Quantifying and enforcing plane symmetry in images of 2D periodic objects

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other projects: Oregon Nanoscience and Microtechnologies Institute, Office of Naval Research, Research Corporation, North-West Academic Computing Consortium, National Science Foundation, National Center for Electron Microscopy Berkeley

Lord Kelvin (William Thompson), 1883:

"I often say that when you can measure what you are speaking about, and express it in numbers, you know something about it;

but when you cannot measure it, when you cannot express it in numbers, your knowledge is of a meager and unsatisfactory kind; it may be the beginning of knowledge, but you have scarcely, in your thoughts, advanced to the state of science."

Outline

1. **Plane symmetry, a well defined mathematical concept, deviations from it are quantifiable**

2. **Experimental and simulated examples:**
   Scanning Tunneling Microscopy (STM), 2D periodic and highly symmetric calibration samples, symmetrizing a blunt STM tip,
   Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), better surface and nano-science, *but problems of deciding between plane groups without prior knowledge*, other limitations

3. **Knowledge of 2D symmetry makes for more sophisticated art (M. C. Escher)**

4. **Summary and Conclusions**

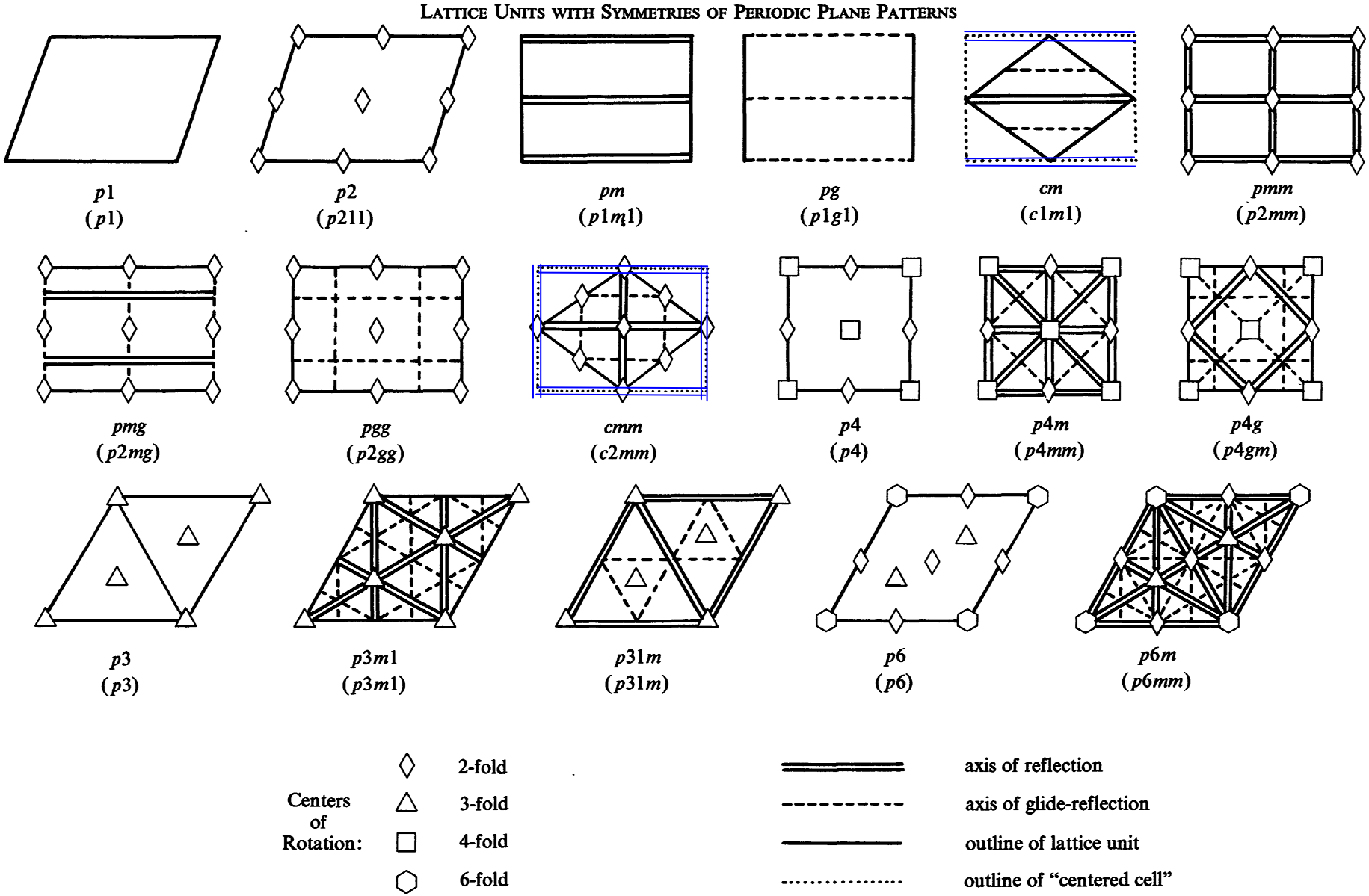


CHART 2. International notation identifies the seventeen two-dimensional crystallographic groups. The short form is given first, with the full notation in parentheses.

D. Schattschneider, *The American Mathematical Monthly* **85** (1978) 439-450, **but modified for centered cells**

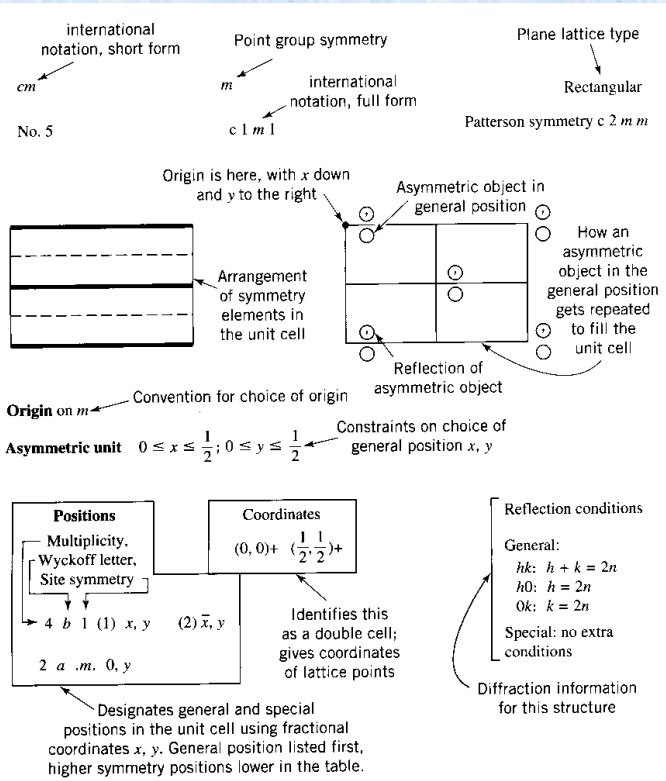


Figure 3.32 Annotated copy of plane group No. 5, *cm*, from the *International Tables for Crystallography*, 1996.

T. Hahn (Ed.), Brief Teaching Edition of Volume A, Space-group symmetry, International Tables for Crystallography, 5th revised edition, International Union of Crystallography (IUCr), Chester 2005.

Robotics and machine vision community favors the direct space approach to plane symmetry detection and quantification, Y. Liu et al. IEEE Transactions on Pattern Analysis and Machine Intelligence 28 (2004) 354-374

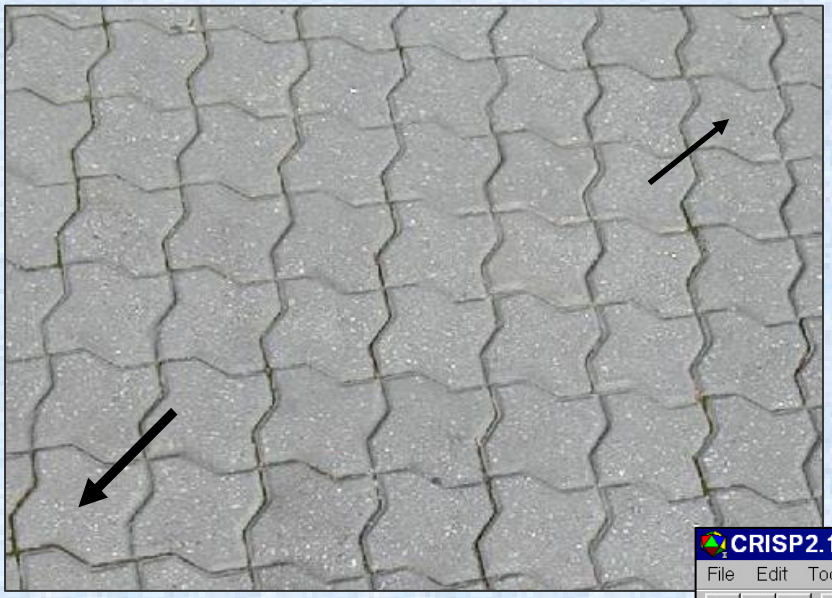
But crystallographic community prefers the reciprocal space, kinematic scattering, Fourier transform approach !

