"The new standard of STM imaging of QC surfaces: flowers and donuts. How analyzing them ?"

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Surface versus bulk : what can we learn from surface studies ?

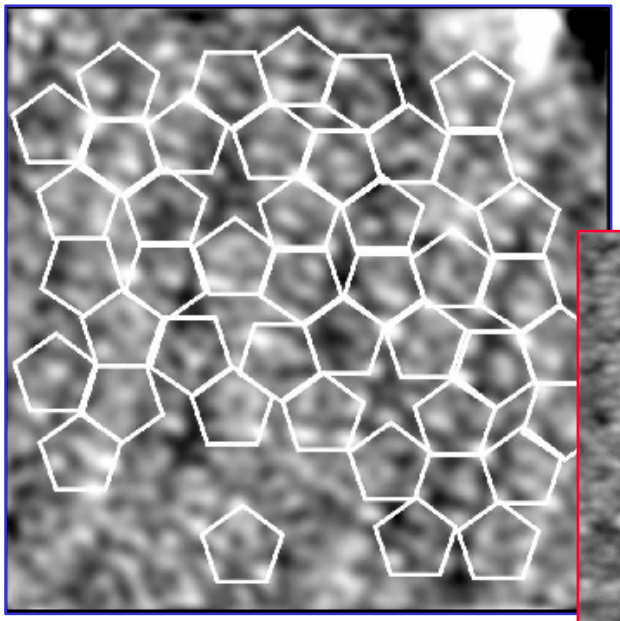
Bulk structural studies :

- **Real space : TEM**
- **Reciprocal space : X-ray / neutron diffraction**

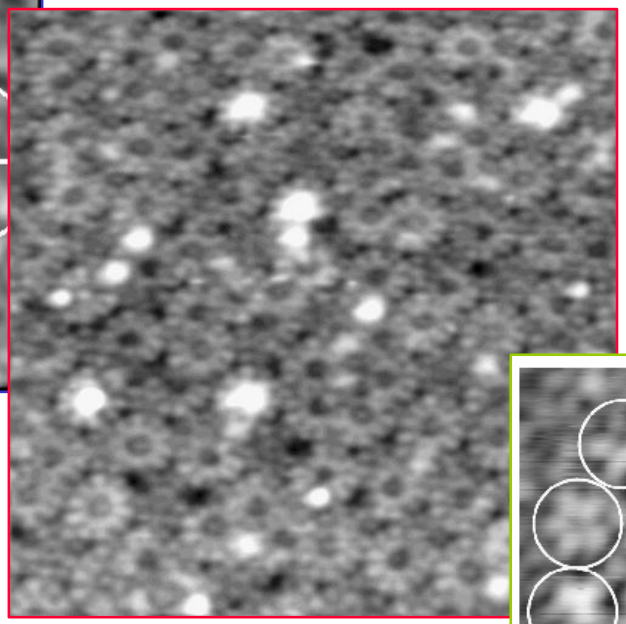
Surface studies :

- Structural information
- Thermodynamics
- Applications ? (tribology)

Fascinating world at the atomic scale !

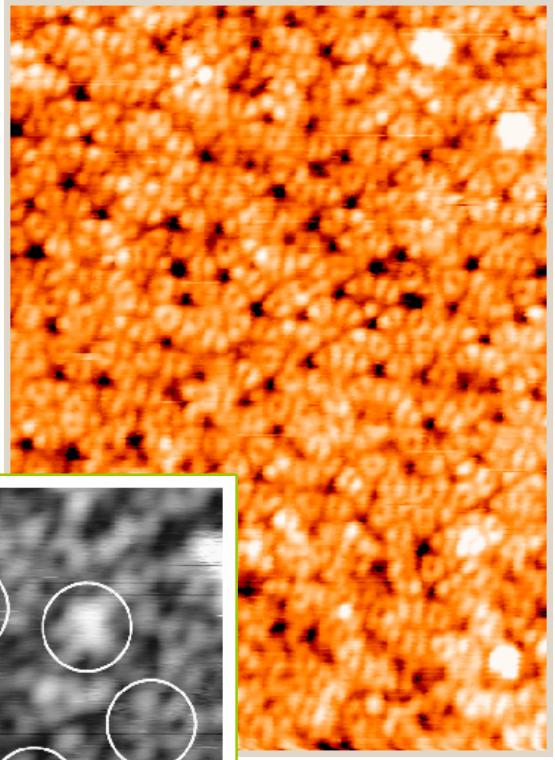


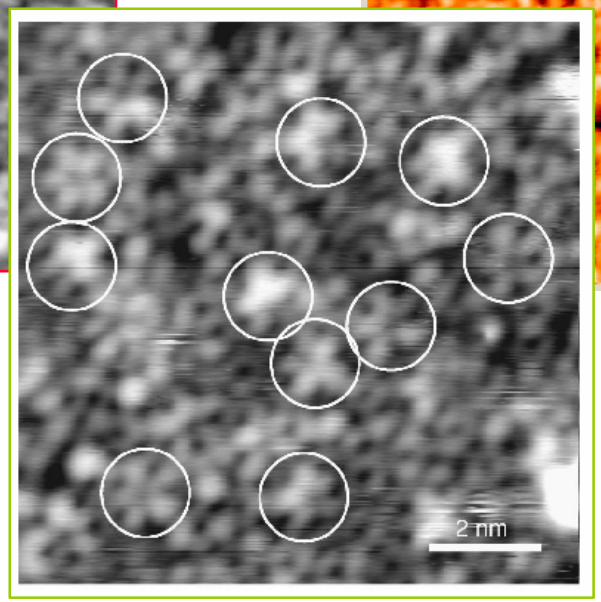
J. Ledieu et al.
SURFACE SCIENCE, **492** (2001) **L729**.



T. Cai et al.
PHYS. REV. B, **65** (2002) 140202.

L. Barbier et al.
PHYS. REV.LETT., **88** (2002) 085506.



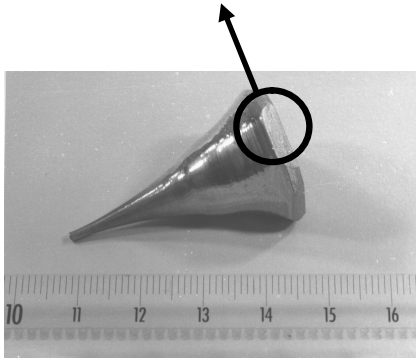


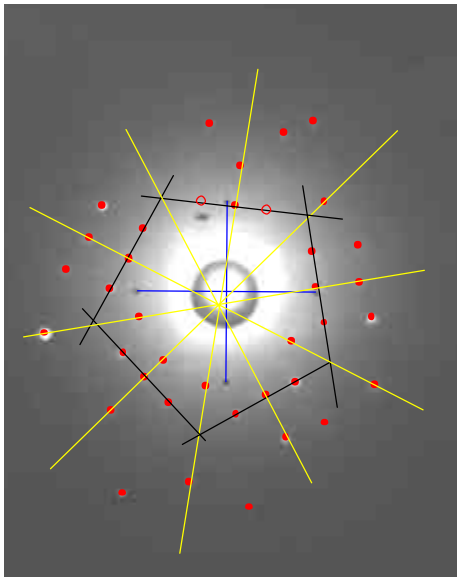
M. Kishida et al.
PHYS. REV. B, **65** (2002) 094208

Focus on 2002 publications ...

Basic surface studies

5-fold growth facet





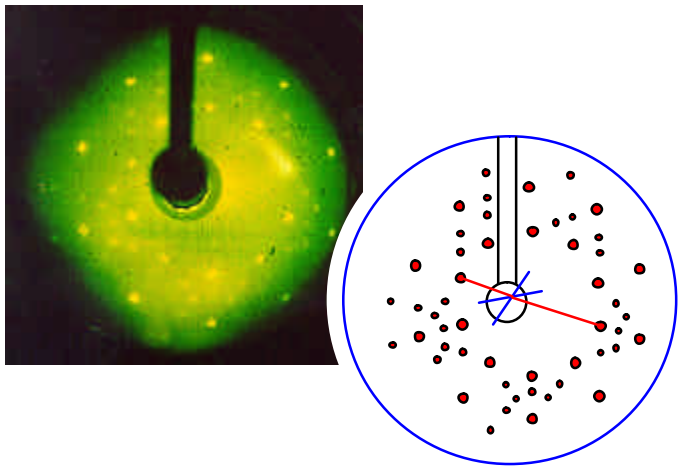
Lauë diagram

$Al_{70.4}Pd_{21.4}Mn_{8.2}$
(^ 5 fold axis)

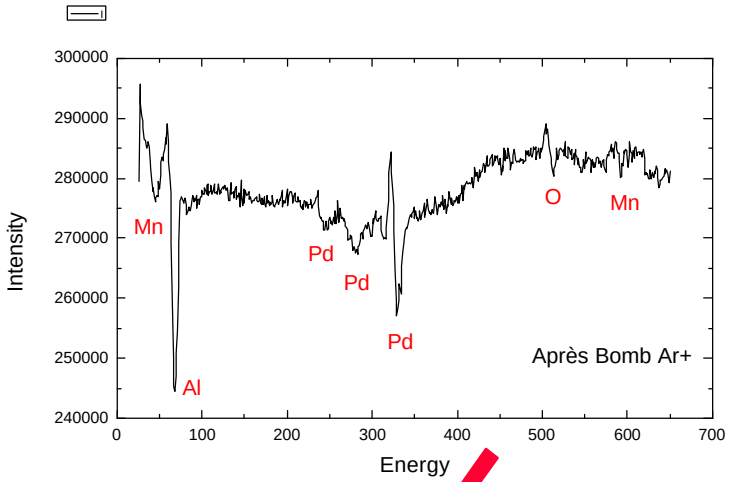
Under UHV :

Ar^+ sputtering (400 eV, 5mA, 1h) / Annealing 923 K

LEED diagram:



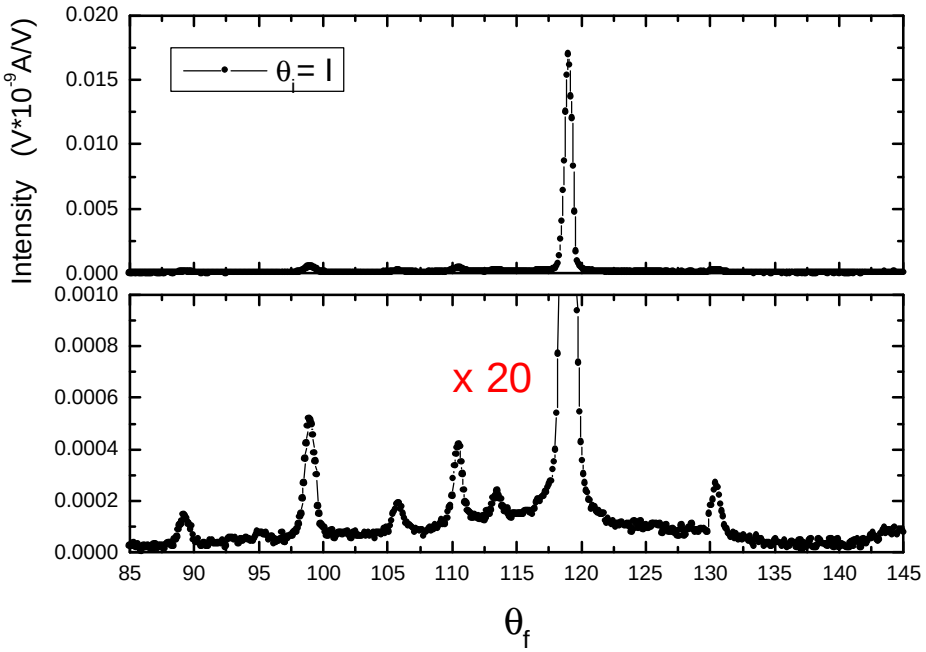
AES spectroscopy
Al-rich surface



5-fold surface
Al-rich

Surface study: neutral He diffraction

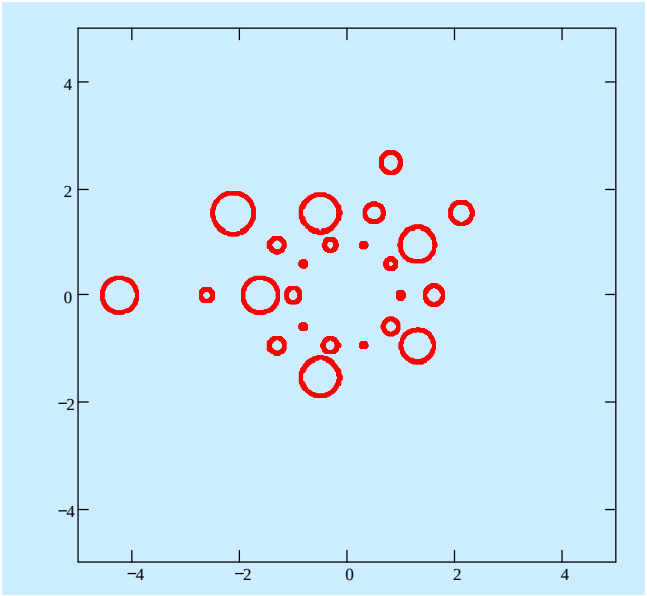
$k = 6.5\ \text{Å}^{-1}, q_i = 60°$



Intense specular peak :
$I(0,0)/I_0$=0.06
Flat surface, not much defects

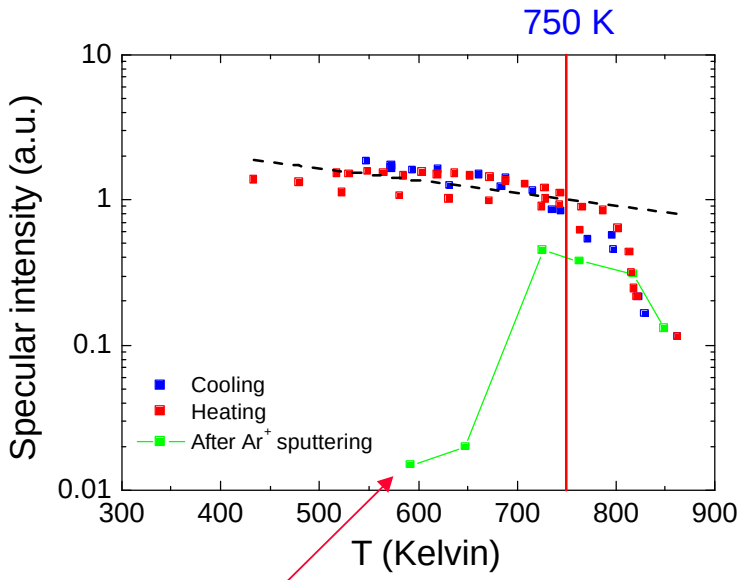
Low intensity of diffraction peaks
I/I(0,0)=0.015
Low corrugation = high density terraces
dh_{He}= 1.9 pm

5-fold symmetry
of the topmost surface plane



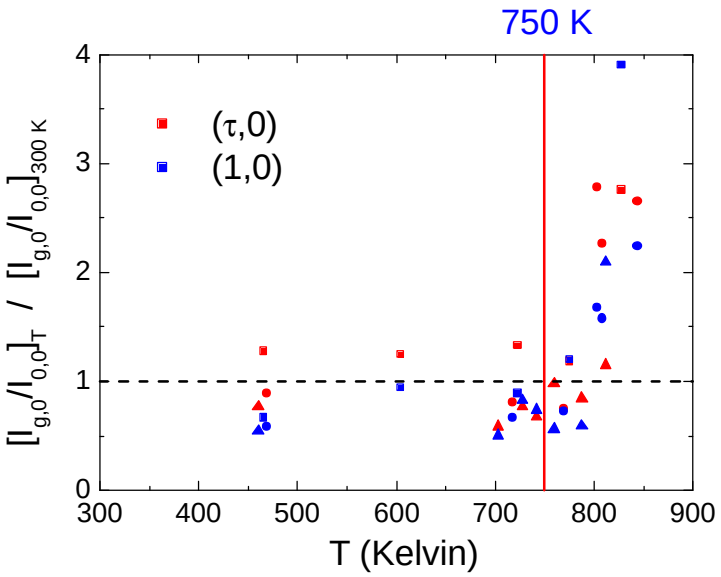
Surface study: He diffraction

Thermal behavior : $I_{0,0}$ =f(T)



