Chapter 3
Imaging with a STM

Objective: to learn the different STM imaging techniques.

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3.1: Imaging principle and techniques

Important parameters

Voltage bias determines the energy range of probed electronic states

$V = V_{tip} - V_{sample} > 0$: e- from sample to tip, occupied states are probed.

$V = V_{tip} - V_{sample} < 0$: e- from tip to sample, empty states are imaged.

Tunnel resistance R_t determines the tip-sample distance. Usually, the parameters are the bias V and the set-point I_t:

$$R_t = \frac{V}{I_t} = 5\,M\Omega \text{ to } 5\,G\Omega$$

Scanning frequency: below the resonance frequency of tubes.
Usual parameters are the points per line and the time per point.

PID regulation parameters: in order to be effective, the regulation time constant should be below the scan time over a characteristic feature.

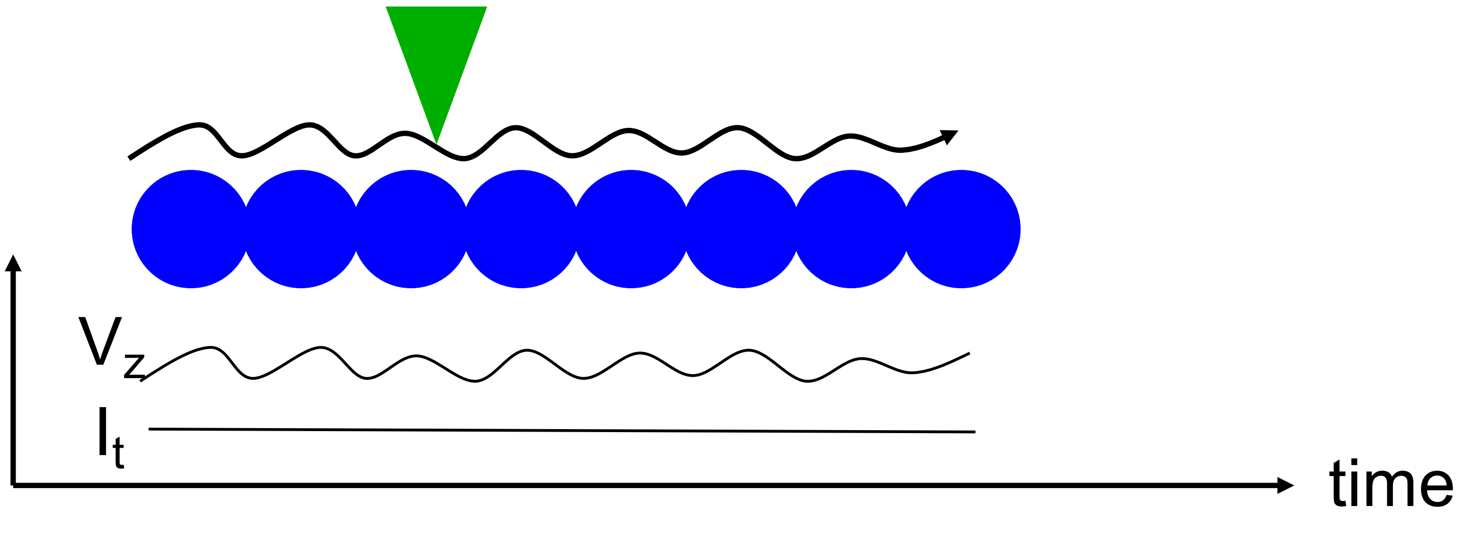
Constant current imaging

Tunnel current regulation is active and effective at every time.

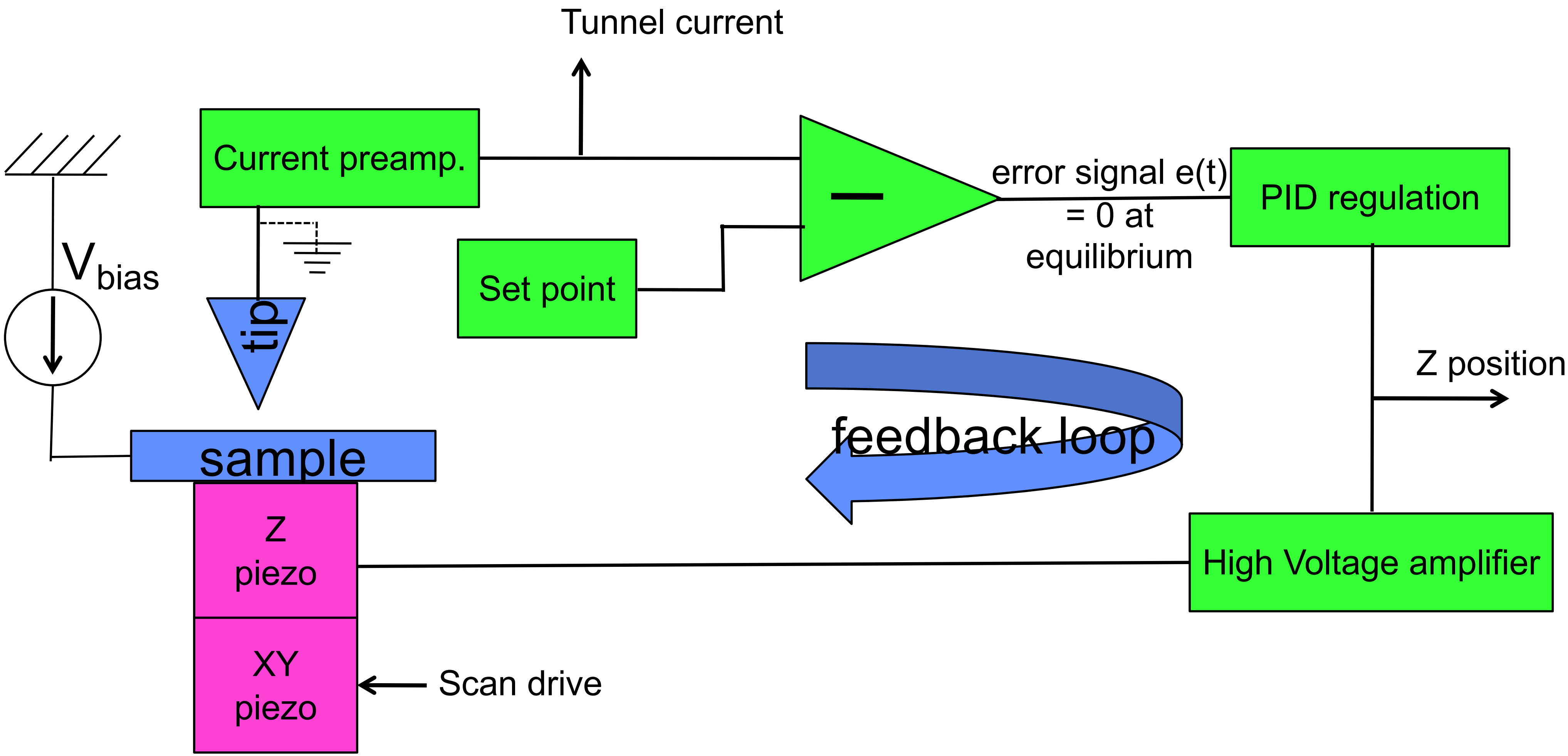
$$\mathbf{I_t = Cst}$$

During the x,y scan, the regulation output V_z is :
- amplified and sent to the piezo
- measured.

$V_z(x,y)$ scaled by the Z-piezo sensitivity gives the topography information



STM electronics



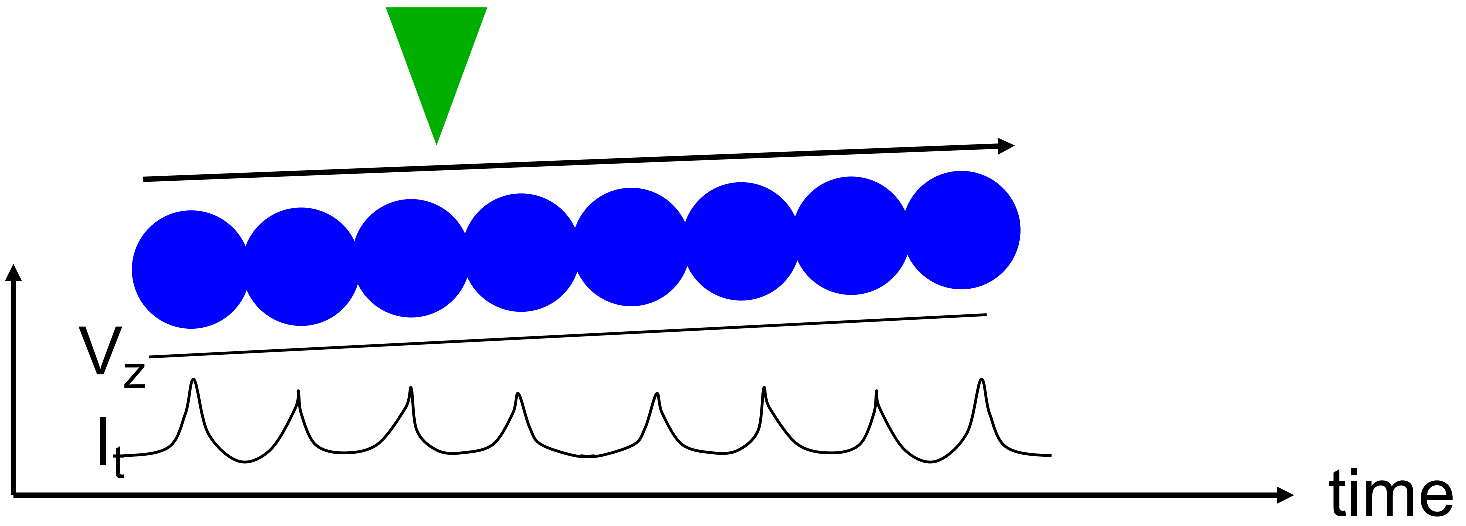
Constant height imaging

Tunnel current regulation is inactive or active with a long time constant so that mean slope is followed.

The regulation output V_z is close to constant, the current I_t is measured.

I_t gives the topography information.

Possible only on atomically-flat surfaces, highly-sensitive but non-linear information. Much less used.



Nanonis simulator

Virtual image of a Si (111) 7x7 surface

During an image, observe current image / z image

Play with PID parameters, scanning speed, scan direction, bias

Current decay with distance : « z spectroscopy », log scale

Tunneling spectroscopy

Can be freely dowmloaded from www.nanonis.com

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3.2: The spatial resolution

The corrugation

For any kind of quantitative topography, corrugation Δd is by definition:

the topography variation amplitude **as** measured by the microscope.

