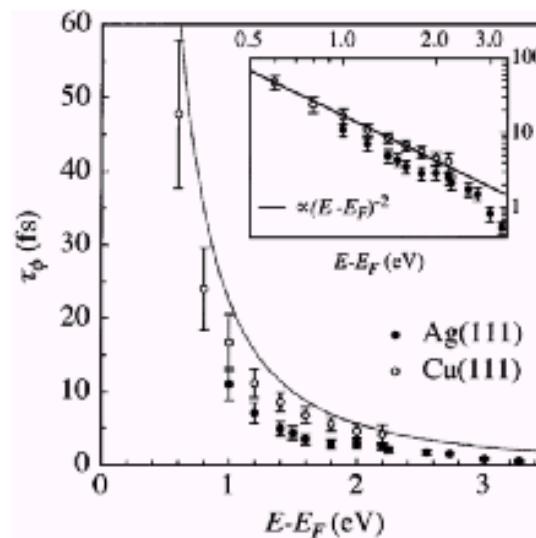
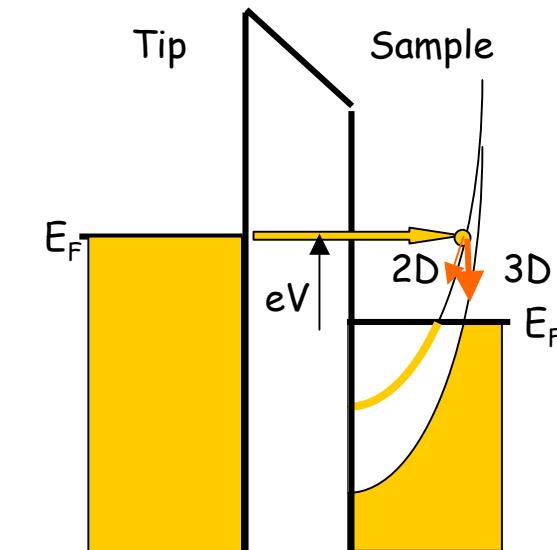
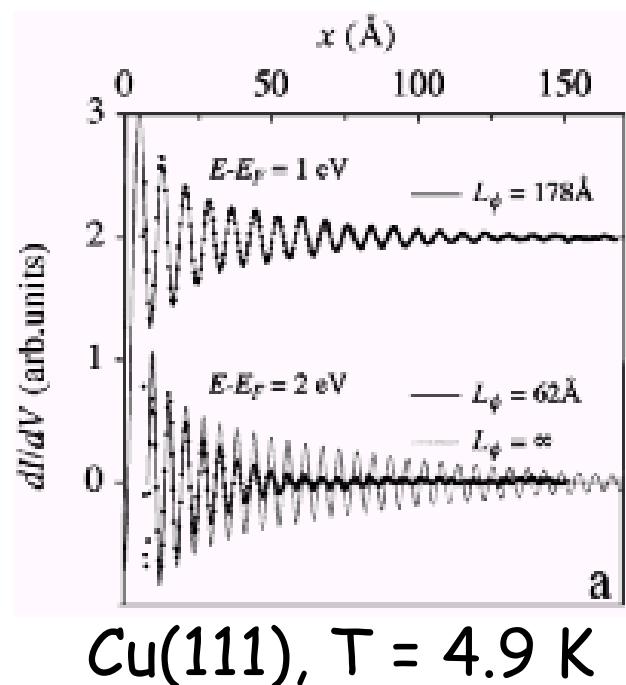
	3.5 K	77 K	178 K
Ag (111)	600	250	
Cu (111)		660	160

Lower limit for $L_\phi(\text{\AA})$

(For Cu k_F is much bigger than for Ag, thus Fermi-Dirac broadening is weak.)

3.10 Quantum interferences - electron lifetime

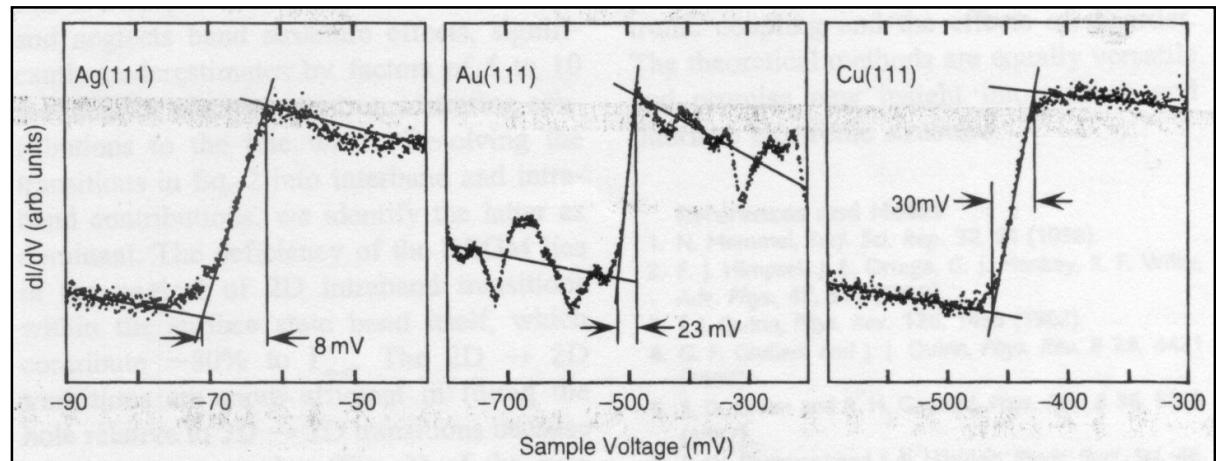
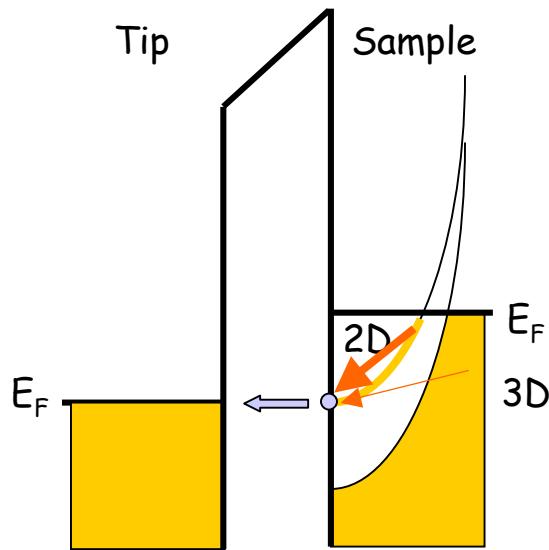
Electron lifetime measurements



τ_ϕ has a $(E - E_F)^2$ behaviour, which is predicted for a 3D free electron gas in the Fermi liquid theory

3.11 Quantum interferences - hole lifetime

Hole life-time measurements at the band edge of different surface states



The width of the onset is directly related to the lifetime of holes at the band edge: $\tau = \beta \frac{h}{4\Delta}$

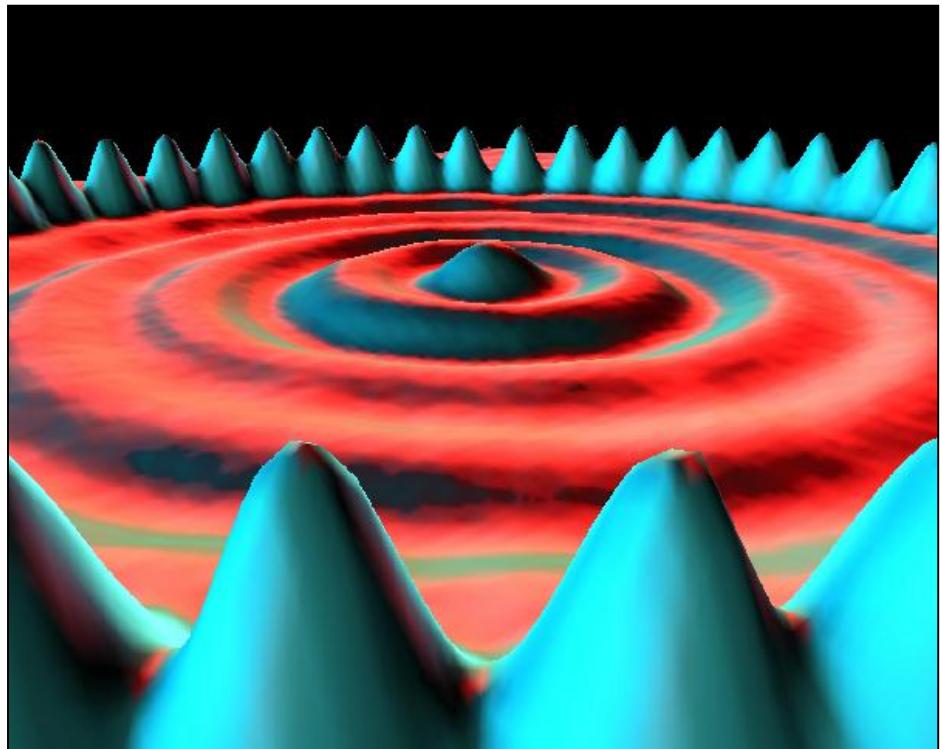
2D decay channels dominate the electron-electron interaction that contributes to the hole decay

4. Quantum resonators

4.1 Quantum resonator - Corrals

Quantum corrals

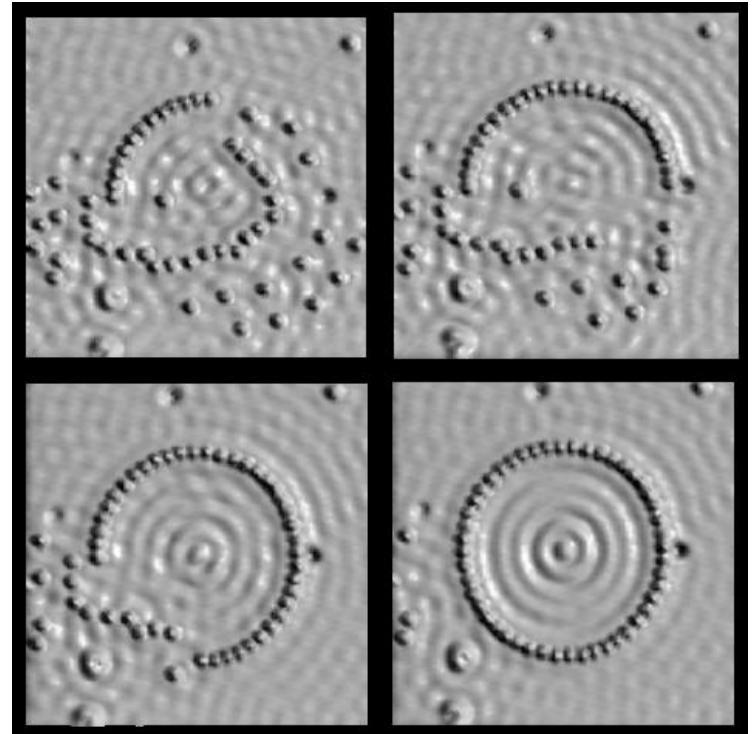
M.F. Crommie, C.P. Lutz, D.M. Eigler



Science, 262 (8 Oct. 93)