Ar⁺ sputttering
(400 eV, 5mA, 1h)
Annealing ➡ 923 K

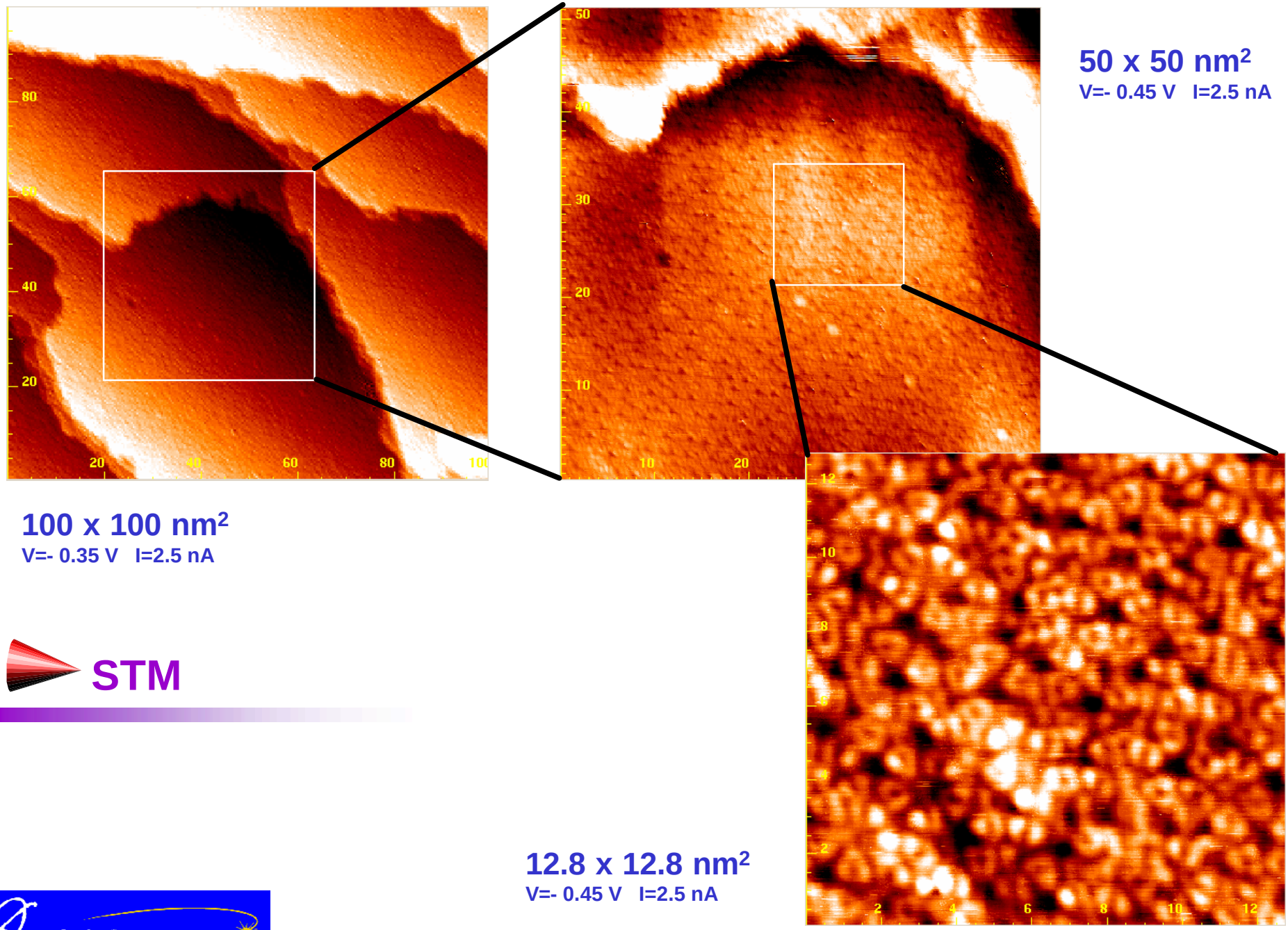
Thermal behavior : $I_{g,0}$ =f(T)



- After Ar+ : Surface flattens at 750 K
- Above 750 K : anomalous attenuation
- higher corrugation

➡ Stable surface
Optimization of the cleaning process

STM observations



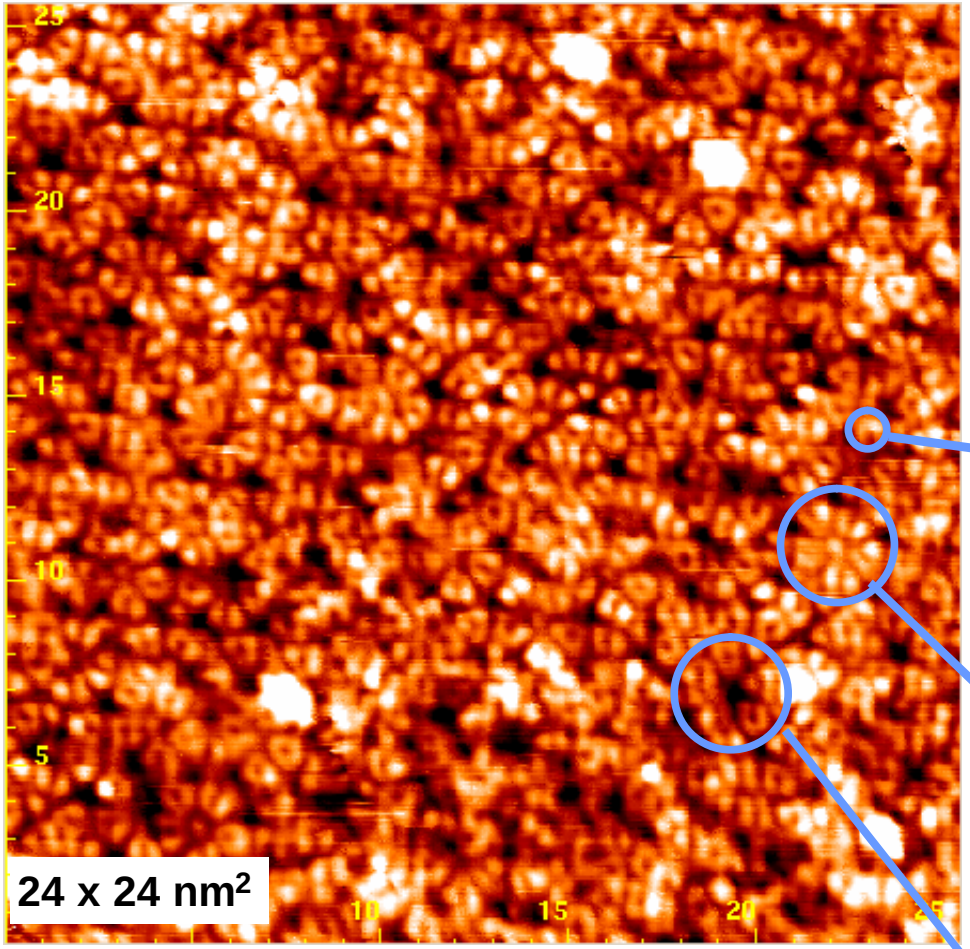
50 x 50 nm²
V=- 0.45 V I=2.5 nA

100 x 100 nm²
V=- 0.35 V I=2.5 nA

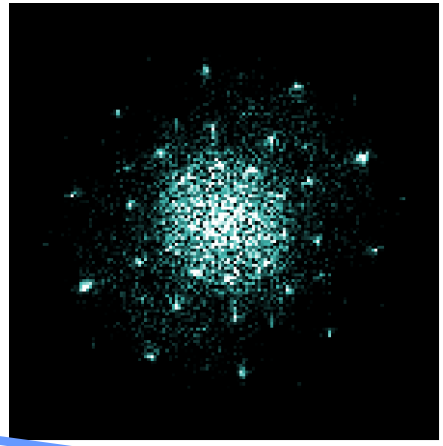
STM

12.8 x 12.8 nm²
V=- 0.45 V I=2.5 nA

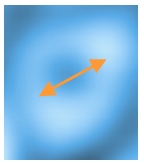
STM observations



Fourier transform
high degree of order

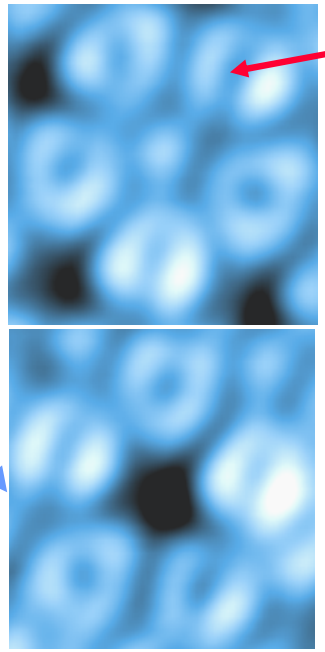


0.55 nm



Donut =
elementary brick ?

Typical local
configurations



Donuts !

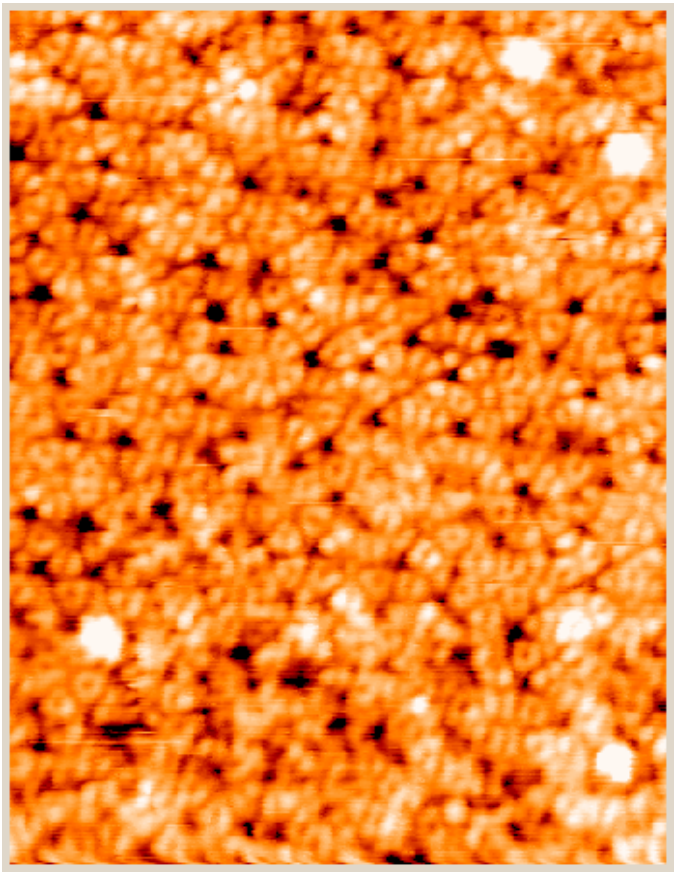
Flowers !

2.4 x 2.4 nm²

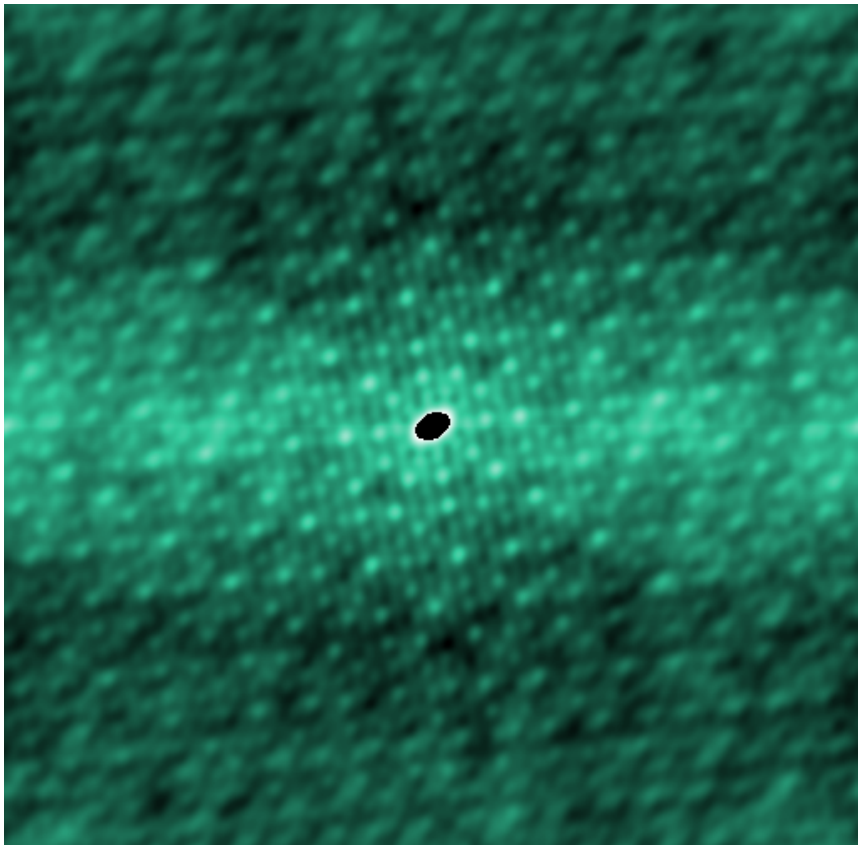
- Saclay -

Auto-correlation function

$$C(r_0) = \iint_r h(r) \bullet h(r - r_0)\, dr = FFT^{-1}\left[FFT \bullet \overline{FFT}\right]$$



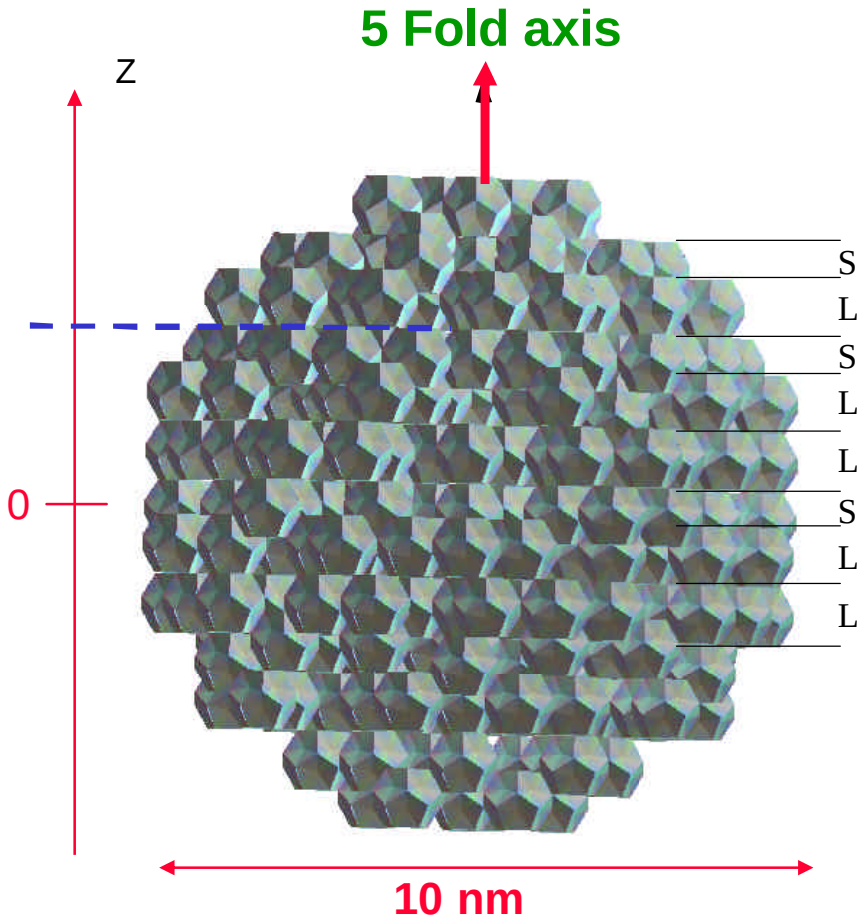
22 x 16 nm^2
(V=- 0.35 V I=2.5 nA)



Long range QC order

How analysing the pictures ?

