Aperiodic surfaces

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Overview

1. Surface structure of quasicrystals
2. Quasicrystal surfaces as templates
3. Other aperiodic surfaces

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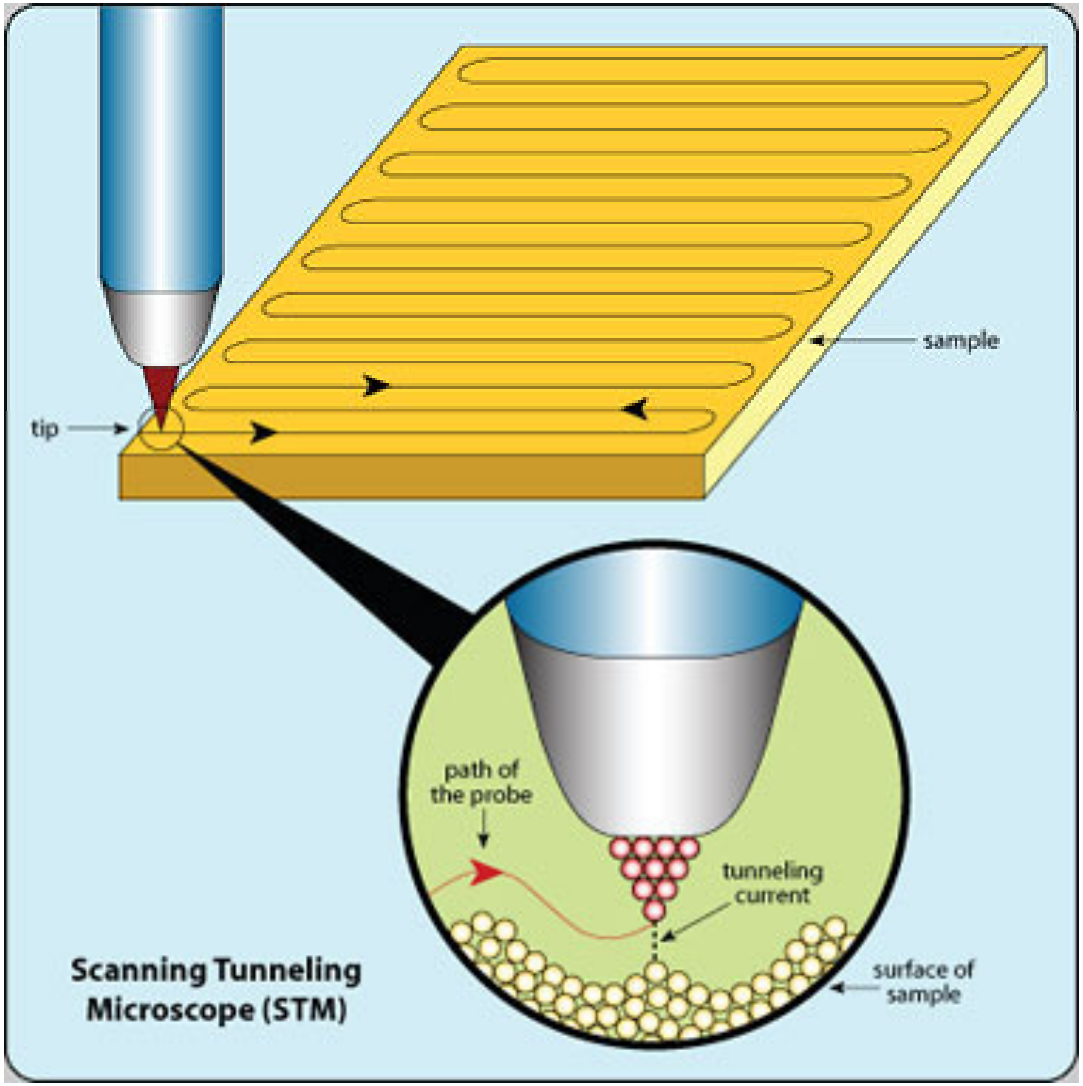
Scanning Tunnelling Microscopy (STM)

- Invented by Binnig and Rohrer at IBM Zurich in 1981-82. -



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First QC surface studies: Real-space atomic structure of a two-dimensional decagonal quasicrystal: $Al_{65}Cu_{20}Co_{15}$

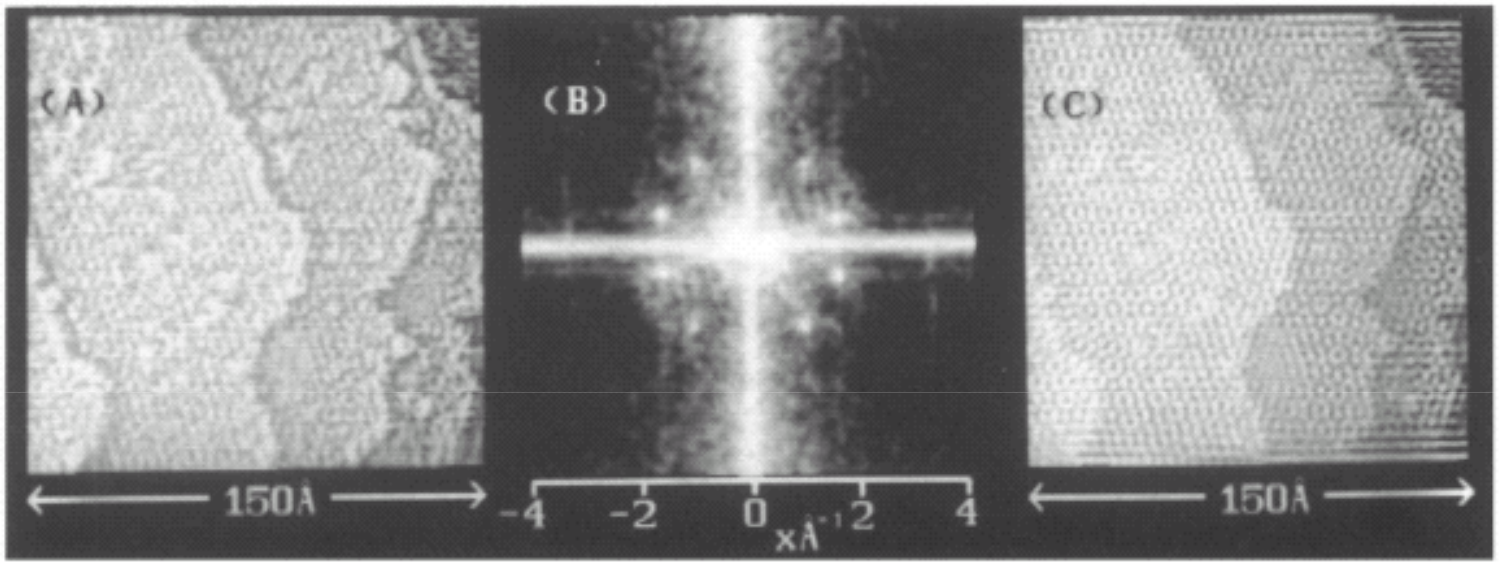

FIG. 1. A tunneling image of the quasiperiodic surface of decagonal $Al_{65}Co_{20}Cu_{15}$. (a) The lateral scale is indicated and the gray scale is derived from local height. (b) Normalized power spectrum of the image, with the wave-vector scale indicated. (c) Small-scale feature enhancement as described in the text.

A. R. Kortan, R. S. Becker, F. A. Thiel, and H. S. Chen, Phys. Rev. Lett. 64, 200 (1990).

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2.1 Case study:

Quasi-Crystalline Structure of Icosahedral $Al_{68}Pd_{23}Mn_9$ Resolved by Scanning-Tunneling-Microscopy

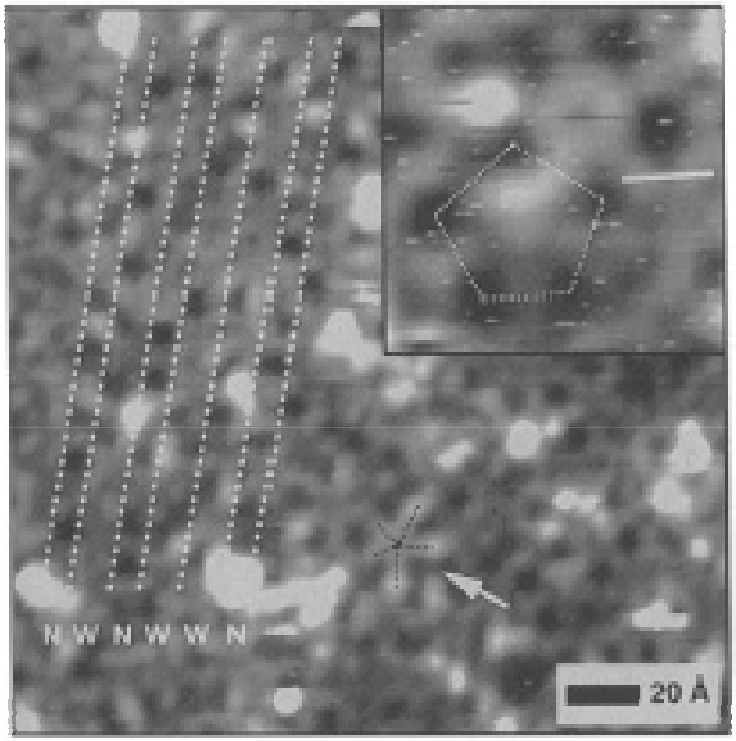

Fig. 3. 200 Å X 200 Å wide STM image of a fivefold terrace on i-AlPdMn. The fivefold symmetry within the terrace is indicated by fivefold 'stars' (arrow), and pentagonal holes, which frequently form larger, self-similar structures like regular pentagons (inset). The edges of most of the holes can be connected by five sets of parallel lines, yielding wide (W, and narrow (N) line separations (Fibonacci-pentagrid).. Size of the inset: 43 Å X43 Å.

Schaub T. M., Bürgler D. E., Güntherodt H. J., Suck, J. B., Phys. Rev. Lett. 73, 1224 (1994).

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Surface structure:

Structural Analysis of the Fivefold Symmetric Surface of the $Al_{70}Pd_{21}Mn_9$ Quasicrystal by Low Energy Electron Diffraction

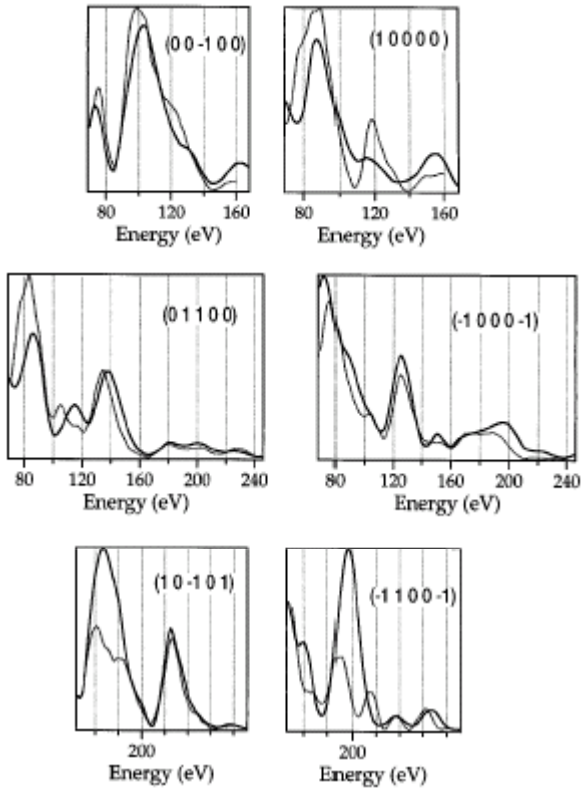

FIG. 2.Best-fit experimental and theoretical IV curves, averaging theory equally over the ten best individual terminations, including relaxations in the top four interlayer spacings of each.

- Approximations were developed to make the structure accessible to LEED.
- Mixture of several relaxed, bulklike terminations is found
- a dense Al-rich layer on top followed by a layer with a composition of about 50% Al and 50% Pd.
- The interlayer spacing between these two topmost layers is contracted by 0.1 to 0.38 Å,
- The lateral density of the two topmost layers taken together is similar to that of an Al(111) surface.

M. Gierer, M. A. Van Hove, A. I. Goldman, Z. Shen, S.-L. Chang, C. J. Jenks, C.-M. Zhang, and P. A. Thiel
Phys. Rev. Lett. 97, 467 (1997).

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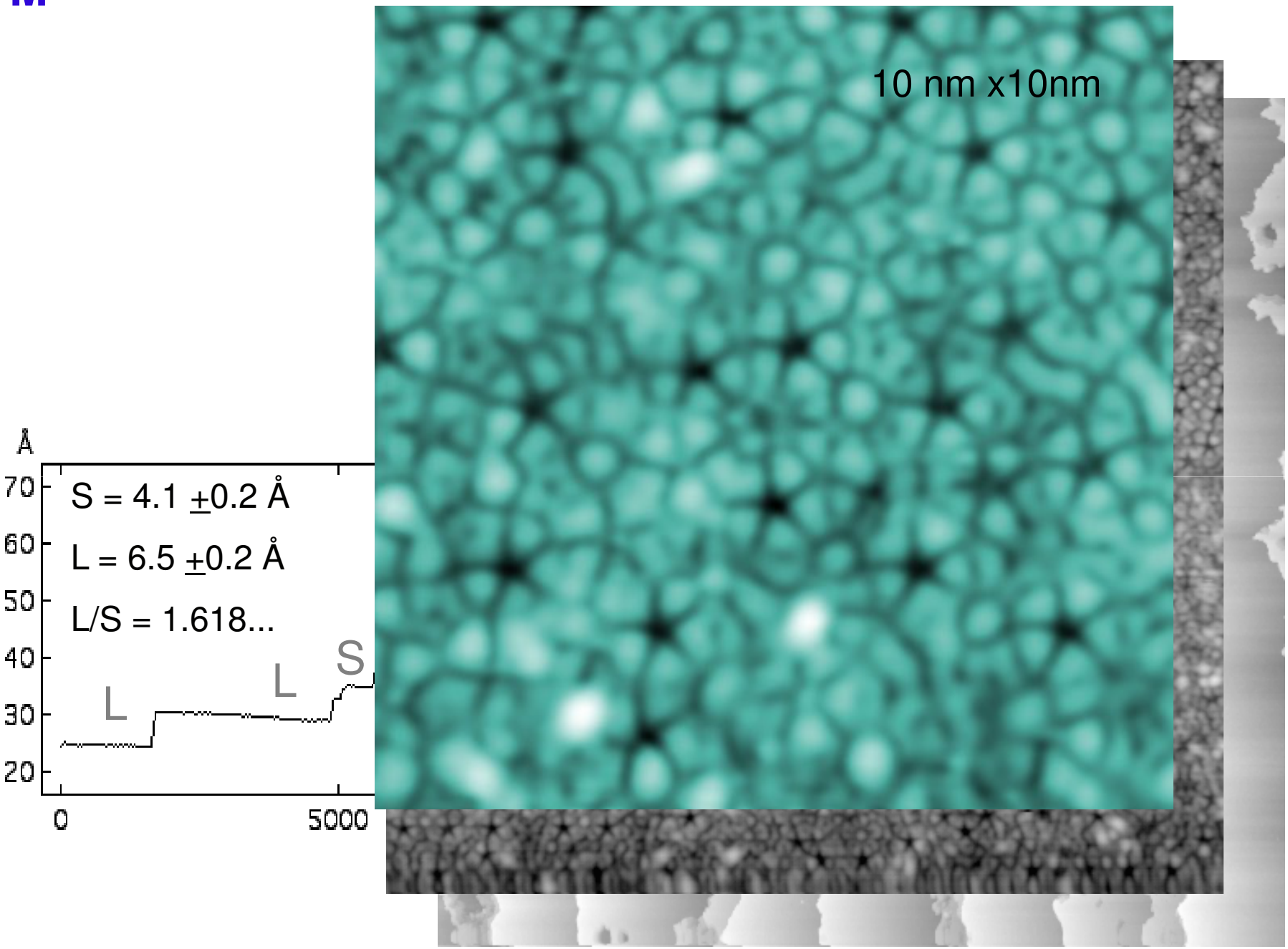
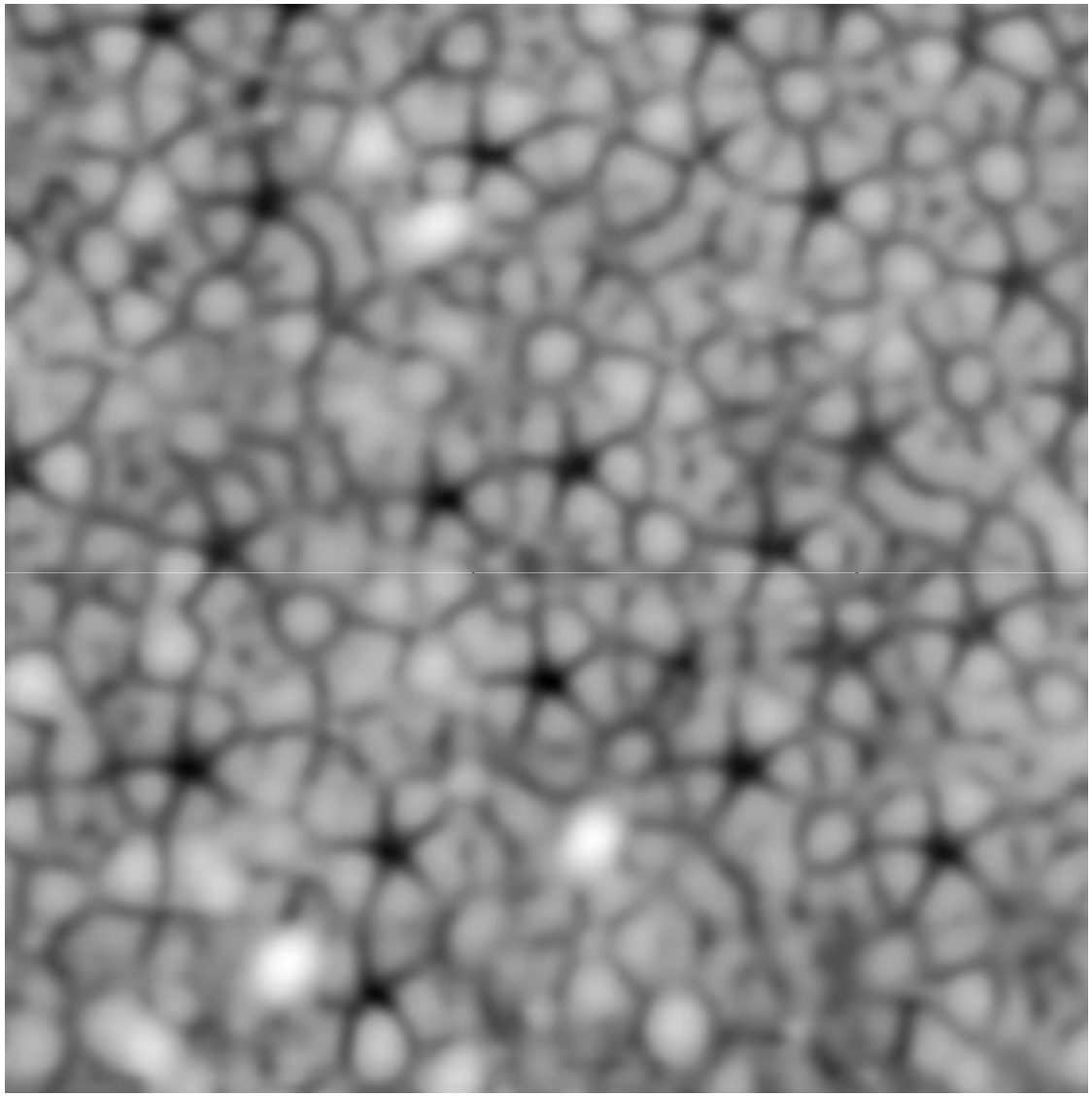
STM





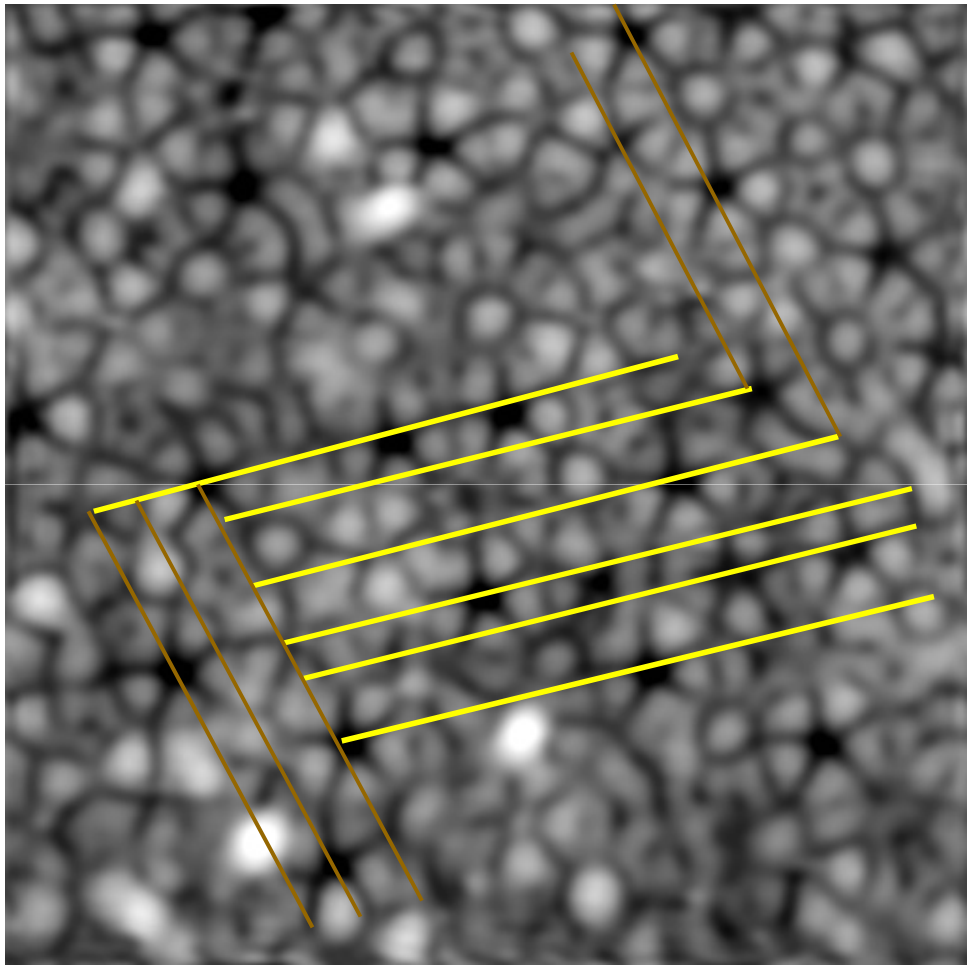
Fibonacci lines - Al-Pd-Mn Surface

...LSLLSL...