Fe/Cu(111)

T=5K

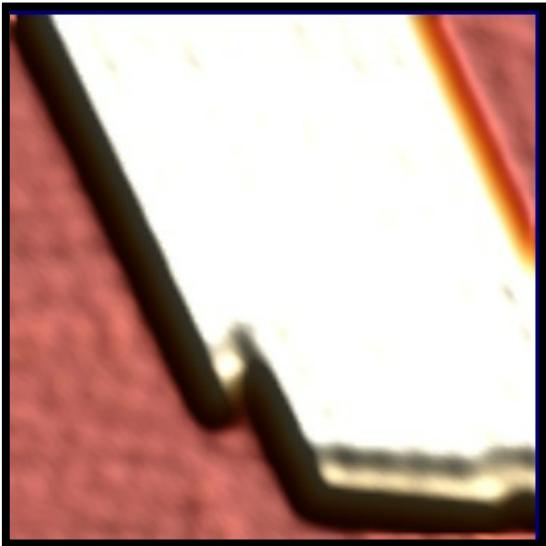


Physics Today 46, 17-19 (1993)

Web address : <http://www.almaden.ibm.com/vis/stm/corral.html>

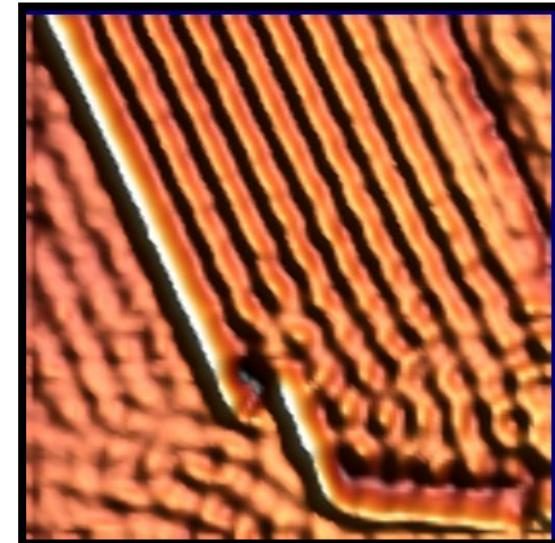
4.2 Quantum resonator - Cu/Cu(111)

Cu island on Cu(111)



25x25 nm²

Topography

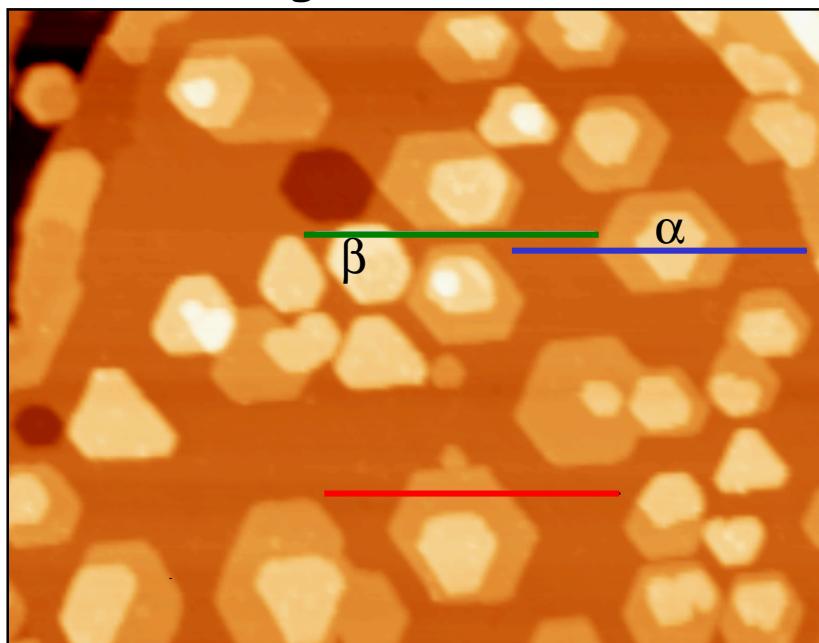


dI/dV at +10 mV

4.3 Quantum resonator - Ni / Cu(111) growth

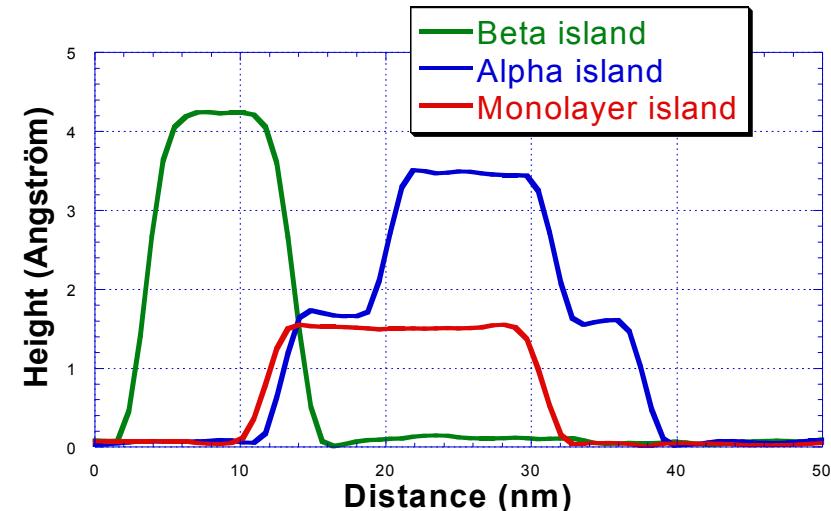
Ni / Cu(111)

- Cu(111) preparation (Ar etching, annealing at 650 K)
- Room temperature deposition : ~ 0.5 monolayer of Ni
- Cooling down at 40K, LT-STM study



Constant current STM image taken at 40 K

$150 \times 125 \text{ nm}^2$
 $V_{\text{sample}} = 150 \text{ mV}$, $I = 1 \text{ nA}$



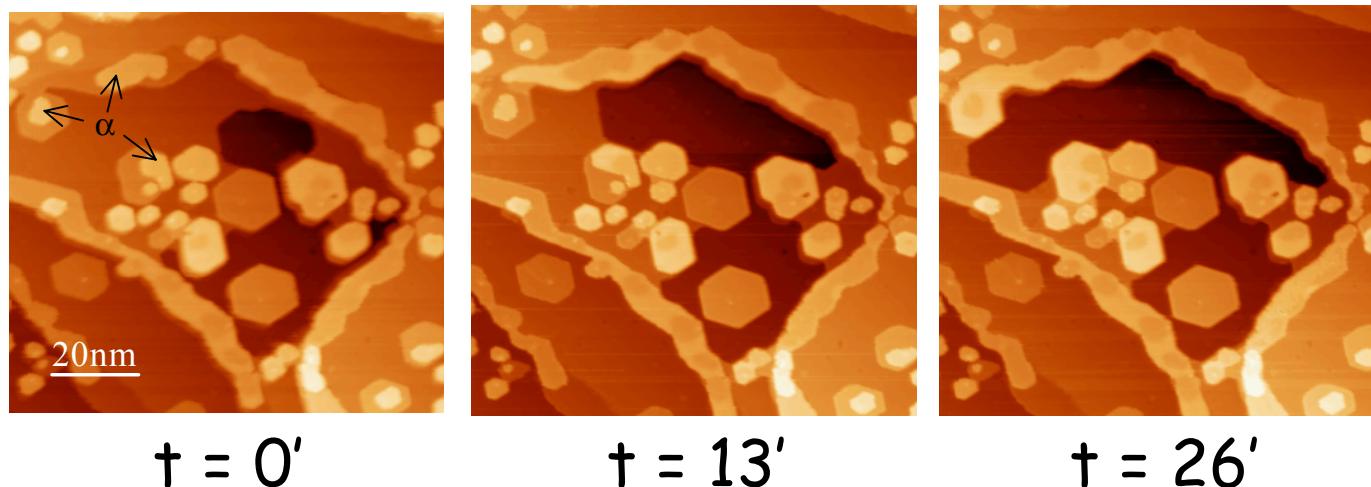
Corresponding height profiles

Two kinds of bilayer islands,
with different apparent height

4.4 Quantum resonator - Ni/Cu(111) - Cu diffusion ?

Room temperature STM movie (real duration 1 h)

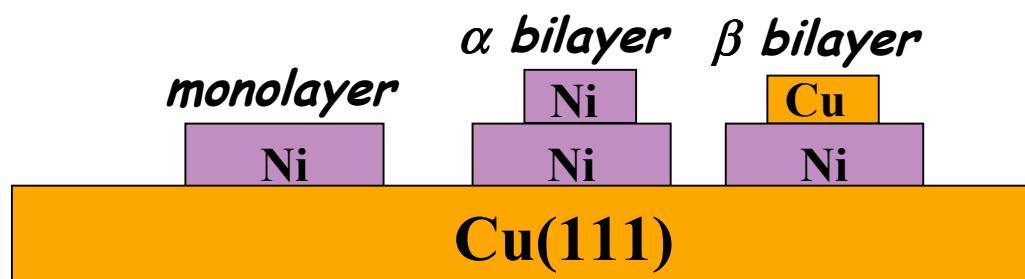
Images extracted from the movie
 $(100 \times 100 \text{ nm}^2)$