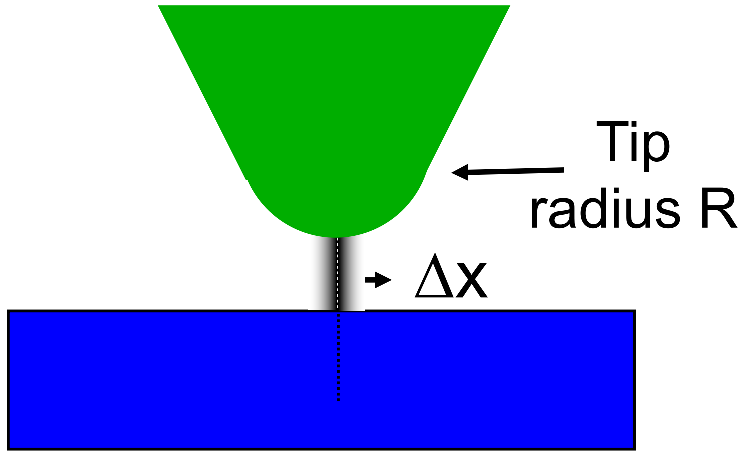
It is a fraction of Angtröm on an atomically flat surface, and can be larger on rougher surfaces.

Depends on every experimental conditions.
Can be decreased by a blunt tip, an inefficient regulation …: not an intrinsic quantity.

Spatial resolution

Binnig (1978); **hypothesis of a continuous media**.

$$I(\Delta x) = I_0 \exp\left(-\alpha \frac{\Delta x^2}{R}\right) \quad \text{where } \alpha = \frac{\sqrt{2mW}}{\hbar}$$



The tunnel current is concentrated on a scale:

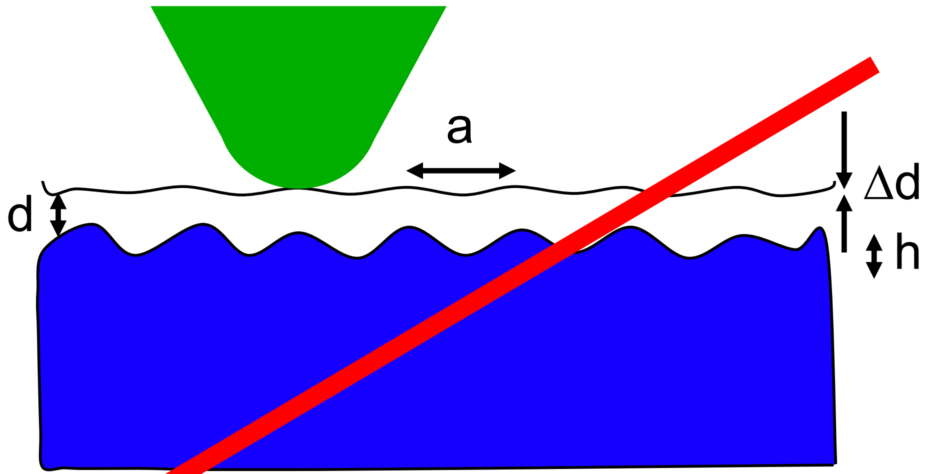
$$\sqrt{\frac{R}{\alpha}} << R$$

R = 10 nm, α = 1 Å^{-1} : current flows on a scale Δx = 1 nm.

Spatial resolution is not limited by the tip radius.

Trying to model the atomic resolution

Model of a **continuous media** surface: homogenous electron gas.



Calculated corrugation Δd_{theo}:

$$\frac{\Delta d_{theo}}{h} = \exp\left(-\pi^2 \left\{\frac{R+d}{\alpha a^2}\right\}\right) \qquad \left(\text{if } a \gg \frac{\pi}{\alpha} \text{ and } d \gg \frac{2}{\alpha}\right)$$

Stoll (1984)

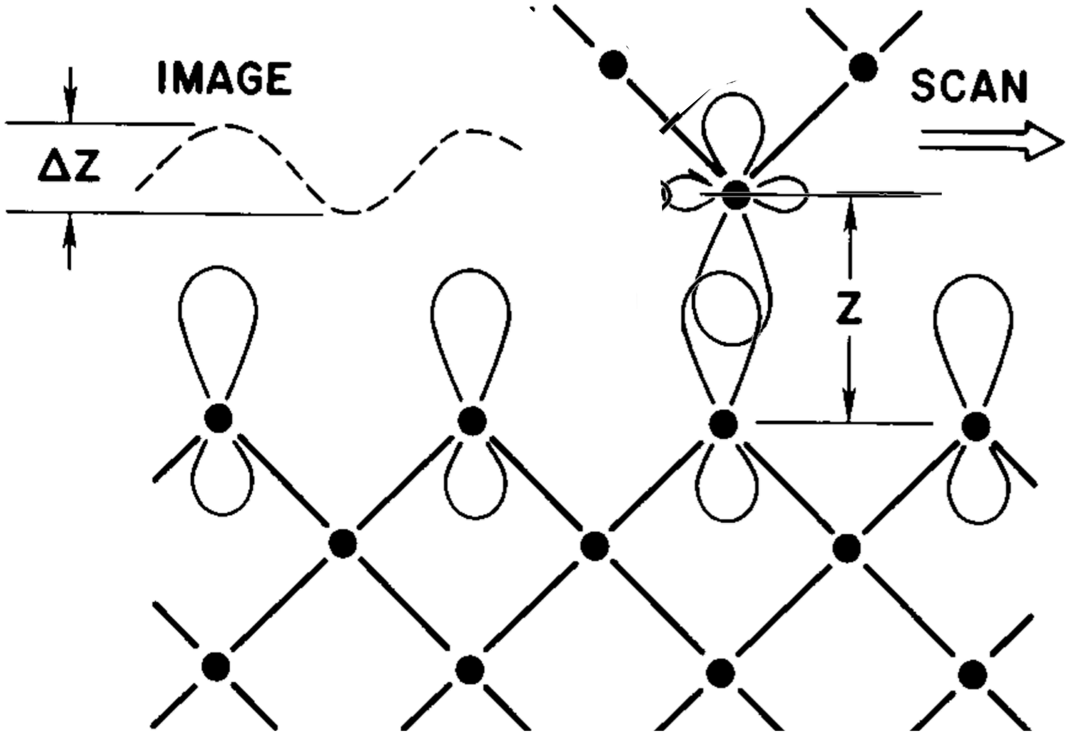
For a metal : a = 2.5 to 3 Å, α = 1 Å^{-1}, h = 3 Å. Tip: R = d = 3 Å

⇨ calculated Δd_{theo} = 0.01 Å: too small compared to experiment!

This model **fails** to describe the atomic resolution: the hypothesis of a continuous media is **incorrect**.

The origin of atomic resolution

Tunneling is related to the overlap of electronic wavefunctions:



Contrast depends on the nature of the tip apex atoms.
Anisotropic wave-functions are preferred.

The origin of atomic resolution

Tunnel matrix element value depends on orbital symmetry:

$$M_{\psi\chi} = \iint_S \left(\chi^* \frac{\partial \psi}{\partial z} - \psi \frac{\partial \chi^*}{\partial z} \right) dS$$

χ wave function on the tip, ψ on the sample

Contrast depends on the nature of the tip electronic wavefunction, and thus on the nature of the apex atoms.

W known to have a d_{z2} surface state.

L. Gross et al, Phys. Rev. Lett. 107, 086101 (2011).

TABLE IV. Tunneling matrix elements.

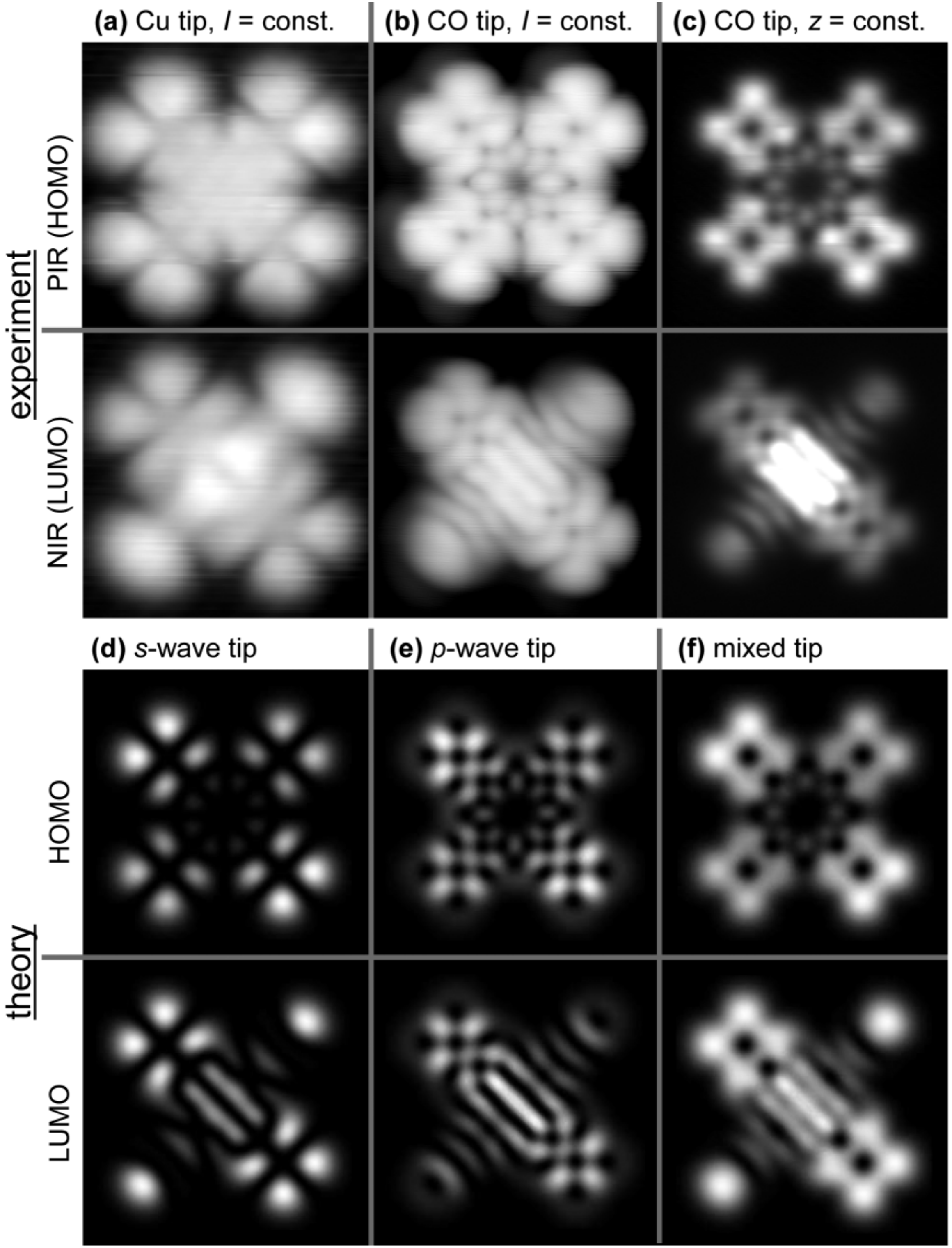
State χ	M
s	ψ
$p\ [z]$	$\frac{\partial \psi}{\partial z}$
$p\ [x]$	$\frac{\partial \psi}{\partial x}$
$p\ [y]$	$\frac{\partial \psi}{\partial y}$
$d\ [zx]$	$\frac{\partial^2 \psi}{\partial z\, \partial x}$
$d\ [zy]$	$\frac{\partial^2 \psi}{dz\, \partial y}$
$d\ [xy]$	$\frac{\partial^2 \psi}{\partial x\, \partial y}$
$d\ [z^2-\frac{1}{3}r^2]$	$\frac{\partial^2 \psi}{\partial z^2} - \frac{1}{3}\kappa^2 \psi$
$d\ [x^2-y^2]$	$\frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi}{\partial y^2}$

Atomic resolution depends on tip's electronic states

Cu tip: s states
Cu tip with a CO molecule adsorbed: p or s+p states

Contrast enhanced and modified with a CO tip.