S = 4.6 Å

L = 7.4 Å

L / S = τ



100Å x 100Å STM image

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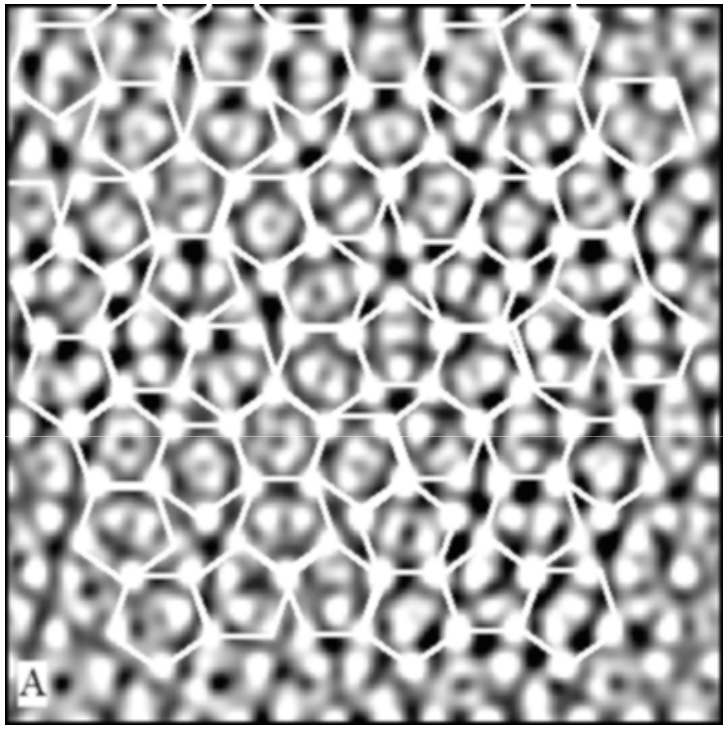
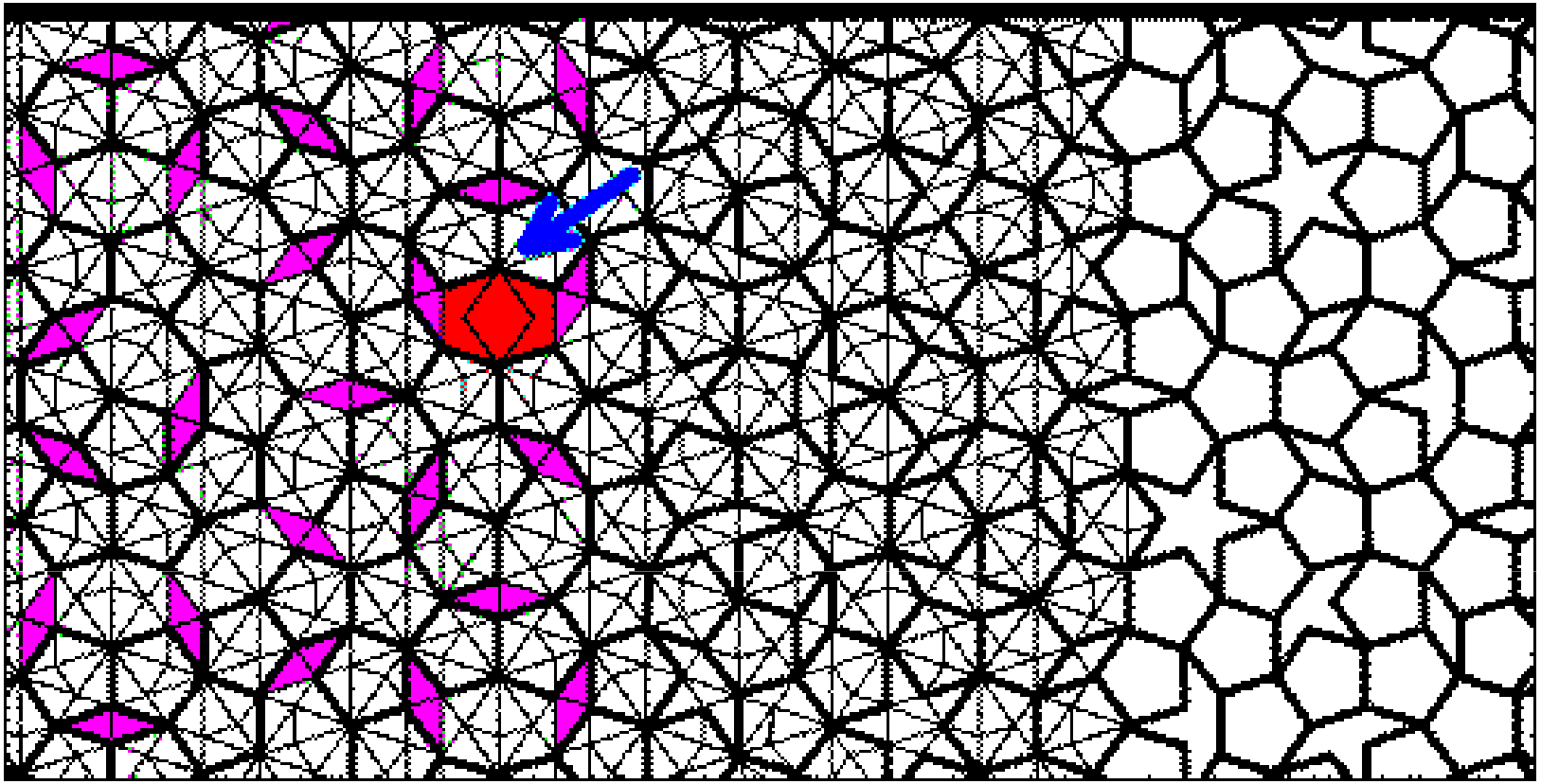
Penrose tiling



100Å x 100Å

•Surf. Sci. Lett. 492/3 (2001), pp L729-L734, Phys. Rev. B 66 (2002) 184207

Comparison with Katz-Gratias-Elser geometric model:



The edge length of the tiles in the model =7.758 Å matches the experimental value 8.0±0.3 Å

J. Ledieu, R. McGrath, R.D. Diehl, T.A. Lograsso, D.W. Delaney, Z. Papadopolos and G. Kasner Surf. Sci. Lett. 492/3 (2001), pp L729-L734, Phys. Rev. B 66 (2002) 184207

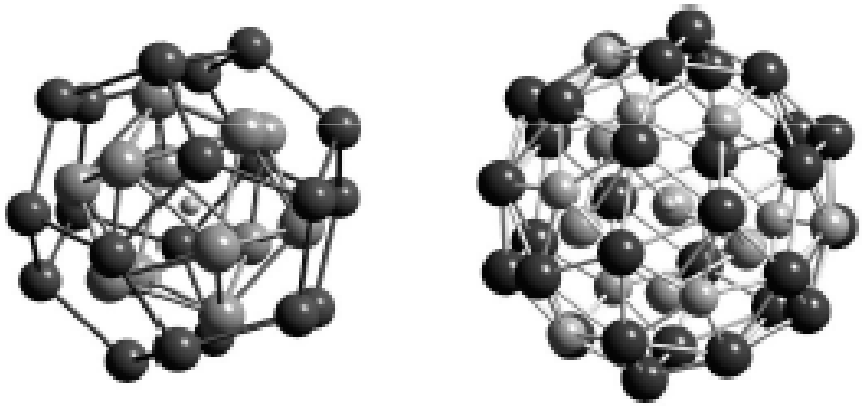
Clusters in the Al-Pd-Mn qasicrystals

PHYSICAL REVIEW B, VOLUME 63, 024202

Atomic clusters in icosahedral *F*-type quasicrystals

Denis Gratias, Frédéric Puyraimond, and Marianne Quiquandon
LEM-CNRS/ONERA, BP 72, 29 Avenue de la division Leclerc, 92322 Châtillon Cedex, France

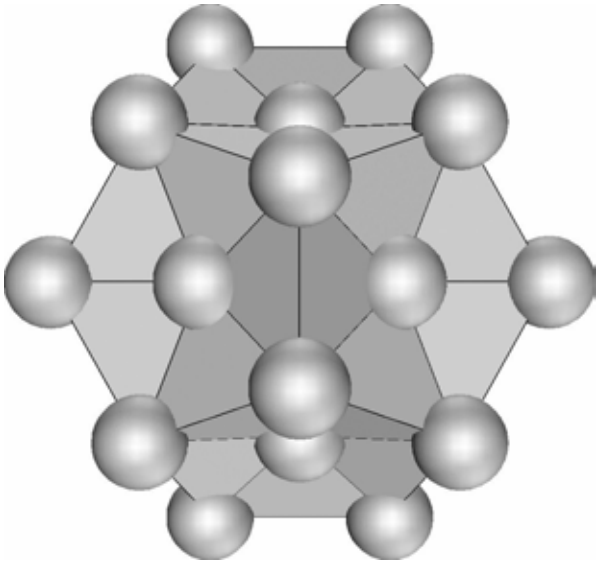
André Katz

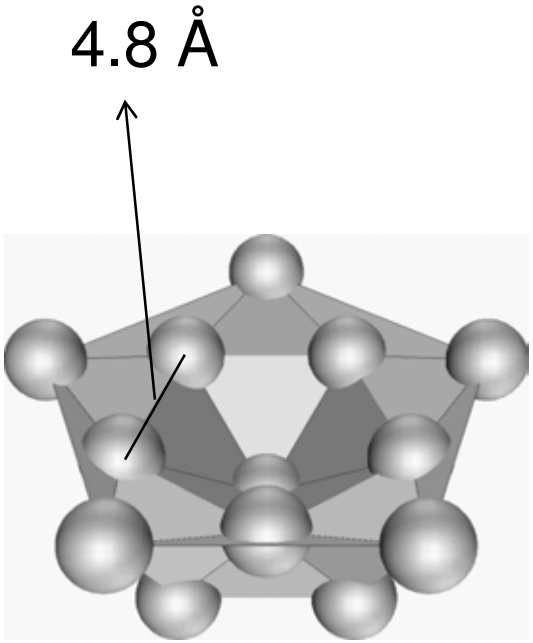


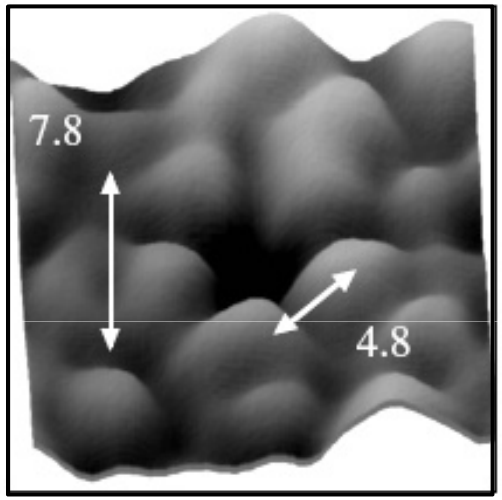
(a) (b)

FIG. 4. (a) 33 atoms *B* cluster; (b) 50 atoms *M* cluster (the central dodecahedron contains only seven atoms). Observe that these two clusters are only similar to the Bergman and Mackay clusters encountered in several complex intermetallic phases.

Cut Bergman: equatorial truncation



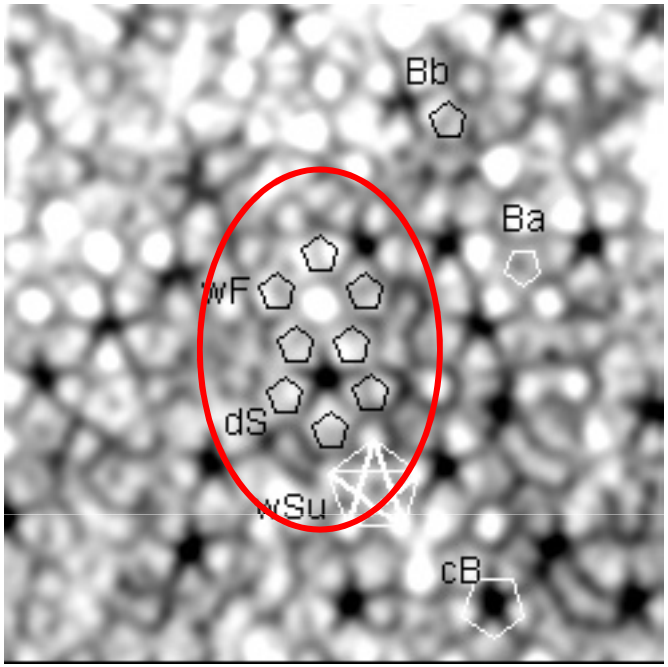


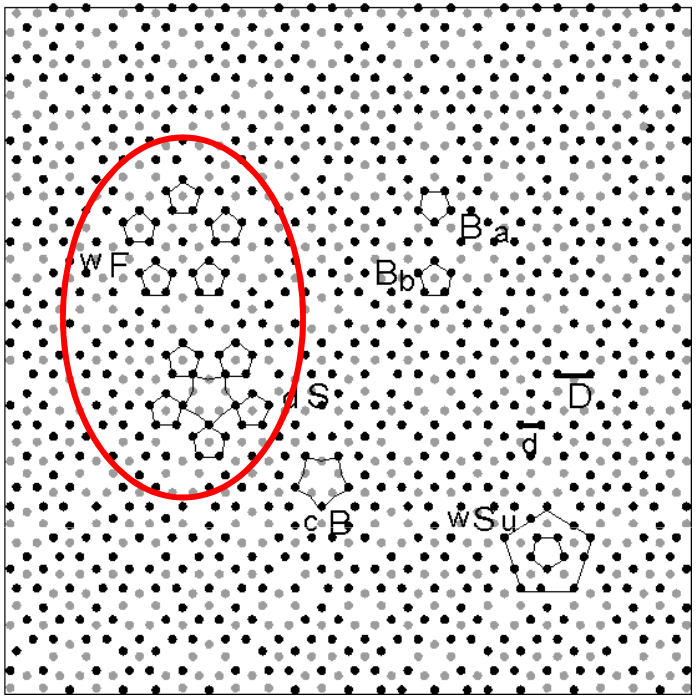


Note: cB indicates a Cut Bergman cluster as the origin of the 5-fold hollow features.

Ledieu and McGrath, J. Phys. Conds. Matter 15 (2003)

Detailed comparison of local features: STM vs geometric model $\mathscr{M}$: the C termination

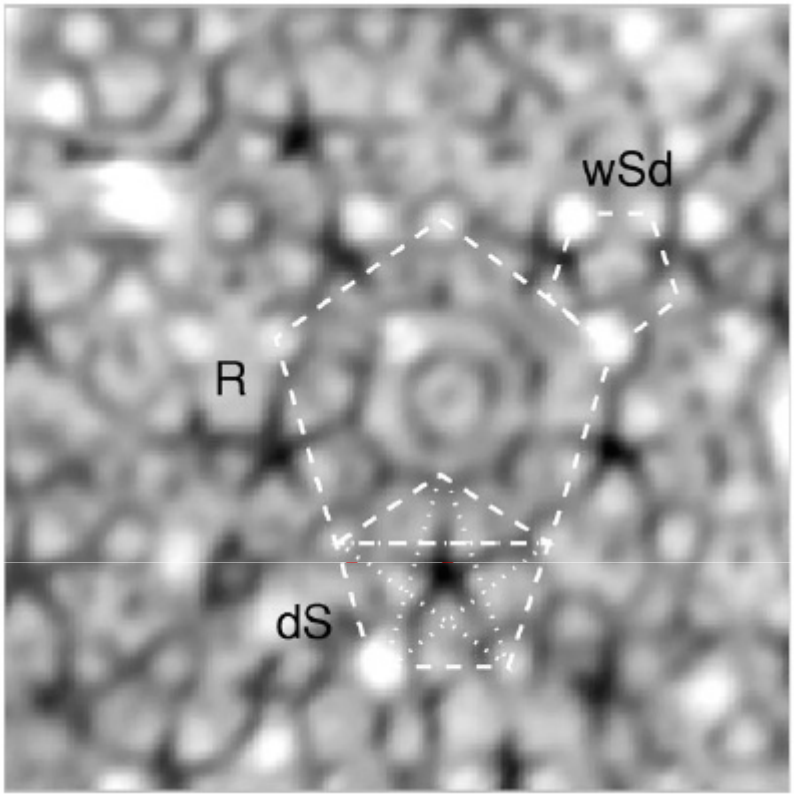


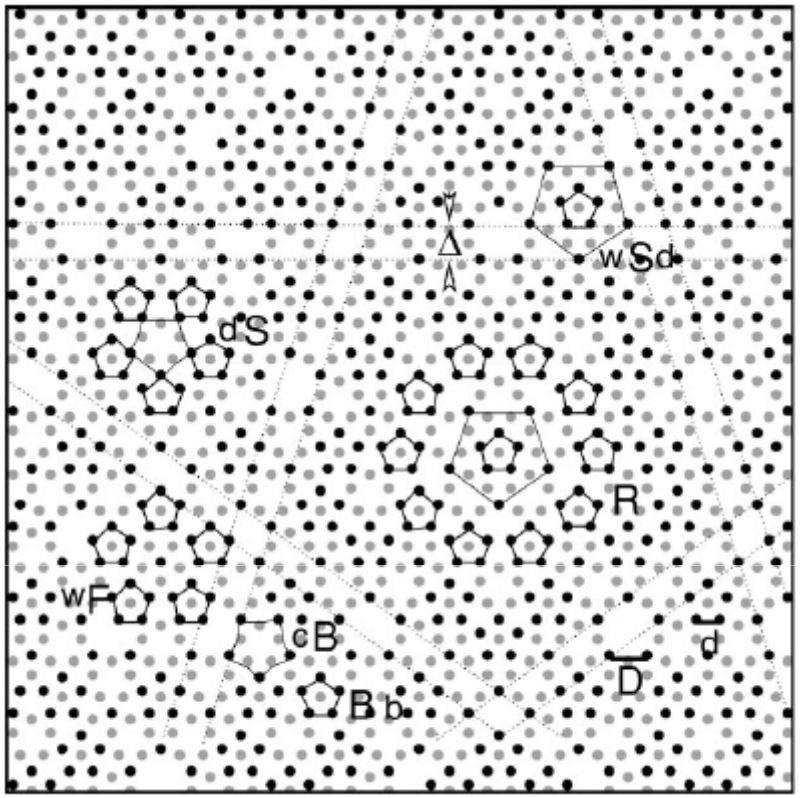


Note: cB indicates a Cut Bergman cluster as the origin of the 5-fold hollow features.

Papadopolos et al. Phys. Rev. B 66 (2002) 184207

Detailed comparison of local features: STM vs geometric model $\mathscr{M}$: the R termination





cB indicates a Cut Bergman cluster as the origin of the 5-fold hollow features.

Papadopolos et al. Phys. Rev. B 66 (2002) 184207

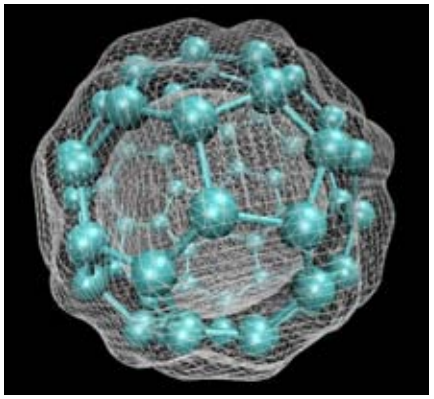
Density functional theory calculations (DFT)

•Last 15 years has seen wide availability of computer codes to solve Schrödinger's equation for large groups of atoms

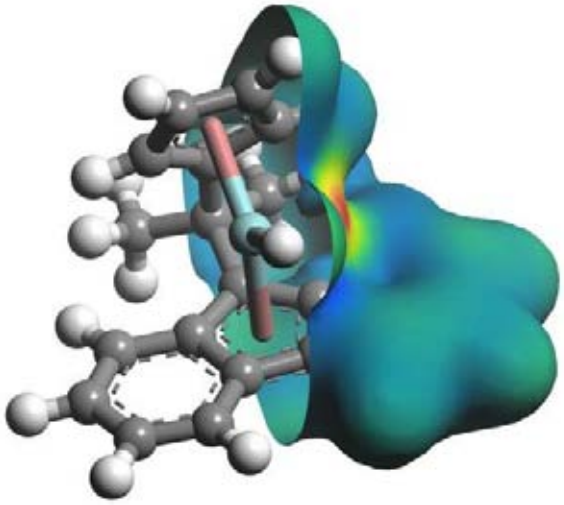
• Based on density functional theory (DFT) using the local density approximation (LDA) and the generalised gradient approximation (GGA)

• Much success in application to minimum energy surface structures to clean surfaces and simple adsorbate systems

• Can be used to create simulated STM data for comparison to aid interpretation of real data



Molecules with isosurfaces of ground state electron density as calculated with **DFT**



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Modelling approach

ab initio density functional calculations using VASP : Vienna *Ab Initio* Simulation Package

But

These codes only work for periodic materials!