$$f(x,y)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}F(H,K)\exp\{-2\pi i(xH+yK)\}dHdK=FT^{-1}\left[F(H,K)\right]$$

The Fourier transform of a 2D periodic object is a discrete set of complex numbers, which contains exactly the same information!

$$f(x,y)^{periodic}=\sum_{-H}^{H}\sum_{-K}^{K}F(H,K)^{discrete}\exp\{-2\pi i(xH+yK)\}$$

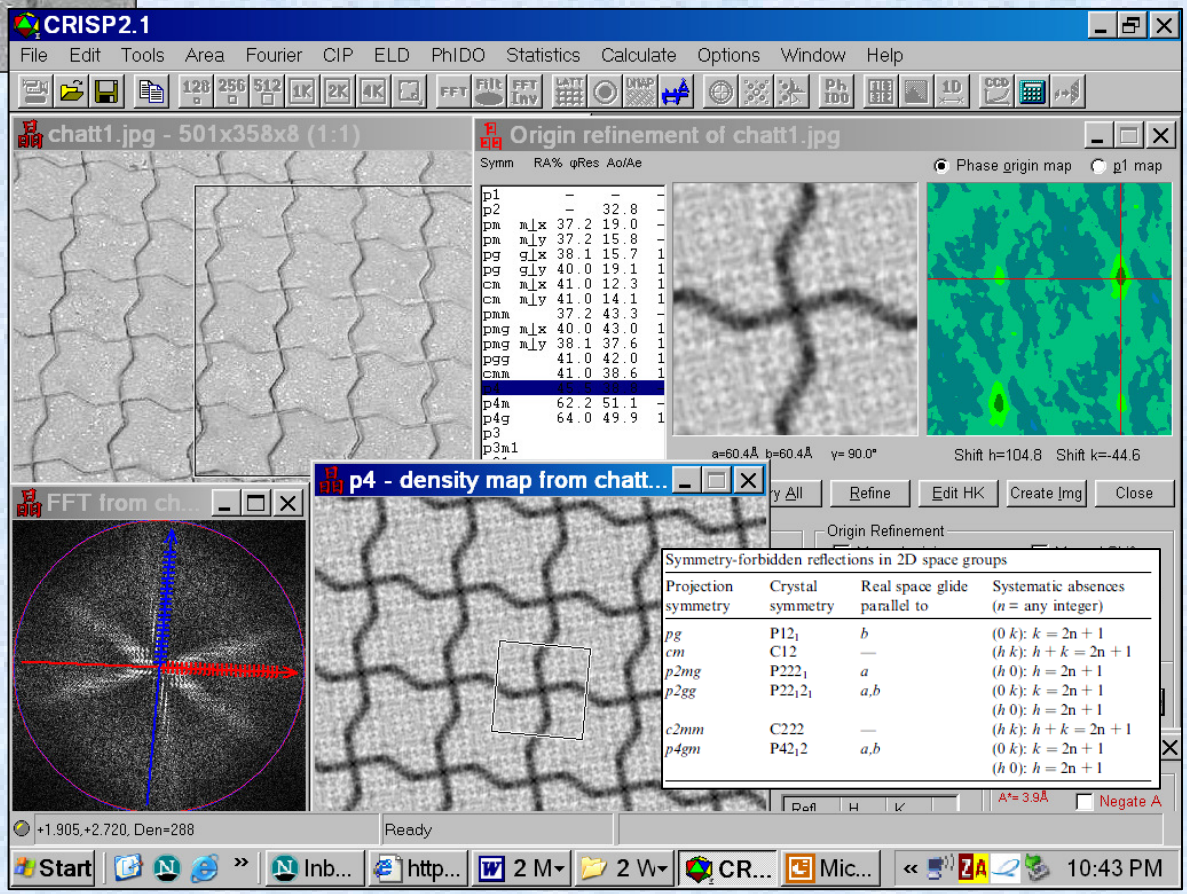
Instead of analyzing the symmetry relations between *each pixel* of a 2D image, it is sufficient to analyze the symmetry relations of *a few Fourier coefficients*, in X-ray crystallography known as “structure factors”!!