L. Gross et al, Phys. Rev. Lett. 107, 086101 (2011).



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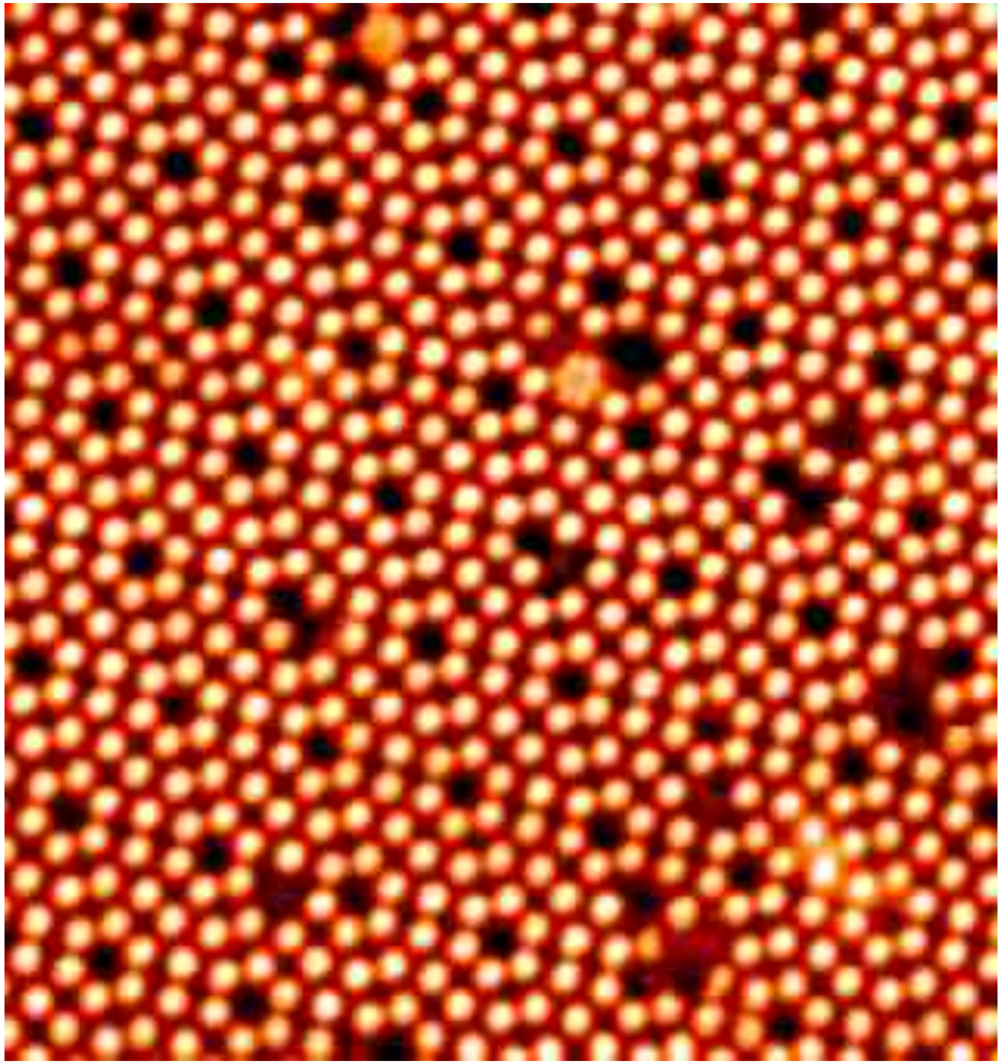
3.3: The STM benchmark Si 7x7

Si (111) 7x7

Si (111) annealed at 1000° C, slow cooling-down.

Single vacancies or adsorbates are visible: true atomic resolution.



Omicron website: http://www.omicron.de/results

Si (111) 7x7 : the model

7x7 reconstruction minimizes nb of pending bonds : 49->19

Miller index refer to the number (= 7) of atomic cells involved.

In STM, the adatoms only are visible, a well as the corner vacancies.

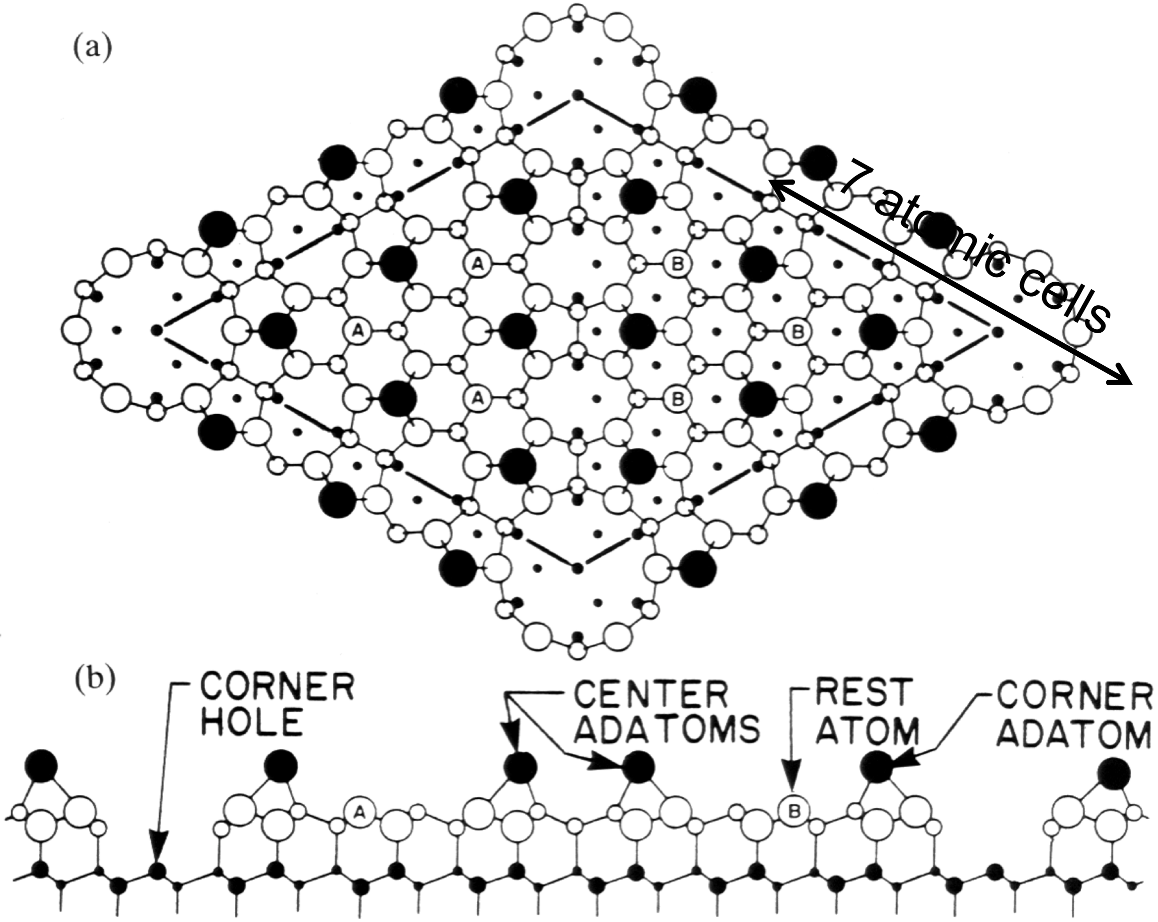
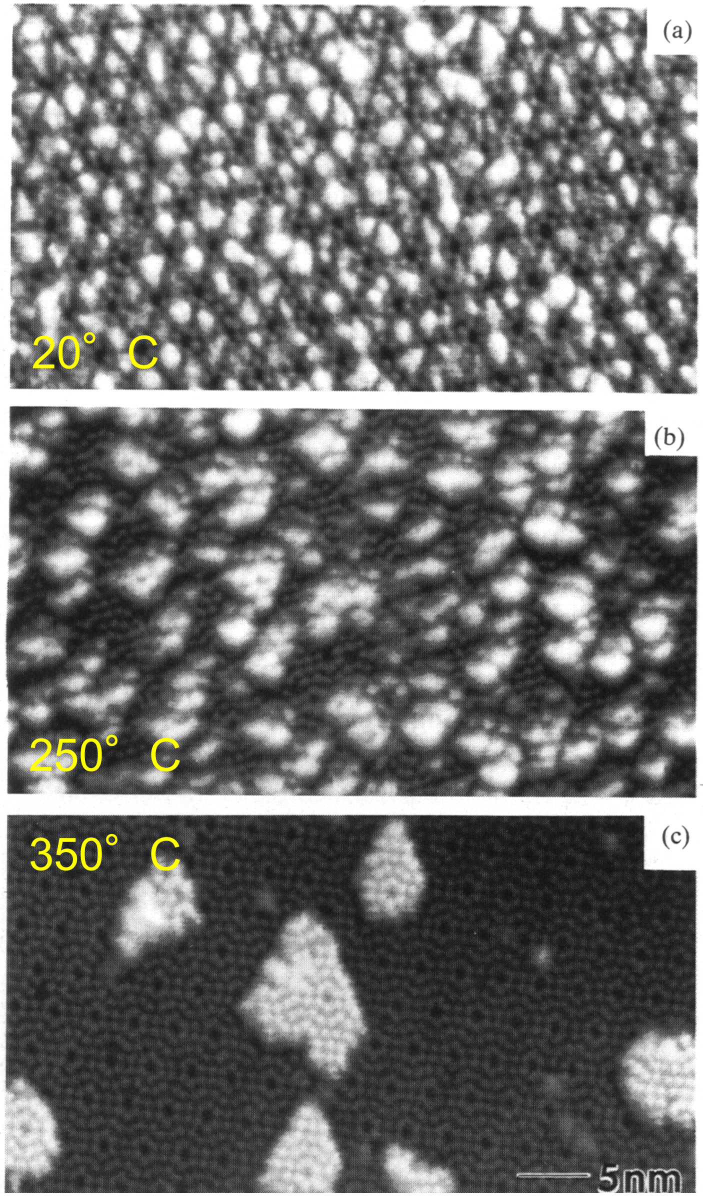


Fig. 4.2. DAS model of the Si(111) (7×7) surface. (*a*) Top view. Atoms o (111) layers at decreasing heights are indicated by circles of decreasing size Heavily outlined circles represent 12 adatoms. Larger open circles represen atoms in the stacking fault layer. Smaller open circles represent atoms in th dimer layer. Solid circles and dots represent atoms in the unreconstructed laye beneath the reconstructed surface. (*b*) Side view. Larger open and solid circle indicate atoms on the ($\bar{1}01$) plane parallel to the long diagonal across the corne vacancies of the (7×7) unit cell. Smaller open and solid circles indicate atom on the next ($\bar{1}01$) plane (Takayanagi *et al.*, 1985b).