Solution: Use Approximants

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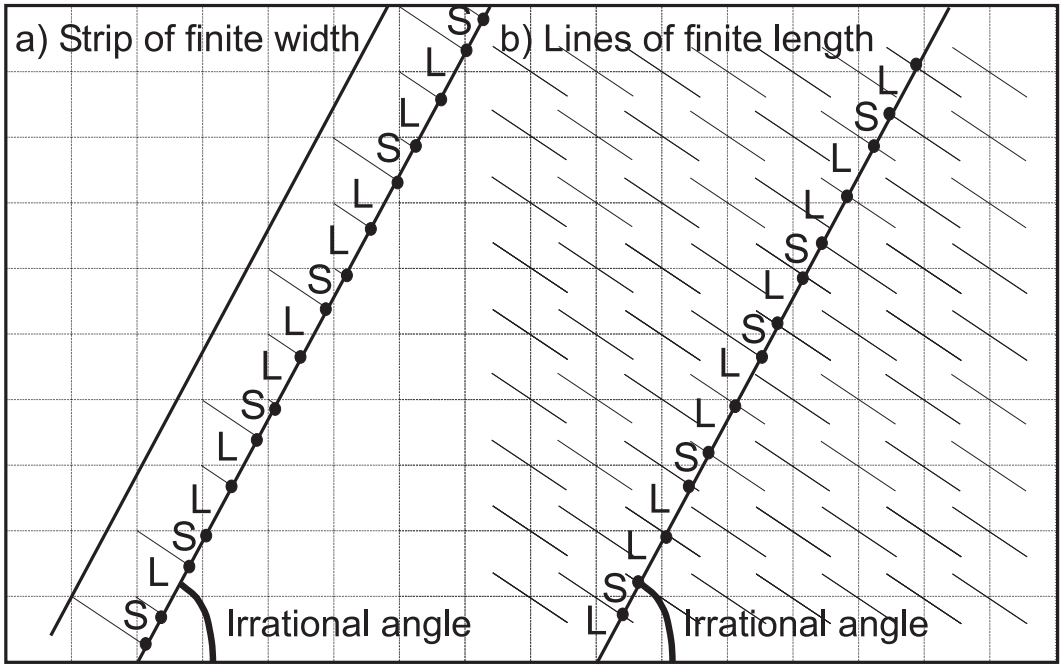
Cut and project method:

A methodology for generating lower dimensional quasicrystal structures from higher dimensional crystalline structures



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Cut and project method

The cut-and-project method can be used with a rational angle to give a periodic quasicrystal approximant. The angle is expressed in terms of the ratio of terms of the Fibonnacci sequence.

e.g instead of $\tan^{-1}\tau$, use $\tan^{-1}$ 3/2 ,

gives the 3/2 approximant

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DFT: calculations of surface structure of AlPdMn quasicrystal

calculations performed on 3/2 and 2/1 rational approximants;
structural relaxations only for 2/1 approximant

TABLE I. Structural data of approximants to *i*-AlPdMn and of the slab models for the fivefold surface. Cell dimensions d_t, $t=x,y,z$ in Å, number of atoms N_a, and chemical composition.

Model	d_x	d_y	d_z	N_a	N(Al)	N(Pd)	N(Mn)
2/1 bulk	20.31	20.31	20.31	544	372	124	48
2/1 MS	23.88	20.31	6.60	205	137	54	14
2/1 M	23.88	20.31	4.08	136	96	36	4
3/2 bulk	32.86	32.86	32.86	2292	1612	472	208
3/2 MS	39.40	32.86	6.60	535	364	132	39
3/2 M	39.40	32.86	4.08	357	251	92	14
5/3 bulk	53.17	53.17	53.17	9700	6844	2012	844
5/3 MS	62.51	53.17	6.60	1401	965	340	96
5/3 M	62.51	53.17	4.08	930	663	236	31

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M. Krajcí and J. Hafner, Phys. Rev. B. 71 (2005) 054202

DFT: calculations of surface structure of AlPdMn quasicrystal: This termination equivalent to the “R” termination in the M model

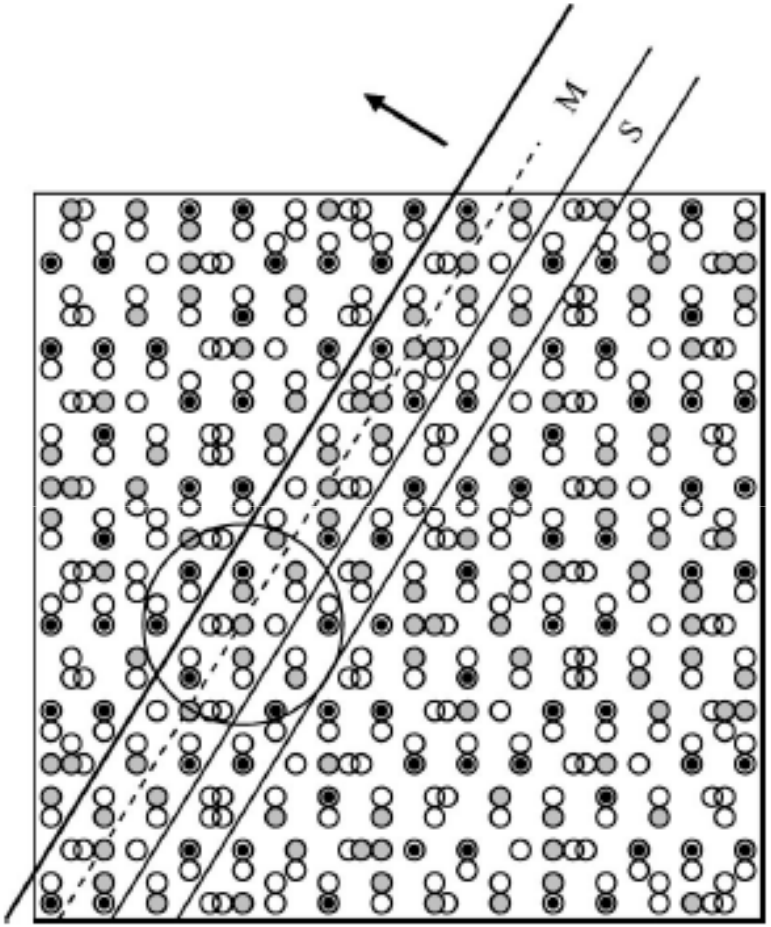

FIG. 3. Side view of the MS and the M models of the *i-AlPdMn* surface derived from the 3/2-approximant.

The M model consists of the M slab only. The dashed line in the middle of the M slab indicates the positions of centers of the *B* clusters. The radius of one B cluster is indicated by the circle. The surface plane dissects the B clusters.

The MS model includes the complete bottom part of the B clusters. The small circles represent projected positions of the atoms

M. Krajcí and J. Hafner, Phys. Rev. B. 71 (2005) 054202

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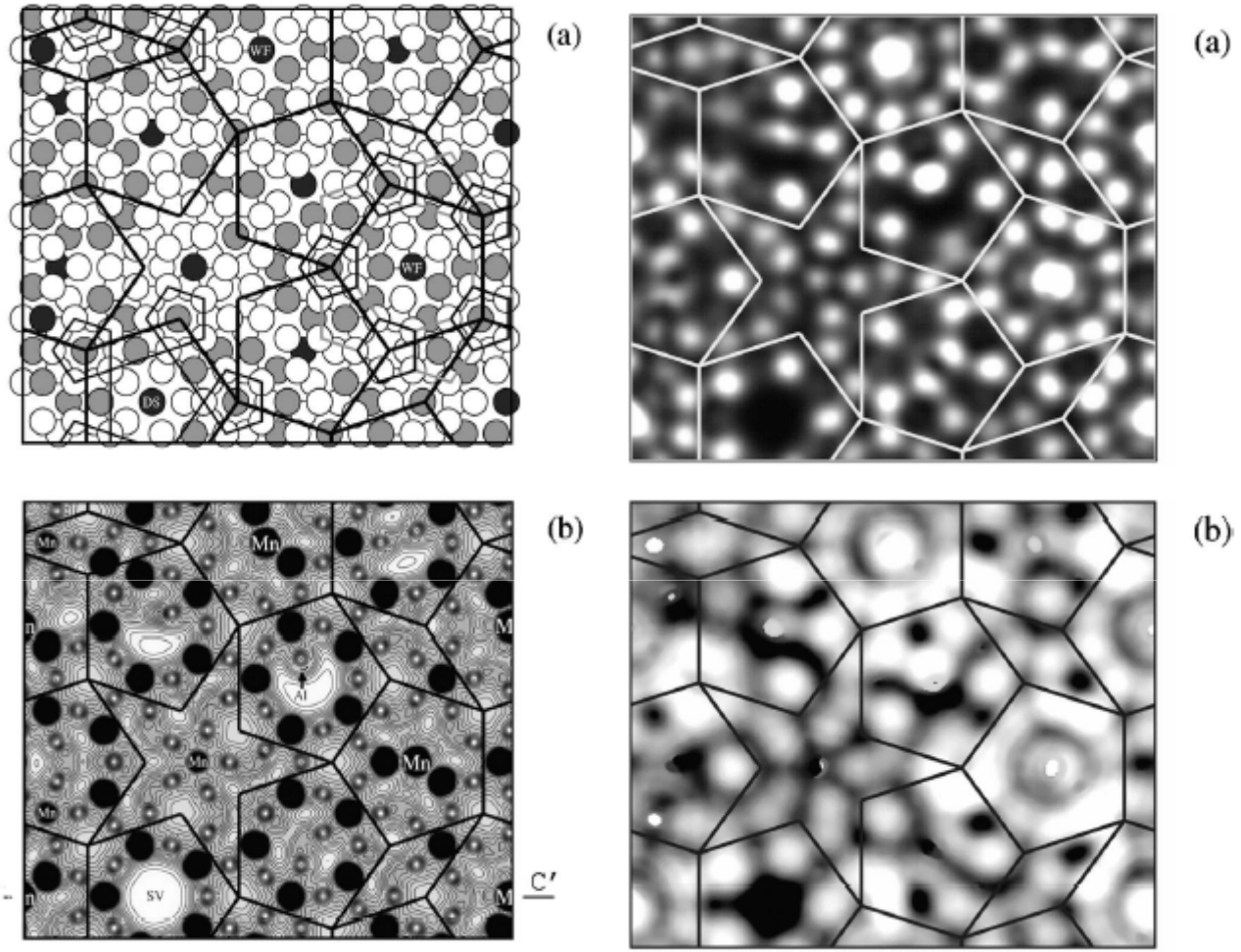
DFT: calculations of surface structure of AlPdMn quasicrystal



M slab, 3/2 approximant: atomic structure, electronic charge density,
Constant height STM, constant current STM simulations
M clusters contained within pentagons; B cluster at vertices

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M. Krajcí et al, Phys. Rev. B. 73 (2006) 024202

DFT: comparison with STM images

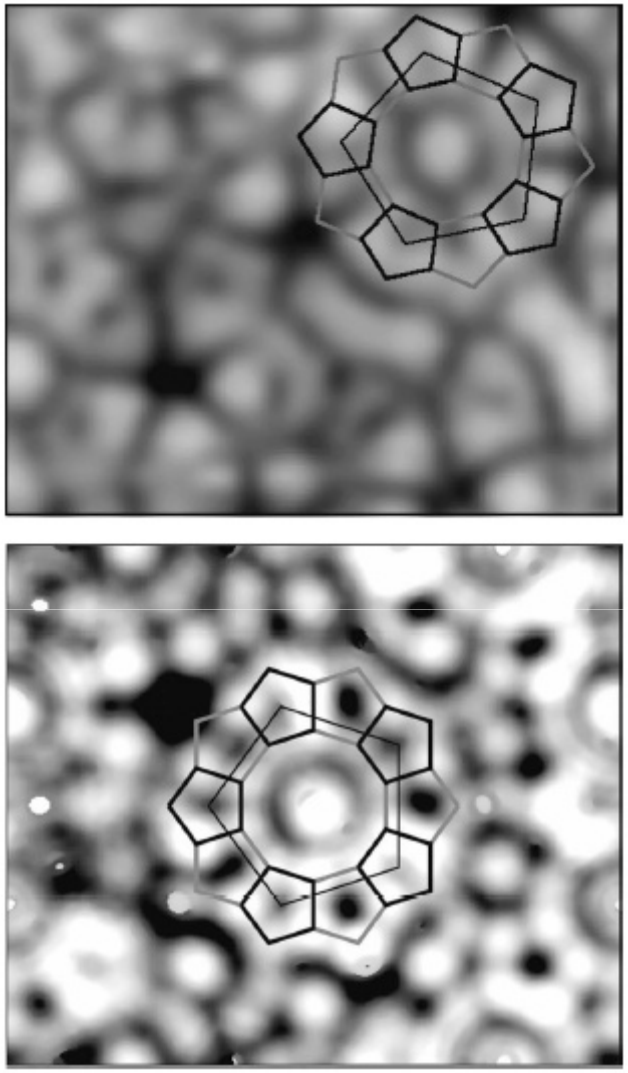

FIG. 4. A comparison of the experimental top and calculated bottom STM images of the white flower WF. The area of the STM image 39.5 Å x 32.9 Å is the same as the size of the structural model. The WF corresponds to a M cluster (the central decagon) surrounded by five B clusters (black pentagons). The skeleton of the WF is formed by five dark and five gray pentagons of size 2.96 Å. The big pentagon marked by the thin line indicates the position of the “top” pentagonal tile of the P1 tiling.

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M. Krajcí et al, Phys. Rev. B. 73 (2006) 024202

DFT: comparison with STM images

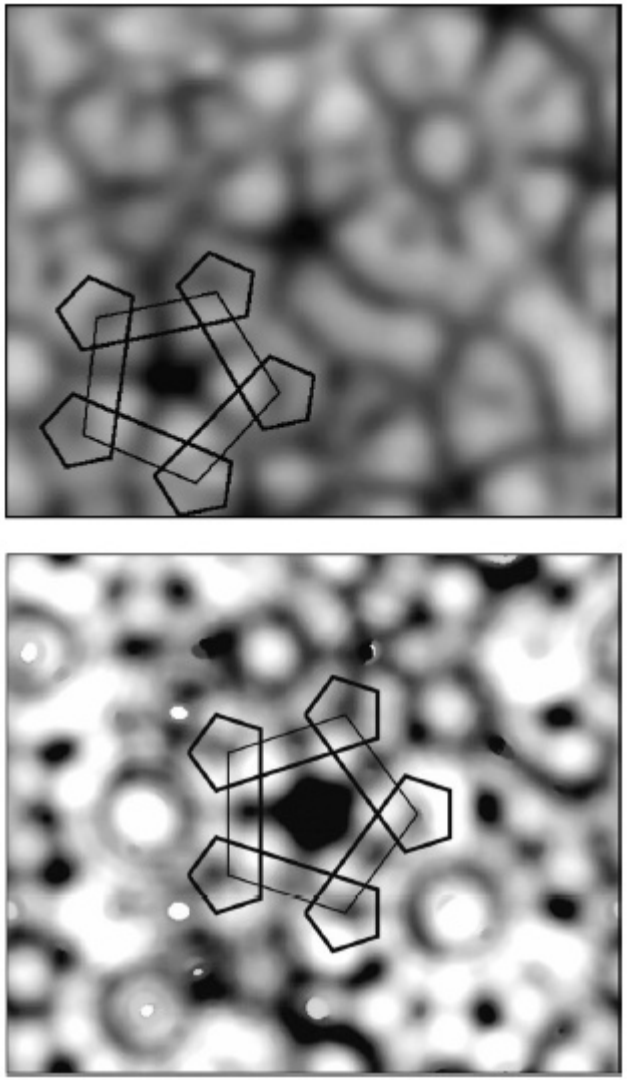

FIG. 5. A comparison of the experimental top and calculated bottom STM images of the dark pentagonal hole—*dark star DS.* The area of the images is 39.5 Åx32.9 Å. The DS is formed by a surface vacancy surrounded by a pentagon of Al atoms separated by 4.79 Å and a pentagon of Pd atoms of the same size forming in the STM image dark “arms” of the DS. The skeleton shown in the figure consists of one central pentagon of 4.79 Å surrounded by five pentagons of 2.96 Å. The big pentagon marked by the thin line indicates the position of the “bottom” pentagonal tile of the P1 tiling.

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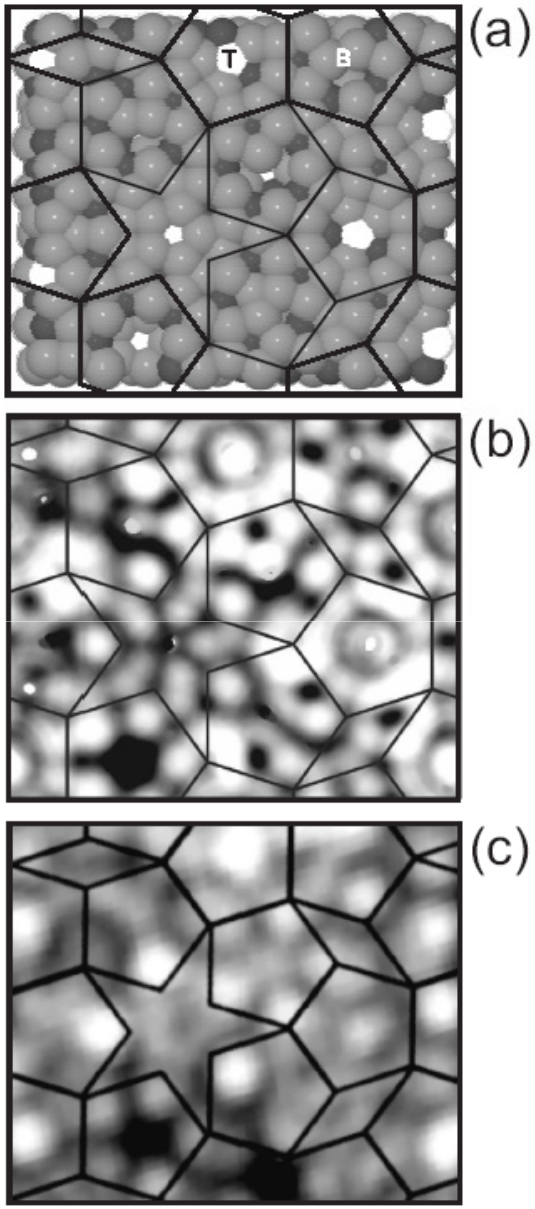
M. Krajcí et al, Phys. Rev. B. 73 (2006) 024202

DFT: comparison with STM images

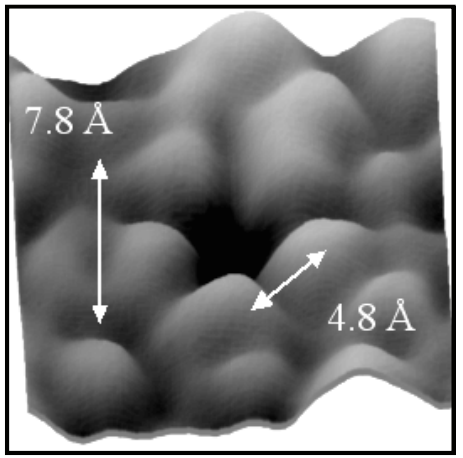


M. Krajcí et al, Phys. Rev. B. 73 (2006) 024202

STM interpretation: DFT simulations

Conclusions:

- Transition metal atoms form a rigid framework
- Al atoms may relax
- Pd atoms not imaged in STM: images are of Al and Mn atoms
- Five-fold hollows may be due to truncated pseudo-Mackay clusters with the Mn atom 2.56 Å below the surface plane (bottom pentagons)
- Top pentagons are truncated pseudo-Mackay clusters with the Mn atom in the surface plane. They have a protrusion at the centre.