1) Need a structural model : based on (bulk) X-ray, neutron diffraction data...



The QC Bergman bowl

From 6-d to 2-d:

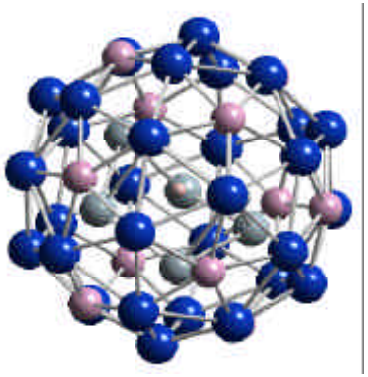
The 6-d Katz-Gratias model based on neutron diff data :

N. Schramchenko (2001)

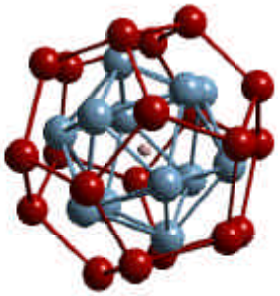
+ Cut algorithm = QC 3-d bowl

Cut ^ to the 5-fold axis

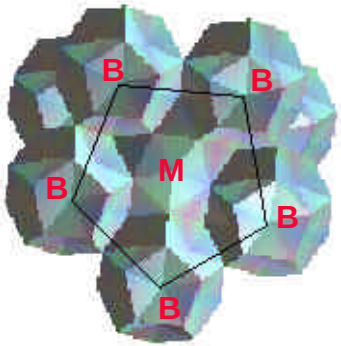
2-d surfaces



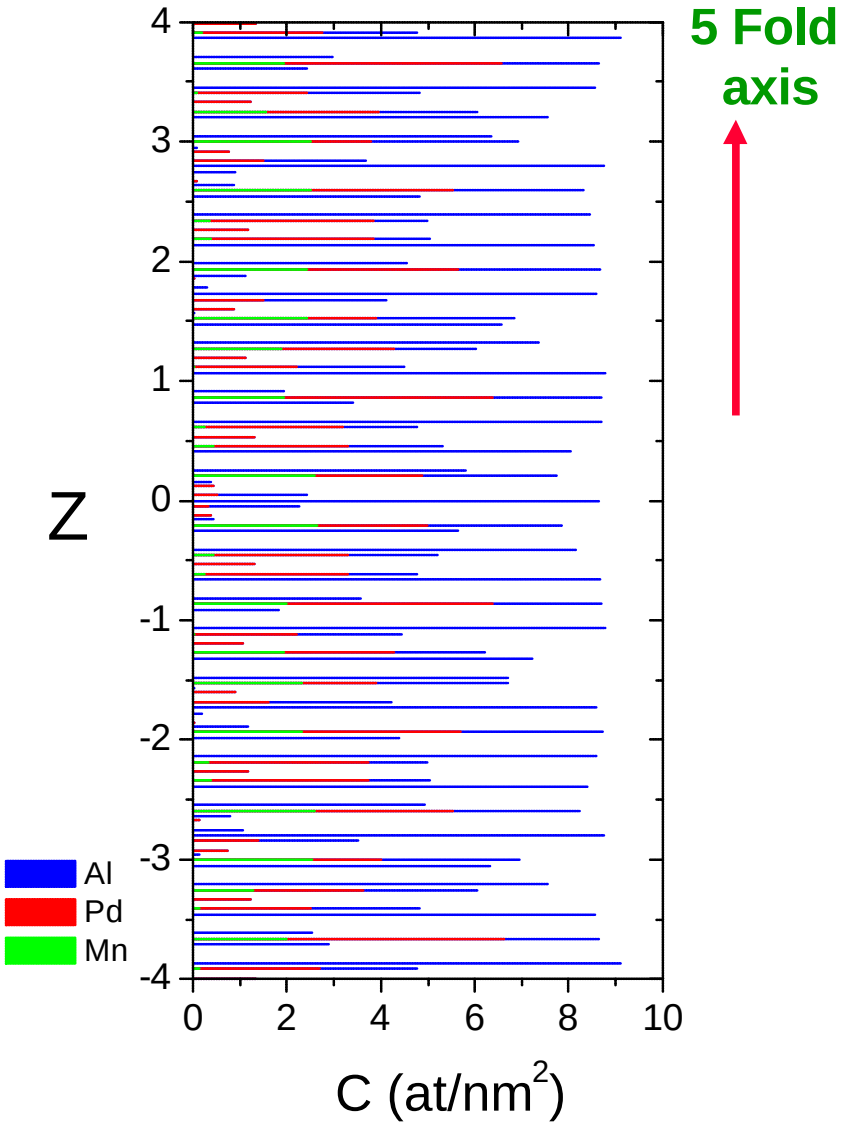
Mackay



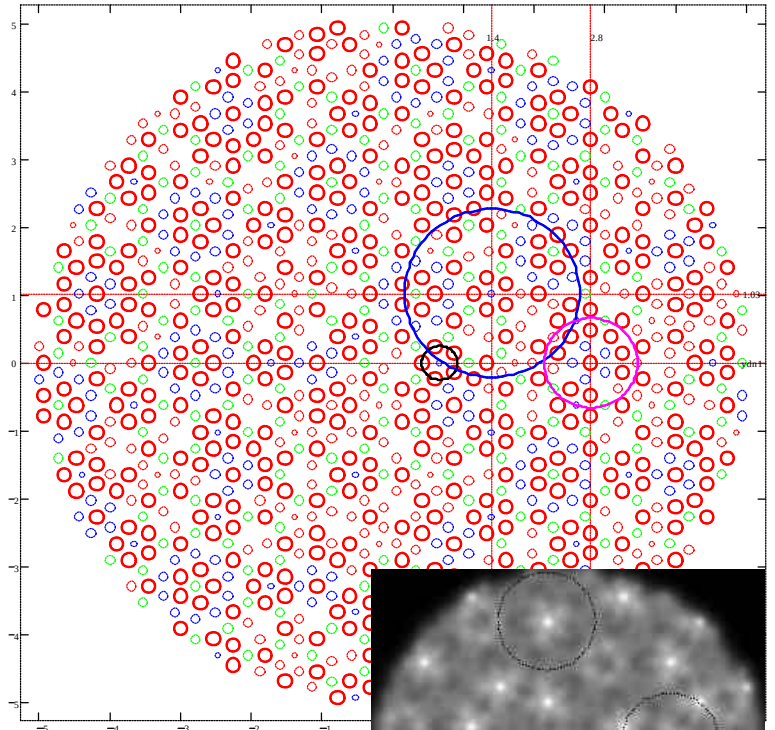
Bergman



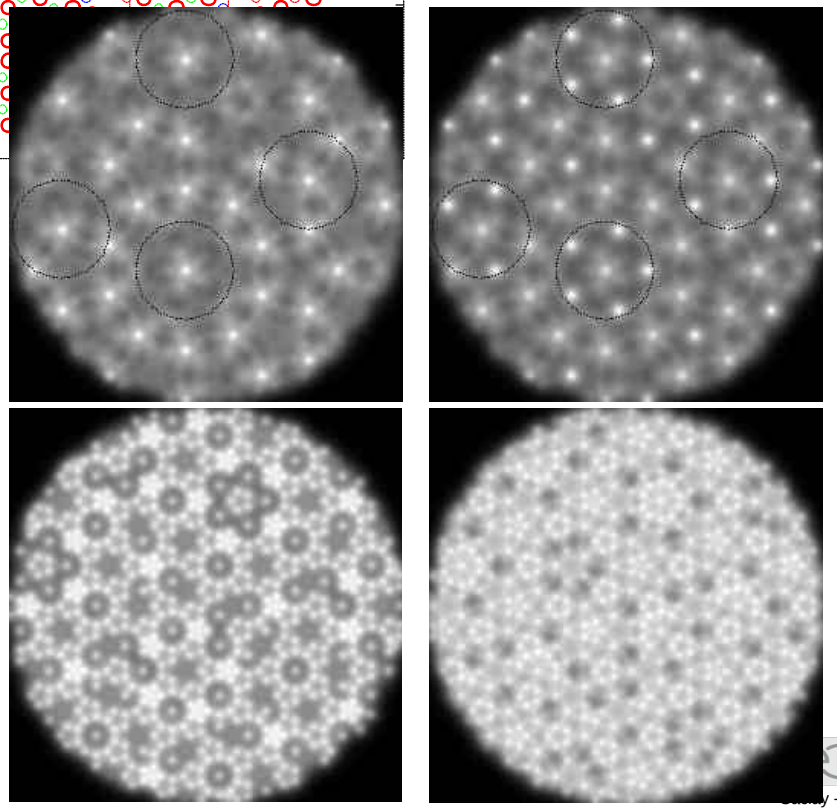
Plane positions and surface configurations



5 Fold axis



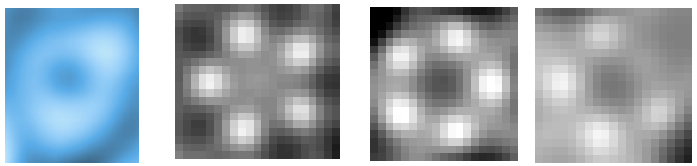
Al
Pd
Mn



Simulation of STM images

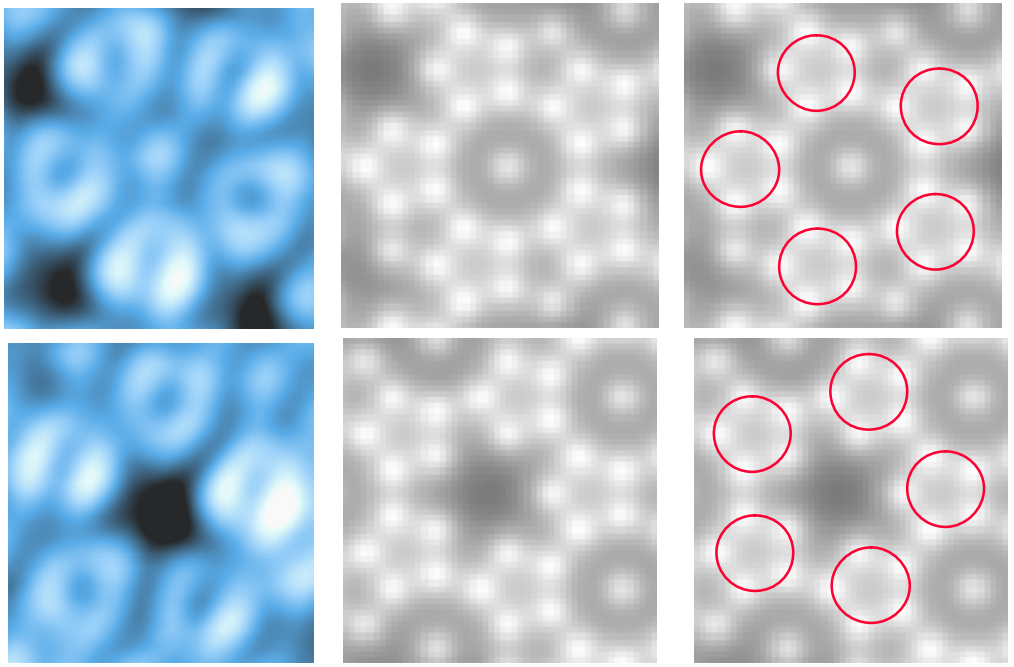
$0.028 < C < 9.93$ at/nm^2

Looking for the identification of local patterns



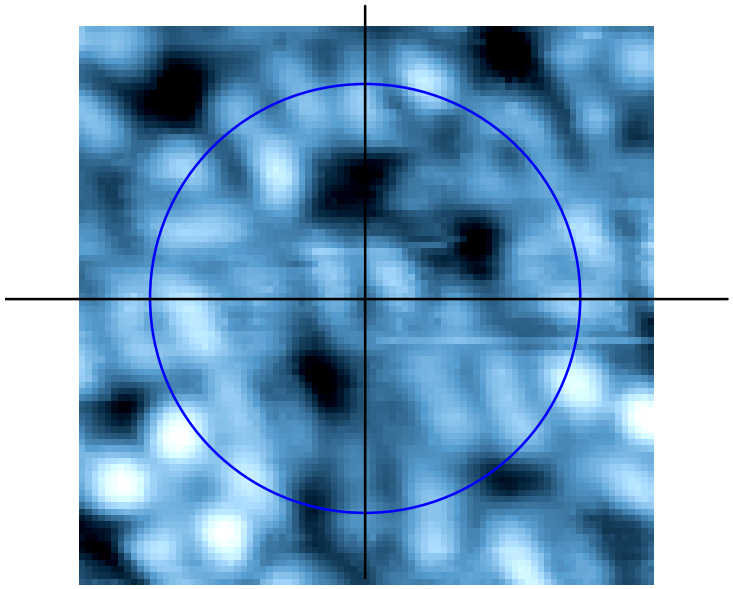
0.7 x 0.7 nm^2

Donuts !

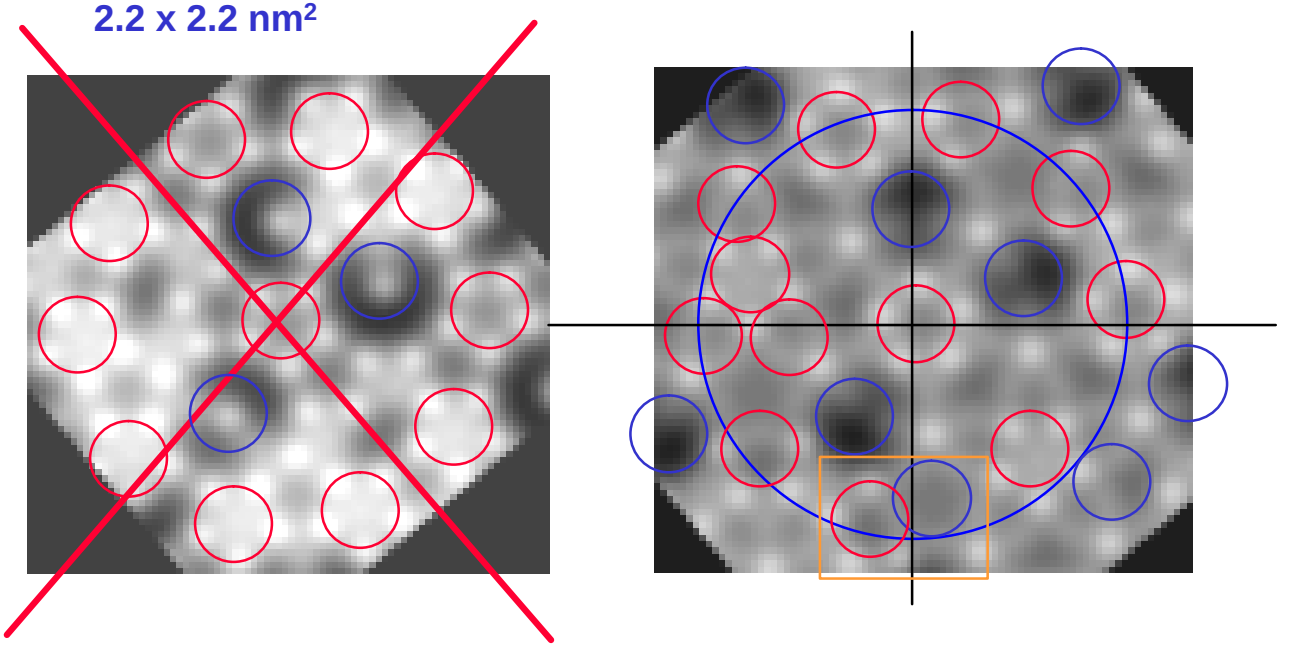


Flowers !