Digital photogram of this street pavement was not recorded perpendicular to the pavement. Note the size difference between pavement bricks marked by arrows.

plane group: p4, point group of motif: 4

Crystallographic Image processing quantifies the plane symmetry correctly. Enforcing this symmetry leads to removal of the “imperfections of the imaging process” and “enhancement of surface details” of the pavement bricks.



$$F_{res} = \frac{\sum_{HK} \left| \left| F_{obs}(H,K) \right| - \left| F_{sym}(H,K) \right| \right|}{\sum_{HK} \left| F_{obs}(H,K) \right|} \qquad \alpha_{res} = \frac{\sum_{HK} w(H,K) \cdot \left| \alpha_{obs}(H,K) - \alpha_{sym}(H,K) \right|}{\sum_{HK} w(H,K)}$$

$$\left| F_{sym}(H,K) \right| = \sum_{j}^{n} \left| F_{obs}{}^{j}(H,K) \right| \Big/ n$$

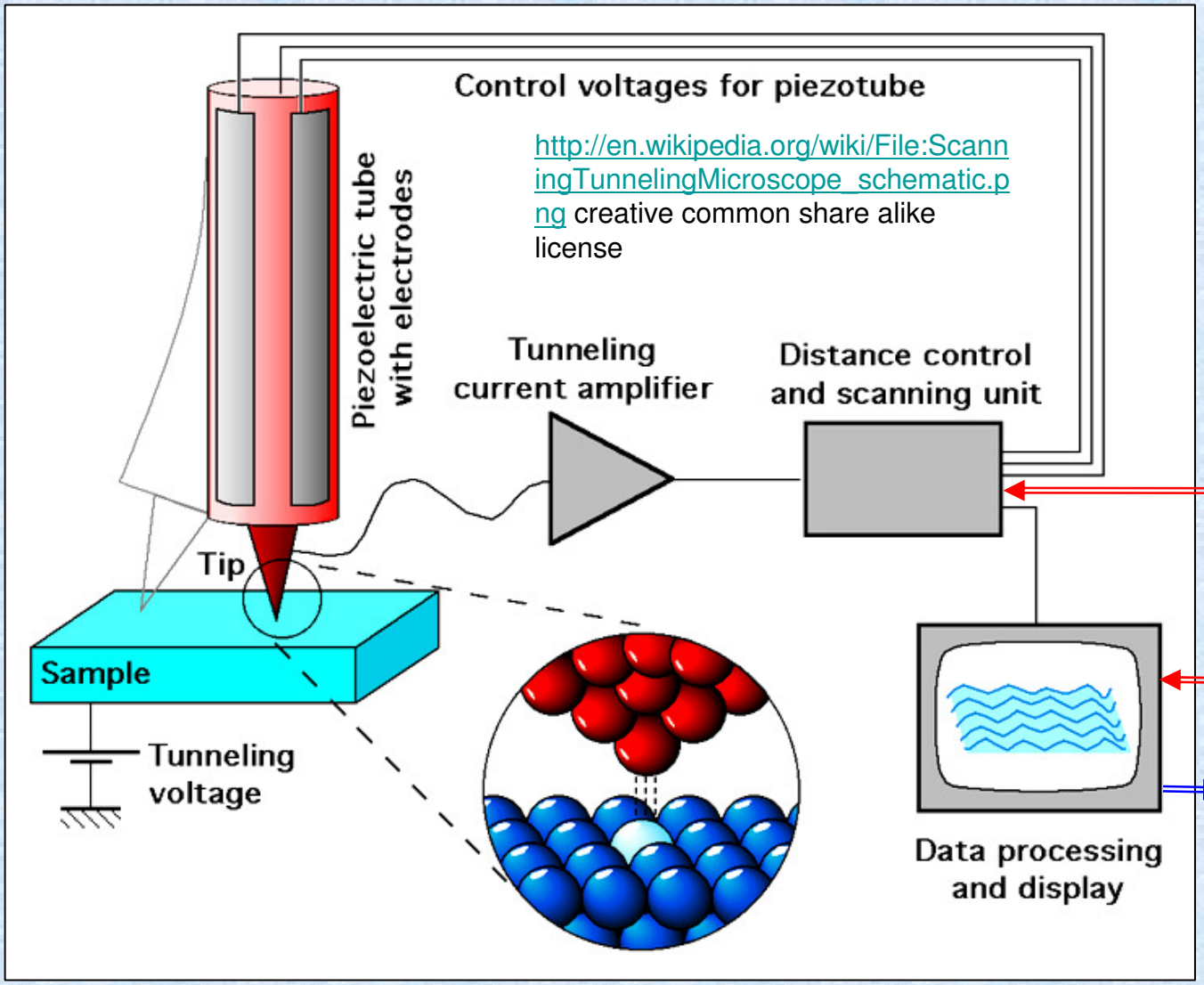
$$\alpha_{sym}(H,K) = \arctan\left[\frac{\sum_j w^j s^j \sin\{\alpha_{obs}^j(H,K)\}}{\sum_j w^j s^j \cos\{\alpha_{obs}^j(H,K)\}} \right] + \left\{ \begin{array}{ll} 0^\circ & [if \sum_j w^j s^j \cos\{\alpha_{obs}^j(H,K)\} > 0] \\ 180^\circ & [if \sum_j w^j s^j \cos\{\alpha_{obs}^j(H,K)\} < 0] \end{array} \right\}$$