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5-fold Al-Pd-Mn quasicrystal surface: structural conclusions

Conclusions:

- Surface is a termination of the bulk structure – all techniques concur
- Surface relaxation of about 0.38 Å occurs
- Discrepancy in the interpretation of local configurations in STM
    - 5 –fold stars are cut Bergmans (Papadopolos et al)
    - 5-fold stars are truncated pseudo-Mackay clusters (Krajci et al)

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Case study:

Surfaces of Icosahedral Ag-In-Yb Quasicrystal

Studied by STM, UPS, XPS and MEIS

Hem Raj Sharma

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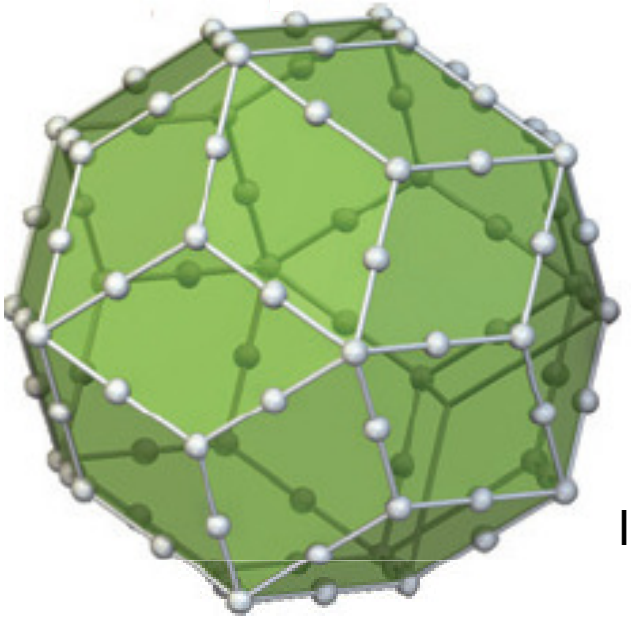
Surface studies of i-Ag-In-Yb quasicrystal

- **Surface atomic structure**
  Using STM, LEED, MEIS
  Comparison with bulk model structure
- S**urface composition**
  Using by XPS and MEIS
- **Valence band structure**
  Using UPS and comparison with calculation
- **Oxidation behaviour**
  Using XPS and comparison with pure elements
- **Reactivity to C_{60}**
- **Growth of Sb, Pb and Sb thin film**
  Pb and comparison with calculation
- **Use of all possible high symmetry surfaces**
  Fivefold, threefold and twofold surfaces

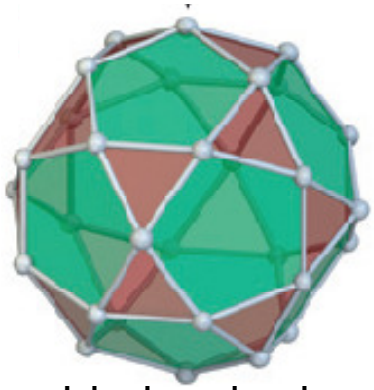
Ag-based QCs vrs Al-based QCs

	Ag-based QCs	Al-based QCs
Building blocks	Isostructral to i-Cd-Yb Rhombic triacontahedral (Tsai-type cluster)	Pseudo-Mackay and Bergman clusters
e/a	2.0	1.7 or 2.1
Structure derived from	Primitive hypercubic lattice (P-type QC)	Face centred hypercubic lattice (F-type QC)
Stability	*sp -d* hybridization	Hume-Rothery mechanism and *s-d* hybridization
Concentration	42%, In: 42%, Yb: 16%	Al ~ 72%,
Surface free energy	Ag: 1.17, In: 0.488, Yb: 0.482 (J/m^2)	Al has lowest surface energy

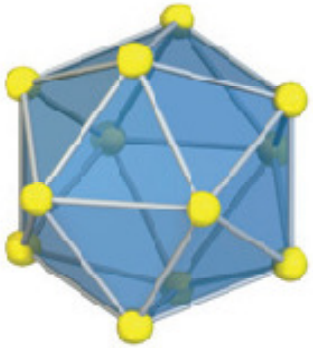
Building Units of i-Cd-Yb



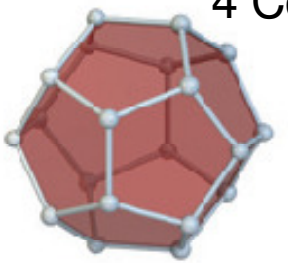
Rhombic triacontahedral
Atoms: 92 Cd atoms
0.78 nm radius



Icosidodecahedron
32 Cd atoms
0.65 nm radius



Icosahedron
12 Yb atom
0.56 nm radius



Dodecahedron
20 Cd atoms
0.46 nm radius

Tetrahedron
4 Cd atoms

Takakura et al., nature materials 2006

- High chemical order and structural perfection
- Full structural solution of i-Cd-Yb was possible
- 93.8% of the total atoms belong to RTH unite, remaining glue atoms
- In i-Ag-In-Yb, Cd is replaced by Ag and In; exact distribution is not known

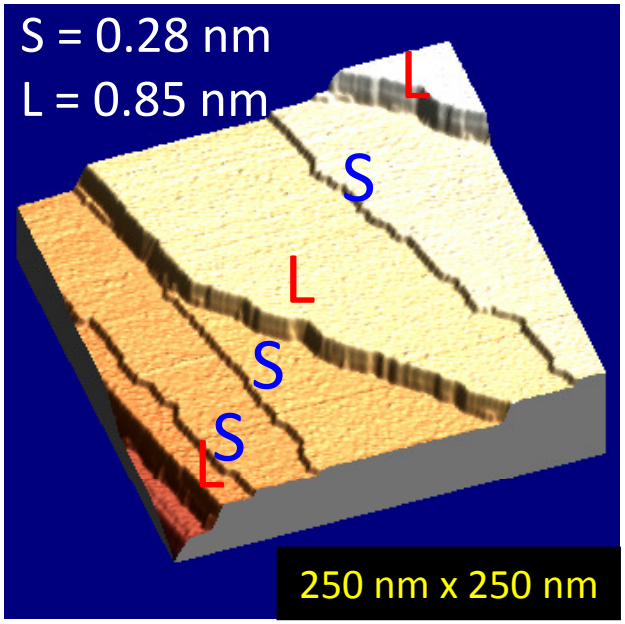
Structure of the Fivefold i-Ag-In-Yb Surface

- STM and comparison with the bulk structure
- Structure analysis by MEIS

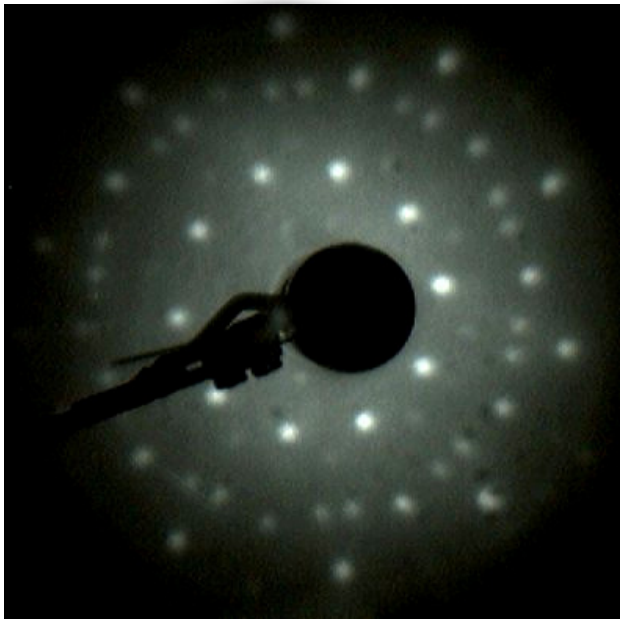
H. R. Sharma, M. Shimoda, K. Sagisaka, H. Takakura, J. A. Smerdon, P. J. Nugent, R. McGrath, D. Fujita, S. Ohhashi and A. P. Tsai
Structure of the fivefold surface of the Ag-In-Yb icosahedral quasicrystal
Physical Review B 80, 12140 (R) (2009)

Fivefold Surface: STM & LEED

STM



LEED



Surface prepared by sputter-annealed @ 440°C

23.4 eV

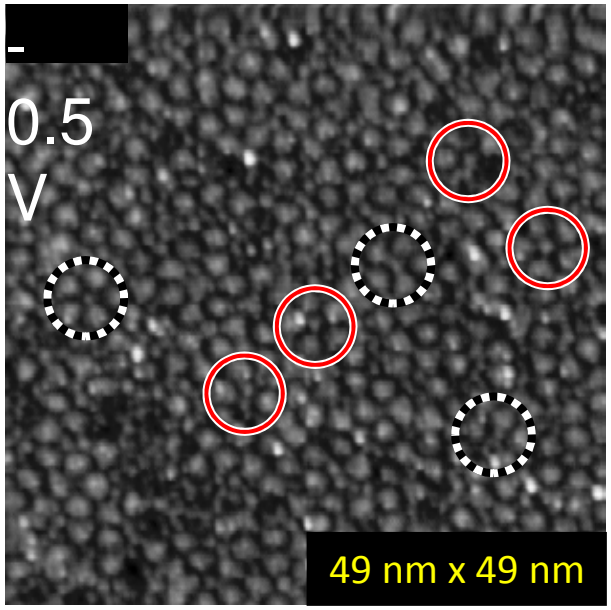
- Large terraces comparable to Al-based QC
- Steps of mainly two different heights

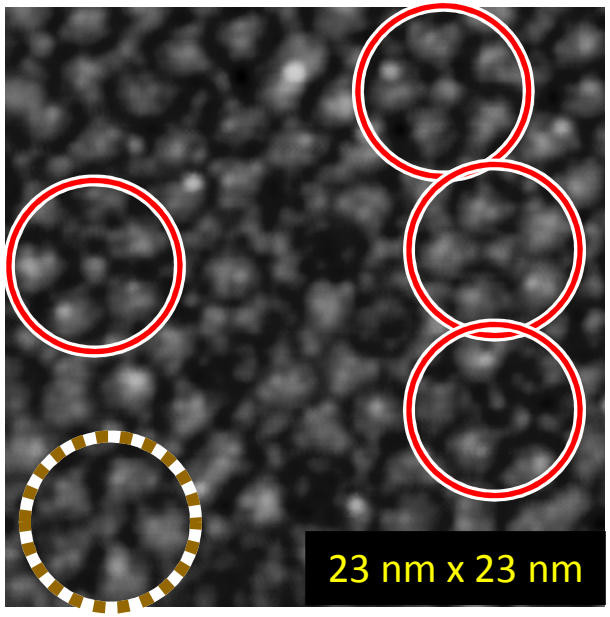
  S = 0.28 nm (σ: 0.04)

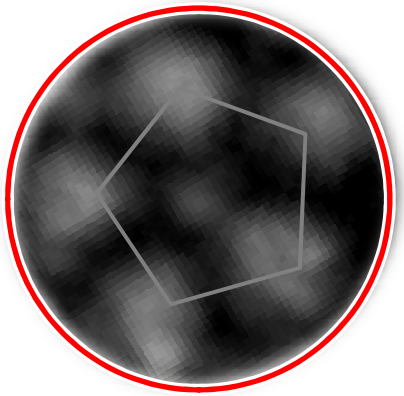
  L = 0.85 nm (σ : 0.05)

LEED reveals quasicrystalline long range order

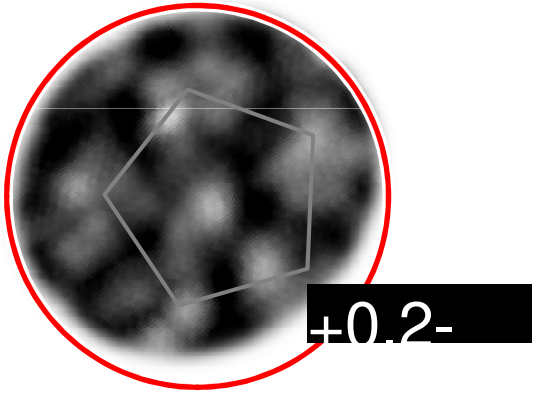
Fivefold Surface: Fine Structure on Terraces

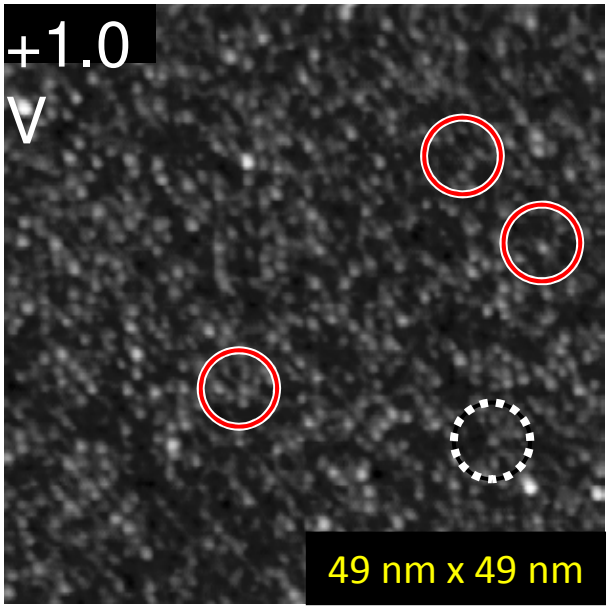


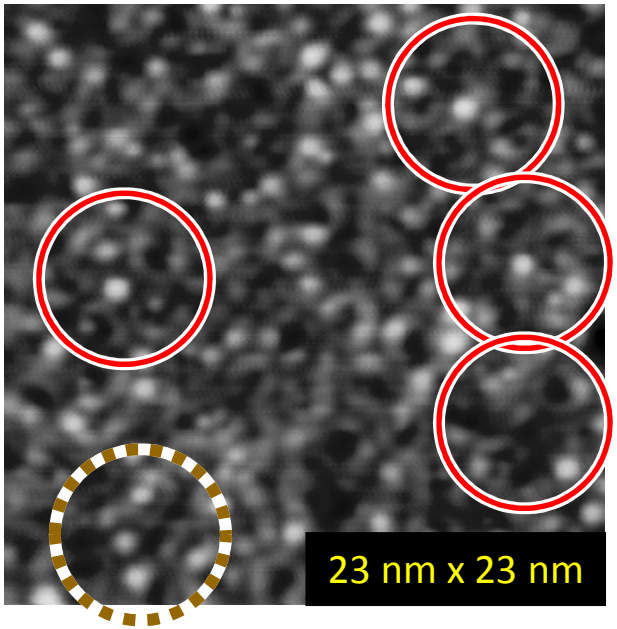


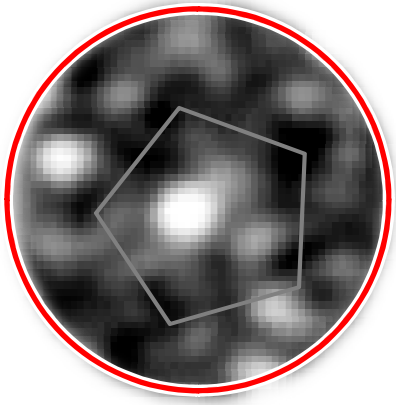


Edge length: 2.5 nm

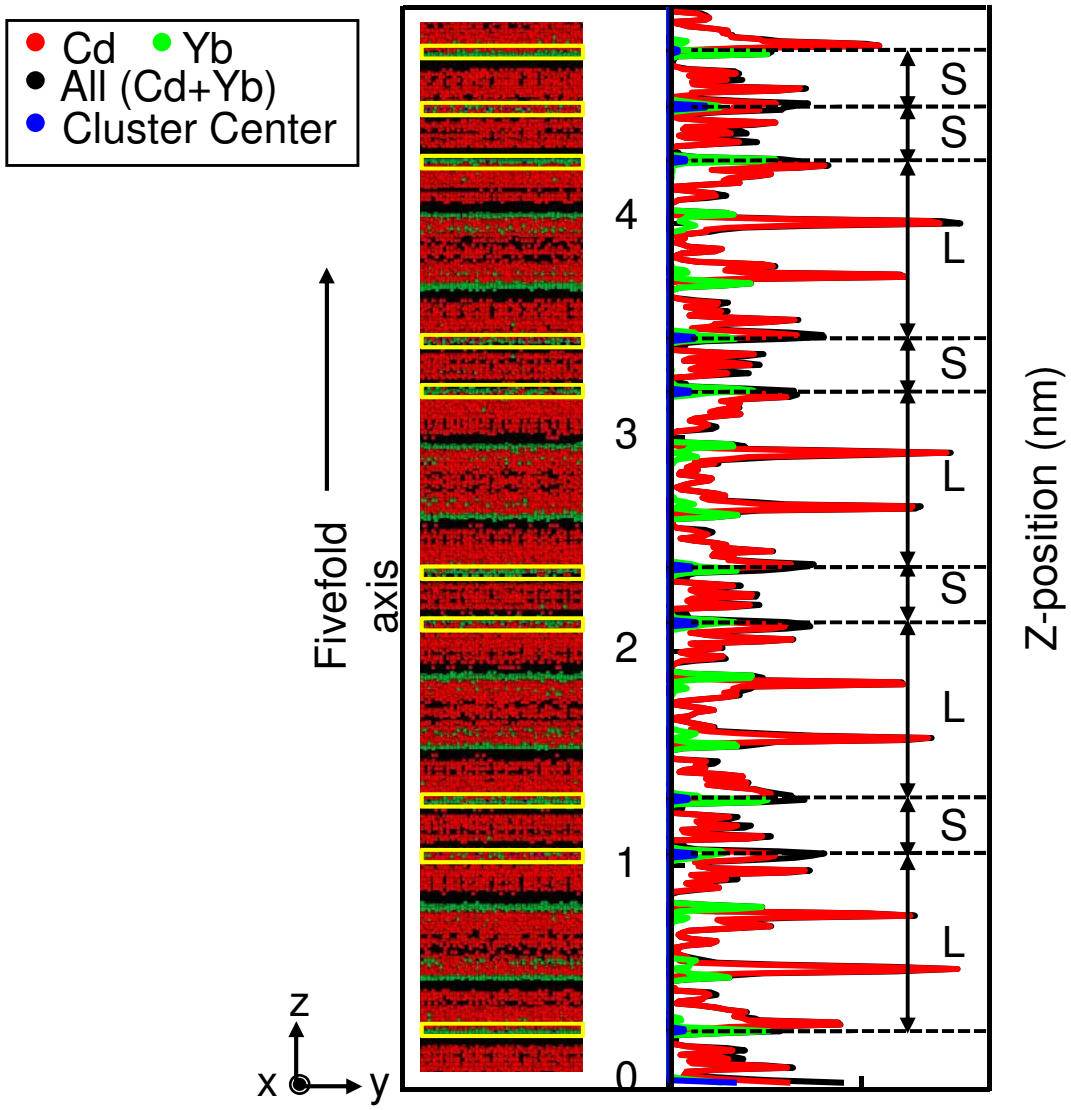




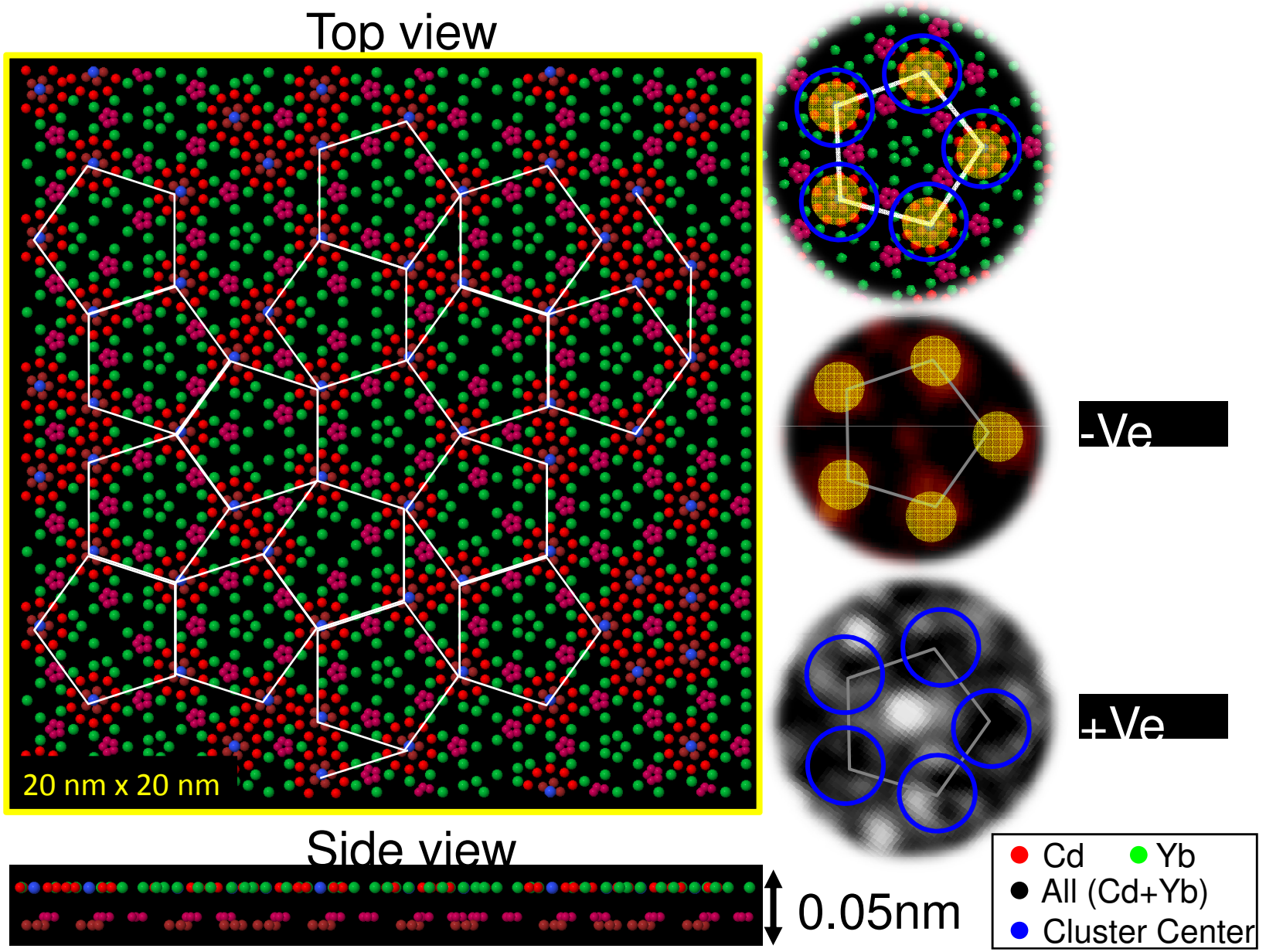




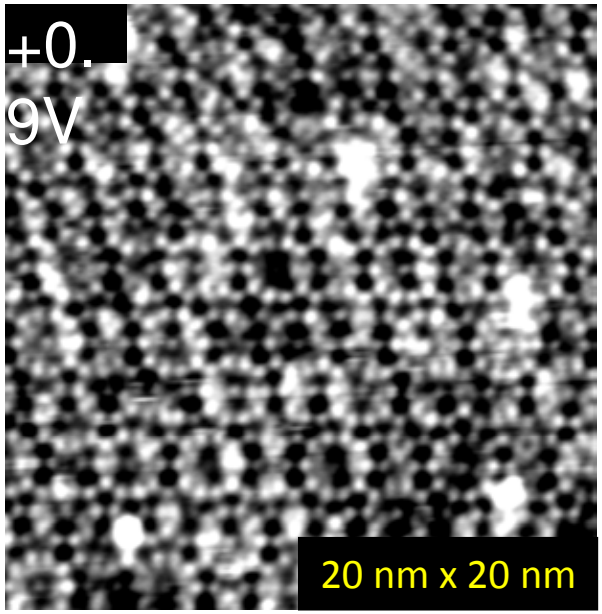
Comparison with Bulk Model



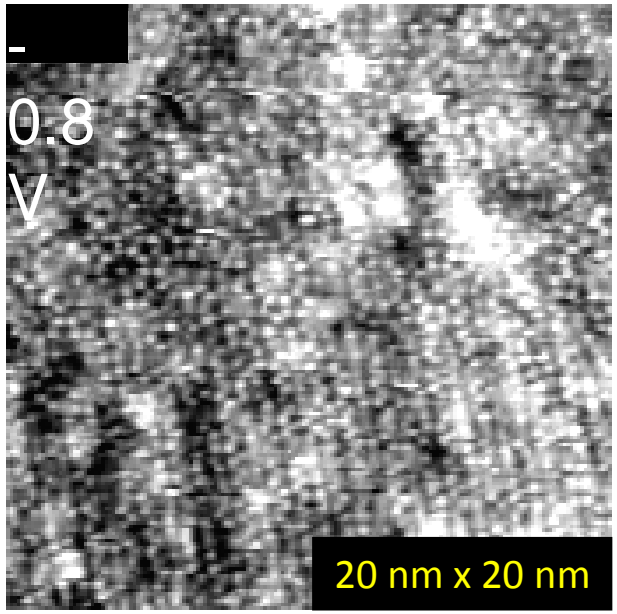
Comparison with Bulk Model



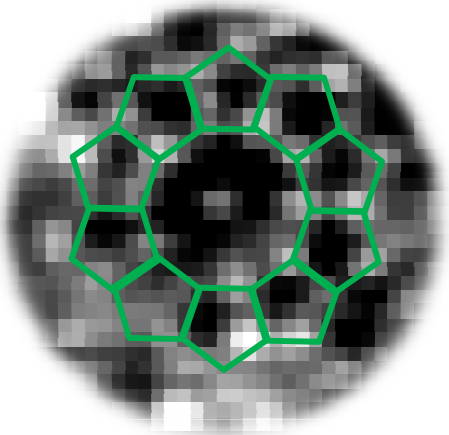
Fivefold Surface: Fine Structure on Terraces