Surface dynamics studies

The higher the temperature, the more mobile atoms are, larger islands are formed.



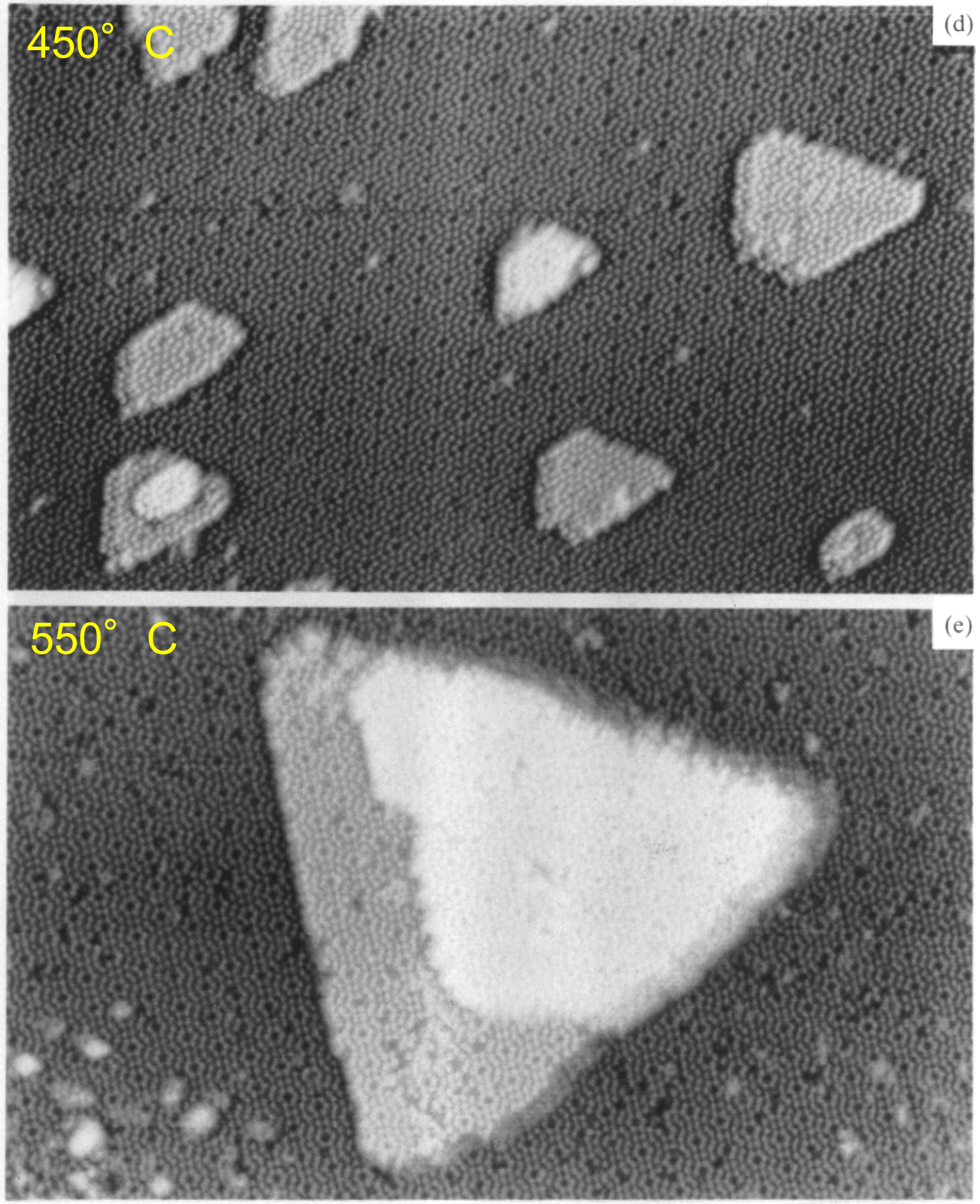
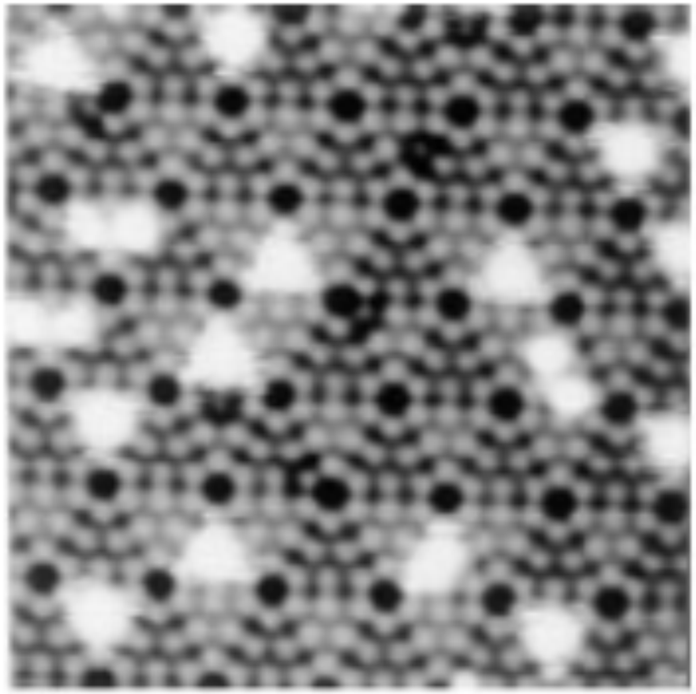


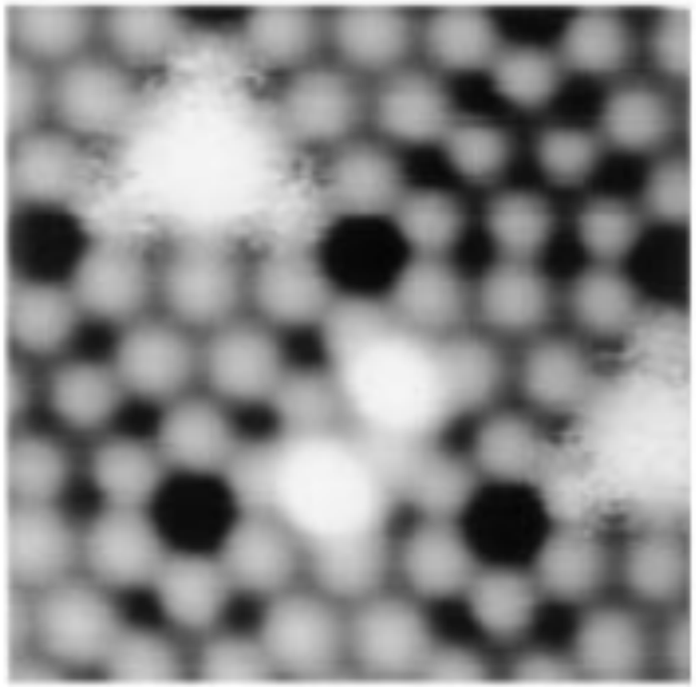
Fig. 4.45. Sequence of STM topographic images showing nucleation of silicon islands on a Si(111) 7×7 surface at different substrate temperature. The area for each is about 20 nm × 40 nm. The amount of silicon deposited is roughly the same for all images: 0.25 ML. The size of a (7×7) unit cell is indicated in (*a*). Substrate temperature during deposition: (*a*) 20 °C, (*b*) 250 °C, (*c*) 350 °C, (*d*) 450 °C and (*e*) 550 °C. On the perfectly triangular island in (*e*) nucleation of the second epitaxial layer is visible (Köhler *et al.*, 1989).

Real-time dynamics of Pb atoms on Si (1)

Atoms on a surface move fast but can be trapped in minima of surface potential.

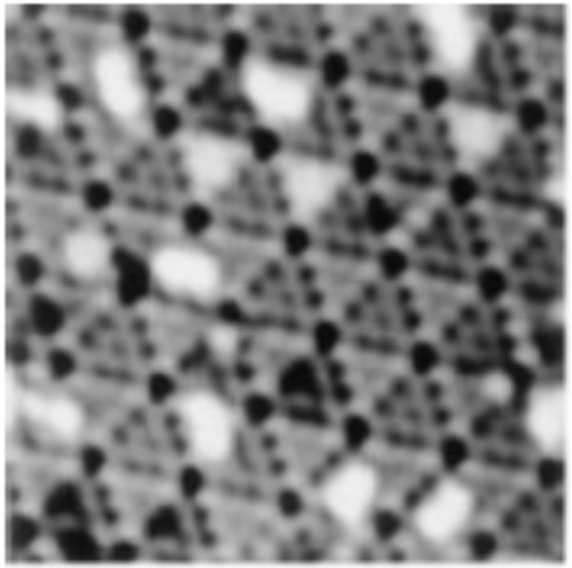


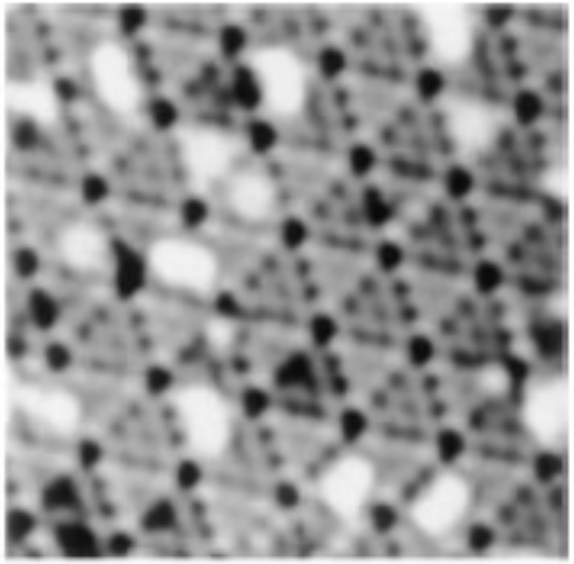
(a)

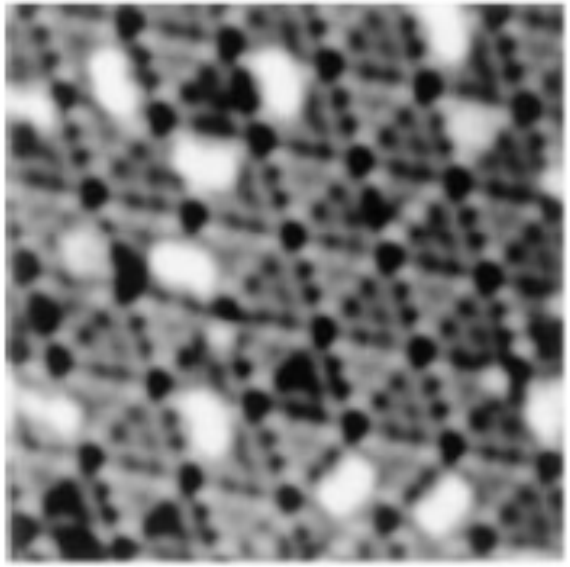


J.-M. Rofriguez-Campos et al, Phys. Rev. Lett. 76, 799 (1996), Institut Néel, Grenoble.