where w^j is a weighting factor, proportional to $\left| F_{obs}{}^{j}(H,K) \right|$; s^j = 1 in the absence of an approximately 180° flipped phase or s^j = -1. For centrosymmetric plane groups finally set to the nearest 0° or 180°.

$\alpha_{sym}(H,K) = \alpha_{obs}(H,K)$ if not symmetry related except for Friedel's law $\alpha_{obs}(H,K) = -\alpha_{obs}(-H,-K)$

$\left| F_{sym}(H,K) \right| = \left| F_{obs}(H,K) \right|$ if not symmetry related except for Friedel's law $\left| F_{obs}(H,K) \right| = \left| F_{obs}(-H,-K) \right|$

Note that known 2D symmetry information about a sample has not been utilized before !!



http://en.wikipedia.org/wiki/File:ScanningTunnelingMicroscope_schematic.png creative common share alike license

Crystallographic processing of an image from a known SPM calibration sample with 2D periodic (and highly symmetric) features in order to
1. Assess the performance of the microscope **(determine prevalent point spread function)** ;
2. Correct subsequently recorded images from unknowns with this point spread function !
(valid for one set of experimental conditions and scanning probe tip at a time)

Scanning Tunneling Microscopy: **left:** state of the art; **right:** our proposed enhancements, provisional patent application pending

Challenge: environmentally stable SPM standards with 2D periodicities at the atomic level, preferably high plane symmetry so that all subgroups can be used for quantification of the performance of the microscope and its proper calibration, HOPG should do !