Cu is removed from
the substrate to cover
some monolayer islands

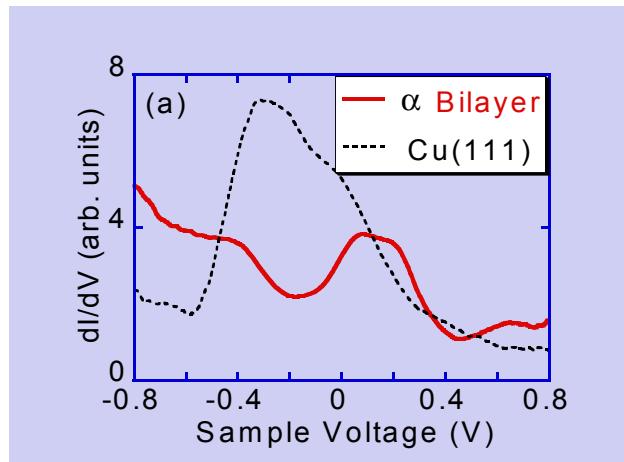


Growth of β islands

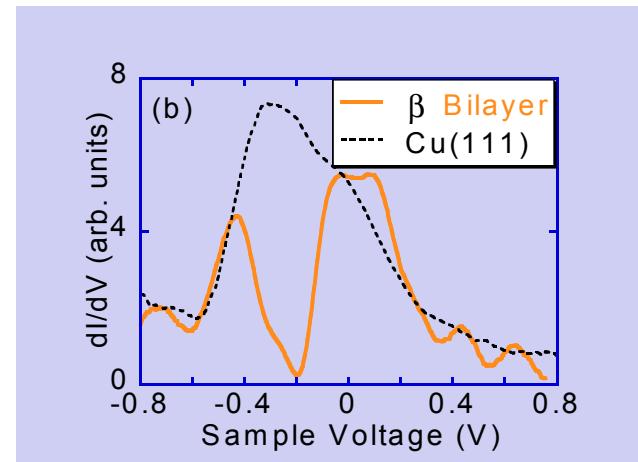


Proposed structure for the islands

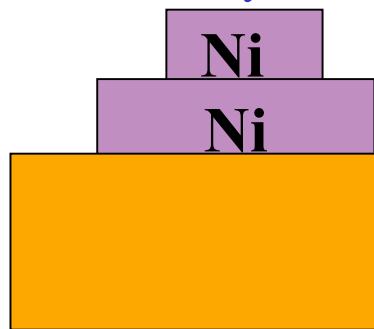
4.5 Quantum resonator - Ni/Cu(111) - STS on bilayer islands



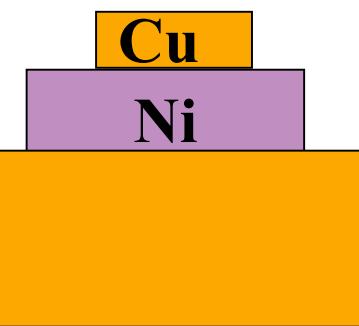
STS
 $T = 40K$



α bilayer



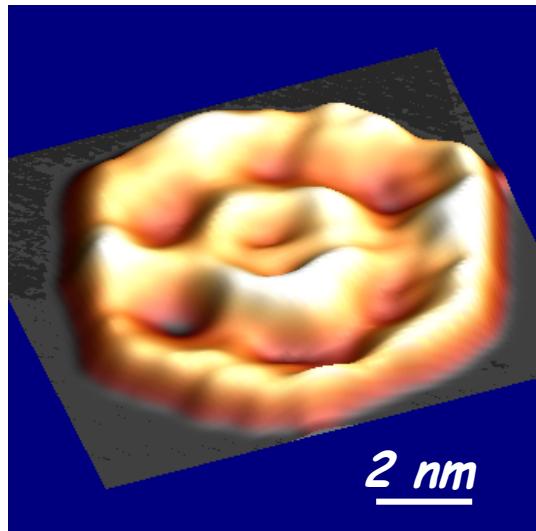
β bilayer



4.6 Quantum resonator - Ni / Cu(111) - Confinement

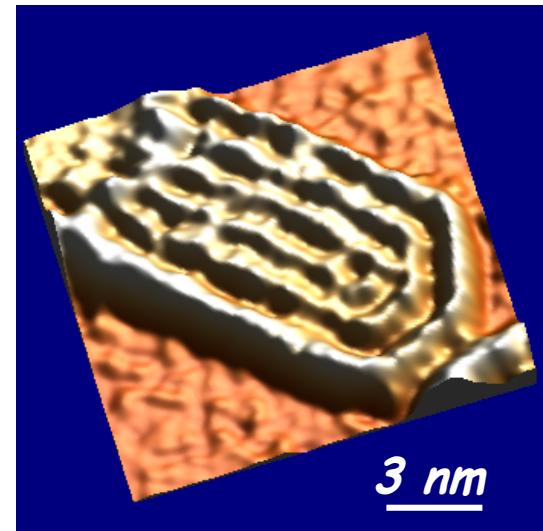
Confinement in both α and β bilayer islands

α Bilayer : Ni/Ni/Cu(111)



dI/dV (+250 mV)
image at 40K

β Bilayer : Cu/Ni/Cu(111)

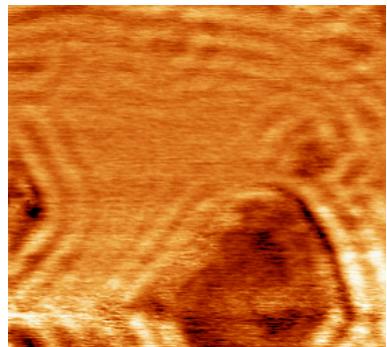
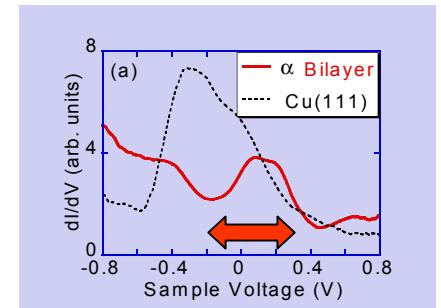
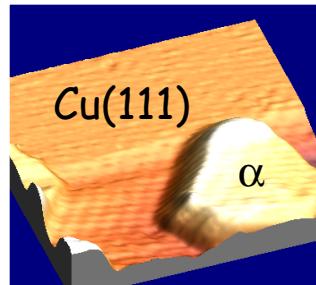


dI/dV (+450 mV)
image at 40K

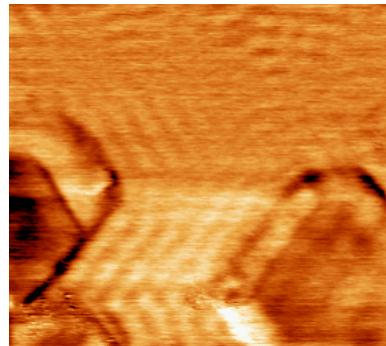
4.7 Quantum resonator - Ni / Cu(111) - Confinement

Confinement in an Ni bilayer island (α)

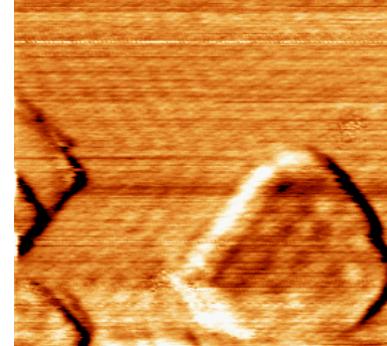
Topography :



-200 mV



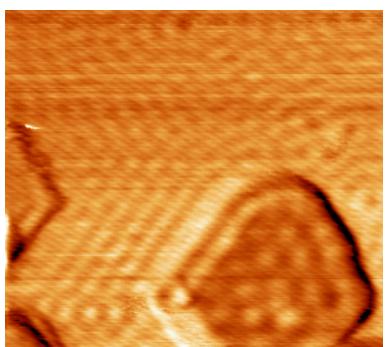
-100 mV



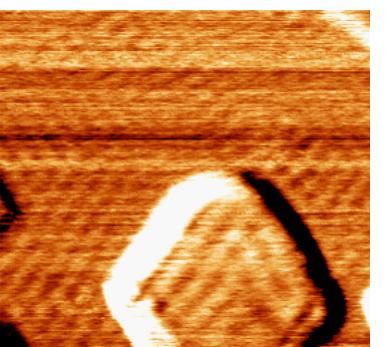
-50 mV

dI/dV images
at 40 K

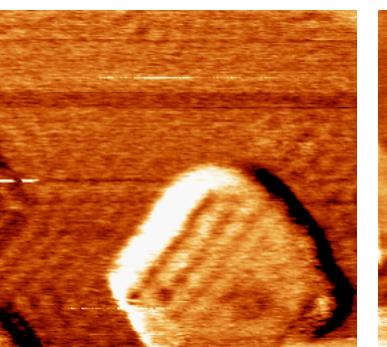
$30 \times 30 \text{ nm}^2$



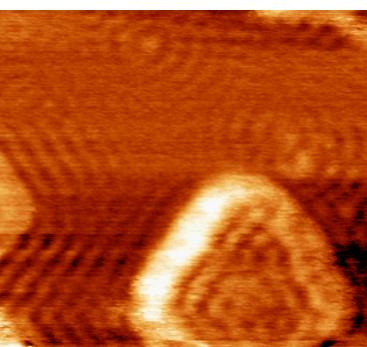
+20 mV



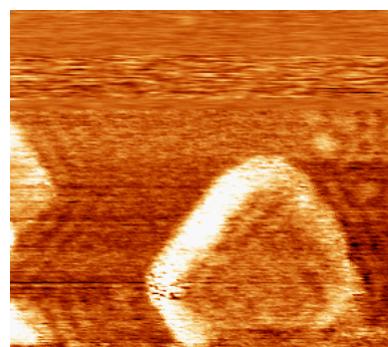
+50 mV



+100 mV

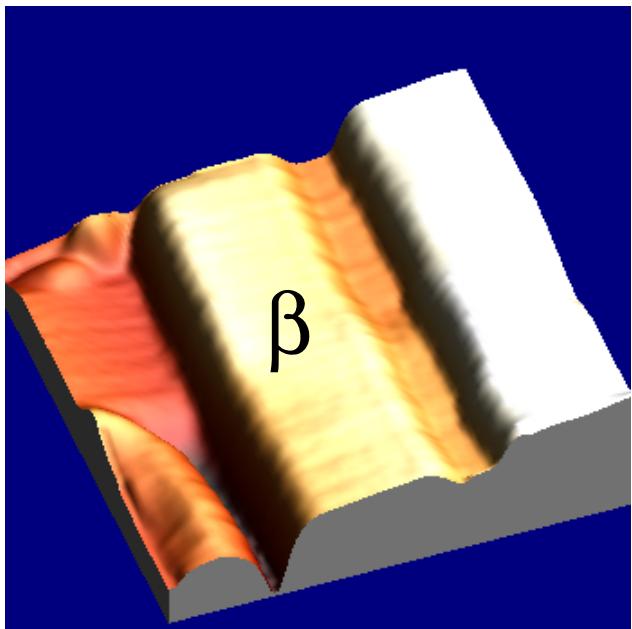


+200 mV



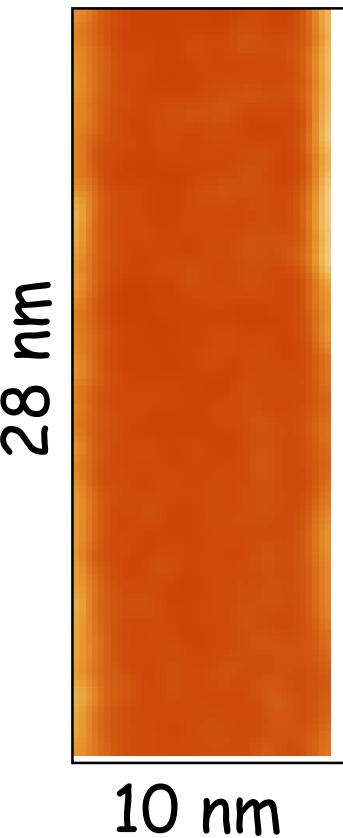
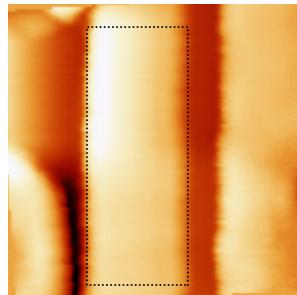
+300 mV