2.2 x 2.2 nm^2



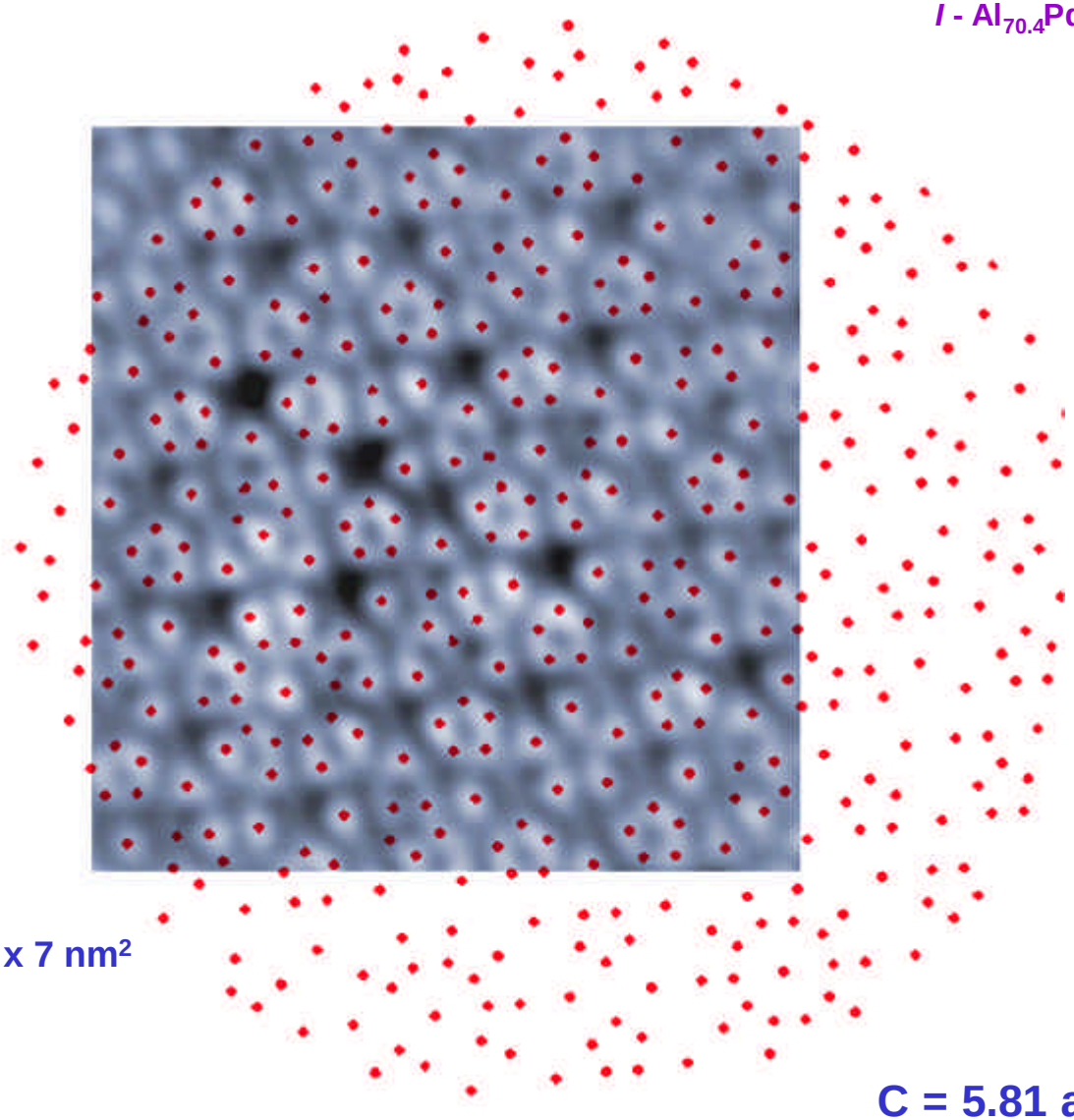
9 x 9 nm^2



Plane selection

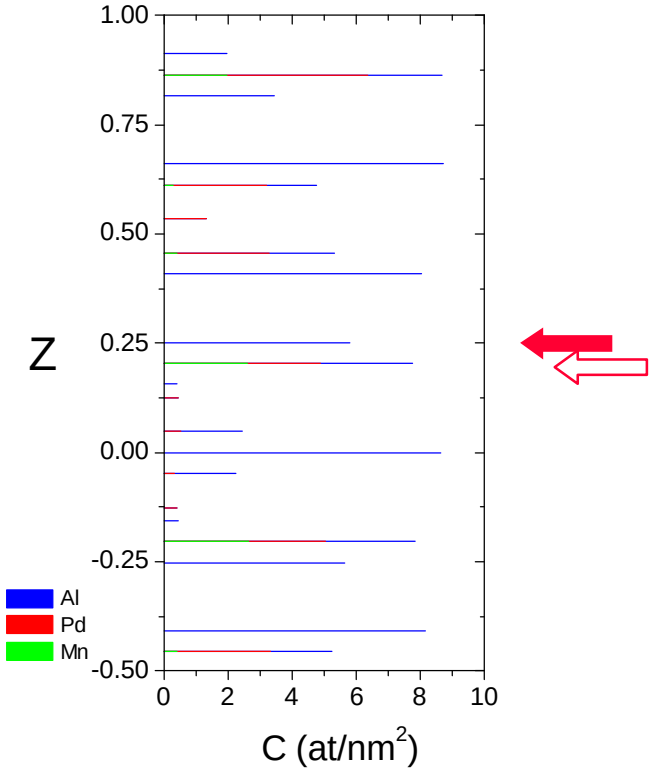
Identification of local configurations:

I - $Al_{70.4}Pd_{21.4}Mn_{8.2}$: single quasicrystal (CNRS-CECM-Vitry)



6.6 x 7 nm²

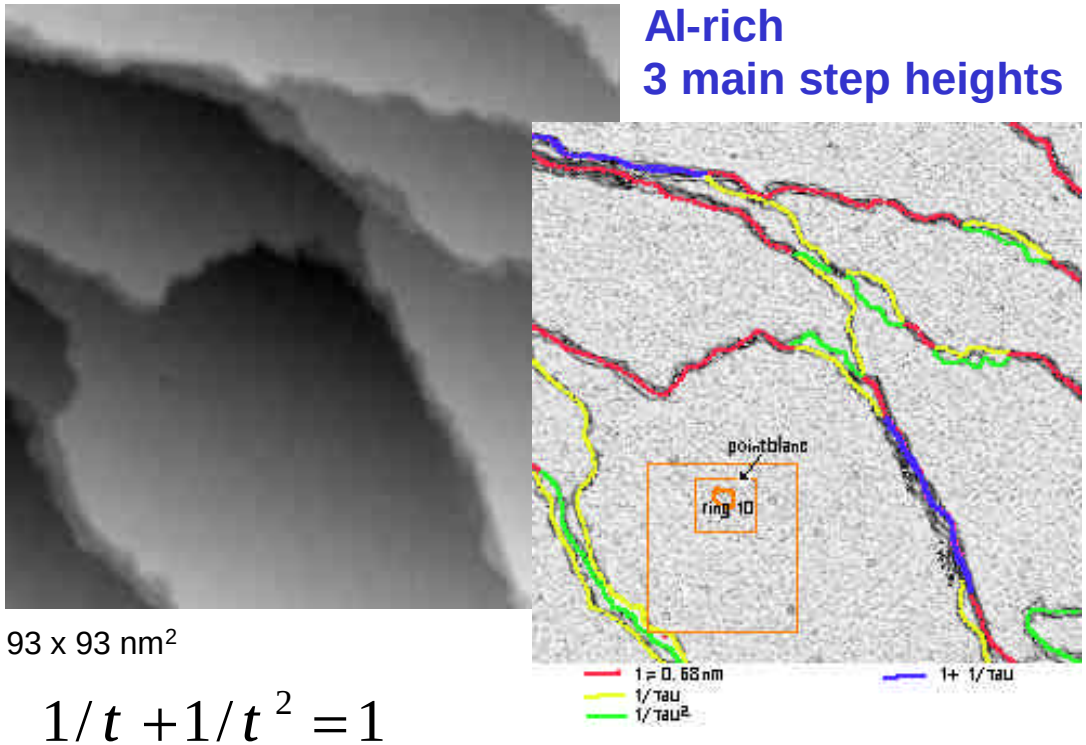
Find the agreement between the model and an extended configuration



C = 5.81 at/nm²

Step heights : Nature of the terraces ?

Surface = dense planes,
Al-rich
3 main step heights



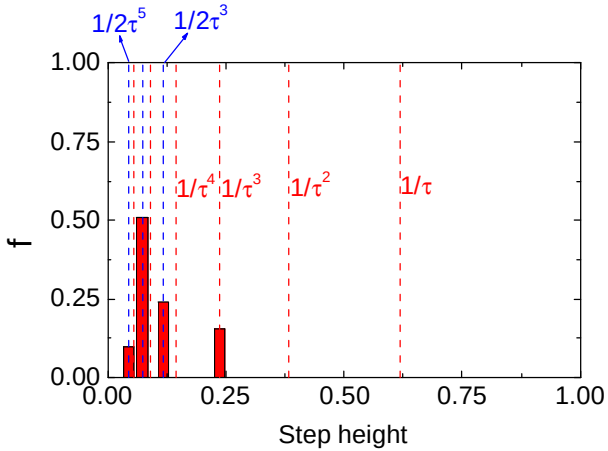
93 x 93 nm²

$$1/t + 1/t^2 = 1$$

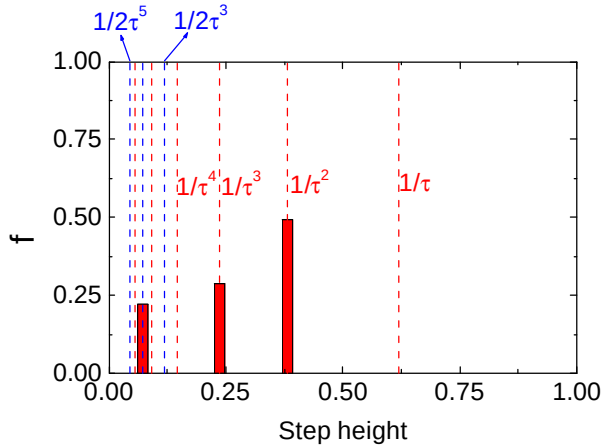
h_3=1.10 nm	$= h_0(1+1/t)$
h_0=0.68 nm	$= h_0$
h_1=0.42 nm	$= h_0/t$
h_2=0.26 nm	$= h_0/t^2$

From the model
histogram of step heights :

All planes:



Between high density planes:



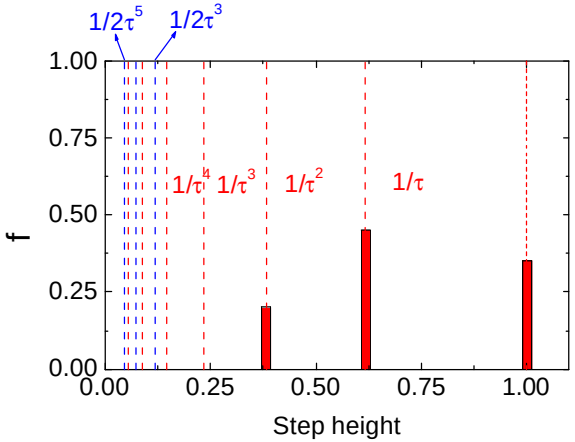
$8 > C_s > 2$ at/nm²

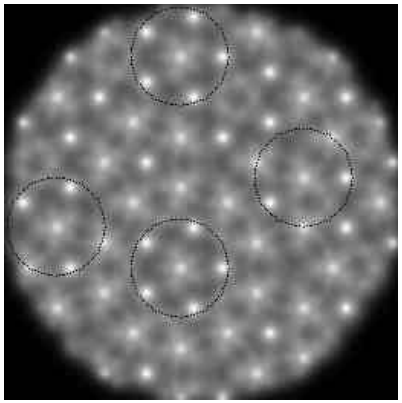
- Saclay -

Need to add some other conditions: Chemical selectivity

(like usual ordered alloys Cu_3Au, Cu_3Pd, Fe_3Al)

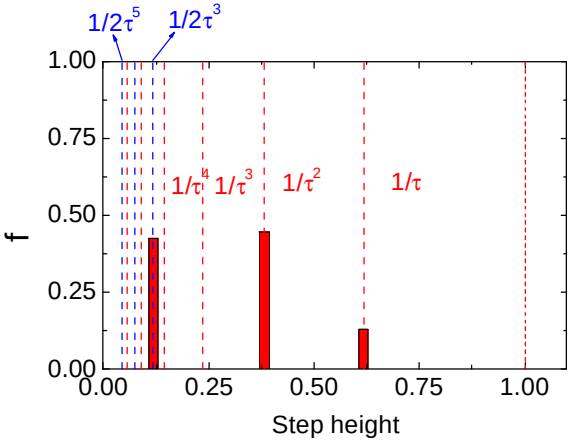
Pure Pd plane ?



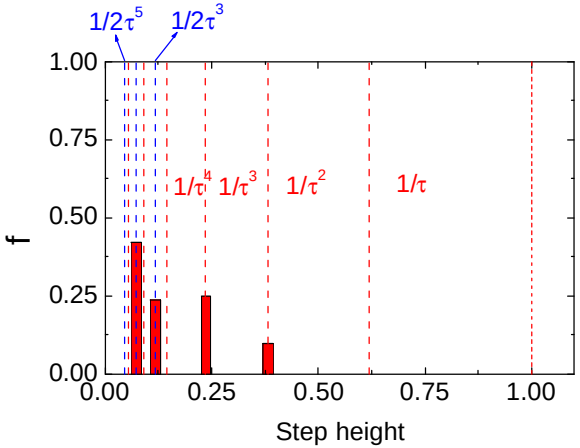


O.K. but low density planes ! (1.3 at/nm^2)

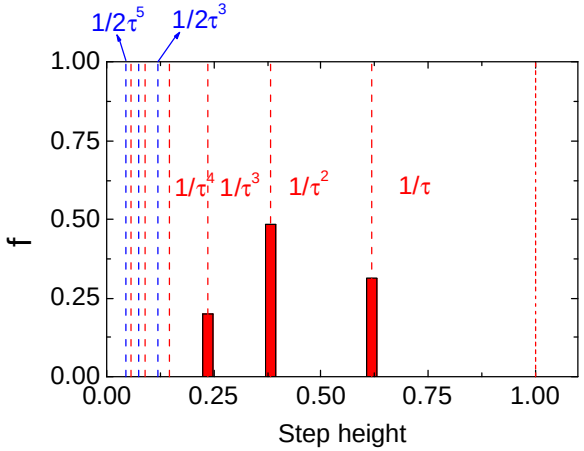
Pd rich plane ?



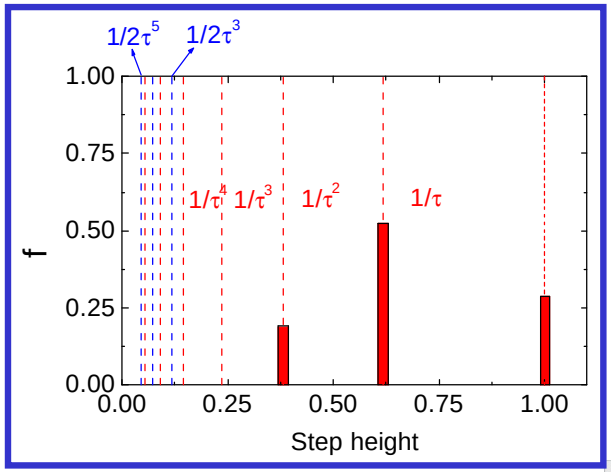
Al rich plane ?



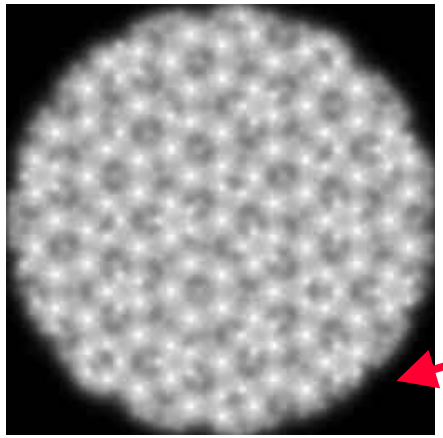
High density pure Al plane ?