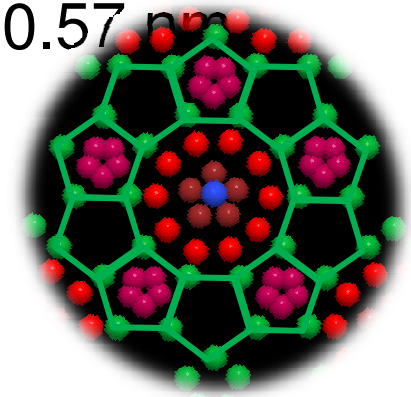
Enhanced by Fourier filtering



Raw data



edge length: 0.57 nm



Model

STM contrast seems to be enhanced by deposition of a small amount of Sb

Overview: Experimental studies of clean surfaces of AlPdMn

Substrate	Technique	Date 1st. pub.	Authors	Ref.
5-f *i*-Al-Pd-Mn	STM	1994	Schaub et al.	[1–3]
		1996	Ebert et al.	[4–7]
		1999	Shen et al.	[8]
		1999	Ledieu et al.	[9–12]
		2002	Barbier et al.	[13, 14]
		2005	Unal et al.	[15]
		2006	Widmer et al.	[15]
	LEED	1996	Jenks et al.	[16–18]
		2003	Kortan et al.	[19]
	LEED I(V)	1997	Gierer al.	[20, 21]
	X-ray techniques	2000	Capello et al.	[22–24]
		2000	Jach et al.	[25]
		1999	Alvarez et al.	[26, 27]
	Ion scattering	2001	Bastasz et al.	[28–30]
		2005	Noakes et al.	[31]
	SEI	1998	Bolliger et al.	[32–34]
	XPD	1999	Naumović et al.	[35–38]
		2004	Zheng et al.	[39]
	Modelling	1999	Papadopolos et al.	[11, 40–42]
		2005	Krajčí et al.	[12, 43]

Overview: Experimental studies of clean surfaces of AlPdMn

2-f *i*-Al-Pd-Mn	LEED	1997	Shen et al.	[18, 44]
	STM	2006	Gröning et al.	[45]
	STM	2006	Reid et al.	[46]
3-f *i*-Al-Pd-Mn	STM	2000	Rouxel et al.	[47]
	LEED	2000	Shen et al.	[18]

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Studies of clean surfaces of d-Al-Ni-Co

Substrate	Technique	Date 1st. pub.	Authors	Ref.
10-f *d*-Al-Ni-Co	STM	2001	Cox et al.	[48]
		2002	Kishida et al.	[49]
		2003	Ebert et al.	[50]
		2004	Yuhara et al.	[51]
		2004	Sharma et al.	[52]
		2004	Cecco et al.	[53]
	LEED I(V)	2004	Ferralis et al.	[54]
		2006	Pussi et al.	[55]
	SPA-LEED	2000	Gierer et al.	[56]
	XPD,RHEED	2000	Shimoda et al.	[57]
	SEI	1998	Zurkirch98,Flückiger et al.	[58, 59]
	Modelling	2006	Krajčí et al.	[60]

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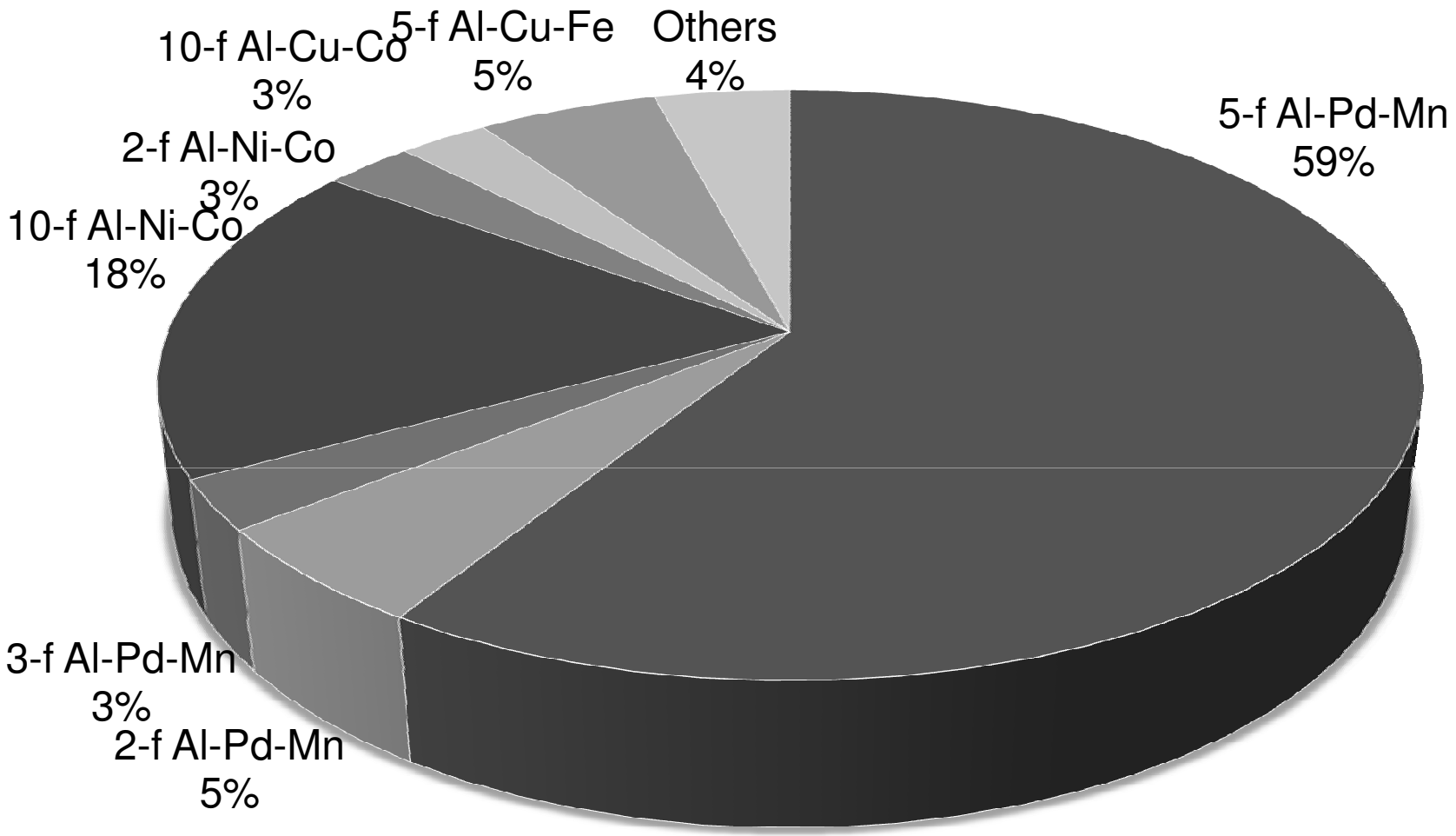
Studies of clean surfaces of other quasicrystals

10-f *d*-Al-Cu-Co	STM	1990	Kortan et al.	[61]
		1990	McRae et al.	[62]
5-f *d*-Al-Cu-Fe	LEED	1997	Shen et al.	[63]
	STM, LEED	2001	Cai et al.	[64, 65]
	STM	2004	Sharma et al.	[52]
5-f *i*-Al-Cu-Ru	STM	2005	Shimoda et al.	[66]
5-f *i*-Al-Ga-Pd-Mn	LEED	2002	Heinzig et al.	[67]
5-f *i*-Ag-In-Yb	STM	2007	Sharma et al.	[68]
2-f *d*-Al-Ni-Co	STM	2005	Park et al.	[69]
	SEI	2003	Flückiger et al.	[59]

Studies of clean surfaces of other quasicrystals



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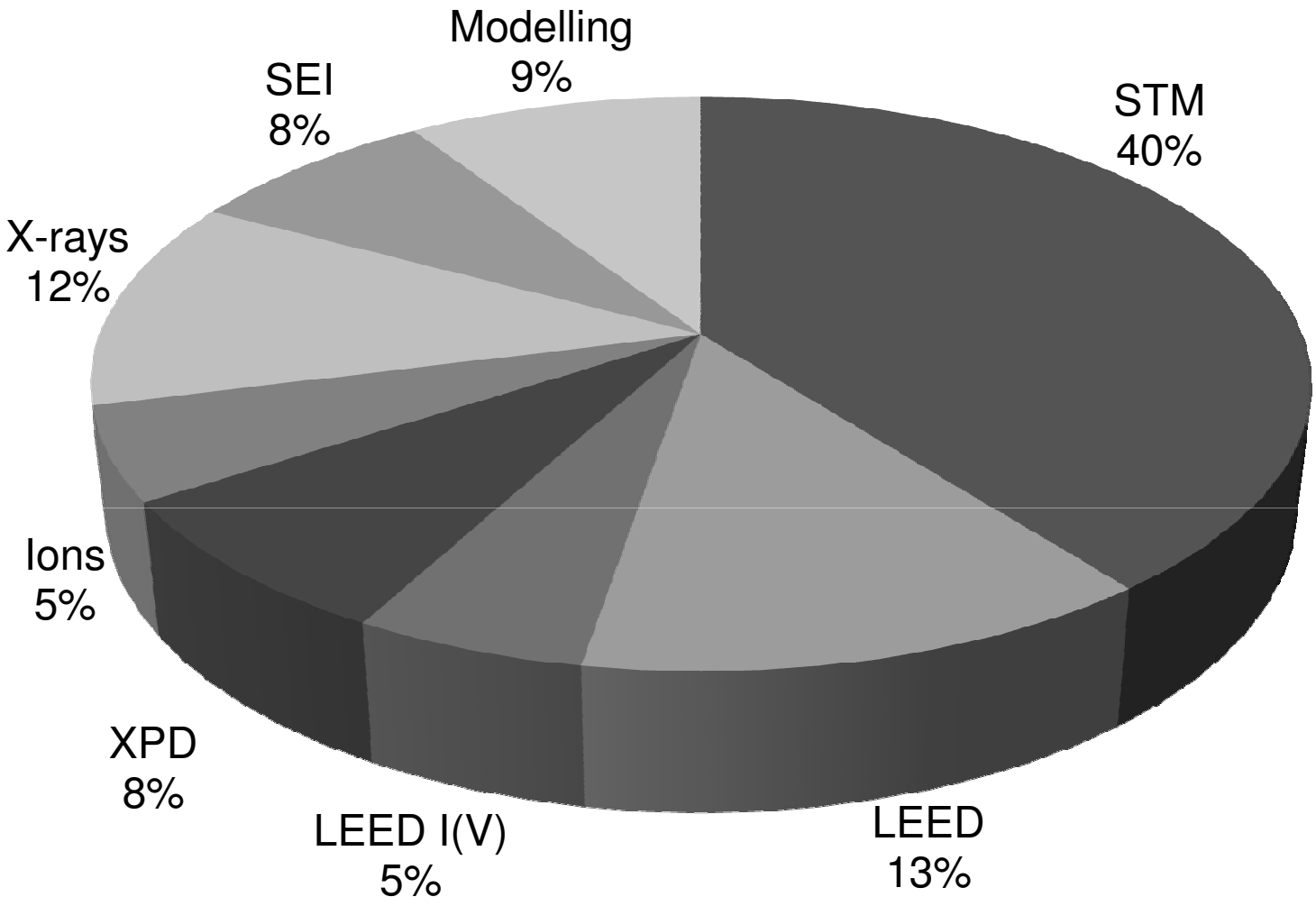
Studies of clean surfaces of other quasicrystals



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Overview

1. Surface structure of quasicrystals
2. Quasicrystal surfaces as templates
3. Other aperiodic surfaces

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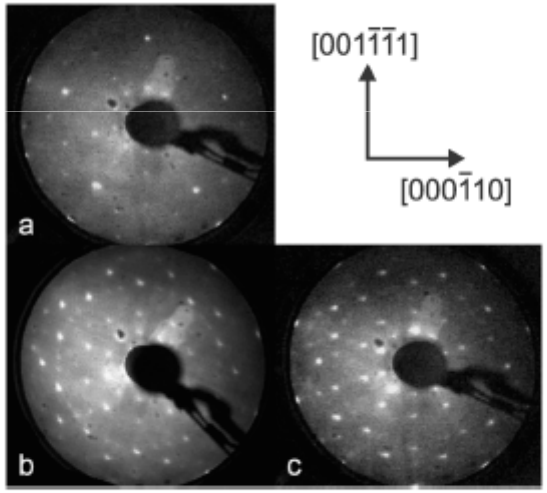
Bi/Al-Pd-Mn

VOLUME 89, NUMBER 15 PHYSICAL REVIEW LETTERS 7 OCTOBER 2002

Quasicrystalline Epitaxial Single Element Monolayers on Icosahedral Al-Pd-Mn and Decagonal Al-Ni-Co Quasicrystal Surfaces

K. J. Franke,[1] H. R. Sharma,[1] W. Theis,[1,*] P. Gille,[2] Ph. Ebert,[3] and K. H. Rieder[1]



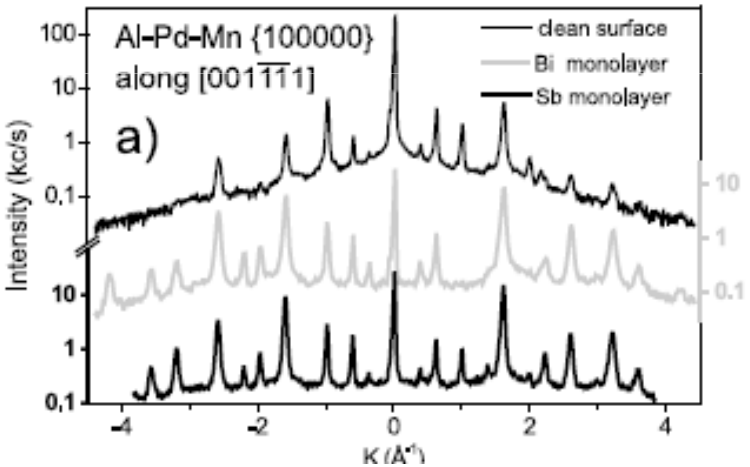


FIG. 2. LEED images from the fivefold Al-Pd-Mn surface with electron energy of 63 eV: (a) clean surface, (b) Sb monolayer, and (c) Bi monolayer. Although the patterns from the monolayers (b),(c) appear tenfold, different electron energies confirm a fivefold symmetry. Indexing follows Ref. [27].

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Quantum Size Effects in Metal Thin Films Grown on Quasicrystalline Substrates

V. Fournée,[1] H. R. Sharma,[2] M. Shimoda,[2] A. P. Tsai,[2,3] B. Unal,[4] A. R. Ross,[4] T. A. Lograsso,[4] and P. A. Thiel[4]

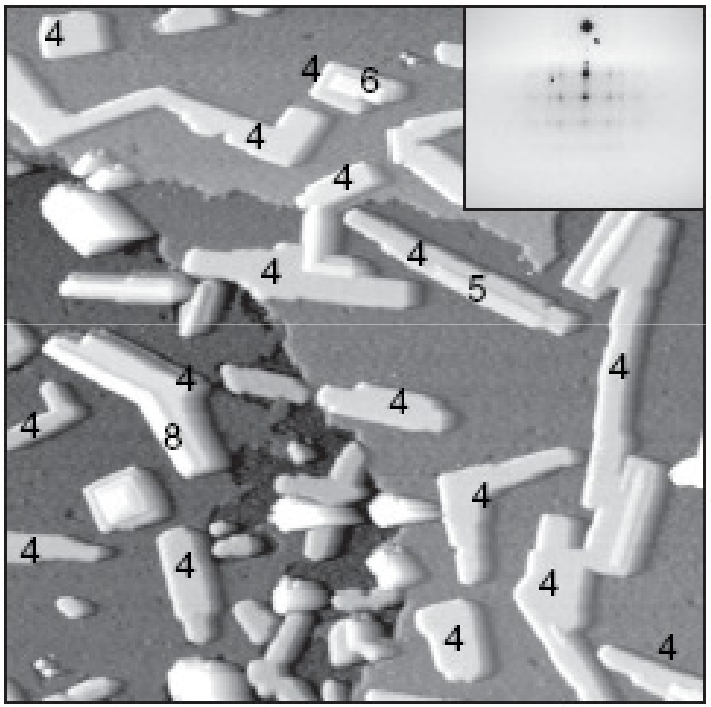
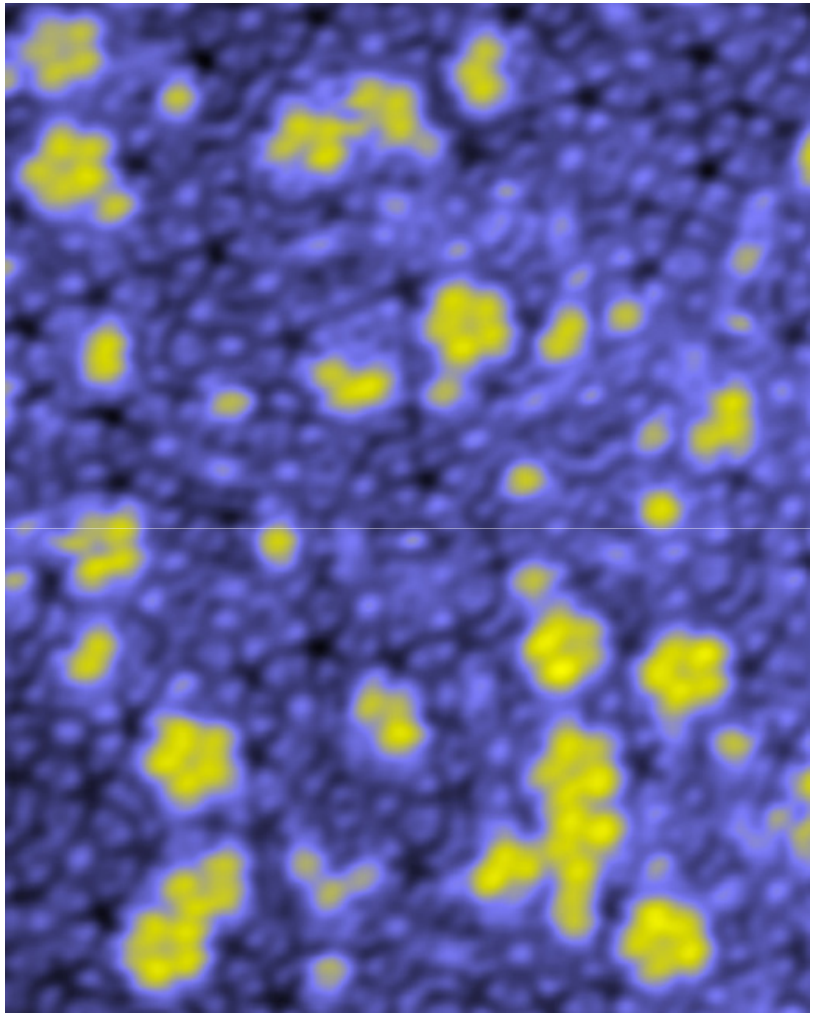


FIG. 2. STM topography (400×400 nm^2) of the fivefold $Al_{63}Cu_{24}Fe_{13}$ surface dosed with 4.5 ML of Bi. Island heights are indicated in units of monolayer. The inset shows a typical RHEED pattern observed for the Bi thin film.