4.8 Quantum resonator - Ni / Cu(111) - Confinement



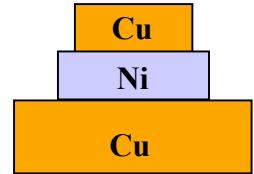
Constant current image

$30 \times 30 \text{ nm}^2$



$T = 40 \text{ K}$

Confinement in a β bilayer island

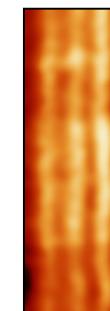


← $dI/dV(V)$ movie
constructed from a
CITS (44 images)

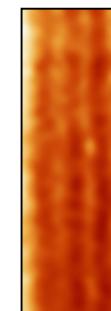
Energy range:
- $300 \rightarrow + 400 \text{ mV}$



- 40 meV

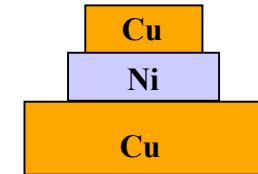


+80 meV

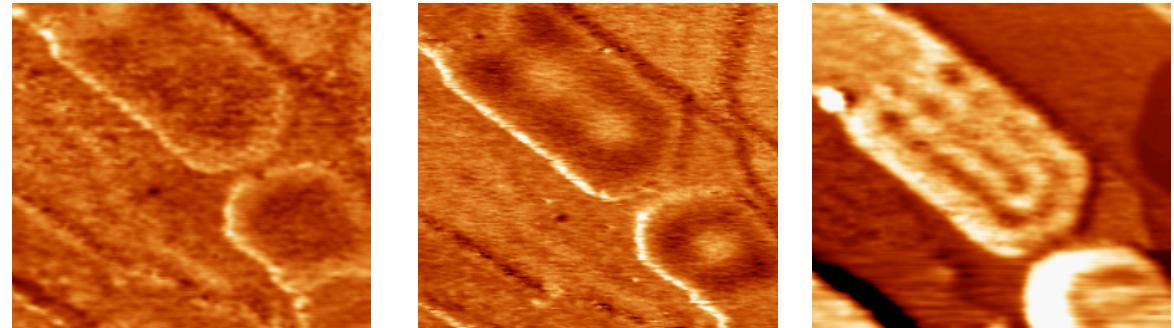
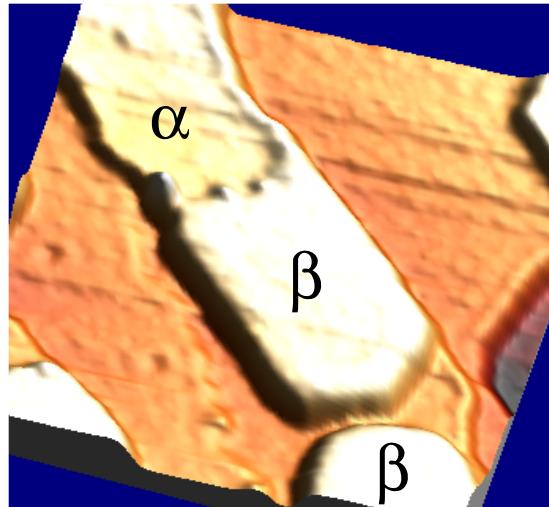


+290 meV

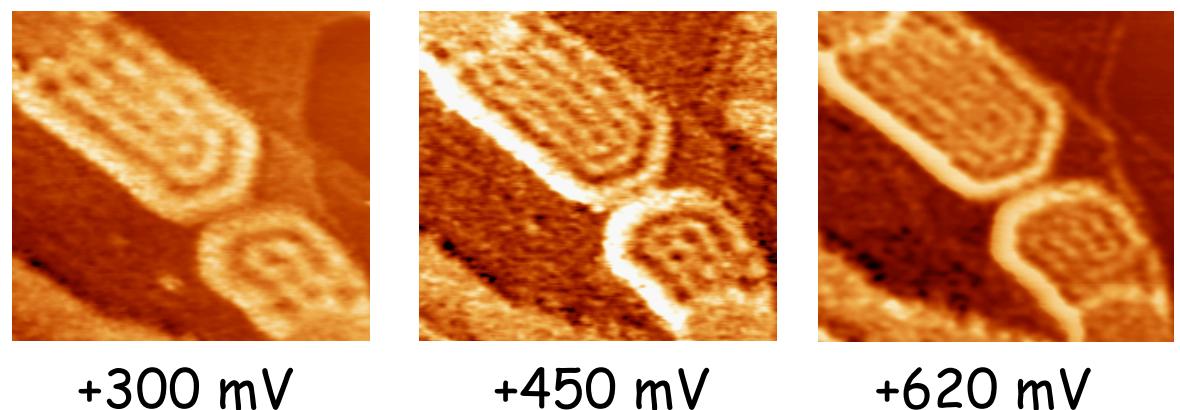
4.8 Quantum resonator - Ni / Cu(111) - Confinement



Confinement in a β bilayer island



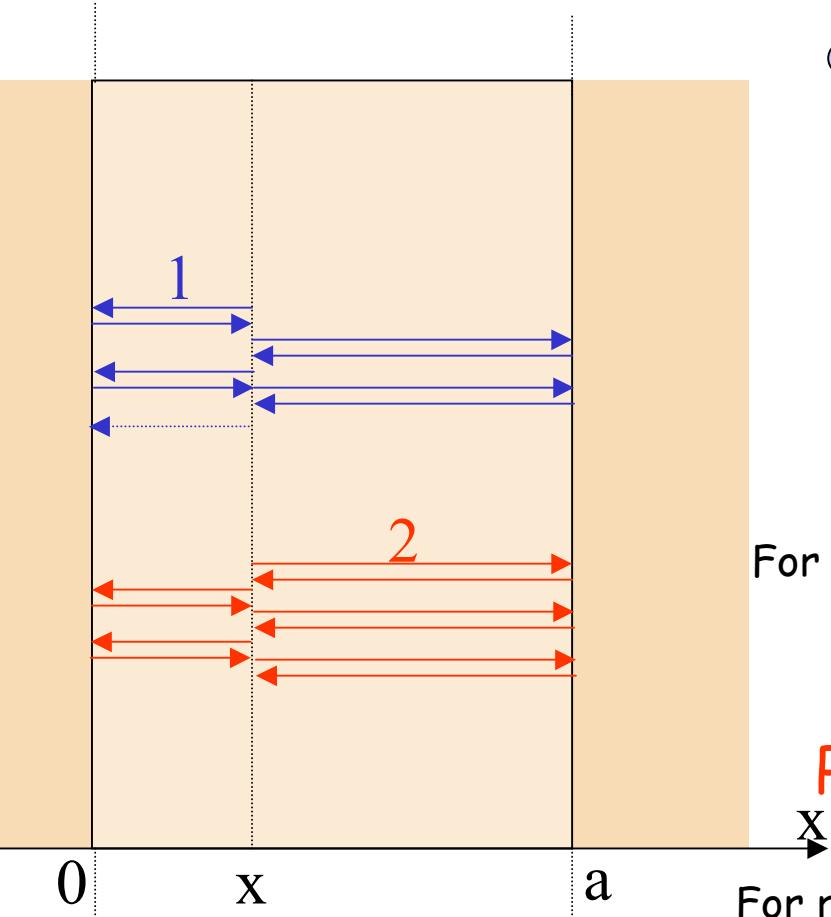
dI/dV images at 40 K
20 x 20 nm²



4.9 Quantum resonator - 1D confinement model

Model for 1D confinement in a resonator of width a

- No inelastic processes except at the boundaries !!! ($a < L_\phi$)
- Steps at $x=0$ and $x=a$ modelled by coherent reflection ($r(k_x), \varphi(k_x)$)



Process 1 :

$$\psi_{1k}(x) = (e^{ik_x x} + r e^{i\varphi} e^{-ik_x x}) \times (1 + r^2 e^{2i\varphi} e^{2ik_x a} + r^4 e^{4i\varphi} e^{4ik_x a} + \dots)$$

For $r \neq 1$:

$$|\psi_{1k}(x)|^2 = \frac{1+r^2 + 2r \cos(2k_x x - \varphi)}{1+r^4 - 2r^2 \cos(2k_x a - 2\varphi)}$$

Process 2 :

$$\text{For } r \neq 1: |\psi_{2k}(x)|^2 = \frac{1+r^2 + 2r \cos(2k_x(x-a) + \varphi)}{1+r^4 - 2r^2 \cos(2k_x a - 2\varphi)}$$

Process 1 is not coherent with respect to process 2

4.10 Quantum resonator - 1D confinement model

incoherent summation : $\rho(k_x, x) = |\psi_{1k}(x)|^2 + |\psi_{2k}(x)|^2$

$$\rho(k_x, x) = \frac{(1+r^2 + 2r\cos(2k_x x - \varphi)) + (1+r^2 + 2r\cos(2k_x x - \varphi))}{1+r^4 - 2r^2\cos(2k_x a - 2\varphi)} = \frac{N}{D}$$