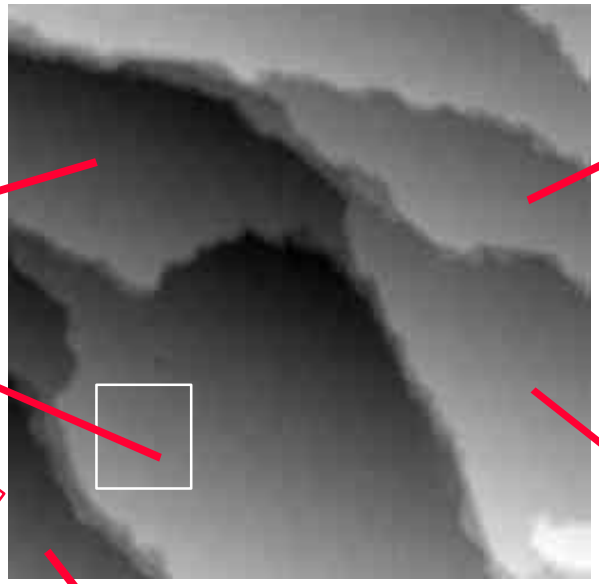
High density pure Al plane + closed second plane ! dh < 1/2t^3

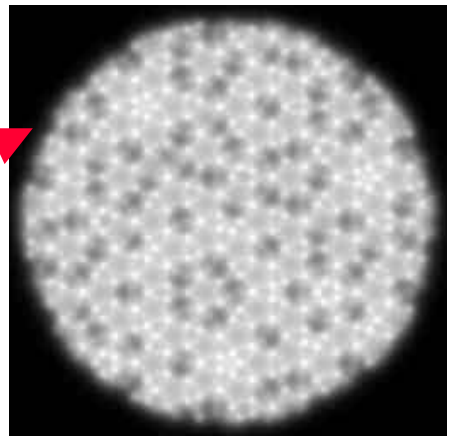


Observed terrace planes are dense pure Al planes in the model

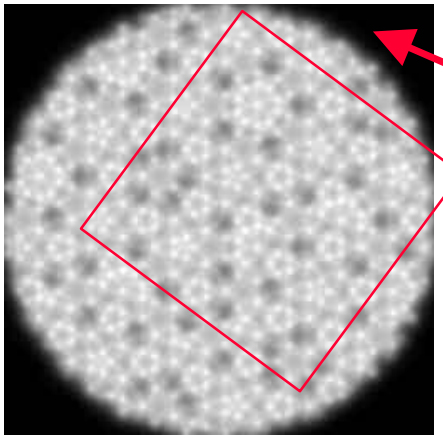


Z=0.91 nm



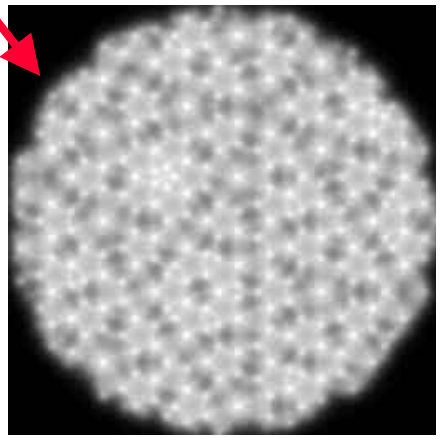


Z=1.98 nm

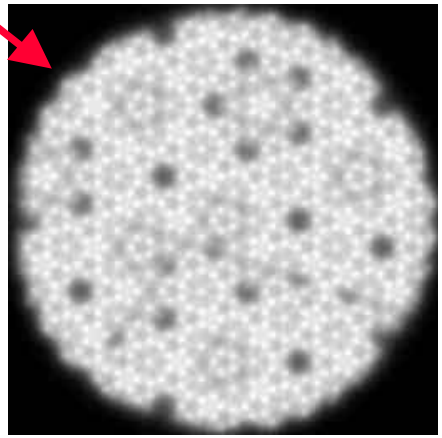


Z=0.25 nm

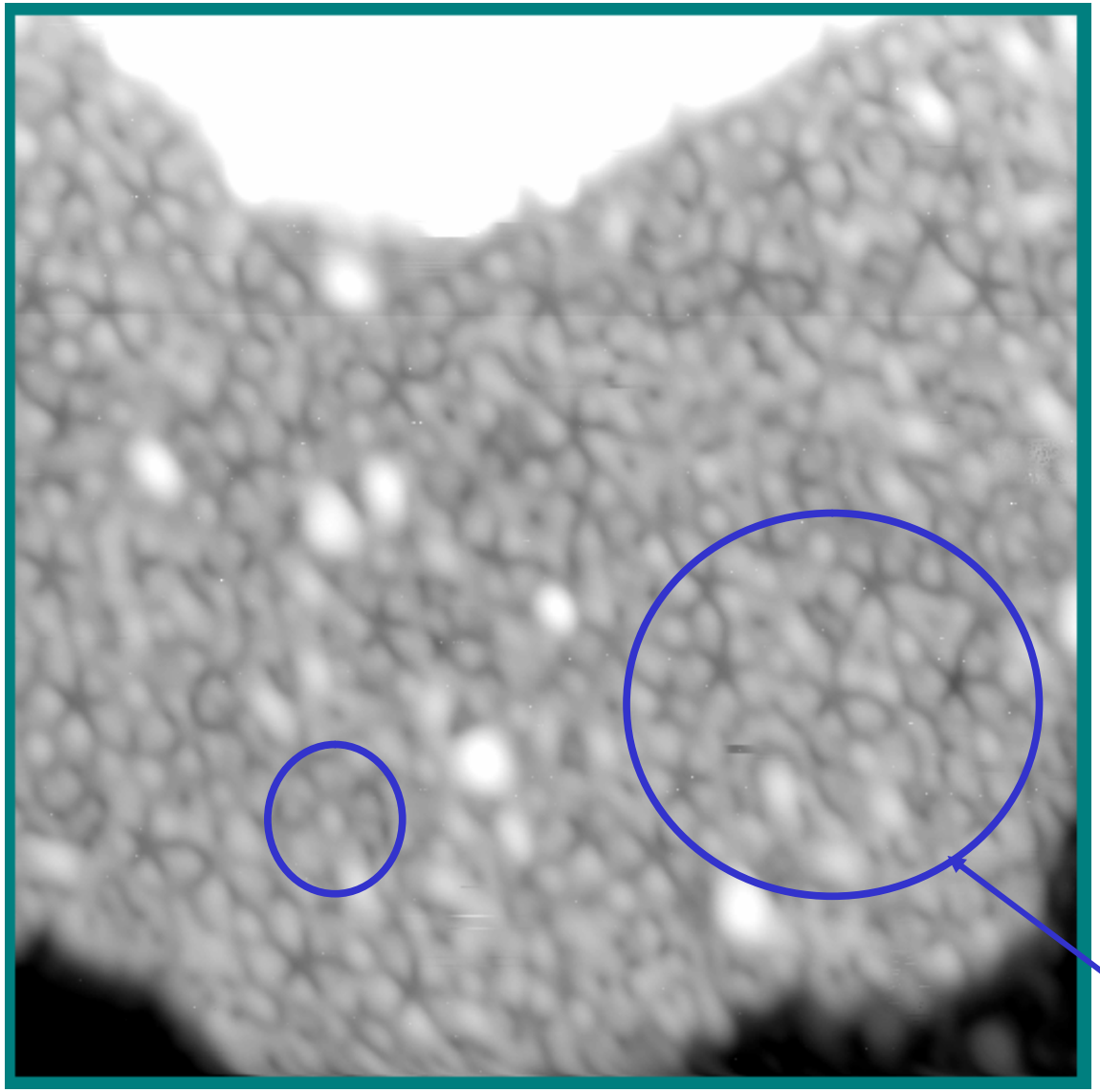
Model
f =10nm

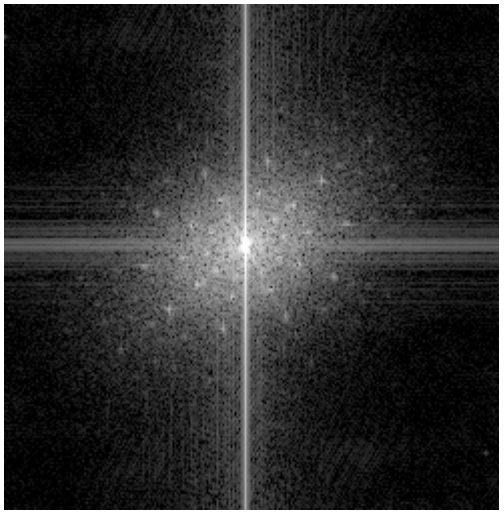


Z=-0.82 nm



Z=1.32 nm





26 nm x 26 nm

Indeed !

Different flowers

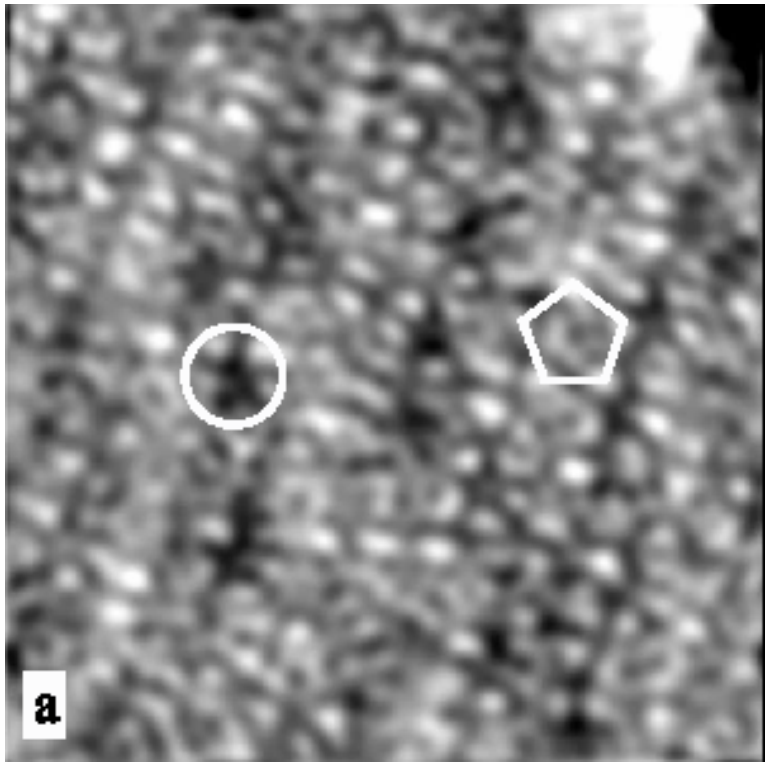
on an other terrace

Tiling of the fivefold surface of $Al_{70}Pd_{21}Mn_9$

J. Ledieu, R. McGrath, R. D. Diehl, T. A. Lograsso, D. W. Delaney, Z. Papadopolos and G. Kasner

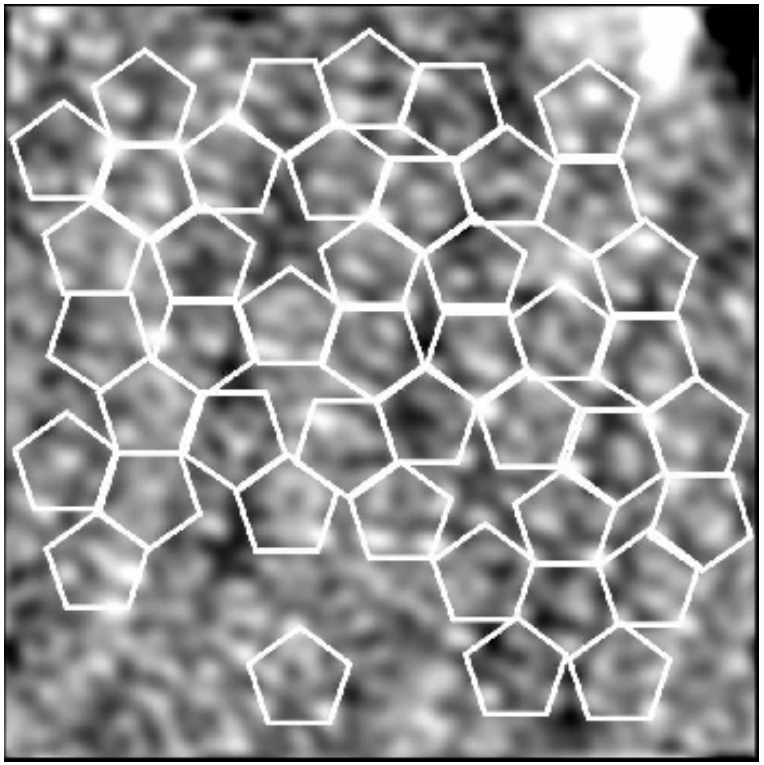
SURFACE SCIENCE, **492** (2001) **L729**.

Surface Science Research Centre, Liverpool

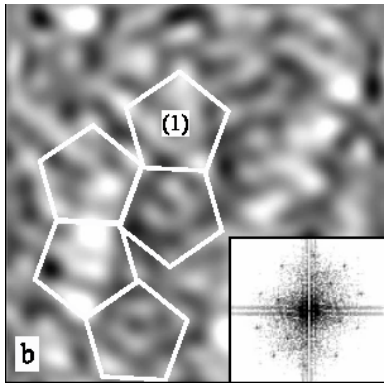


(10 x 10 nm^2)

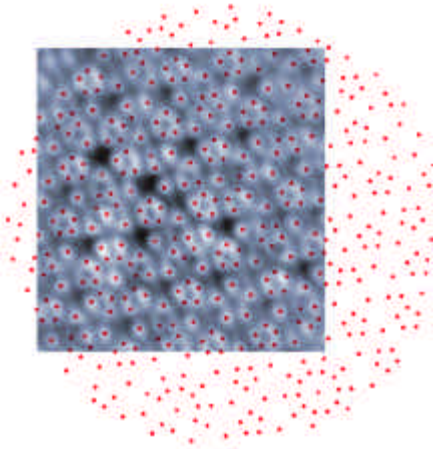
5-fold *i*-Al-Pd-Mn

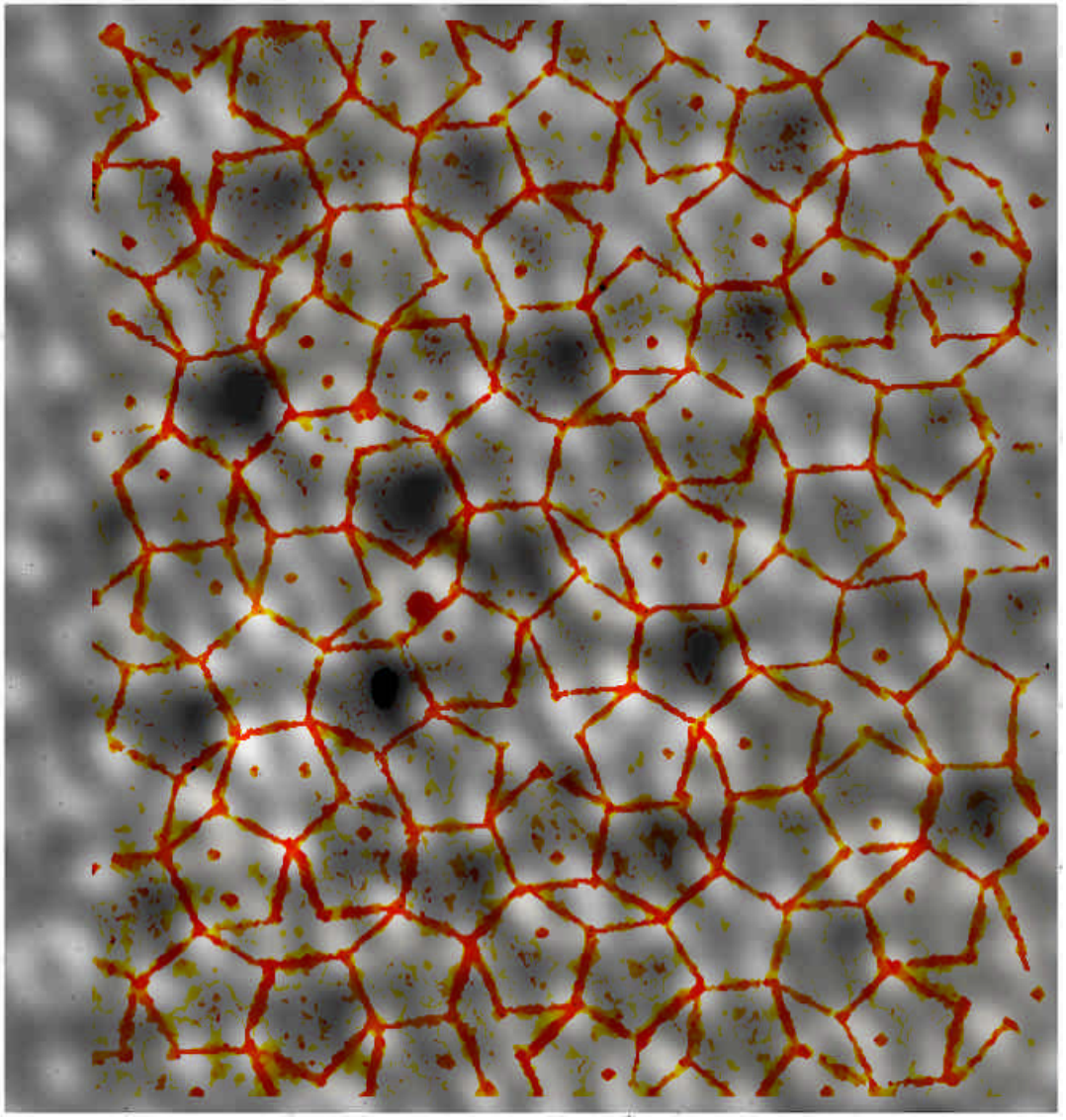


Geometrical tiling



Exact tiling versus 6-d model:



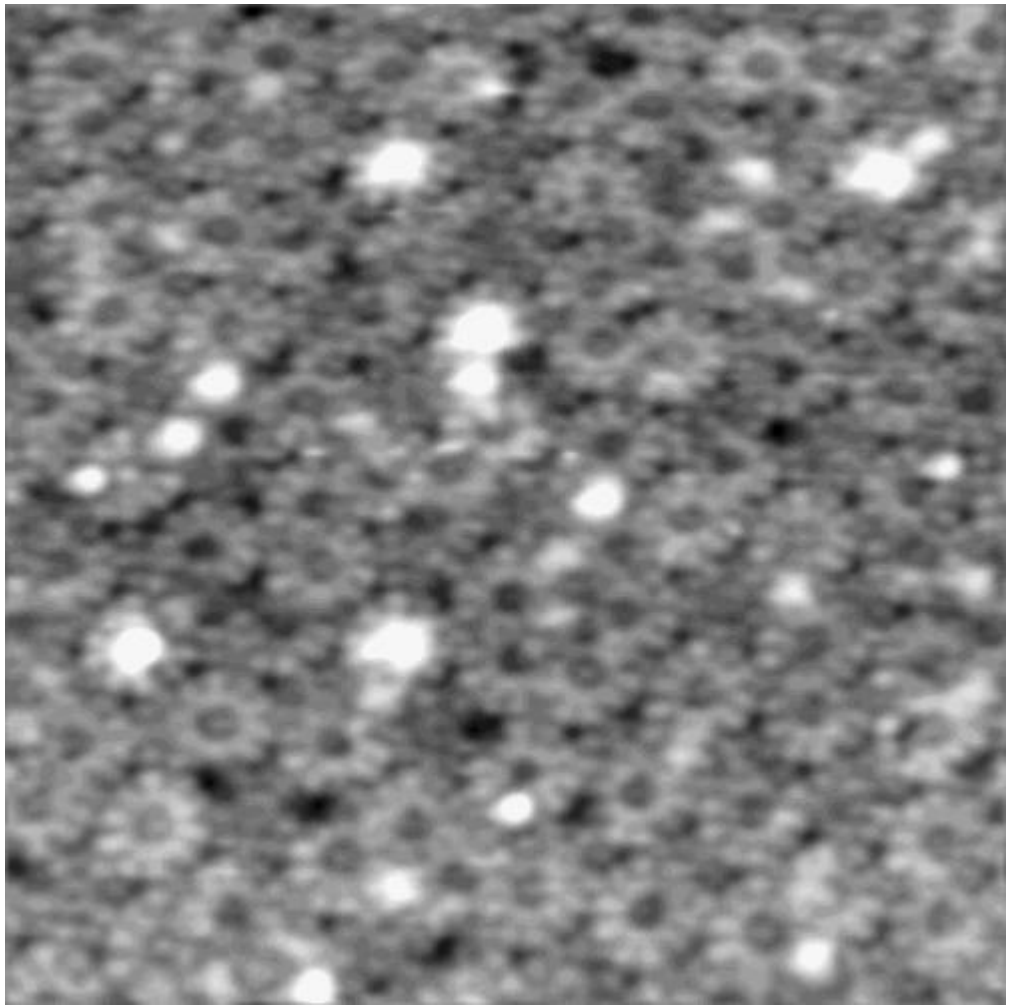


Exact tiling over STM picture
(Z. Papadopoulos, Private com.)

STM study of the atomic structure of the icosahedral Al-Cu-Fe fivefold surface

T. Cai, V. Fournée, T. Lograsso, A. Ross, and P. A. Thiel PHYS. REV. B, **65** (2002) 140202.

Ames Laboratory, Iowa State University, Ames, Iowa 50011



(20 x 20 nm^2) 5-fold *i*-Al-Cu-Fe

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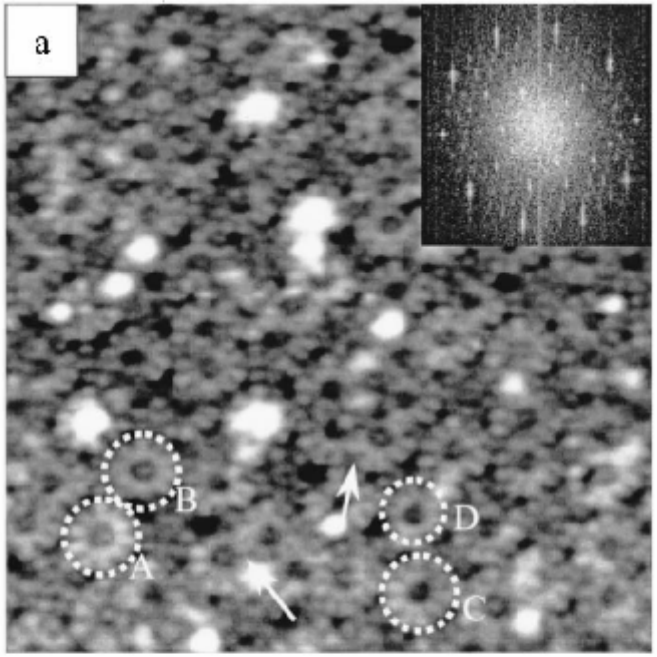
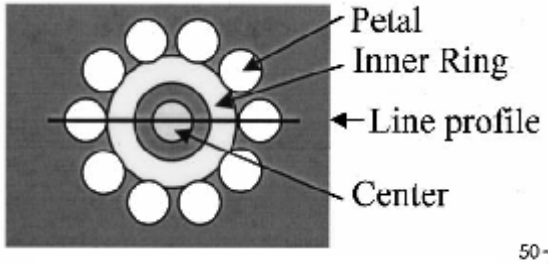
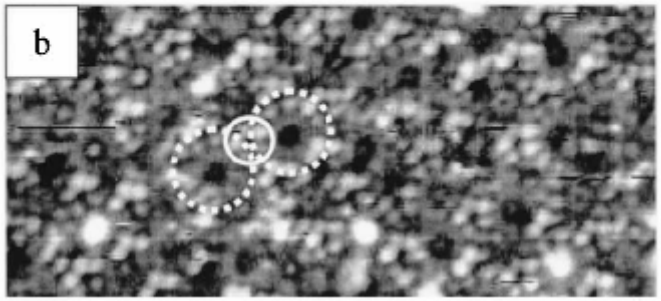
Surface = Bulk terminated



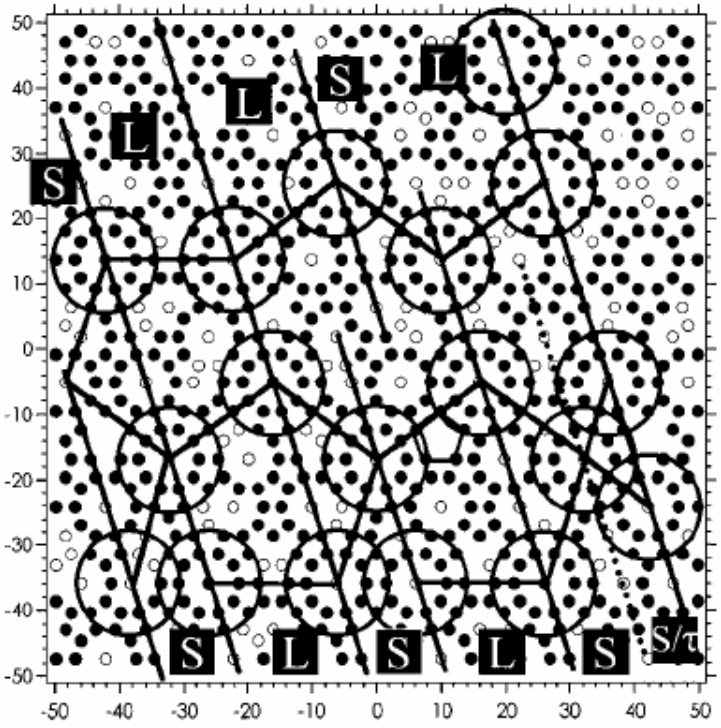


(20 x 20 nm^2)



(10 x 20 nm^2)

5-fold *i*-Al-Cu-Fe



(10 x 10 nm^2)

Bulk model : M. Boudard et al.

J.Phys.: Condens. Matter 4 (1992) 10149.

- Saclay -

STM study of the atomic structure of the icosahedral Al-Cu-Fe fivefold surface

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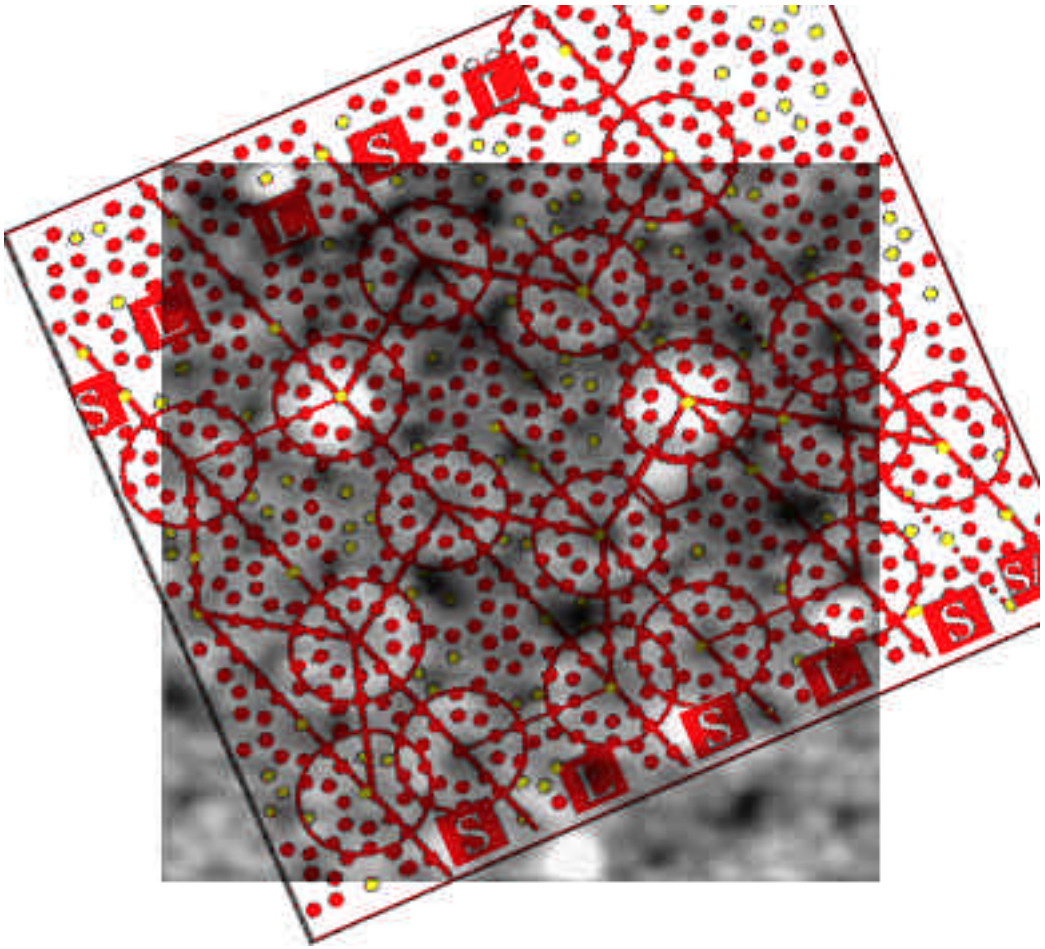

+ Boudard et al. bulk model
Cut at the level of an Al-rich surface plane

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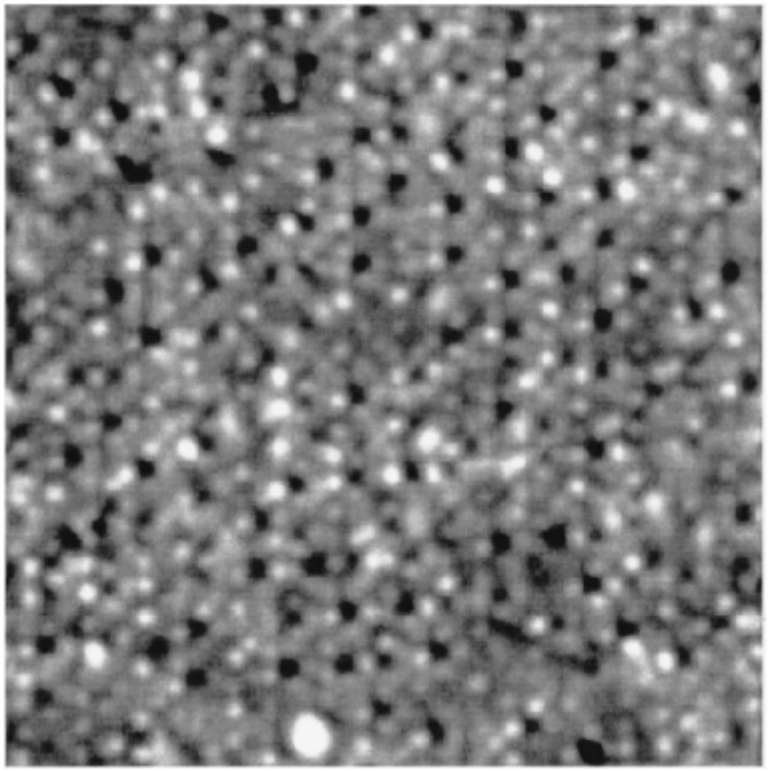