Real-time dynamics of Pb atoms on Si (2)

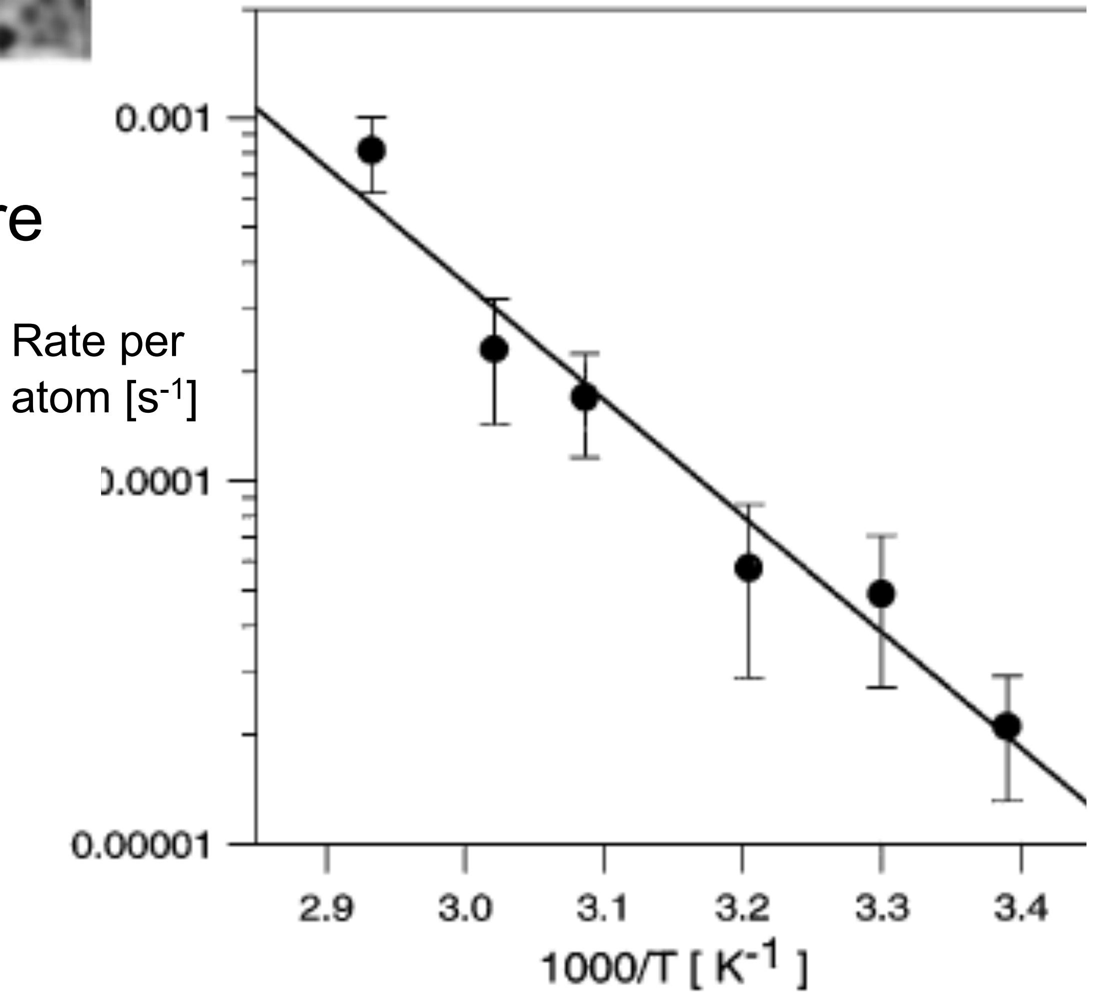

(a)


(b)


(c)

Rate temperature dependence reveals an Arrhenius behavior:

$$r = r_0 \, e^{-E_a/k_B T}$$



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3.4: Imaging at different bias

The chemical contrast: GaAs (110)

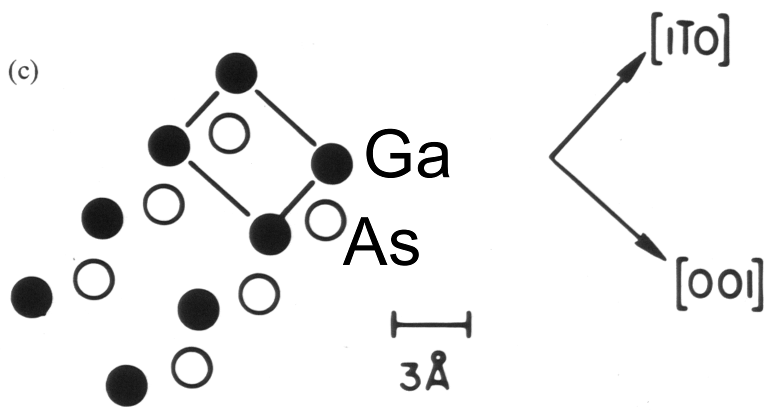
Two superposed images:

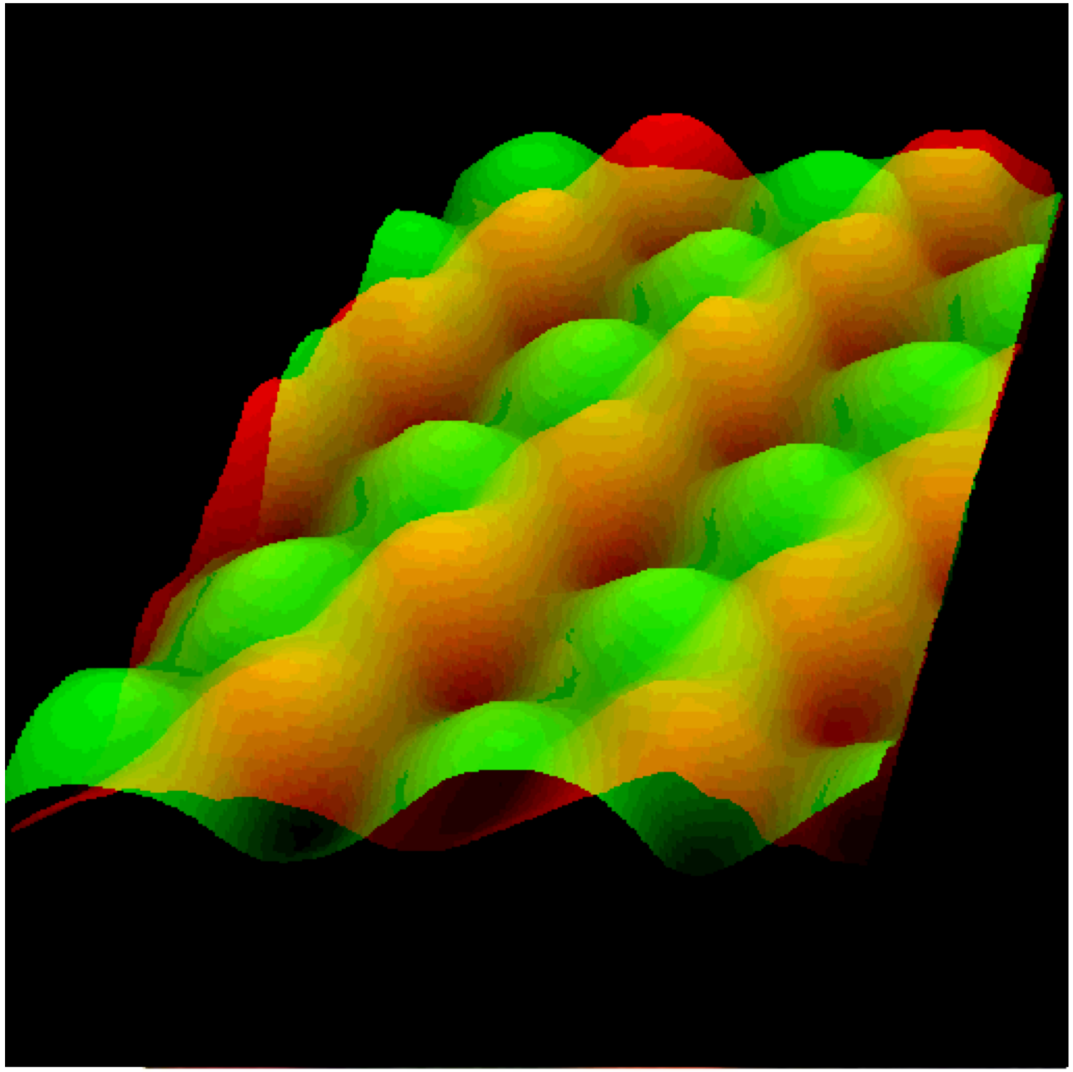
occupied states: $V_{sample} < 0$, red: As.

+

empty states: $V_{sample} > 0$, green: Ga

Images are taken simultaneously to avoid hysteresis effects between two succesive images.