N : term of interferences due to single scattering at $x=0$ and $x=a$

D : broadening term due to multiple scattering in the resonator

$\frac{1}{D}$ is maximum when $\cos(2k_x a - 2\varphi) = +1$ \iff

$$2k_n a = 2n\pi + 2\varphi$$

Stationary phase
condition

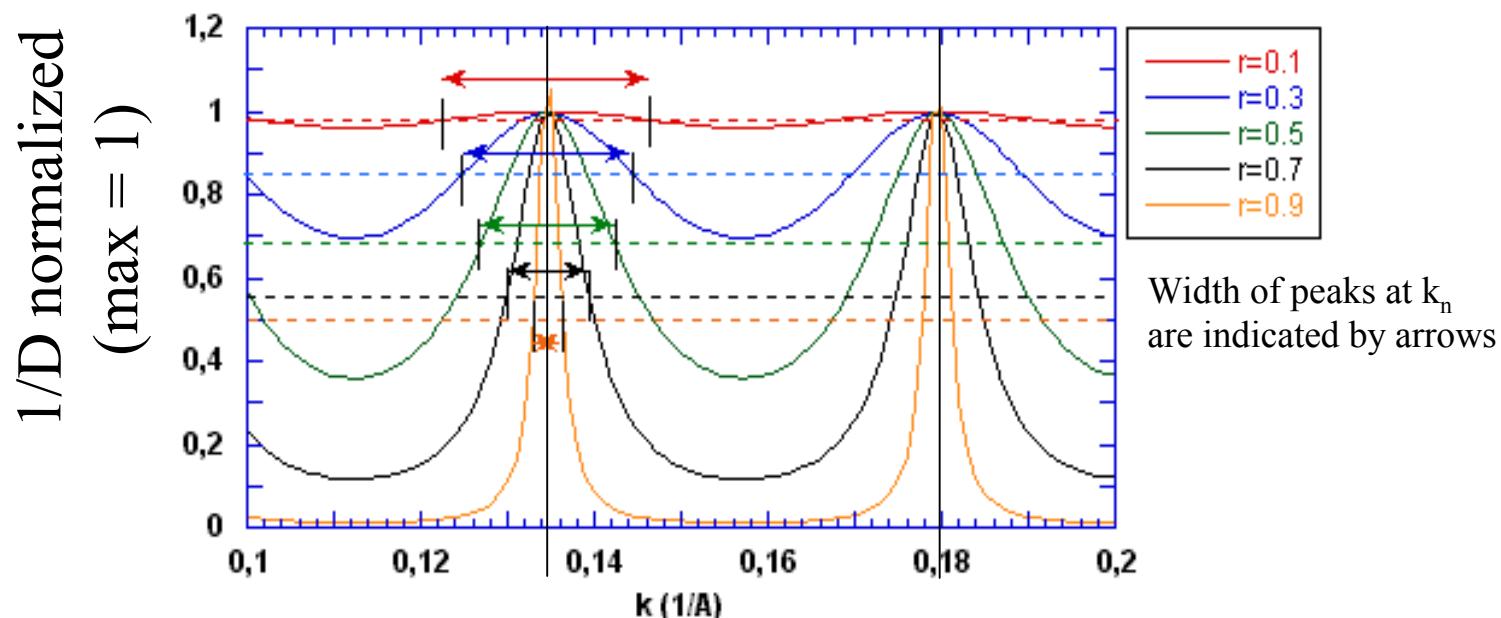
If k_x does not satisfy this condition, destructive interferences due to multiple scattering decrease N/D.
 r governs the strength of the destructive interferences →

4.11 Quantum resonator - 1D confinement model

For $r \leq 1$, and $k_x - k_n \ll \pi/a$:

$$\frac{1}{D} \approx \frac{1}{(2ar)^2} \frac{1}{(k_x - k_n)^2 + \left(\frac{1-r^2}{2ar}\right)^2}$$

Lorentzians centered in k_n with HWHM $\Gamma = \frac{1-r^2}{2ar}$



4.12 Quantum resonator - 1D confinement model

Calculation of $\rho(E)$ is obtained only by numerical integration:

$$\rho(E,x) = \frac{L_0}{\pi} \int_0^k \frac{1}{\sqrt{k^2 - k_x^2}} \rho(k_x, x) dk_x \quad (**)$$

Particular wave numbers k_n imply maxima of ρ at energies defined by :

$$E_{0n} = E_0^{2D} + \frac{k_n^2}{2m^*} \quad \text{with} \quad 2k_n a = 2n\pi + 2\varphi$$

Inelastic processes at step ($r \neq 1$) introduce a broadening of $\rho(E)$ at E_n ($n=0,1,2\dots$).

What is the role of φ ?

$\varphi \neq \pi$ → shifts the energy levels of the resonator
 → spatially shifts the maxima of the LDOS
 (toward the numerator of $\rho(k_x, x)$).

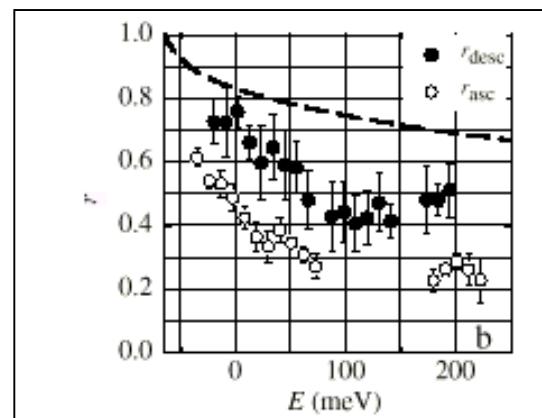
4.13 Quantum resonator - Ag 1D resonator

Confinement in a \sim 1D Ag resonator

Symmetric resonator

- Determination of $\varphi = -\pi \pm 0.3$ (independant of E)
- $dI/dV(x)$ profile is fitted with $\rho(E,x)$ (defined by equation (**)) for each energy
→ Determination of $r_{asc}(E)!!$

Asymmetric resonator → Determination of $r_{desc}(E)$

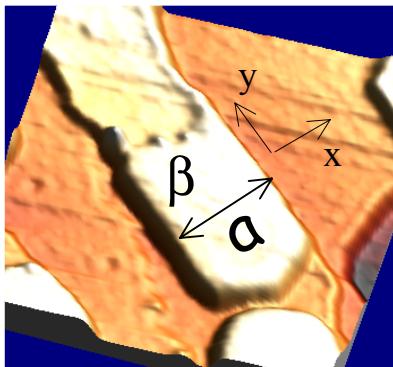
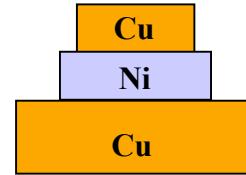


Reflection amplitude is strongly reduced at high energy
→ coupling to bulk states (absorption) becomes important

Absorption is more efficient for an ascending step

4.14 Quantum resonator - Cu/Ni 1D resonator

Model for confinement in an elongated β bilayer island



Contrary to Ag resonator, m^* and E_0^{2D} are not known a priori.

hypothesis

- 1D confinement model
- Parallel steps : infinite potential walls ($r(k_x)=1$, $\varphi=\pi$)



1D : quantization of $k_x = (n+1)\pi/a$

Energy levels :

$$E_{0n} = E_0^{2D} + \frac{1}{2m^*} \frac{(n+1)^2 \pi^2}{a^2}$$

surface LDOS :

$$\rho(E,x) \propto \sum_{i=0}^n \sin^2 \left[\frac{(i+1)\pi x}{a} \right] \times \frac{1}{\sqrt{E - E_{0i}}}$$

For $E_{0n} < E < E_{0(n+1)}$

$\rho(x)$ shows up $(n+1)$ maxima

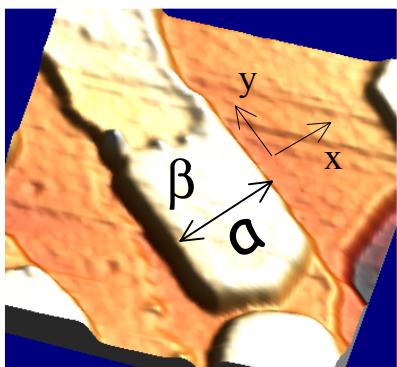
4.15 Quantum resonator - Cu/Ni 1D resonator

Parameters (independent of the island)

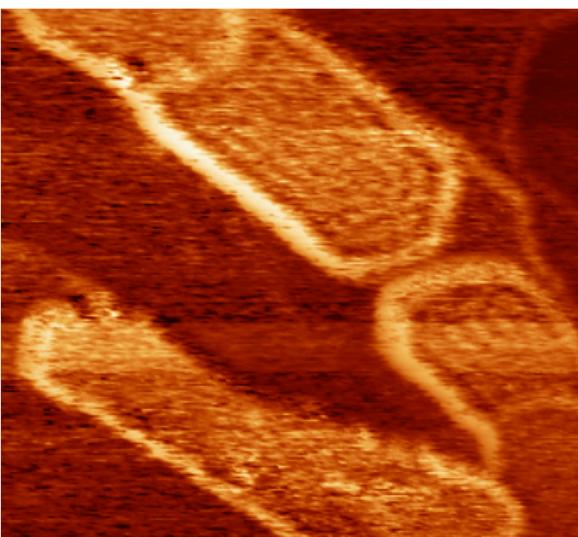
$$E_0^{2D} = -140 \pm 20 \text{ meV} \quad m^* = (0.33 \pm 0.05) m_e$$

For this island:

$$a \approx 90 \text{ \AA}$$

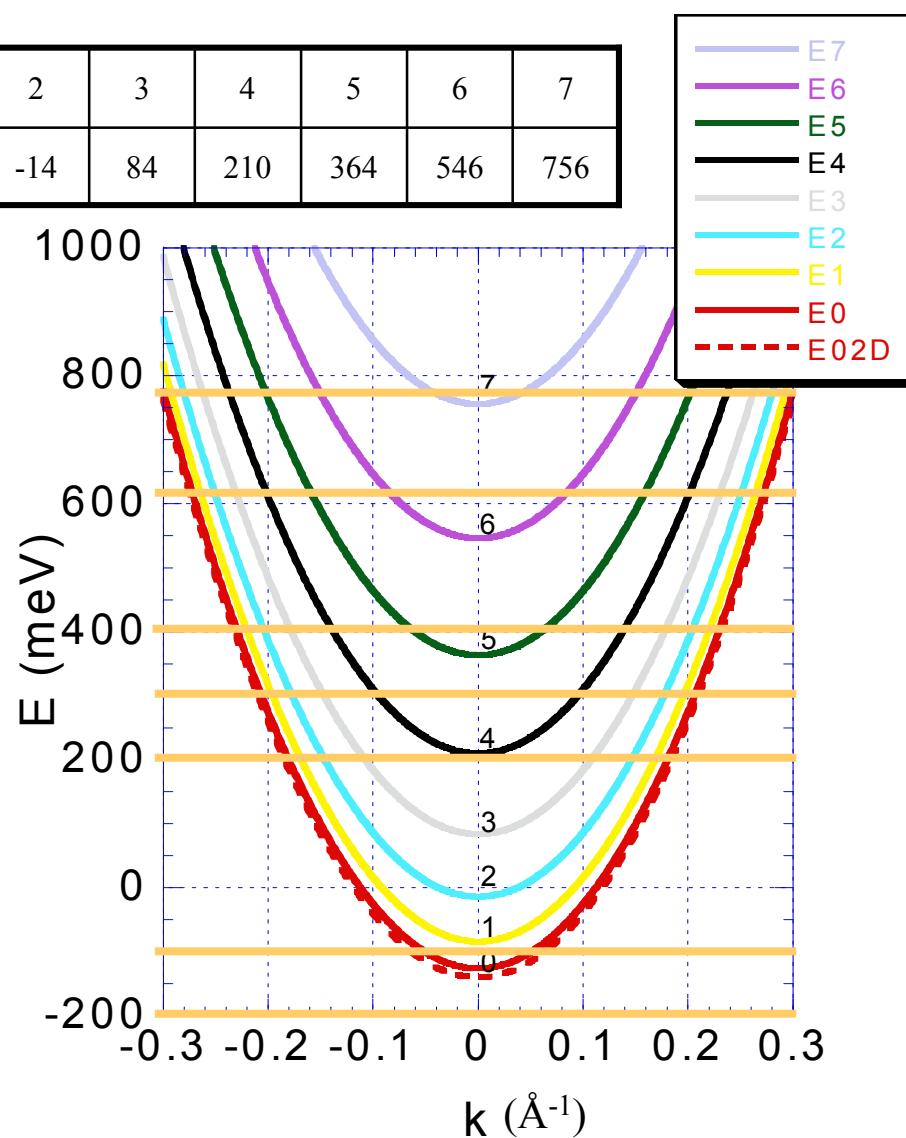


Constant current image
30 x 30 nm²
(1nA, +0.6 V)

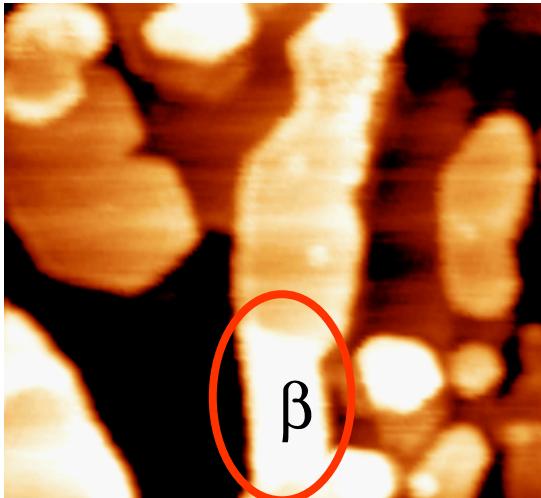


$$+ 620 \text{ mV}$$

n	0	1	2	3	4	5	6	7
E_{0n} (meV)	-126	-84	-14	84	210	364	546	756



4.16 Quantum resonator - Cu/Ni 1D CITS



Topography $50 \times 50 \text{ nm}^2$

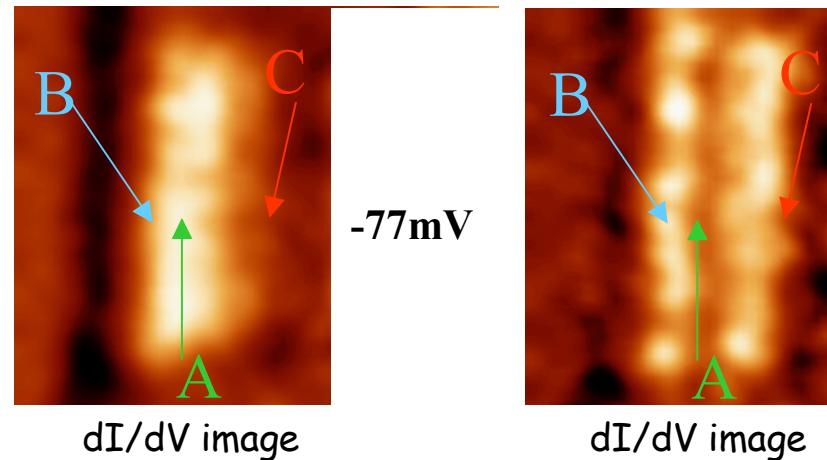
$$E_0^{2D} = -135 \text{ meV}$$

$$m^* = 0.32 m_e$$

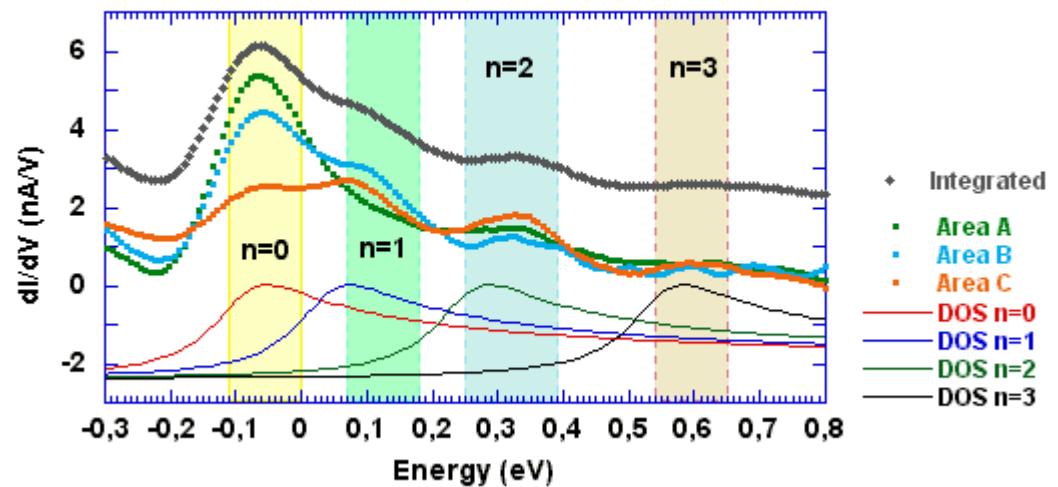
$$a = 5.3 \text{ nm}$$

n	0	1	2	3
$E_{0n} (\text{meV})$	-93	+34	+246	+542

$T = 40\text{K}$



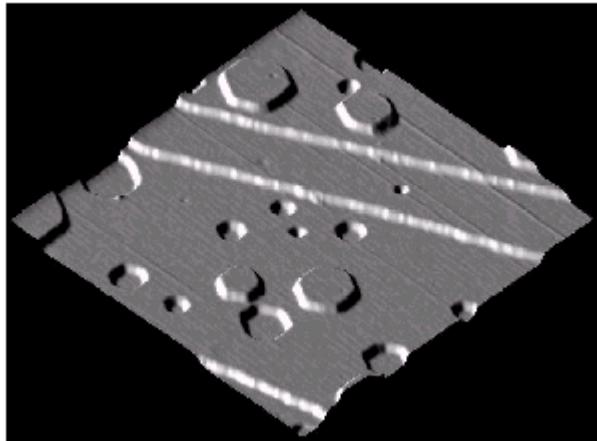
Spectroscopy on a β island, CITS C014.



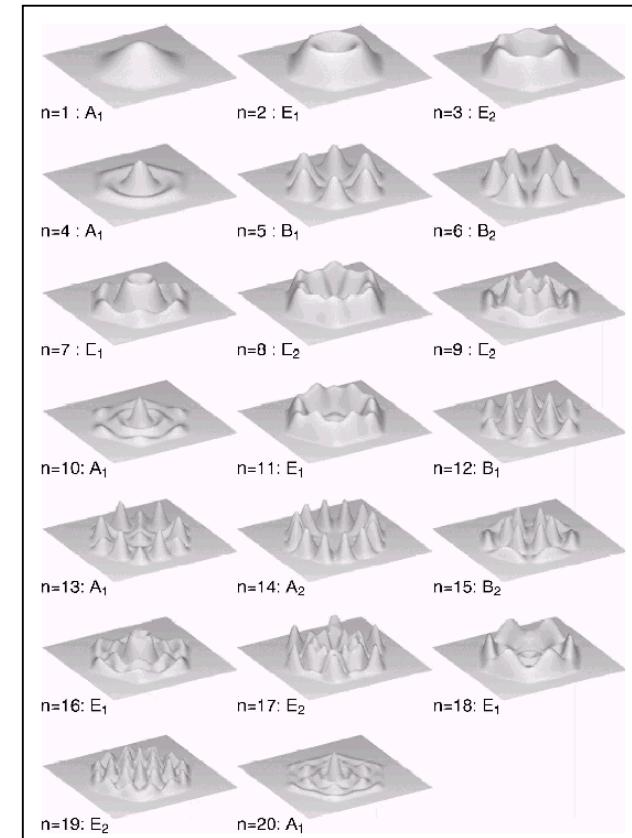
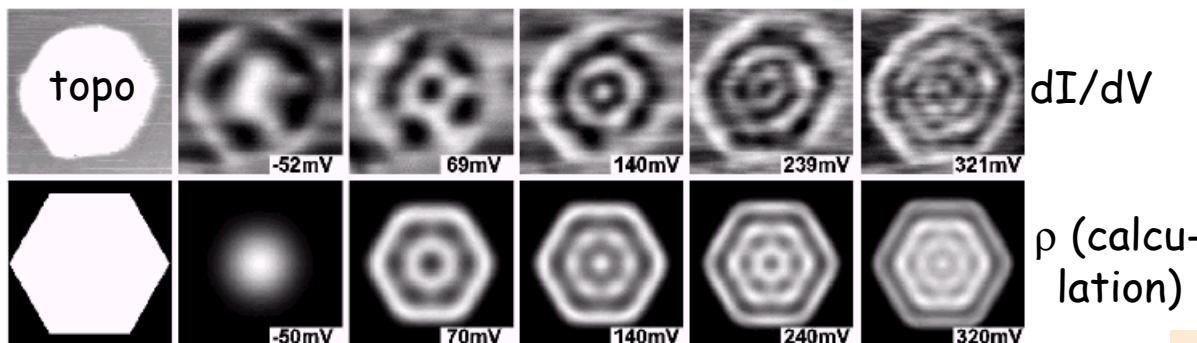
Calculated LDOS is broadened at E_n by a Lorentzian function with HWHM : $\Gamma=70 \text{ meV}$