Bi/Al-Pd-Mn



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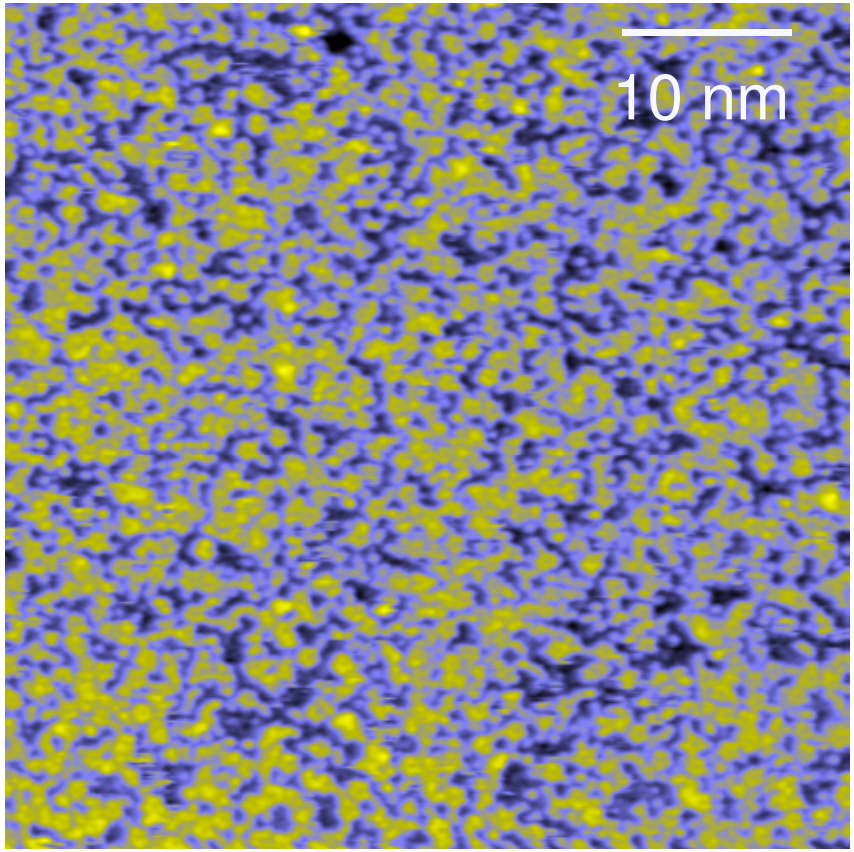
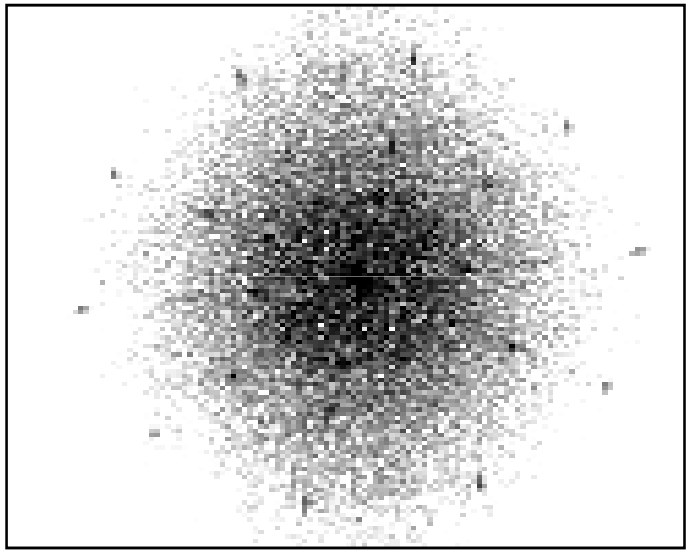
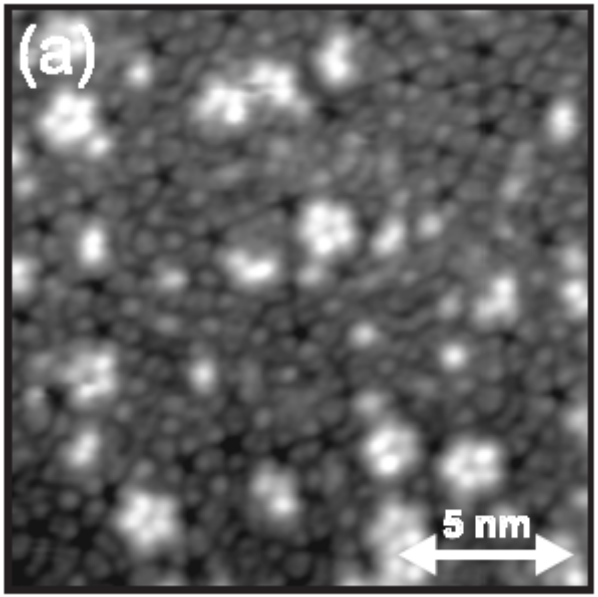
STM of Bi/AlPdMn – low coverage



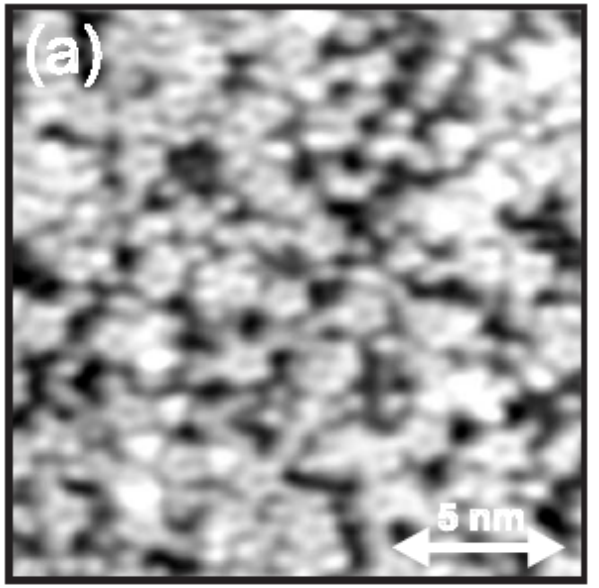


At sub-monolayer coverages, there is a high degree of order in the overlayer discernible by STM

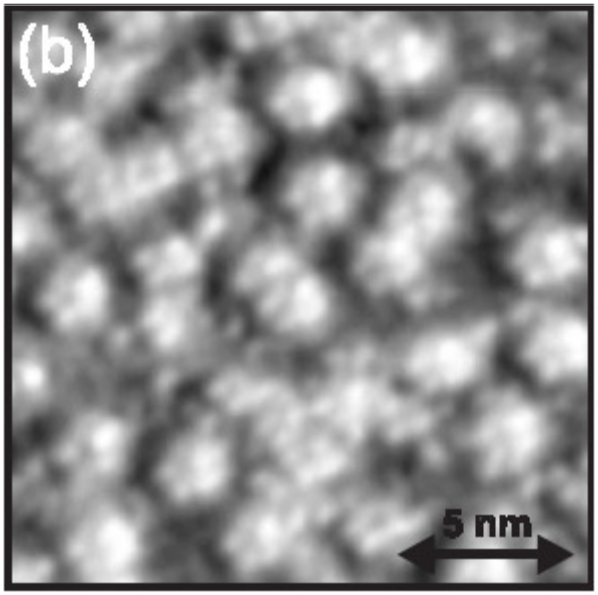
Bi/Al-Pd-Mn



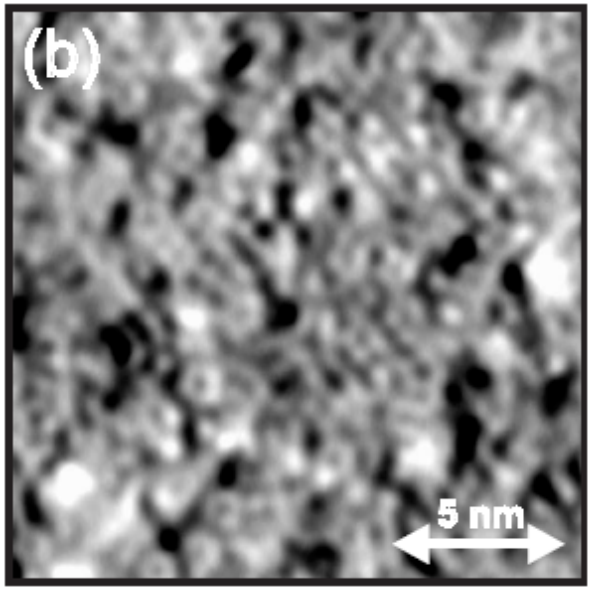
0.13 ML



0.54 ML



0.38 ML



0.9 ML

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Bi/Al-Pd-Mn

- System follows the classic nucleation and growth mechanism
- Initially, *pure nucleation regime*, where island size does not change with coverage
- Transition to takes place at around 0.5 ML to the *pure growth regime*
- These results indicate a single nucleation site for the cluster formation
- Can we identify this site?

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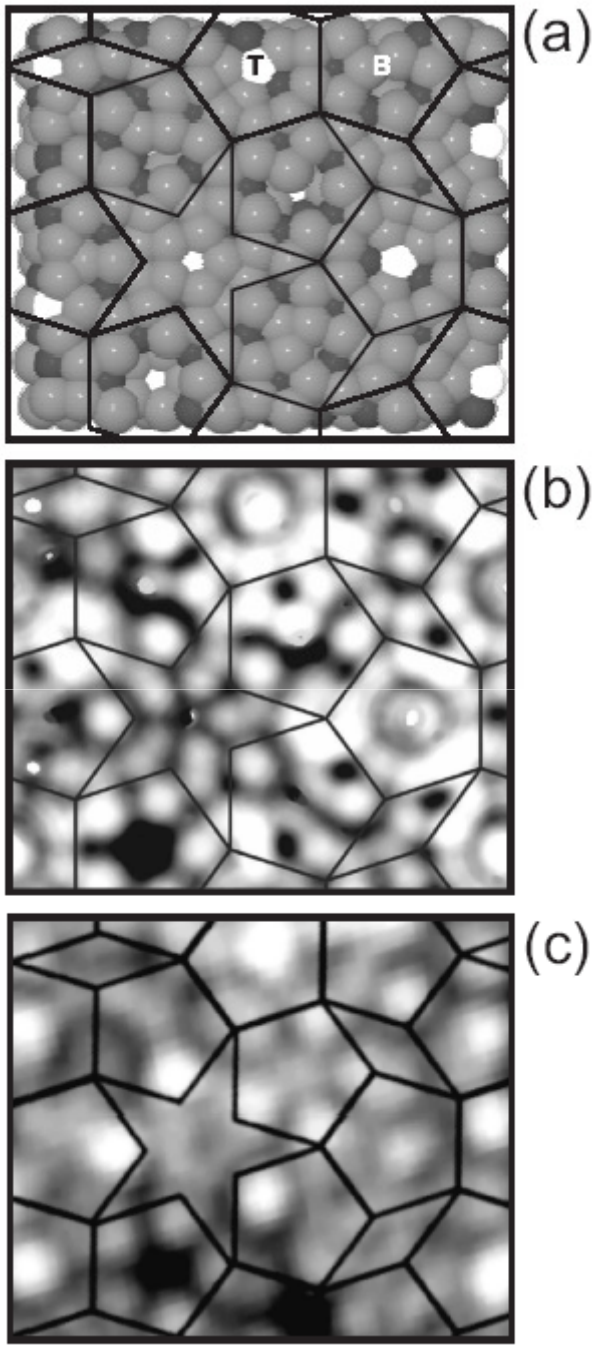
- Recap of interpretation of the clean surface:
- Pentagons have edge length 7.8 Å
- Top pentagons contains Mn
- Bottom pentagons contain 5f stars
- Top and bottom pentagons share a side
- Pentagons of similar orientation share a vertex



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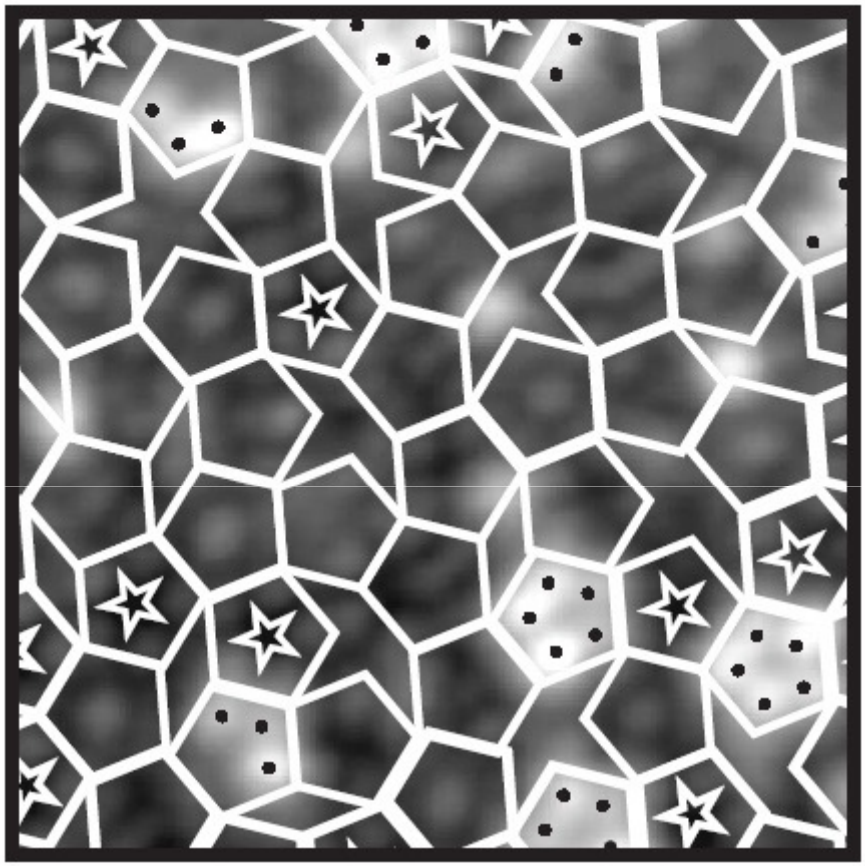

- Surface may be ``tiled“ to include all the Bi pentagons in the same orientation of tile.
- These are opposite in orientation to those containing the 5-f stars.

•The relative frequencies of the pentagon, rhomb, star and boat tiles in the infinite Penrose P1 tiling are
72.4:14.6:4.0:9.0

Here:

72.6:14.5:0.9:12.0.

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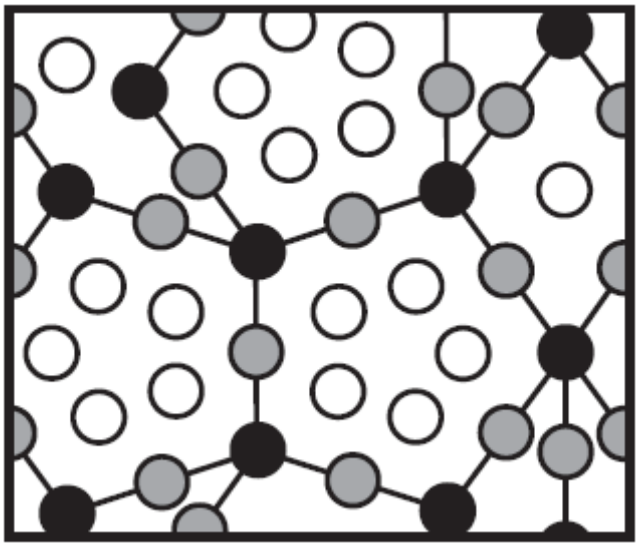

- Predictions made using DFT:
- Vertex site is most favourable:
- Mid-edge next most favourable
- Pentagons are then filled with equal probability

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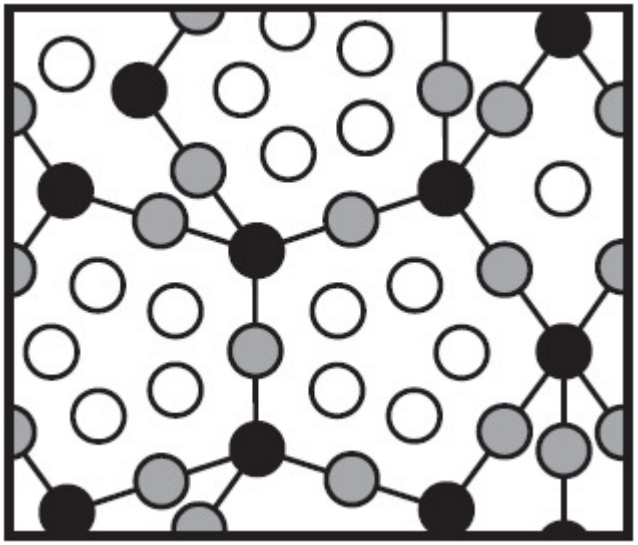
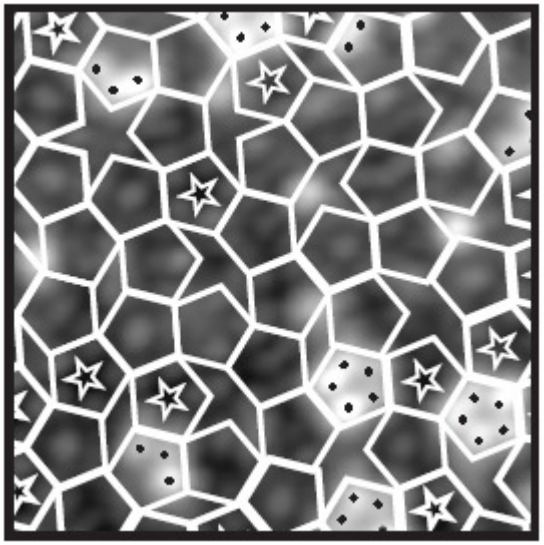
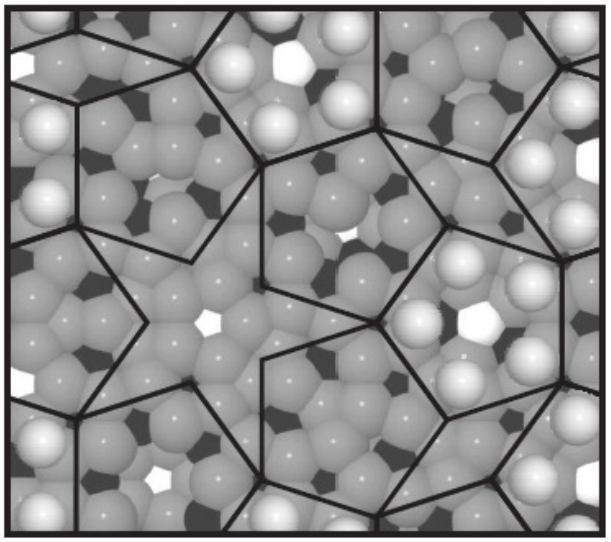
Krajci and Hafner , Phil. Mag., 86 (2005) 825



Predicted using DFT



Observed using STM



Deduced from STM

Smerdon, Parle, Wearing, Lograsso, Ross, McGrath, Phys. Rev. B, 78 (2008) 075407

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- Leads to a simple nucleation and growth mechanism for pseudomorphic monolayers
- Helps rationalise previous results for Al and Si growth

Smerdon, Parle, Wearing, Lograsso, Ross, McGrath, Phys. Rev. B, 78 (2008) 075407

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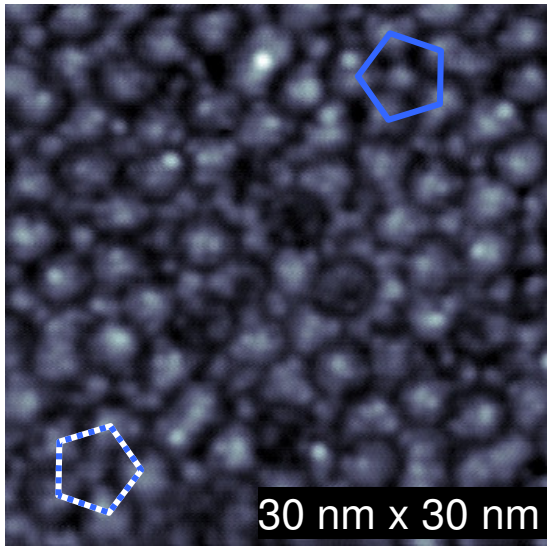
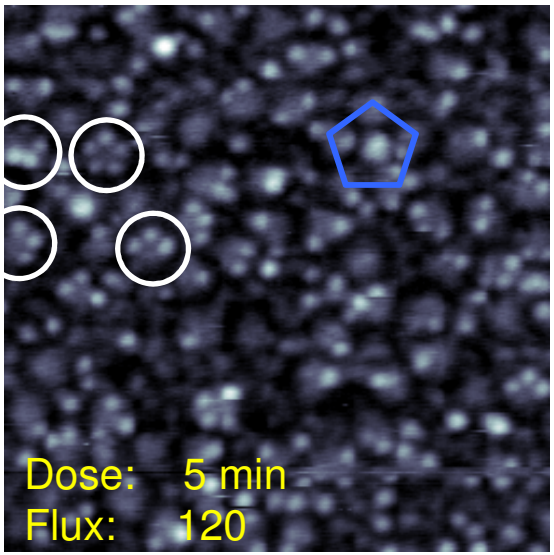
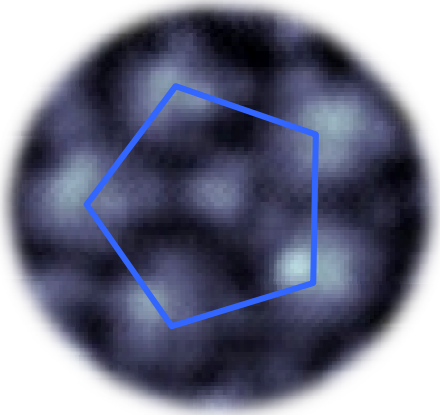
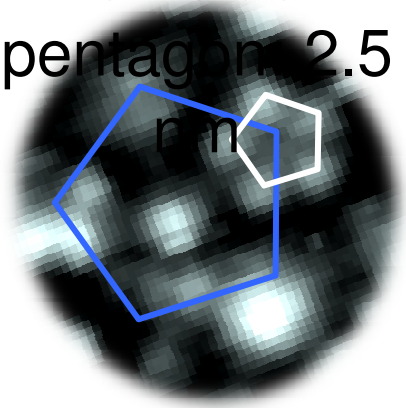
Growth of Pb on i-Ag-In-Yb