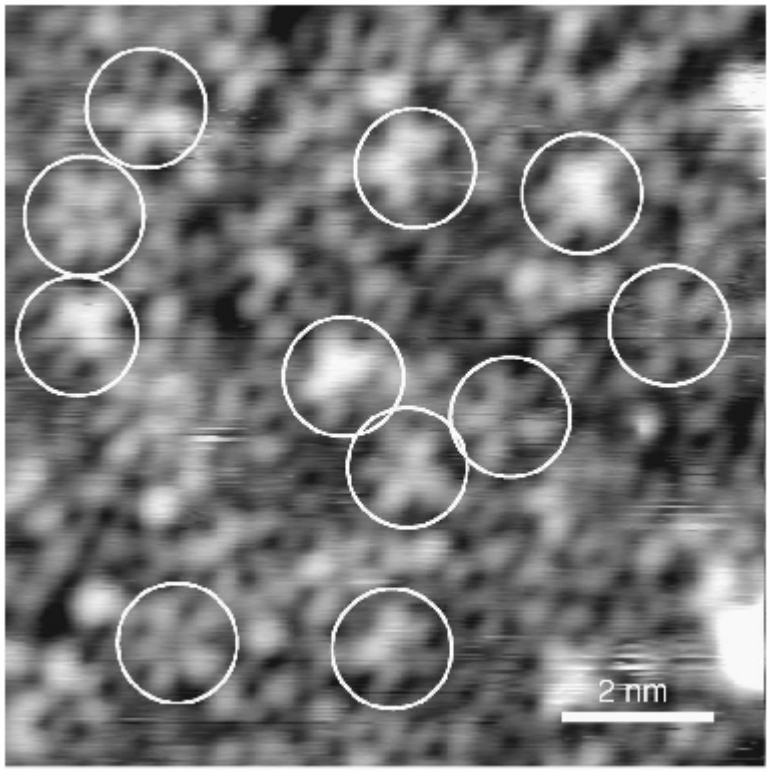
(20 x 20 nm^2)

i-Al-Pd-Mn

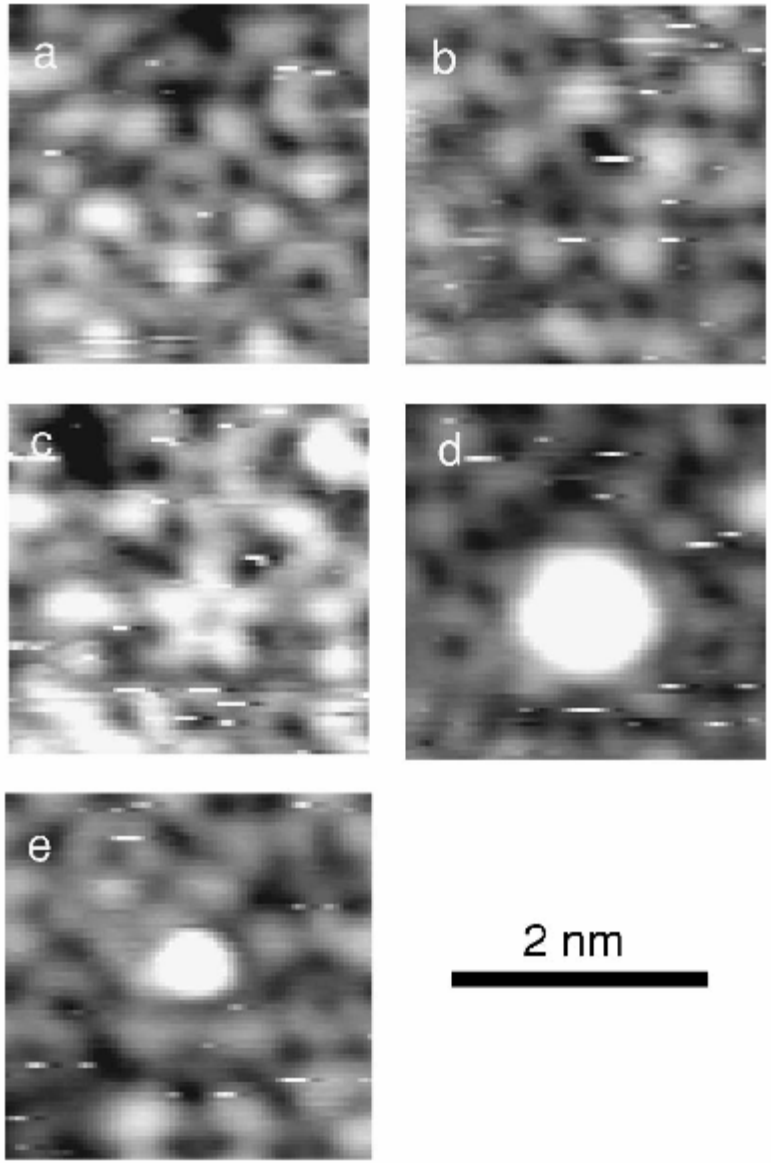
Scanning tunneling microscopy of an Al-Ni-Co decagonal quasicrystal

M. Kishida, Y. Kamimura R. Tamura, K. Edagawa, S. Takeuchi, T. Sato, Y. Yokoyama
J. Q. Guo and A. P. Tsai, PHYS. REV. B, **65** (2002) 094208

The University of Tokyo



Al-Ni-Co decagonal
10-fold plane



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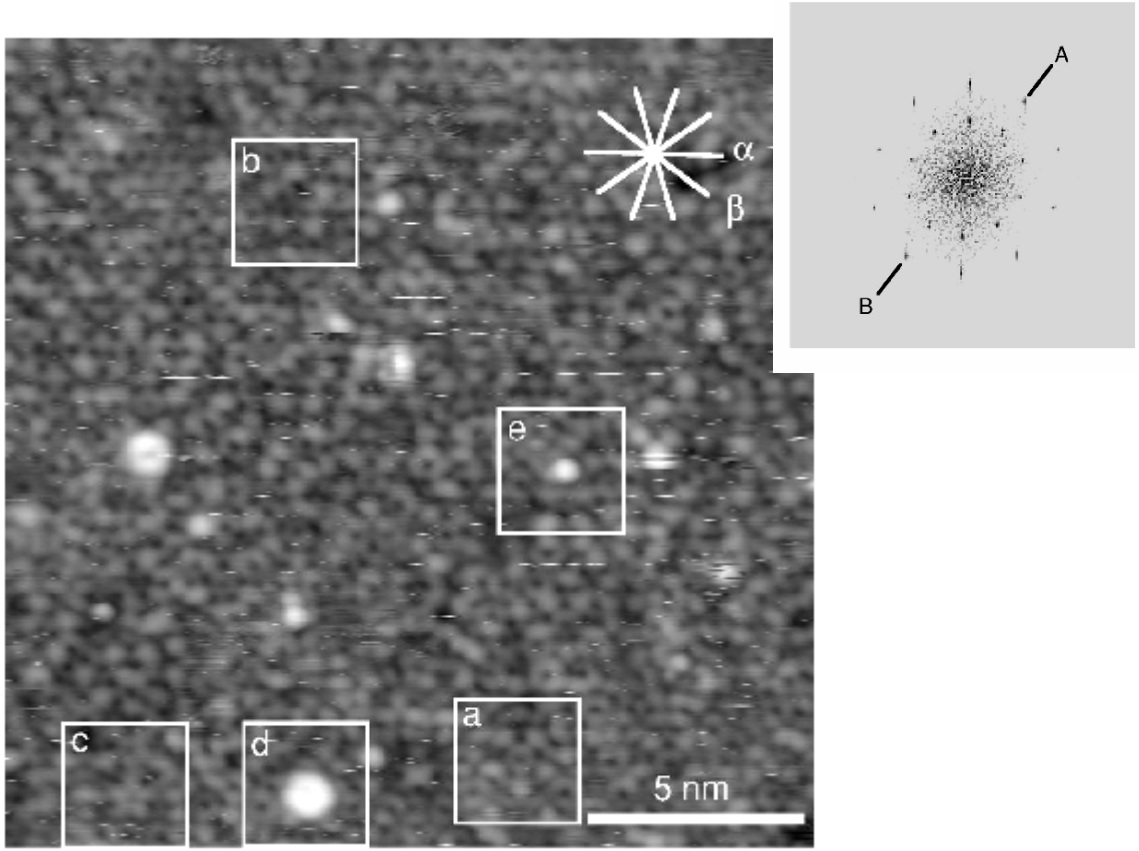
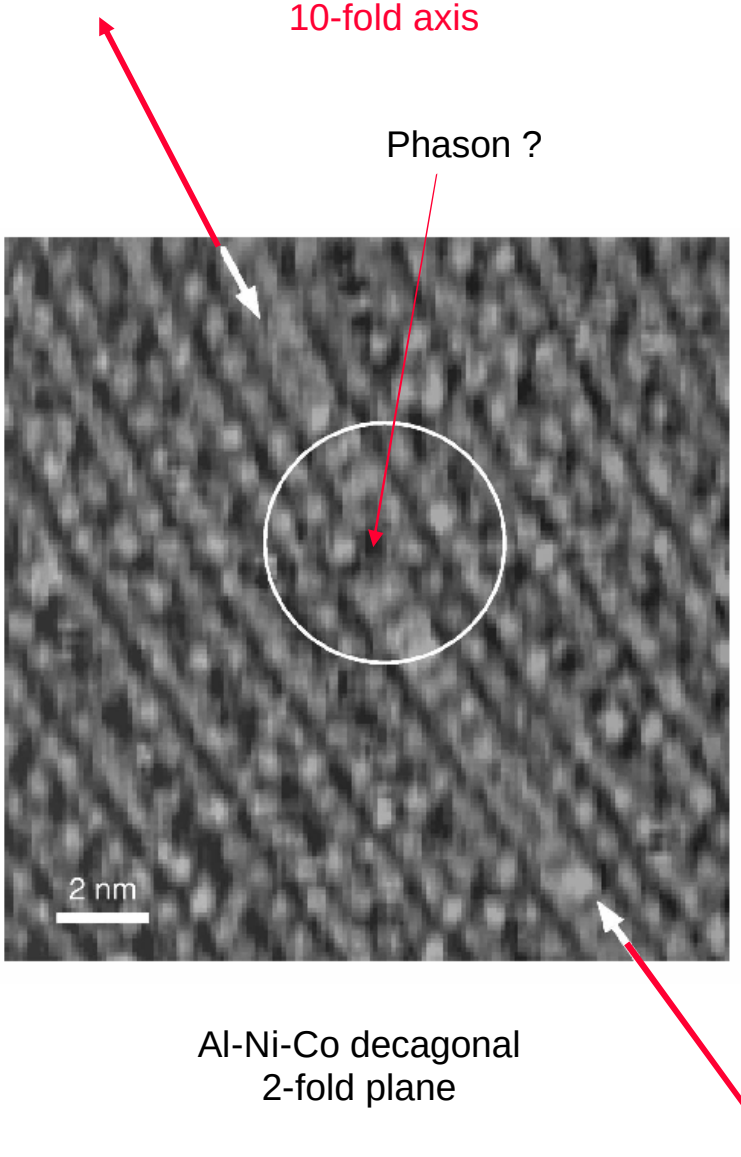


(18 x 18 nm^2)

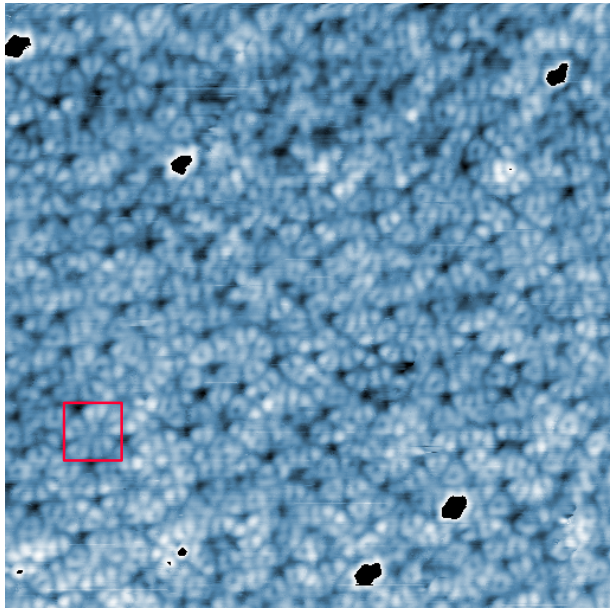
Al-Ni-Co decagonal
5-fold plane



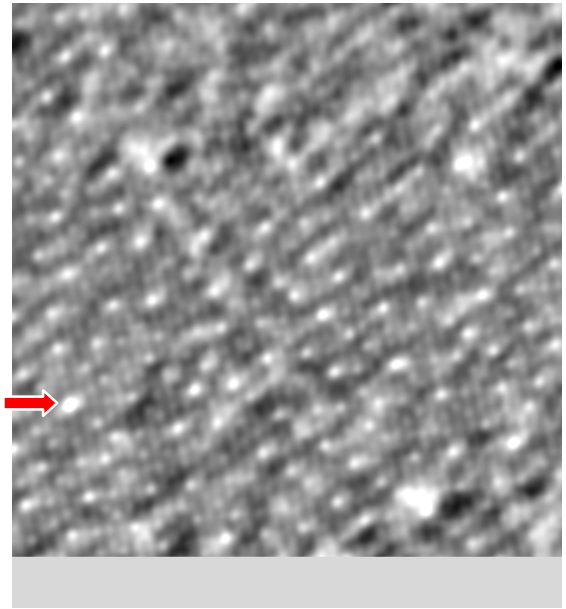
Al-Ni-Co decagonal
2-fold plane

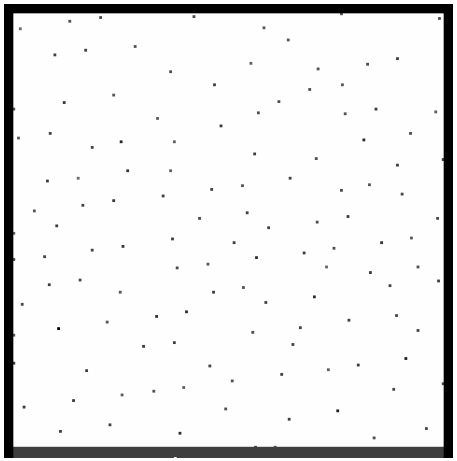
Looking for defects ! ...