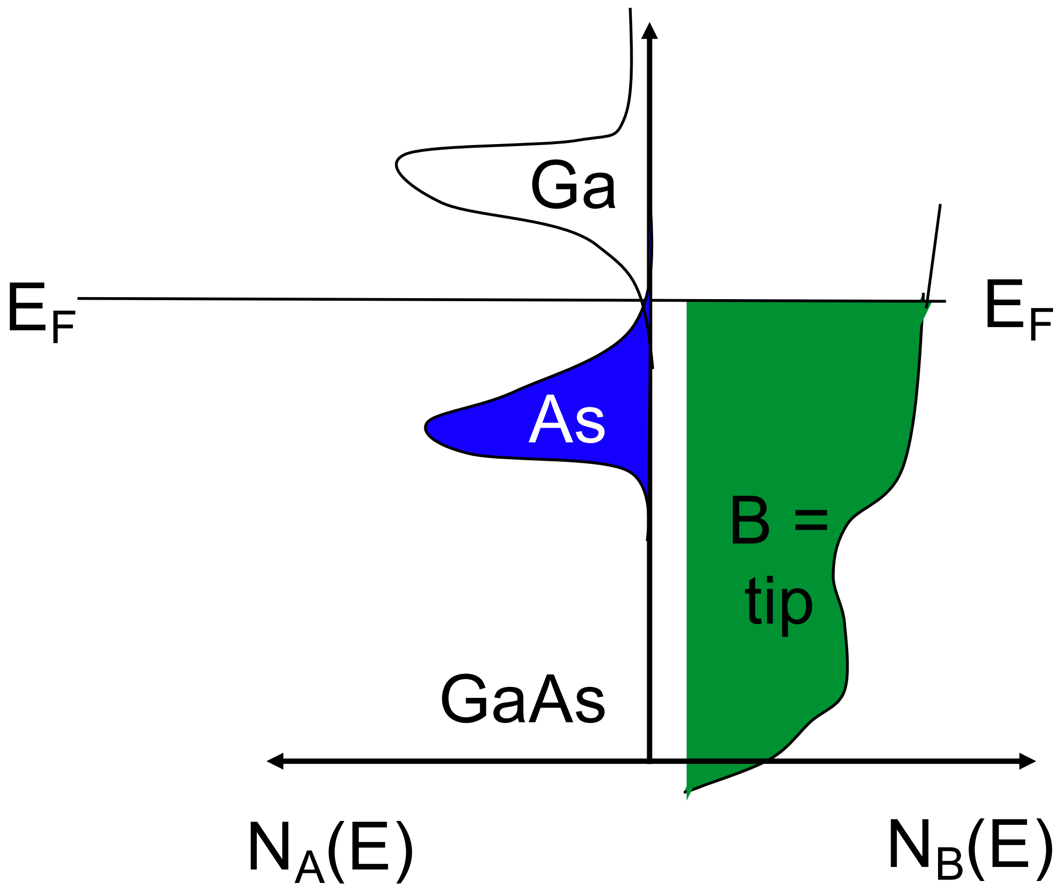




R. M. Feeinstra, J. Stroscio et al, Phys. Rev. Lett. 58, 1192 (1987).

Occupied / empty states: a naive picture

As potential more attractive than Ga.
Close to Fermi level, occupied states are on As, empty ones on Ga.



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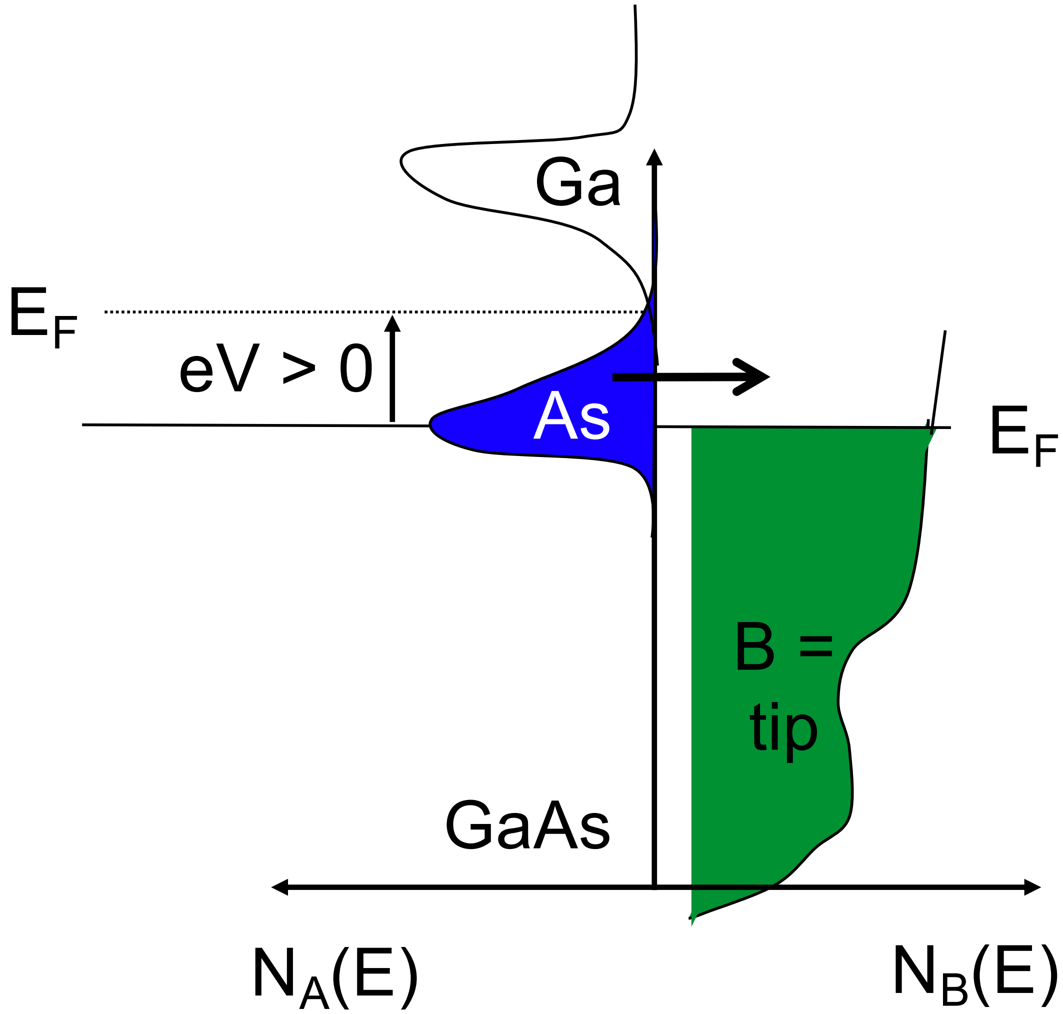
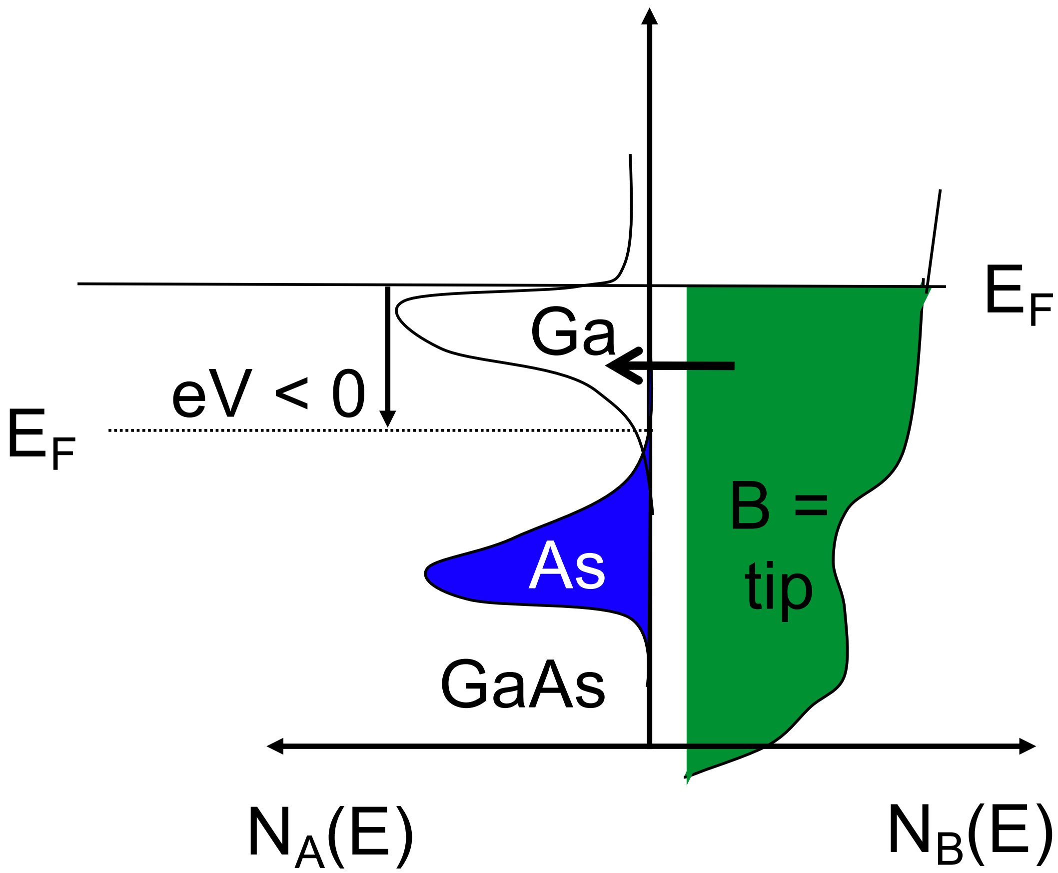


eV > 0: As atoms are imaged.

Occupied / empty states: a naive picture

As potential more attractive than Ga.
Close to Fermi level, occupied states are on As, empty ones on Ga.



eV > 0: As atoms are imaged.
eV < 0: Ga atoms are imaged.

Depending on bias, occupied or empty states participate to tunneling: complementary information can be accessed.

Real-time dynamics of Pb atoms on Si

A different contrast is obtained, depending on bias.