white atoms not clearly visible

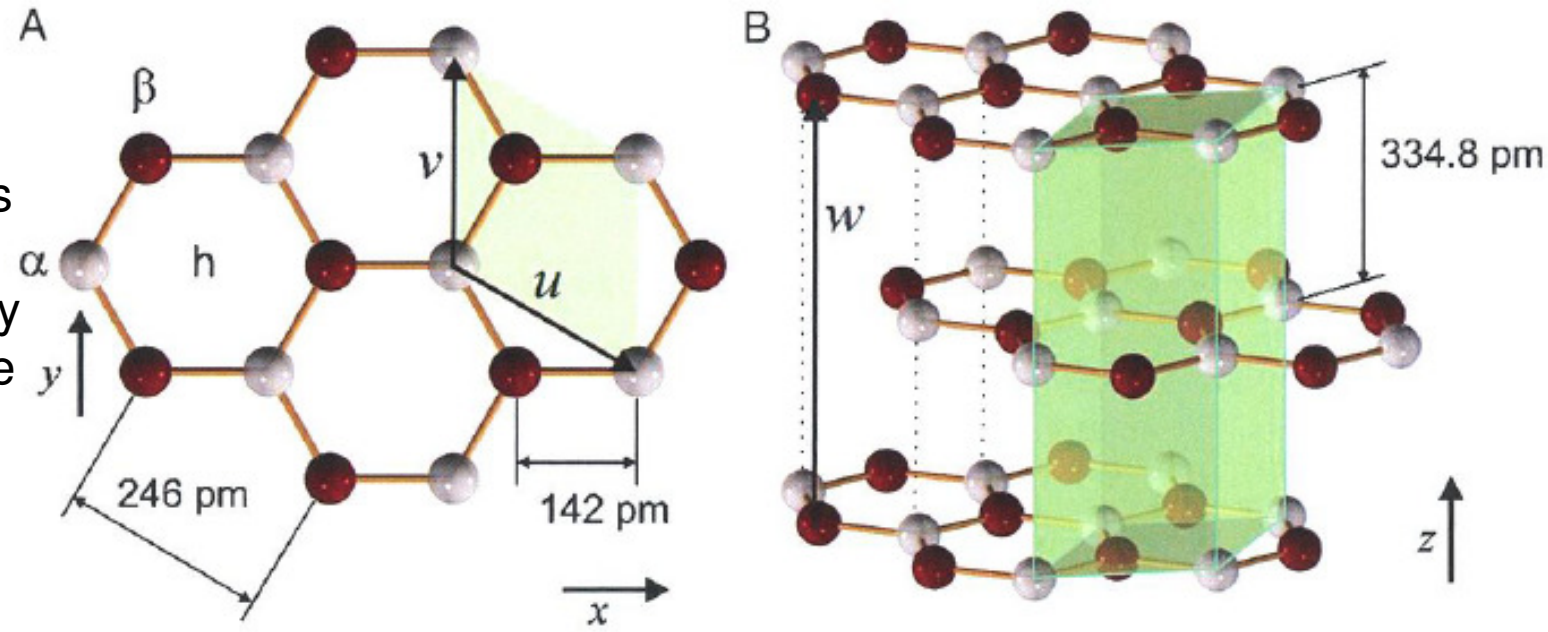
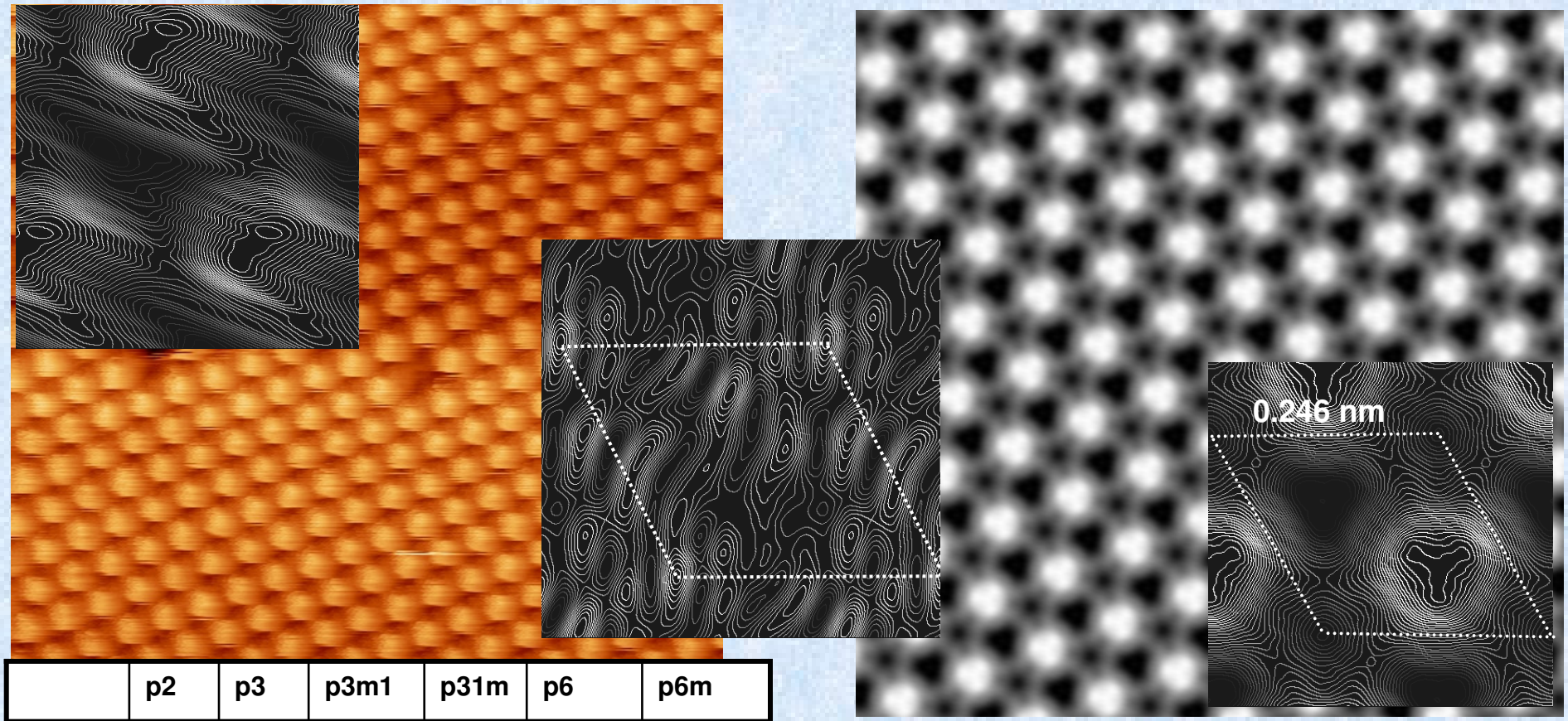