Looking for defects

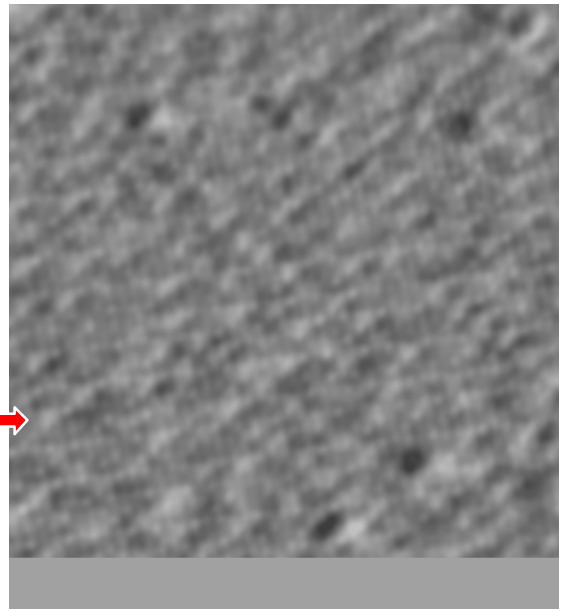


Original flower

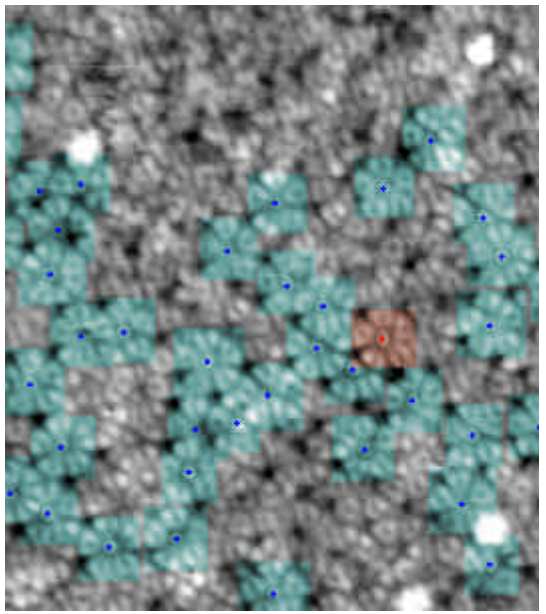




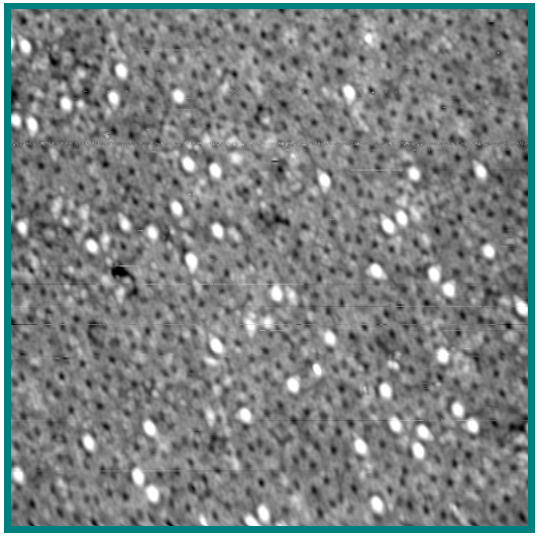
Inverted flower



Within one plane
all flowers have the same orientation



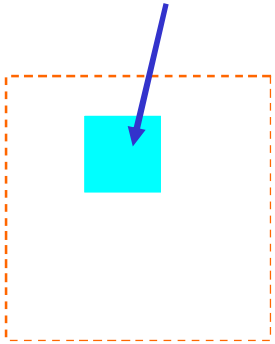
- Saclay -



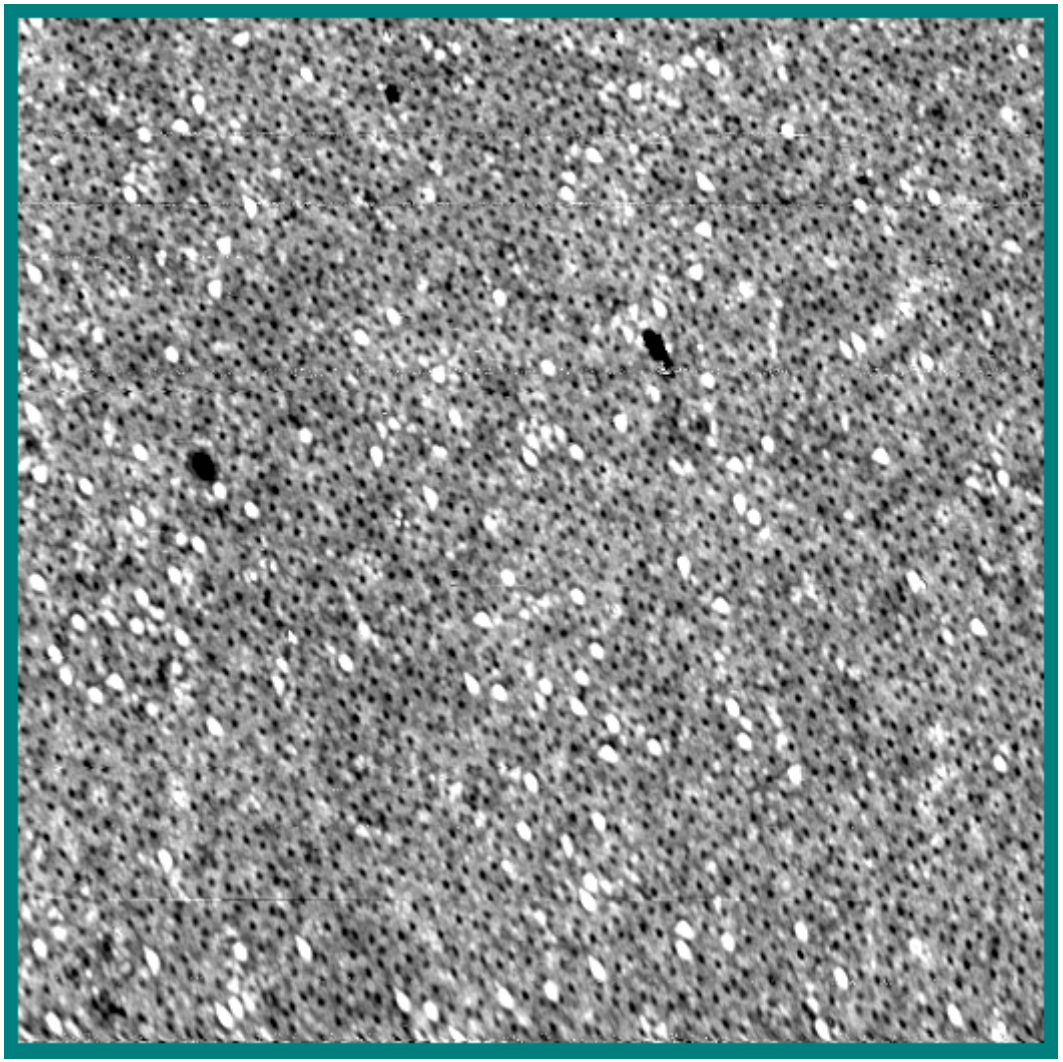
51 x 51 nm² !

T.F.

interpreted configuration



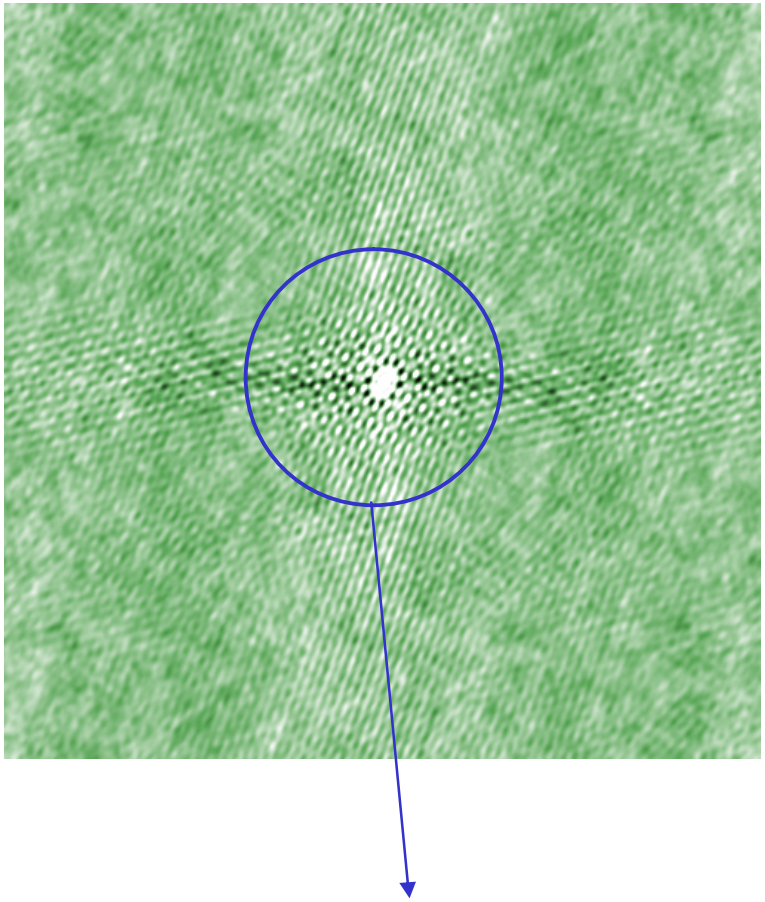
Same scale : Size of the precedent picture



102 x 102 nm² !

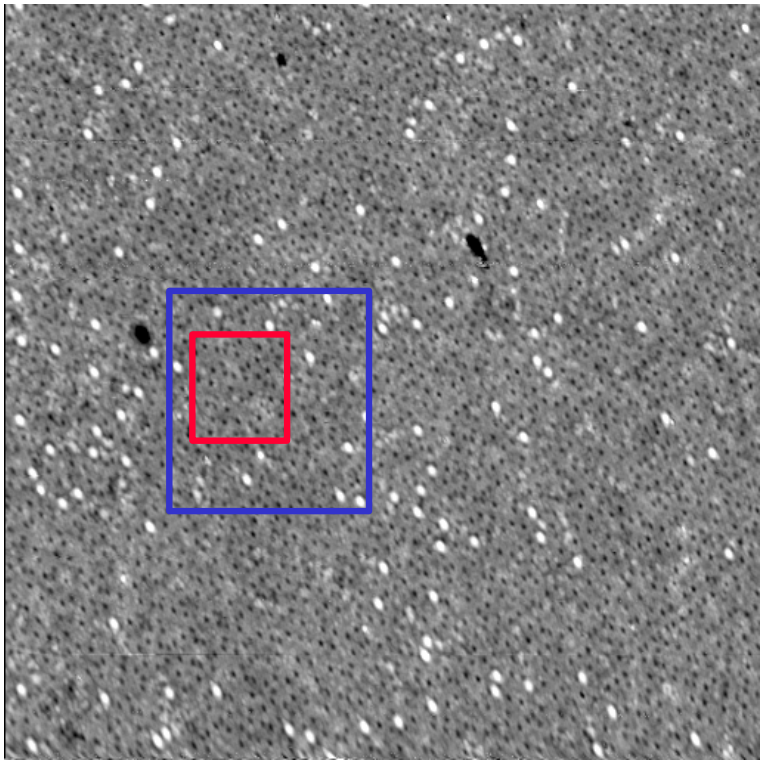
Autocorrelation function

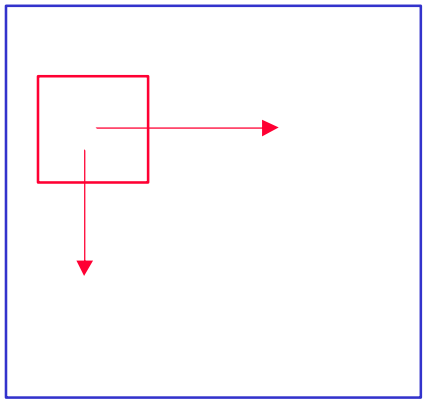
$$C(r_0) = \iint_r h(r) \bullet h(r - r_0)\, dr = FFT^{-1}\left[FFT \bullet \overline{FFT}\right]$$



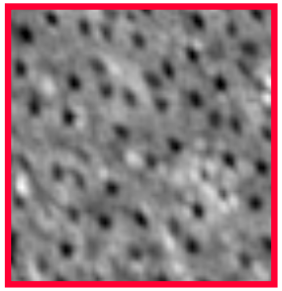
Locally well correlated

102 x 102 nm

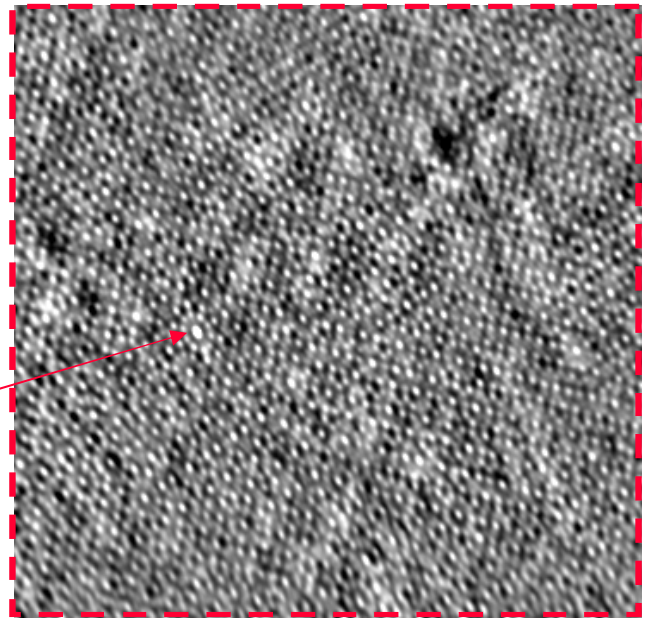




Small selection

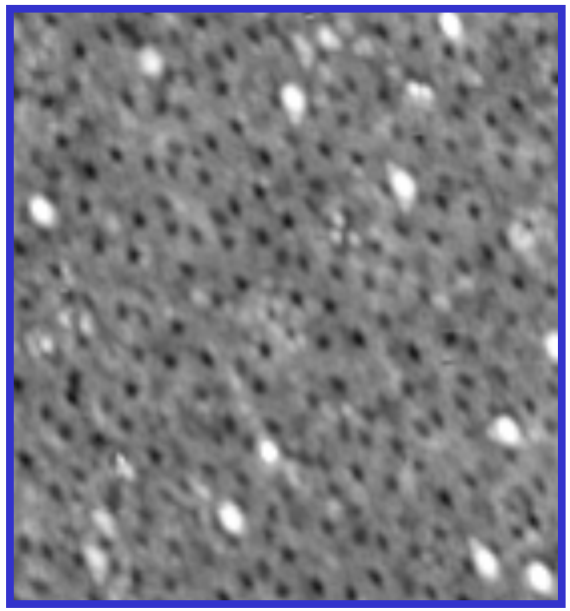


12 x 12 nm

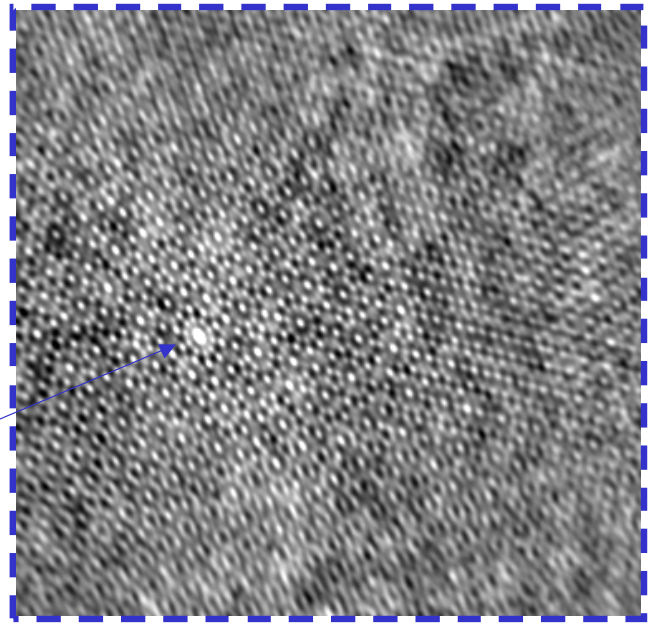


Selection center

Larger selection

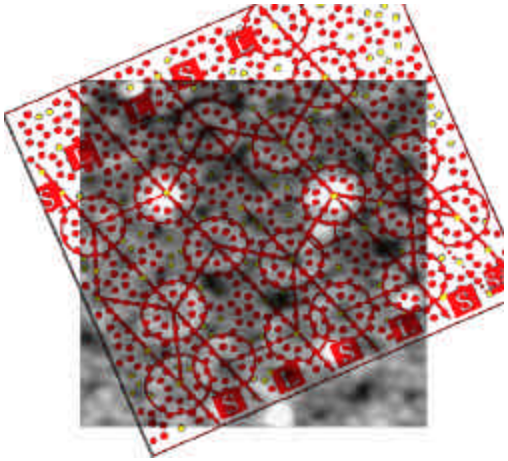


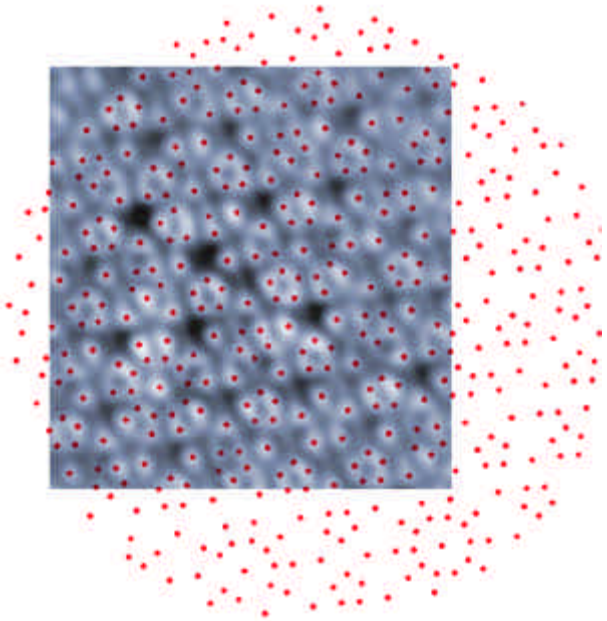
26 x 26 nm



Conclusion

- Surface structure = Bulk truncation structure !





- Local configurations can be identified

- Terraces are dense planes + chemically selected

- Looking for structural defects
  Correlation methods could help ?

- Phasons and surface defects ?