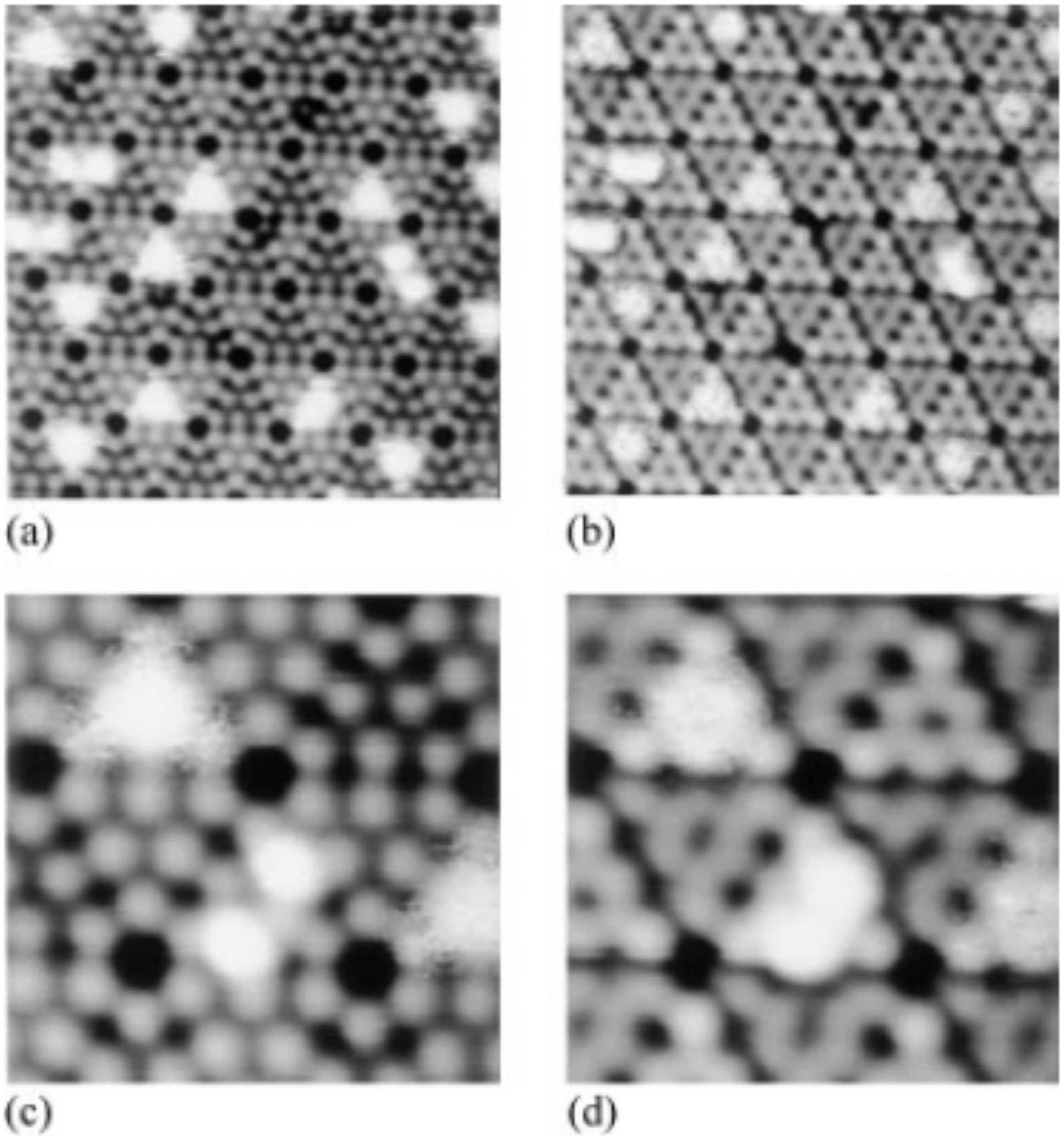


FIG. 1. Filled and empty state STM images of 0.01 ML Pb on Si(111)-(7 × 7) measured at room temperature. The scanning areas are 16.25 × 16.25 nm^2 [(a) and (b)] and 6.0 × 6.0 nm^2 [(c) and (d)]. Sample voltages are +2 V [(a) and (c)] and −2 V [(b) and (d)]. Tunnel current is 0.2 nA for all images.

J.-M. Rofriguez-Campos et al, Phys. Rev. Lett. 76, 799 (1996), Institut Néel, Grenoble.

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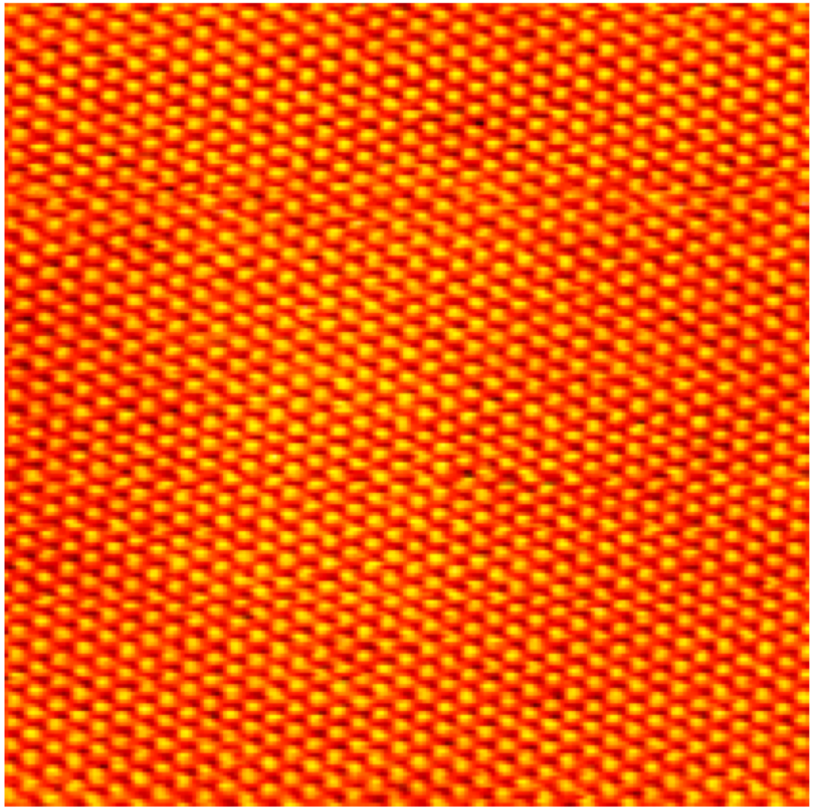
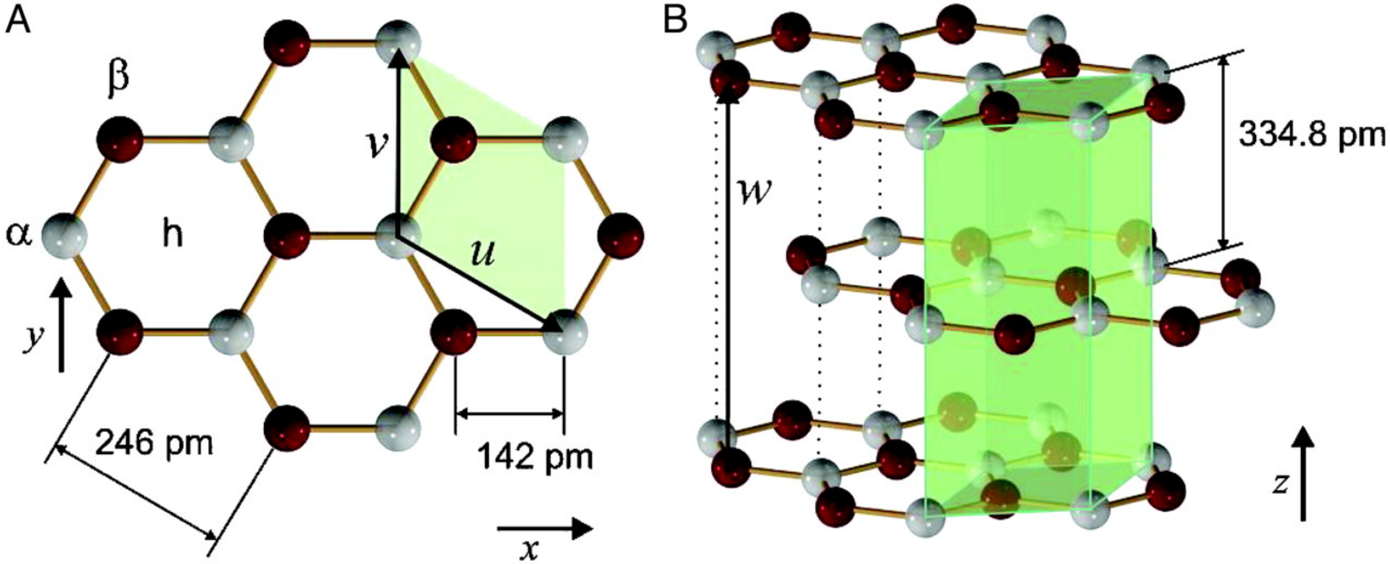
3.5: HOPG,
Highly Oriented Pyrolitic Graphite,
Graphene

Three / six-fold symmetry in graphite



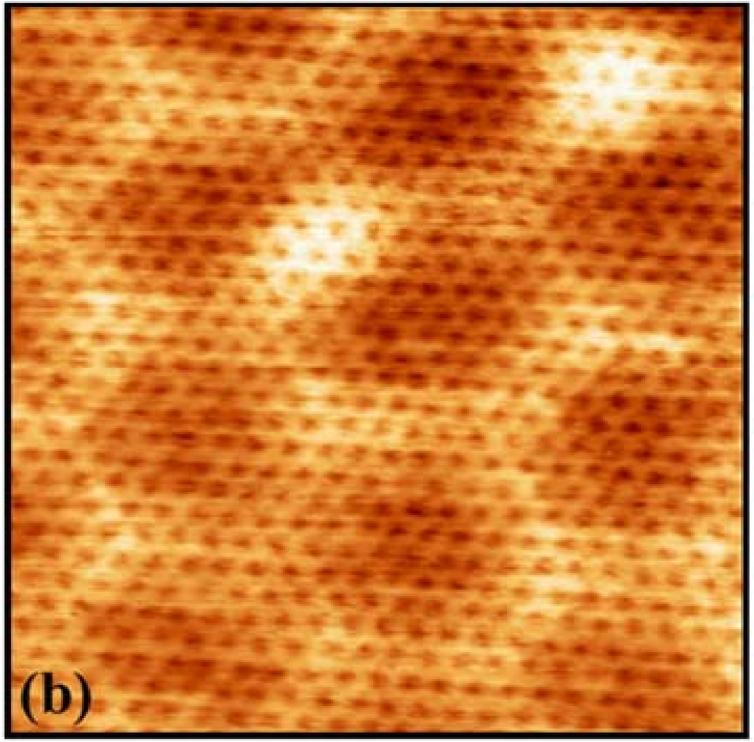


Clean surface thanks to the layered structure and scotch technique.

Images = a triangular lattice, not a hexagonal one:
coupling with the second layer make every other two atom “different”.

STM images not the atoms but the electronic clouds.