4.17 Quantum resonator - 2D hard wall model Ag Berndt

2D confinement in Ag/Ag(111) hexagonal islands



$160 \times 160 \text{ nm}^2$ constant current
STM image, $T = 50\text{K}$

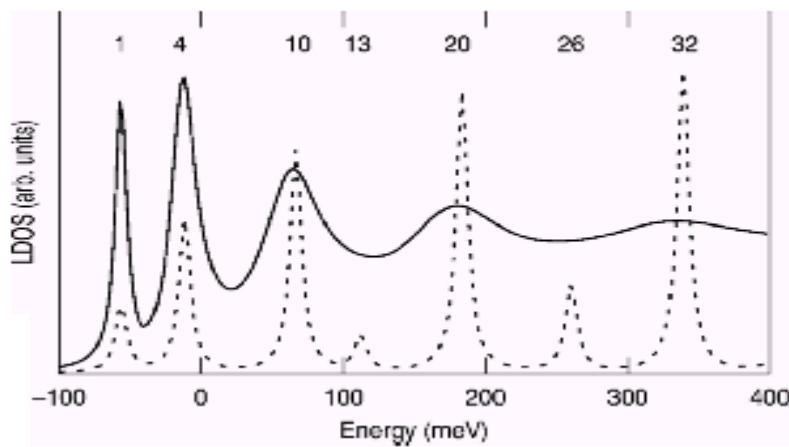
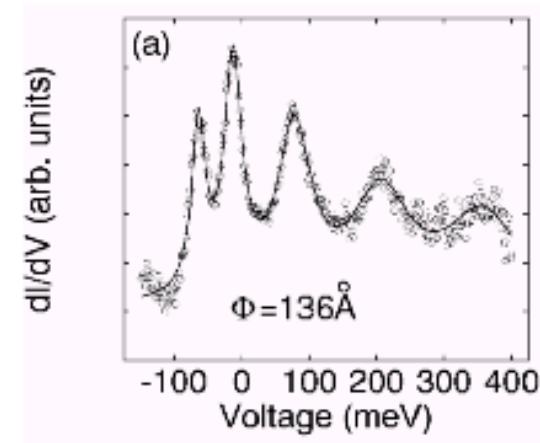
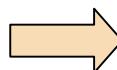


$\rho(E)$ maps computed for the eigenvalues E_n

$$E_n(\text{meV}) = E_0^{2\text{D}} + 76,2 \lambda_n / m^* \cdot \Omega(\text{nm}^2)$$

Probing the inelastic scattering processes :

STS above the centre of a hexagonal island



Calculated spectrum

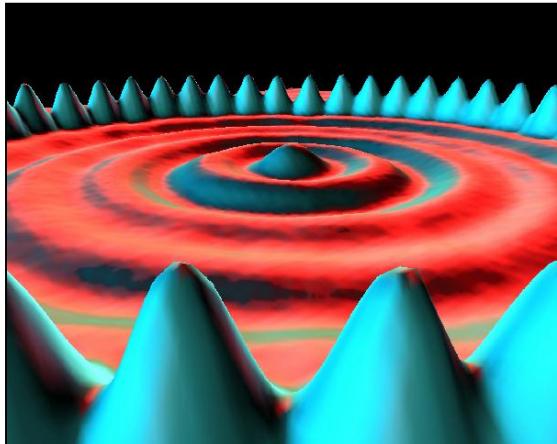
Spectra are decomposed into a series of Lorentzians with increasing linewidth :

$$\Gamma_n \approx 0.2 (E_n - E_0)$$

The width of each energy level Γ_n implies a finite lifetime for the confined electrons.

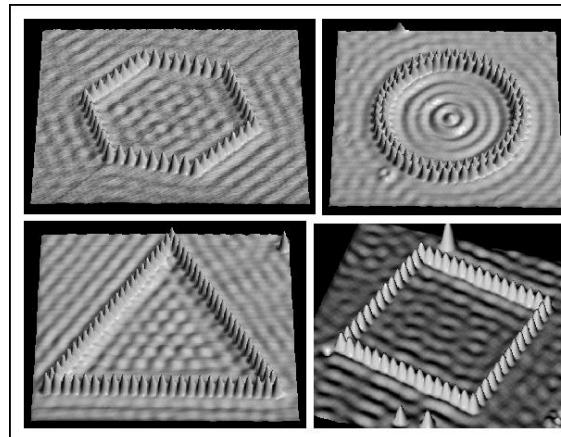
→ Scattering at island edges into bulk states

4.19 Models for Quantum Corrals



Science, 262 (8 Oct. 1993)

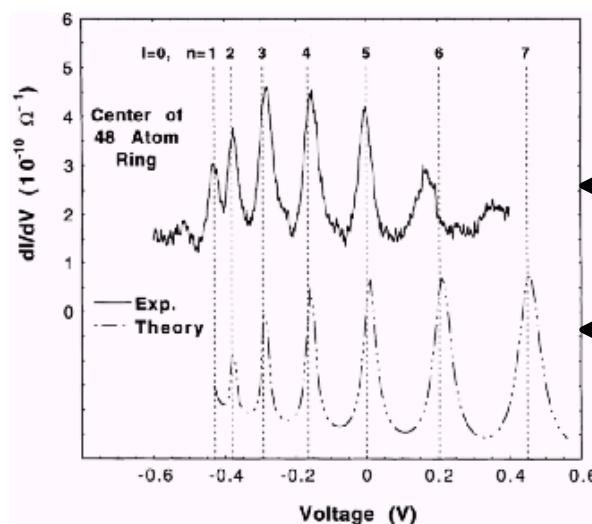
M.F. Crommie, C.P. Lutz, D.M. Eigler, E.J. Heller



Physics Today 46 (11), 17-19 (1993)

ring of 48 Fe atoms
(diameter : 146 Å)

Vertical dashed lines :
Eigenstates given by the
hard-wall model



*M.F. Crommie, J. of electron spectroscopy
109, 1 (2000)*

dI/dV (V)
at the centre

Black dot model :
incoming s-wave amplitude is totally
absorbed (probably coupling with bulk
states) by the scatterer

The black dot model gives a fairly good account of the broadening of the measured dI/dV peaks !!!

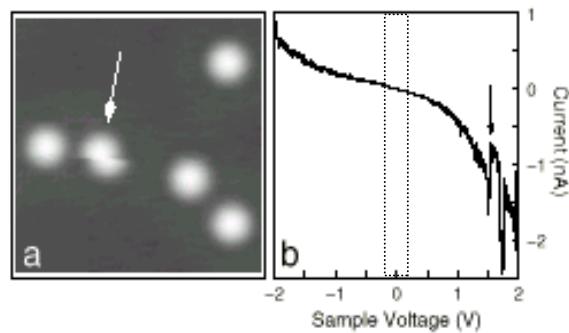
Fe atoms on Cu(111):
With the hard wall
model, the problem is
reduced to finding the
eigenstates of a par-
ticle confined in a box

5.0 Interaction adsorbate - surface state

5. Interaction adsorbate - surface state

5.1 Interaction adsorbate \leftrightarrow surface state - Berndt

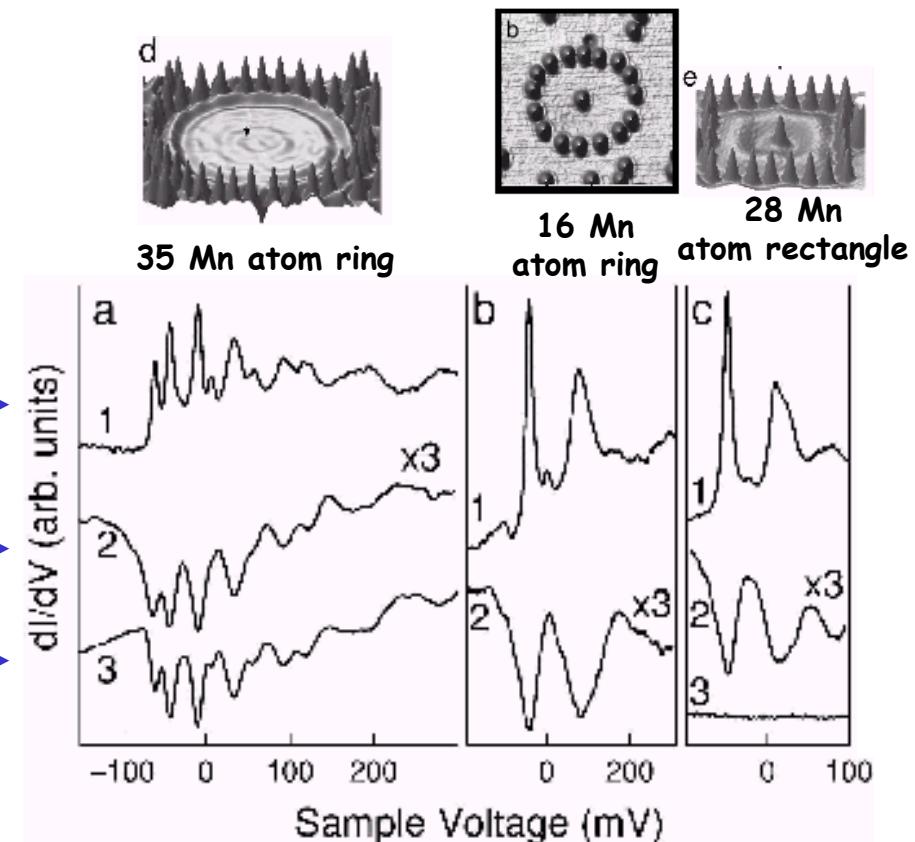
LDOS of an adsorbate centered to a quantum corral



$60 \times 60 \text{ \AA}^2$
topo
Mn/Ag(111)

I/V
spectrum
on single
Mn atom

1. Without central Mn
2. With central Mn
3. Without, inverted and scaled

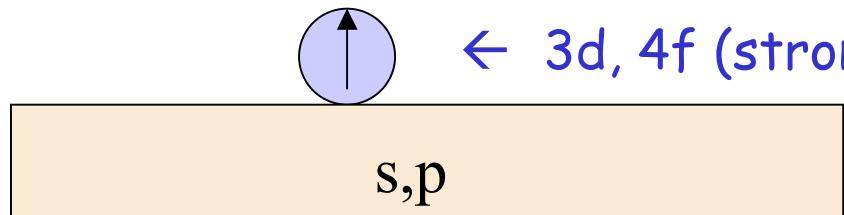


Spectra 2: inverted structure characteristic of a strongly coupled adsorbate level, \`a priori s level (cf calculations)

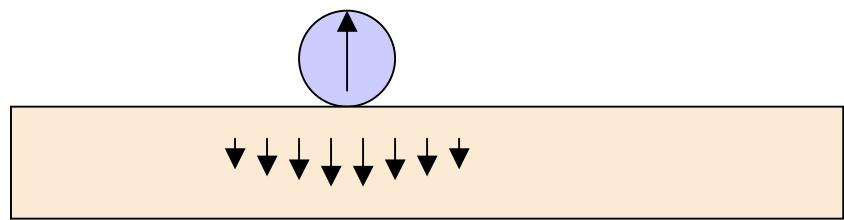
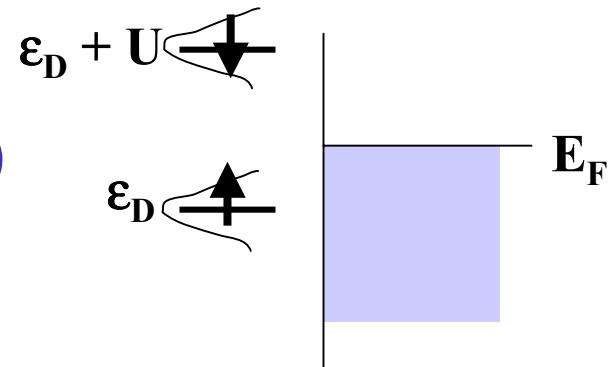
Controlled modification of adsorbate electronic structure !!!