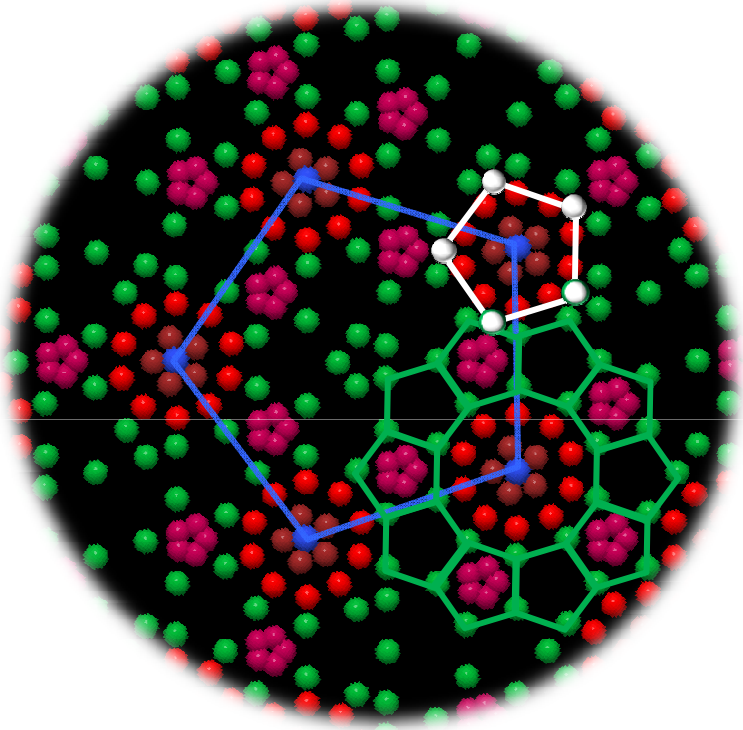




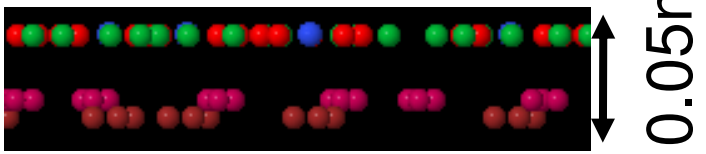
edge length of blue pentagon: 2.5 nm



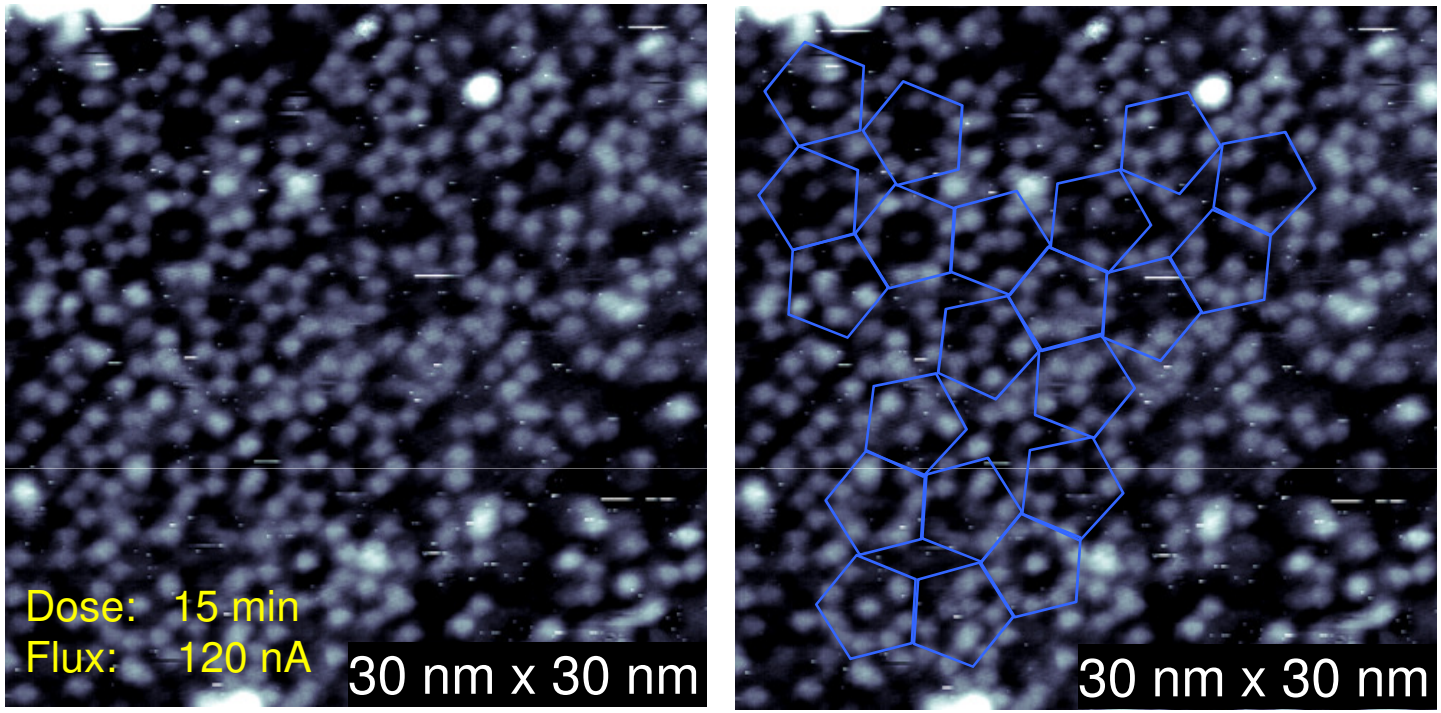
Top view



Side view

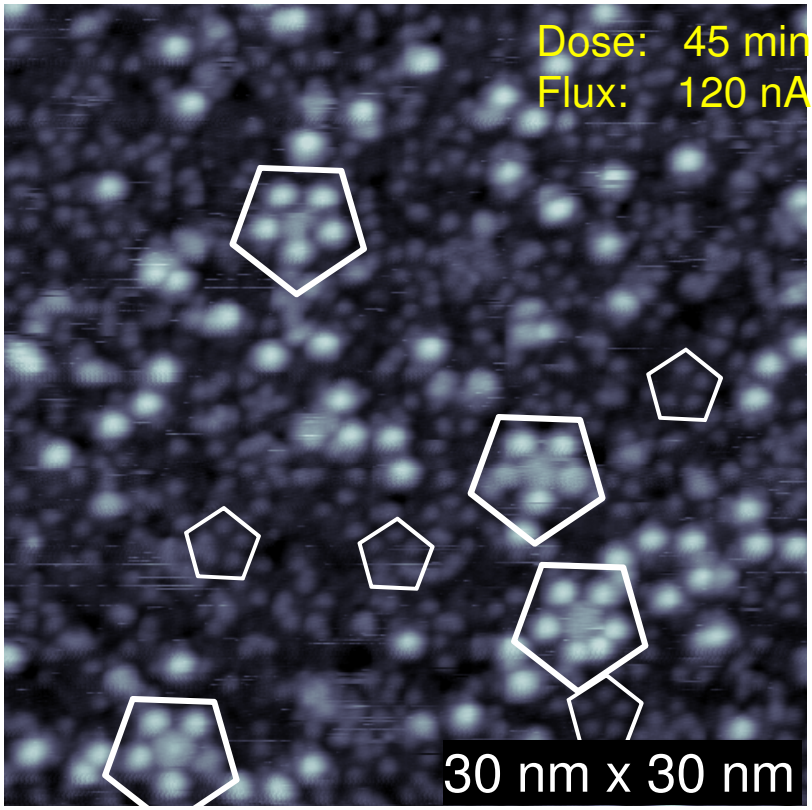


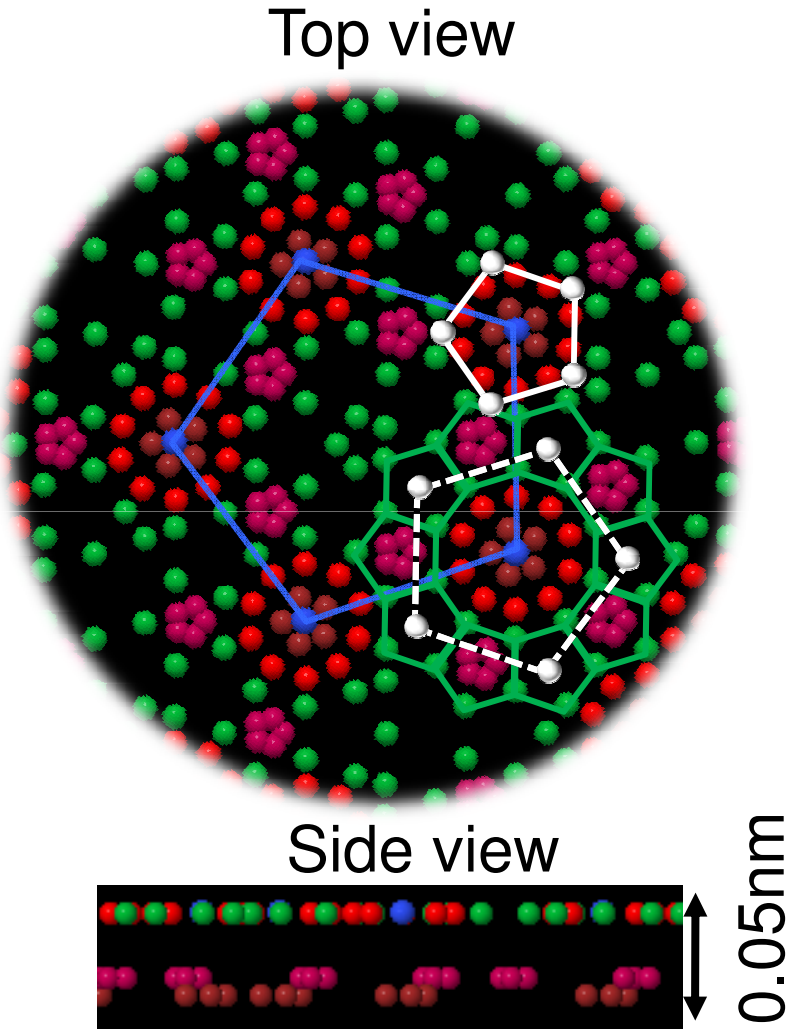
Growth of Pb on i-Ag-In-Yb



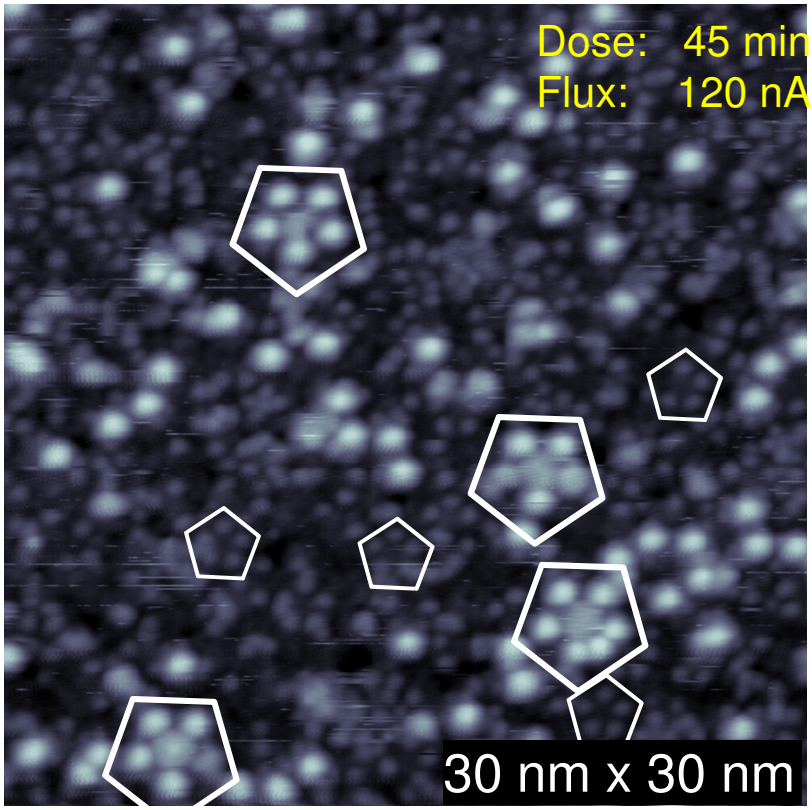
- Density of Adatoms is 0.60 atoms/nm^2 which is comparable to the density of the adsorption sites expected from the model structure
- The adatom density is far less than the density of the substrate, which is about 8 atoms/nm^2