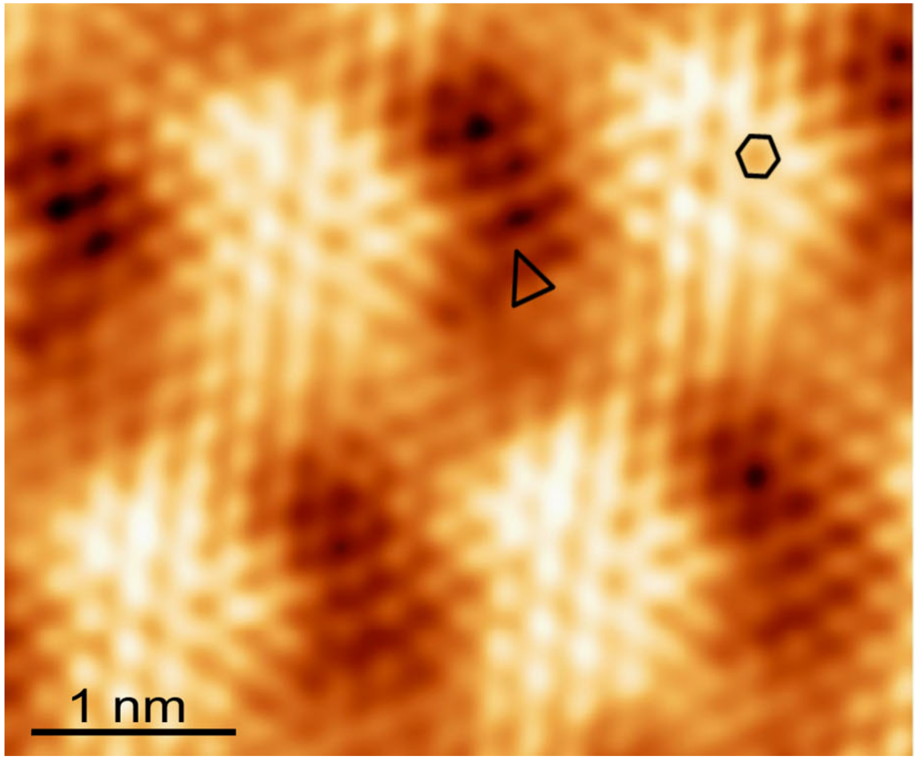
Images of graphene



UHV annealing of SiC,

epitaxy on Re:

formation of a graphene sheet on a crystalline substrate.



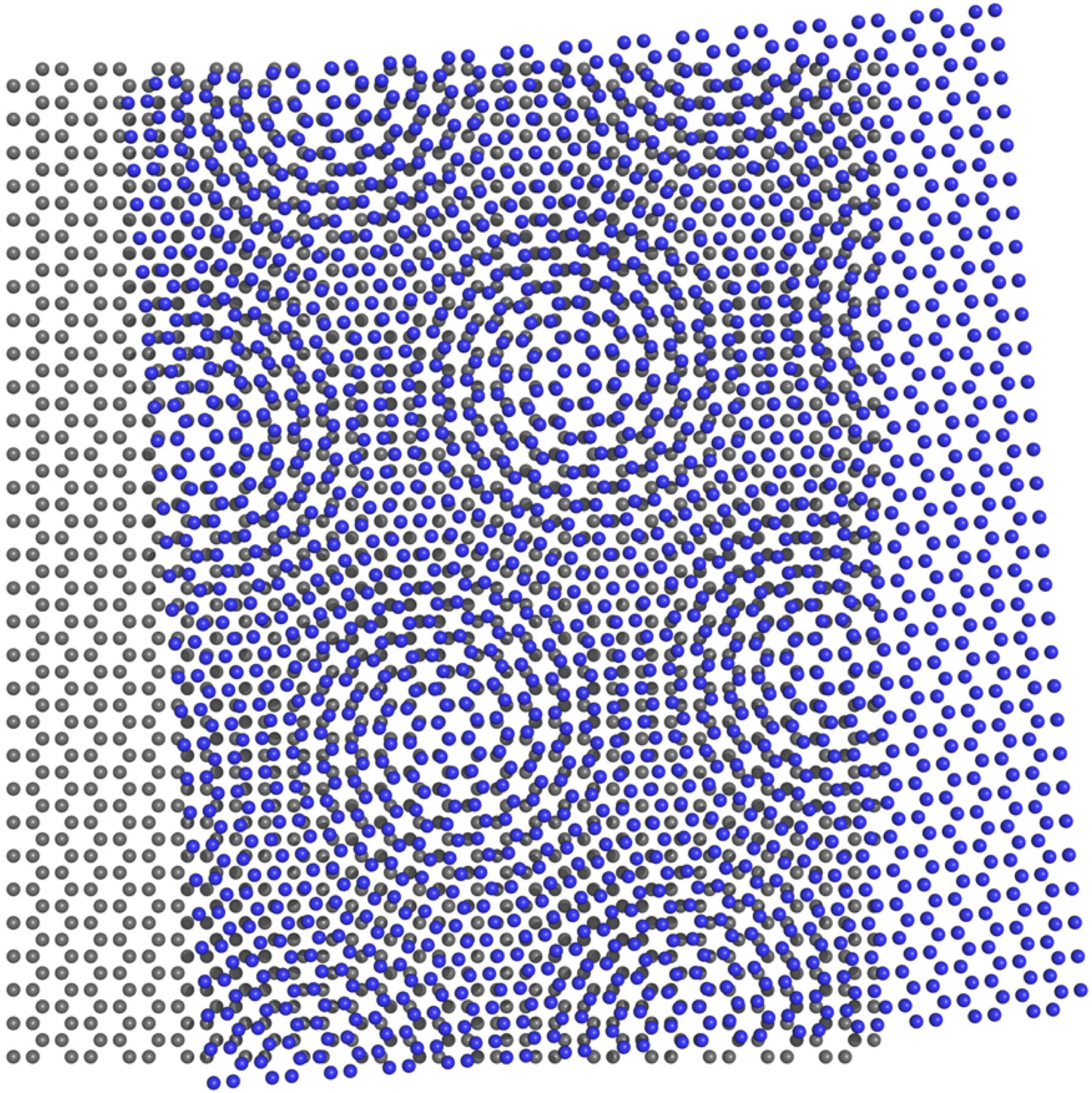
Atomic lattice visible, 6-fold periodicity.

P. Mallet, J.Y. Veuillen et al, Phys. Rev. B 76, 041403(R) (2007), Institut Néel. C. Tonnoir, C. Chapelier et al, Phys. Rev. Lett. 111, 246805 (2013), INAC.

Moiré

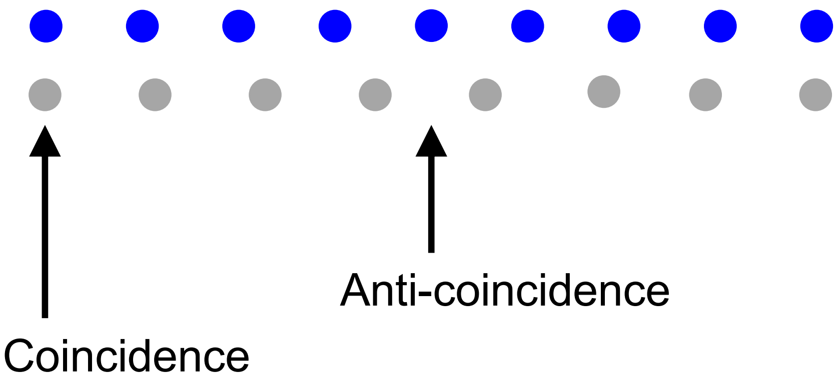
Pattern created when two identical patterns are overlaid while displaced or rotated a small amount from one another.

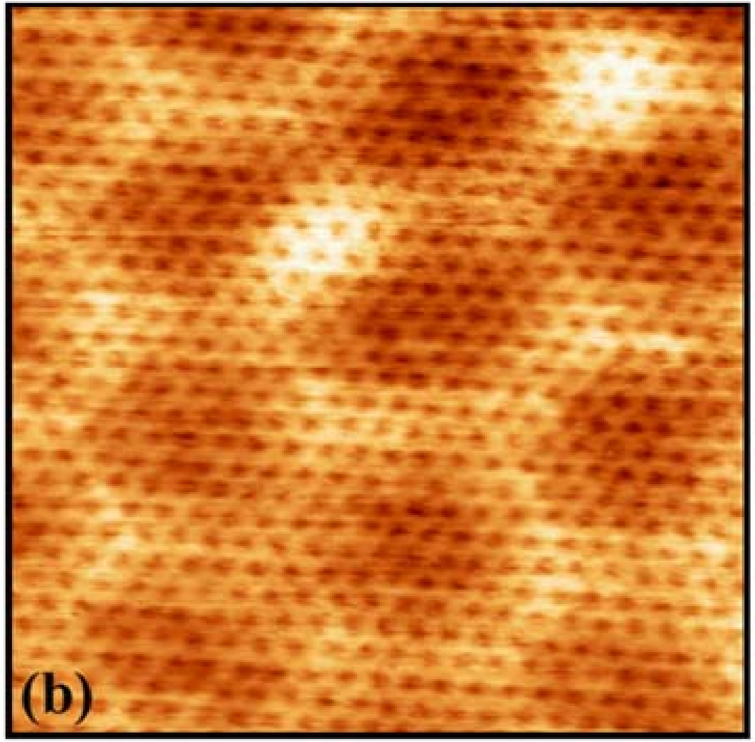
Similar effect with small difference in lattice parameter.

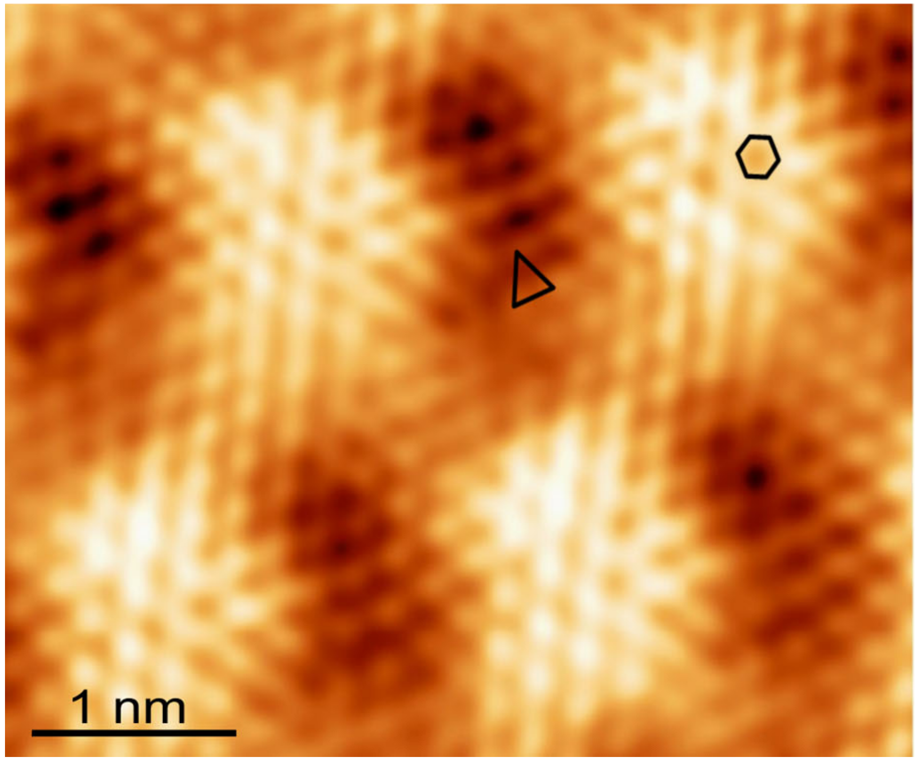


Moiré in graphene

Images shows electronic interference effects with the buffer layer: moiré.







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Conclusion

STM imaging usually carries other information than “pure” topography, that is related to electronic properties.