5.2 Interaction adsorbate \leftrightarrow surface state - Kondo effect

Kondo effect

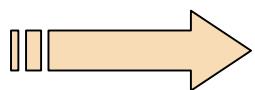


$$T > T_K$$



$T < T_K$ Highly correlated ground state in the electron gas, with screening the adsorbate spin.

Spin dependant scattering
(with spin flip)



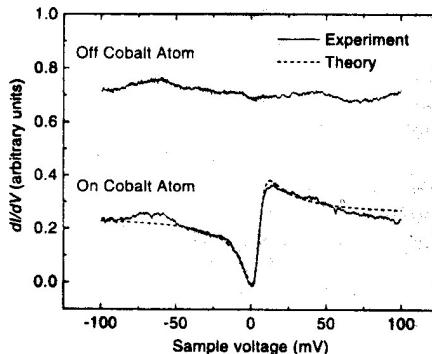
narrow resonance located at E_F , HWHM $\sim T_K$

$$kT_K \approx D^3 \rho(E_F) Jv^{1/3} \exp\left(\frac{1}{3\rho(E_F) Jv}\right)$$

A.C. Hewson, *The Kondo Problem to heavy fermions*, Cambridge University Press, NY 1985)

Kondo effect probed by STS

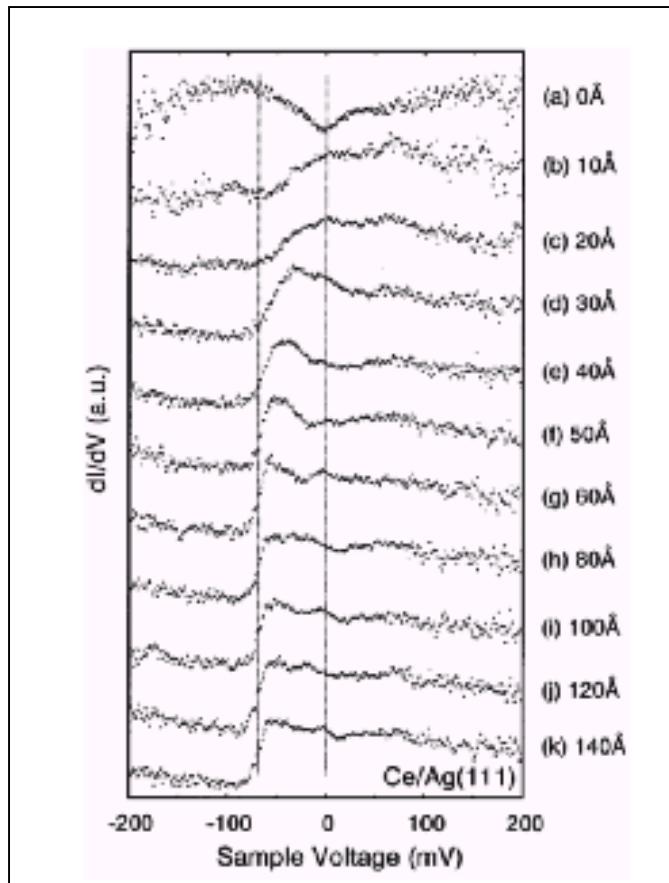
Co / Au(111) : $T_K = 70K$



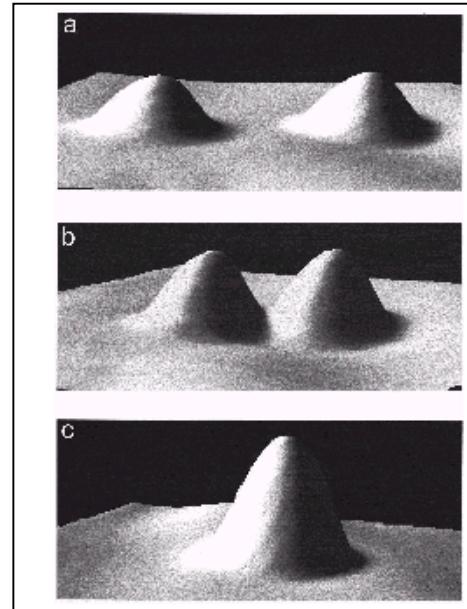
V. Madhavan, W. Chen, T. Jamneala,
M.F. Crommie, N.S. Wingreen

Science 280, 567 (1998)

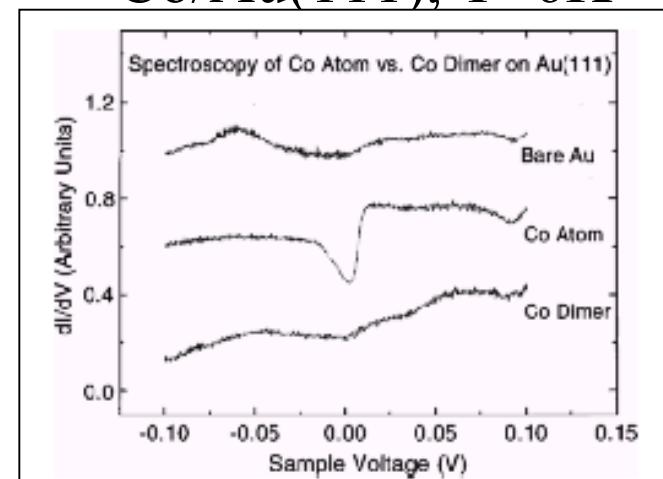
Kondo effect probed by STS



J. Li, W-D Schneider, R. Berndt & B. Delley,
Phys. Rev. Lett 80, 2893 (1998)



Co/Au(111), T=6K

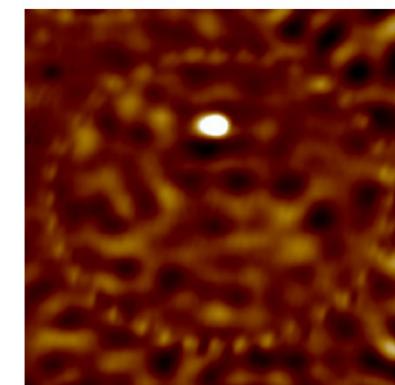
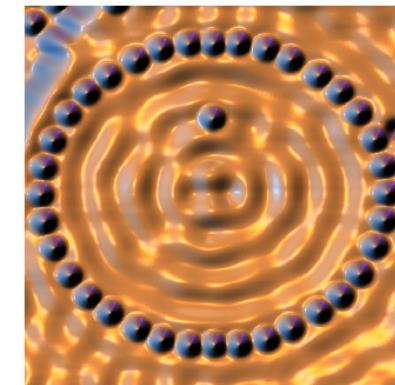
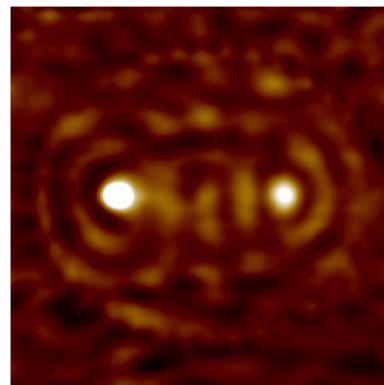
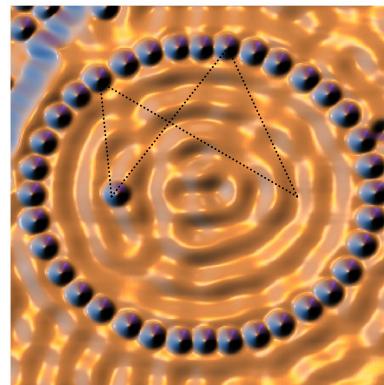
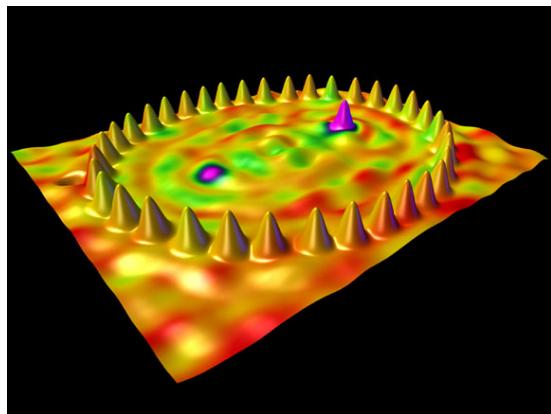
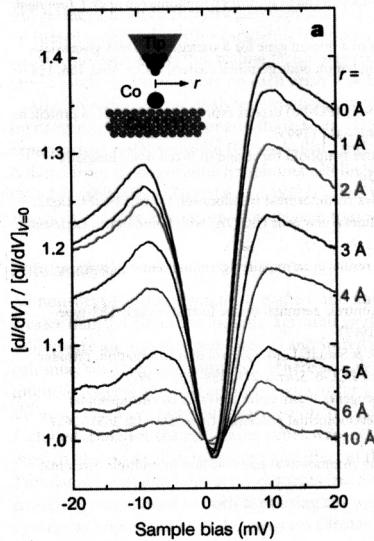


W. Chen, T. Jamneala, V. Madhavan & M.F. Crommie
Phys. Rev. B 60, R8529 (1999)

5.4 Interaction adsorbate \leftrightarrow surface state - Quantum Mirage

Quantum mirage

36 + 1 Co atoms / Cu(111), T=4K



H.C. Manoharan, C.P. Lutz and D. Eigler Nature, 3 Feb. 2000

Conclusion

Scattering of surface states electrons :
low temperature STM study

- Determination of 2D shockley-like surface state parameters
- Study of inelastic processes (e-e and e-phonons interactions)
- Confinement in nanostructures:
quantitative study of scattering processes at defects (steps, adsorbates)
- Interaction adsorbate - confined electron gas :
construction game with atoms
+ driving of the electronic properties at atomic scale !!!