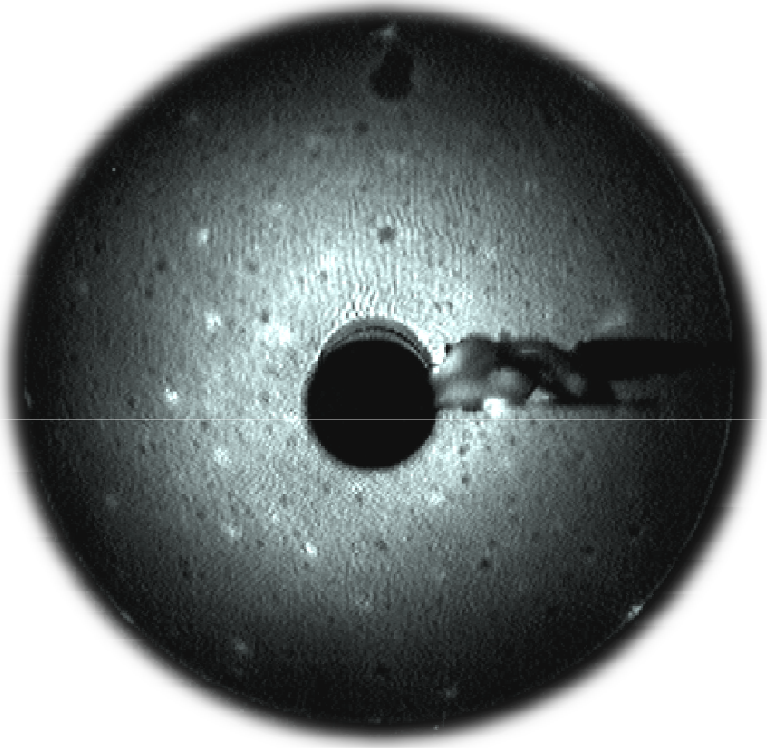
Growth of Pb on i-Ag-In-Yb





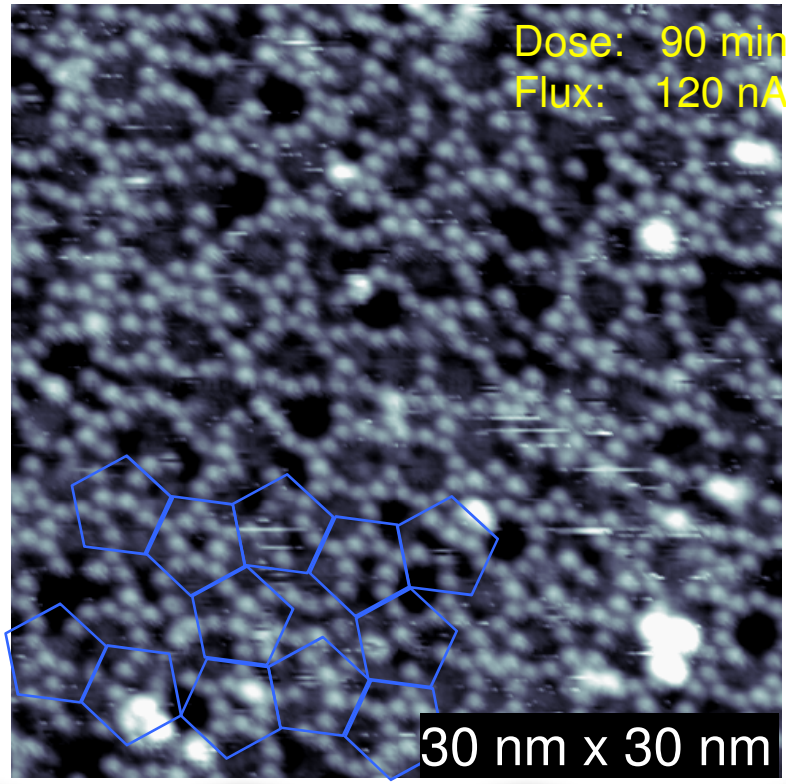
Growth of Pb on i-Ag-In-Yb

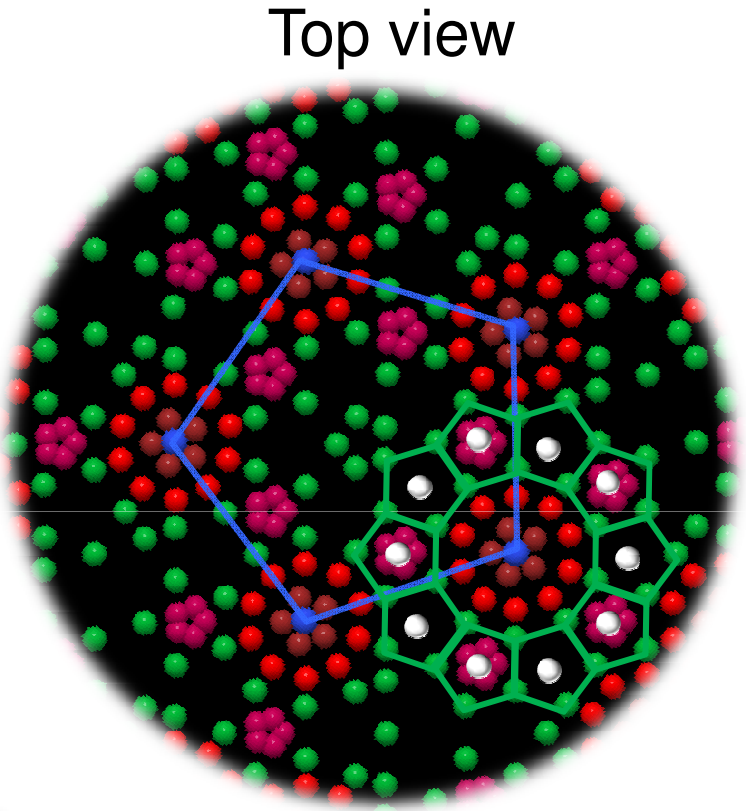


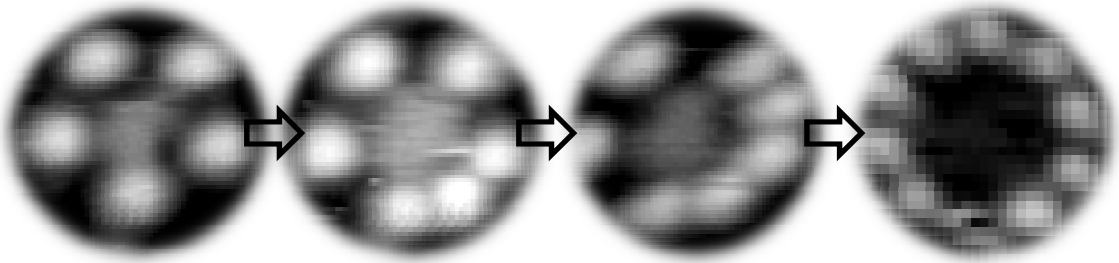


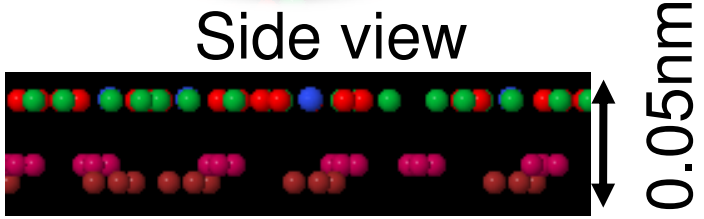
38 eV

Growth of Pb on i-Ag-In-Yb

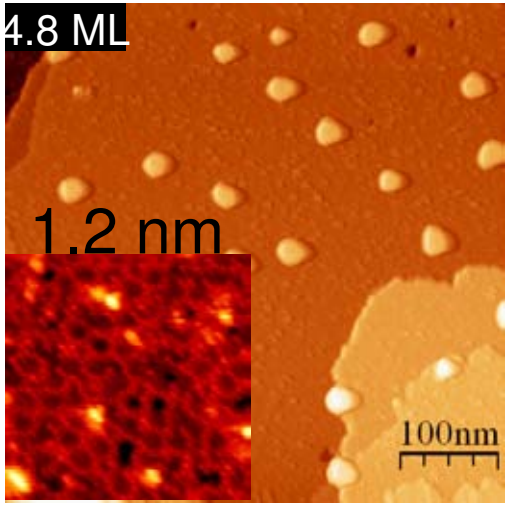


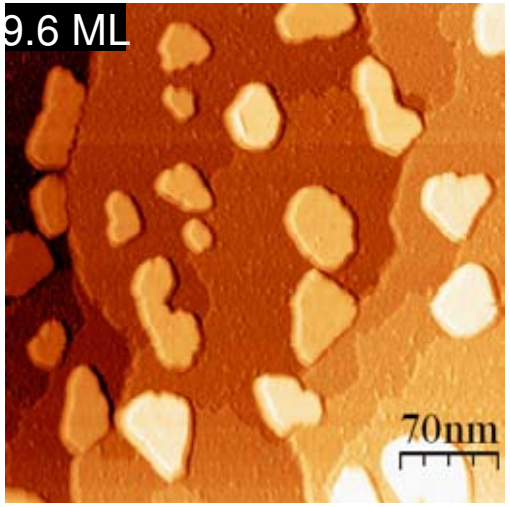


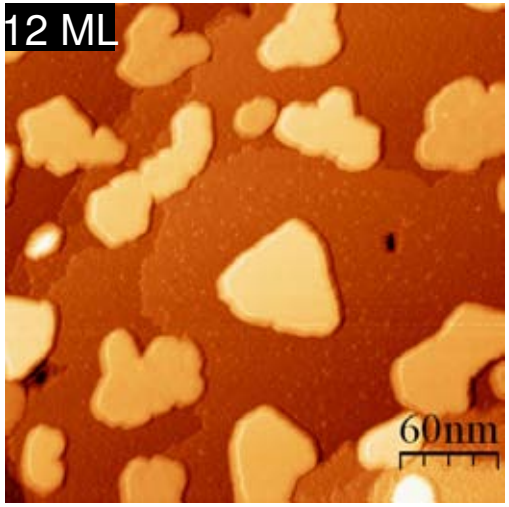




Growth of Pb on i-Ag-In-Yb

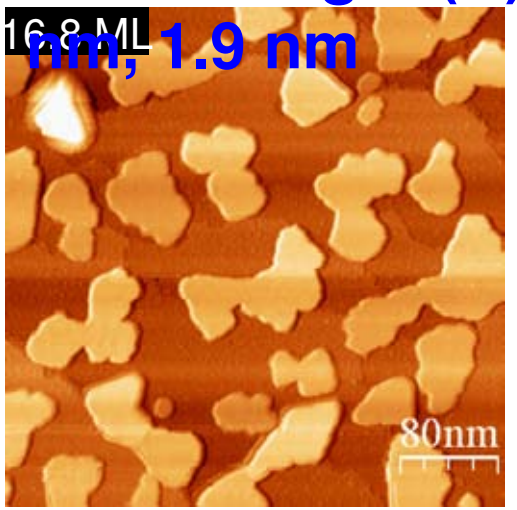


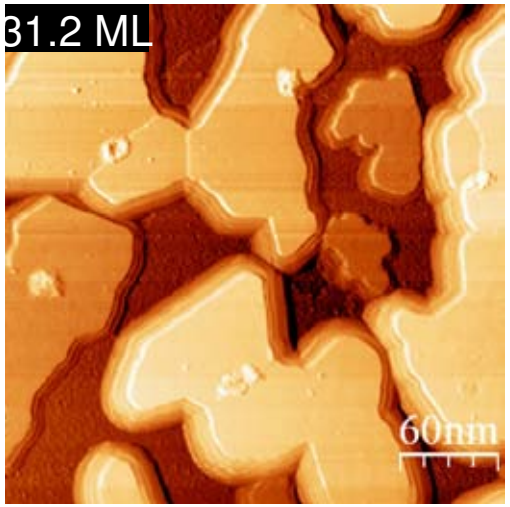


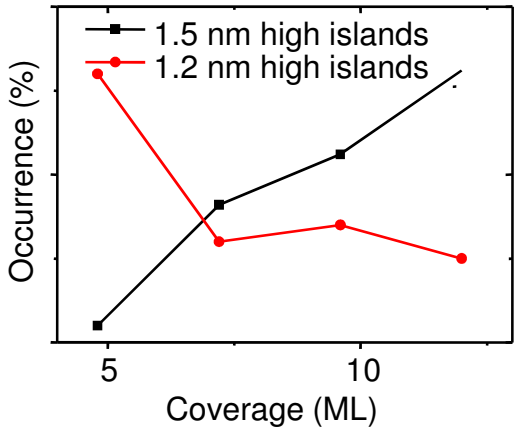


Island height (H): 1.2 nm, 1.55 nm, 1.9 nm

d_{111} for Pb: 2.86Å







Adsorbates on quasicrystals:

Substrate	Adsorbate	Pseudomorphic monolayer	Suggested site	Pentagonal cluster	Ref.
i-Al-Pd-Mn	C_{60}	-	hollow	-	[18]
	Si	-	truncated *M*	-	[44]
	Pb	✓	-	4.9	[21]
	Bi	✓	truncated *M*	4.9	[31, 35]
i-Al-Cu-Fe	Al	-	hollow	5.1	[27]
	Sn	✓	hollow	11.0	[40]
	Bi	✓	-	6.9	[41]
d-Al-Ni-Co	Pb	✓	-	-	[43]
	Si	-	hollow	4.2	[42]

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Smerdon et al. JPCM 2008

Overview

1. Surface structure of quasicrystals
2. Quasicrystal surfaces as templates
3. Other aperiodic surfaces

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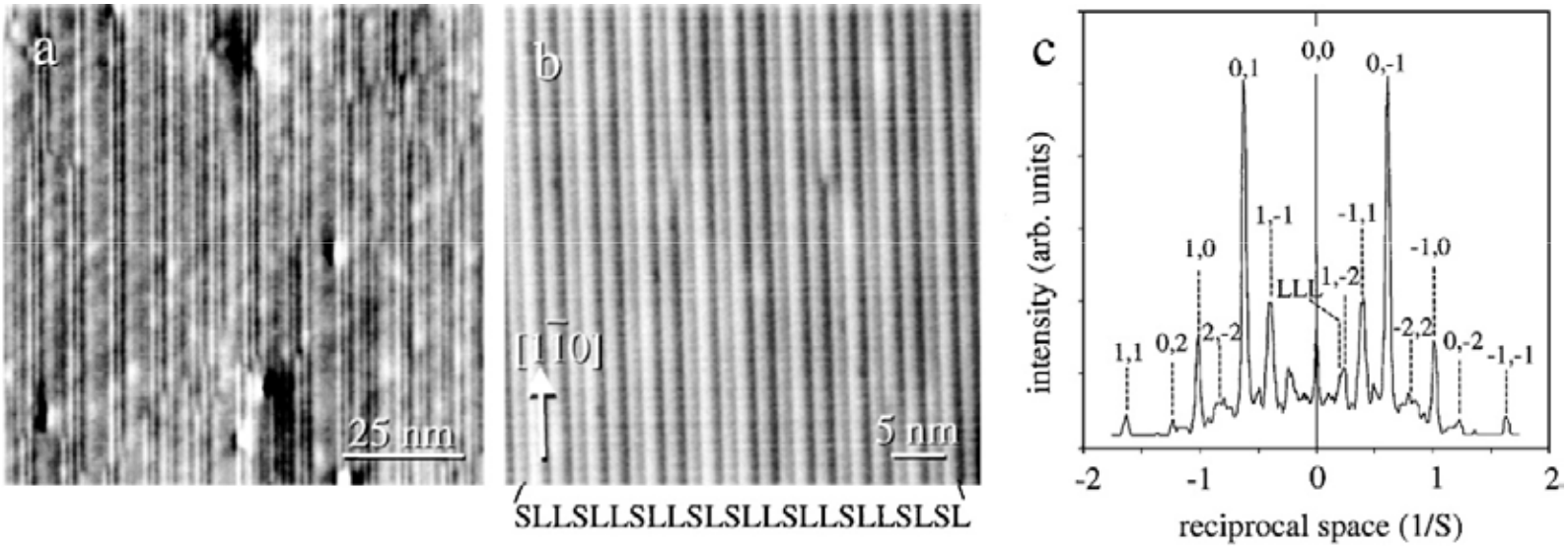
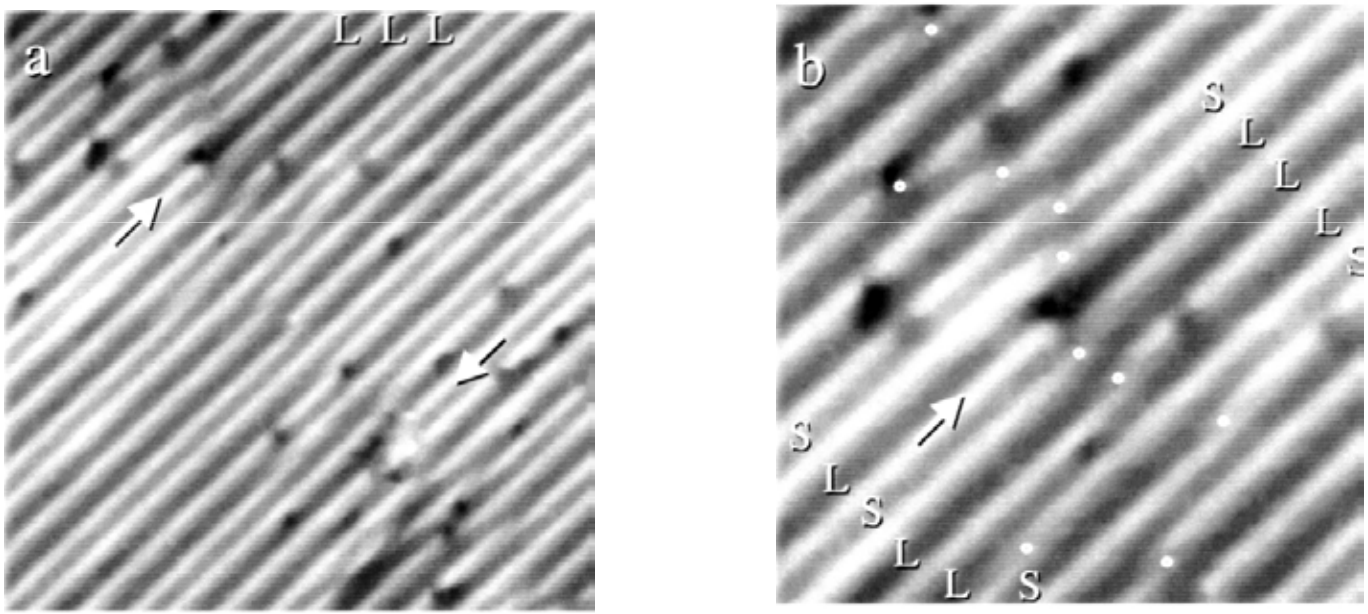
One-dimensional quasiperiodic superstructure of a thin Ag film on GaAs(110) surfaces



Ph. Ebert, K.-J. Chao,Q. Niu, and C. K. Shih, Phys Rev Lett 83 (1999) 3222

obtained by depositing 1.5 to 1.7 nm thick Ag layers at 135 K on freshly cleaved GaAs(110) surfaces in ultrahigh vacuum

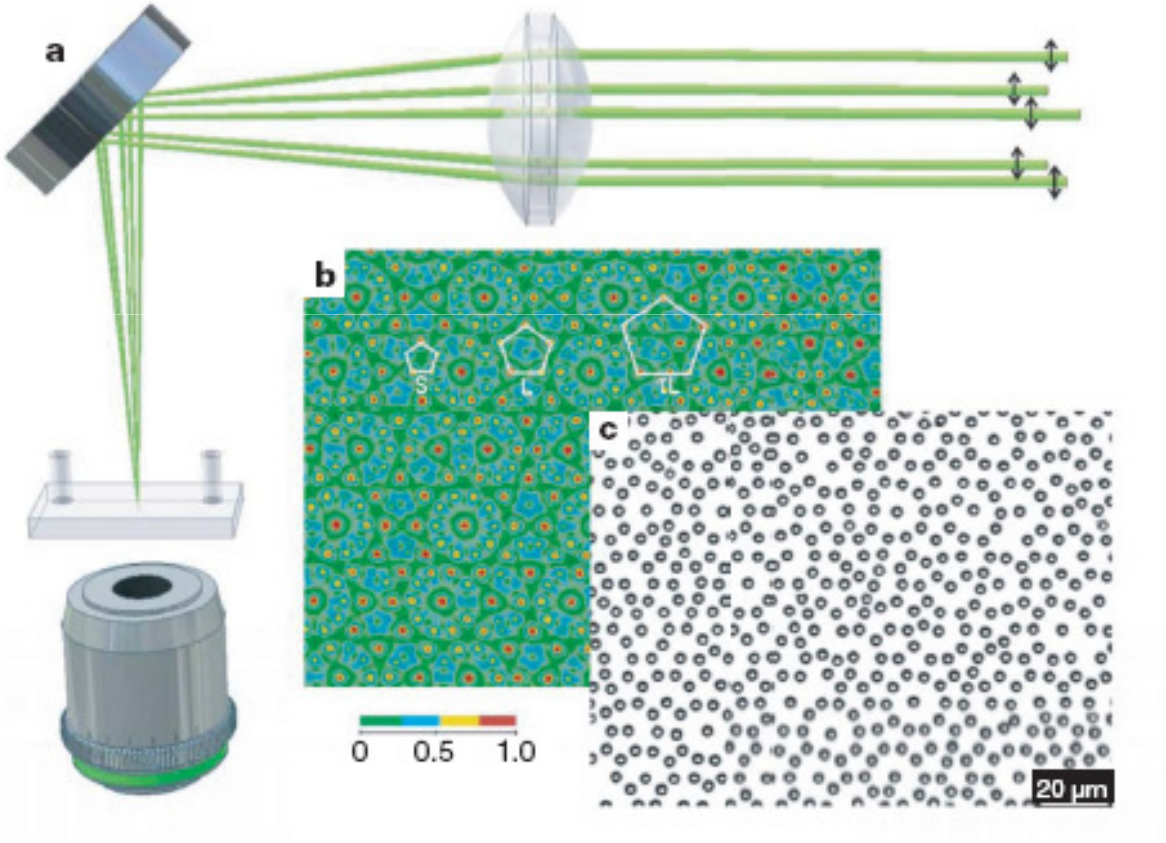
films were annealed at room temperature



Ph. Ebert, K.-J. Chao,Q. Niu, and C. K. Shih, Phys Rev Lett 83 (1999) 3222

Archimedean-like tiling on decagonal quasicrystalline surfaces

Jules Mikhael[1], Johannes Roth[2], Laurent Helden[1] & Clemens Bechinger[1,3]



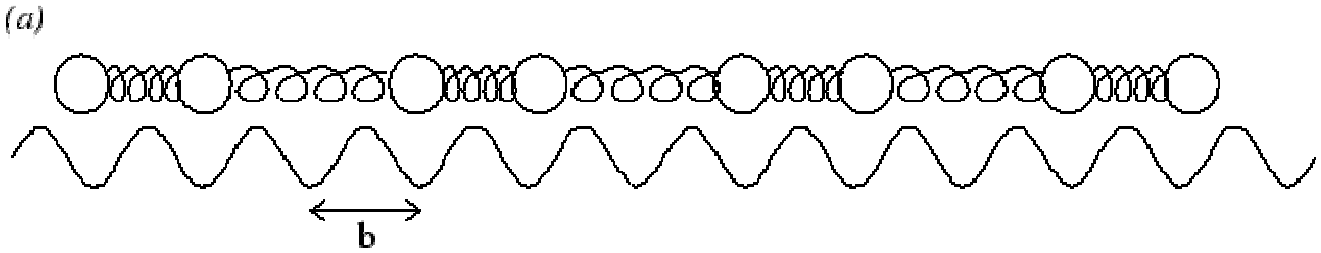
NATURE| Vol 454|24 July 2008 p.501

two periodicities q_1 and q_2 are incommensurate if they cannot be expressed as a ratio of two integers:

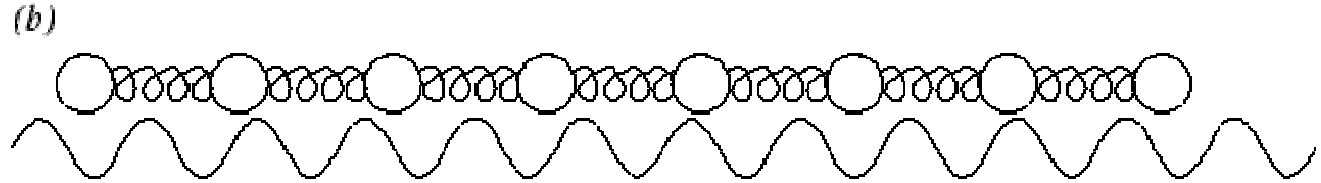
$$\frac{q_1}{q_2} \neq \frac{M}{N} \qquad M, N = 1, 2, 3....$$

Incommensurate phases the result of a conflict between various competing forces within a system. A simple model commonly used to illustrate this is shown below:

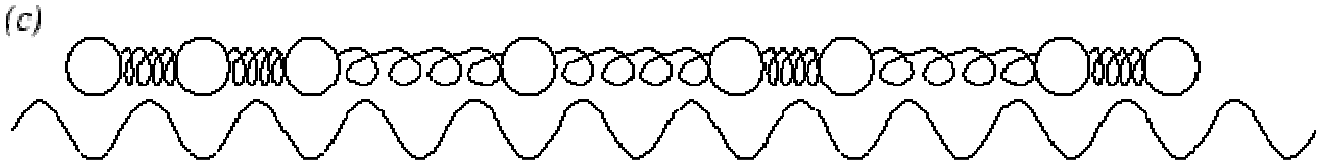
Frenkel and Kontorova model



commensurate



incommensurate



chaotic

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Orientational Epitaxy—the Orientational Ordering of Incommensurate Structures

Anthony D. Novaco*†
Lafayette College, Easton, Pennsylvania 18042, and Brookhaven National Laboratory,‡ Upton, New York 11973

and

John P. McTague†§
University of California, Los Angeles, California 90024, and Brookhaven National Laboratory,‡ Upton, New York 11973

PRL 38 (1977) 1286
(317 citations)

A new class of structures is predicted to exist for monolayer films on solid surfaces. These structures involve two incommensurate lattices—the monolayer lattice and the surface lattice— which have a preferred relative orientation. The precise orientation depends upon the lattice constant and symmetry of each lattice. We believe this orientationally ordered incommensurate phase to be present in many physisorbed films. In particular, the existence of this phase appears to explain recent low-energy electron diffraction data for rare gases adsorbed on homogeneous substrates.

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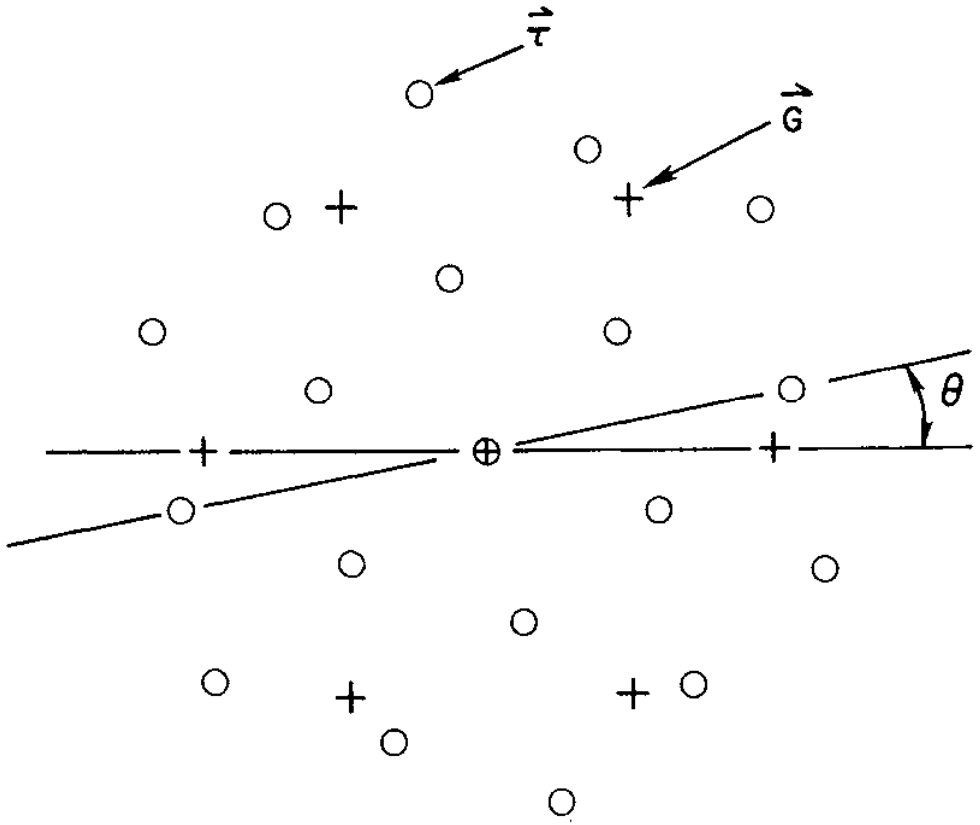

FIG. 1. The reciprocal-lattice vectors $\{\vec{\tau}\}$ for the monolayer lattice and $\{\vec{G}\}$ for the graphite lattice. The angle θ is the angle of rotation relative to the superlattice orientation.