Fig. 1. Crystal structure of graphite. The unit cell is shaded in green. (*A*) Top view on the surface layer. The hexagonal surface lattice is defined by two unit vectors, *u* and *v*, in the *xy* plane with a length of 246 pm and an angle of 120° forming a honeycomb web of hexagonal rings. The basis of the lattice consists of two carbon atoms α (white) and β (red) with a distance of 142 pm. (*B*) Perspective view, showing the layered structure. The distance between layers is 2.36 times the next-neighbor distance of atoms within one layer, and the bond between layers is weak. The α atoms (white) are directly above an α atom in the layer directly underneath at a distance of 334.8 pm; the β atoms (red) are over a hollow sites (h). The unit vector *w* is parallel to the *z*-axis with a length of 669.6 pm.

S. Hembacher, et al., Revealing the Hidden Atom in Graphite by Low-Temperature Atomic Force Microscopy, Proceedings of the National Academy of Sciences of the United States of America, Vol. 100, No. 22 (Oct. 28, 2003), pp. 12539-12542

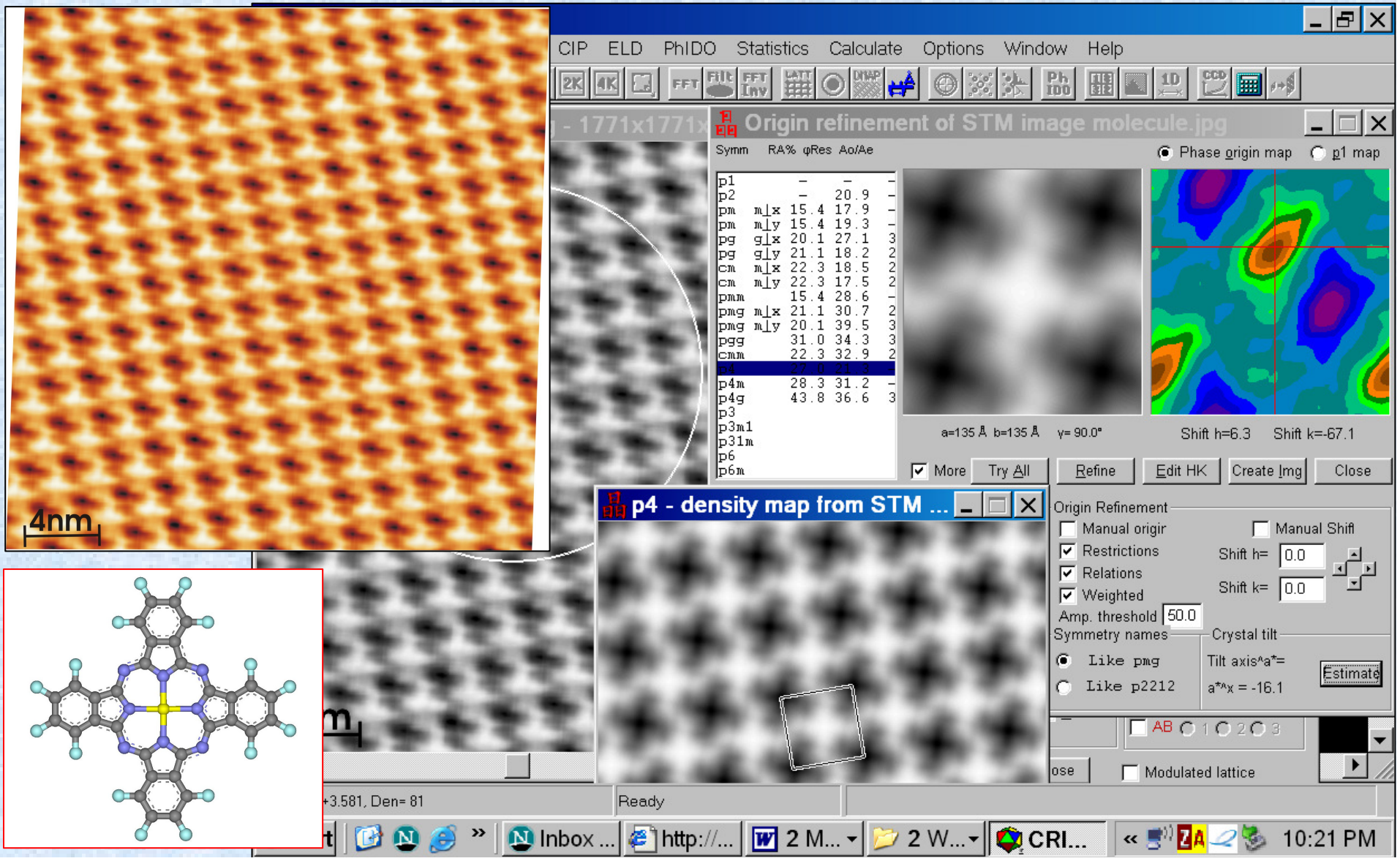


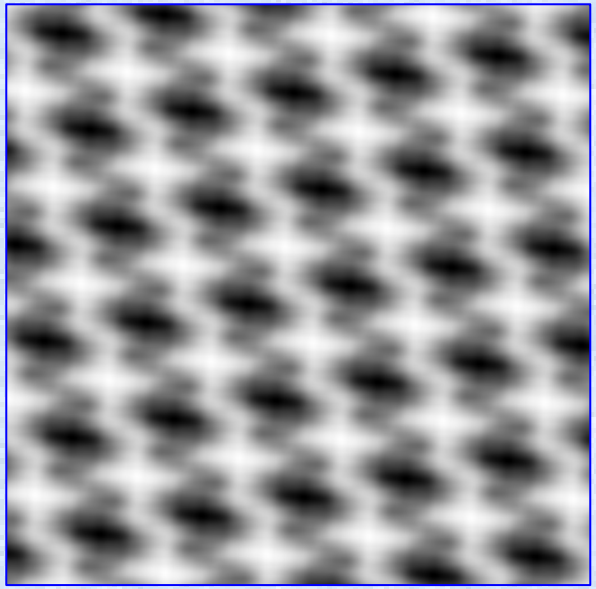
	p2	p3	p3m1	p31m	p6	p6m
F_{res} [%]		50.4	51.3	51.3	50.4	51.3
α_{res} [°]	19.9	14.2	17.1	29.2	31.3	32.2

The relative high amplitude residuals are due to a unit cell angle of 63.7° in the raw image.

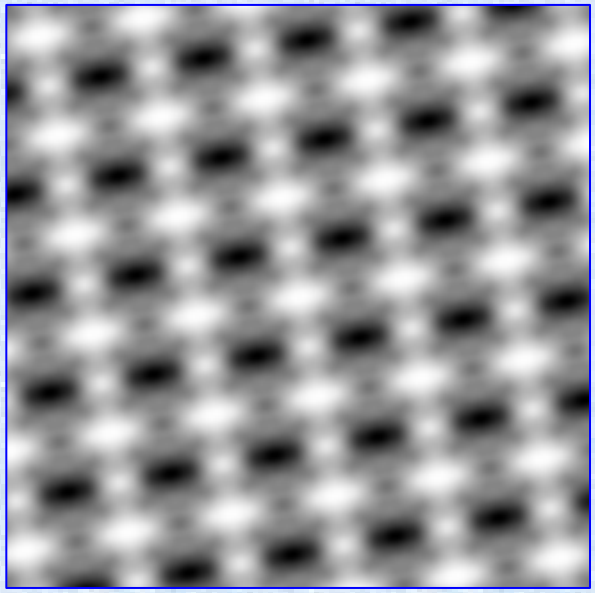
STM images of HOPG **(a)** raw data with 512 by 512 pixels, constant current mode, tungsten tip, 1 V bias, 0.15 nA (left) and **(b)** p3m1 enforced version of raw data (right). Note that there are atomic vacancies in the raw data. While the carbon atom at position ($^2/_3$,$^1/_3$) is clearly revealed, its counterpart at position (0,0) is rather faint, but at a higher intensity than the “empty spot” at position ($^1/_3$,$^2/_3$).

Scanning Tunneling Microscopy Image of a mono-layer of fluorinated cobalt phthalocyanine ($F_{16}CoPc$) on graphite, UHV and 20 K, tungsten tip bias 1 V, constant 0.1 nA tunneling current !

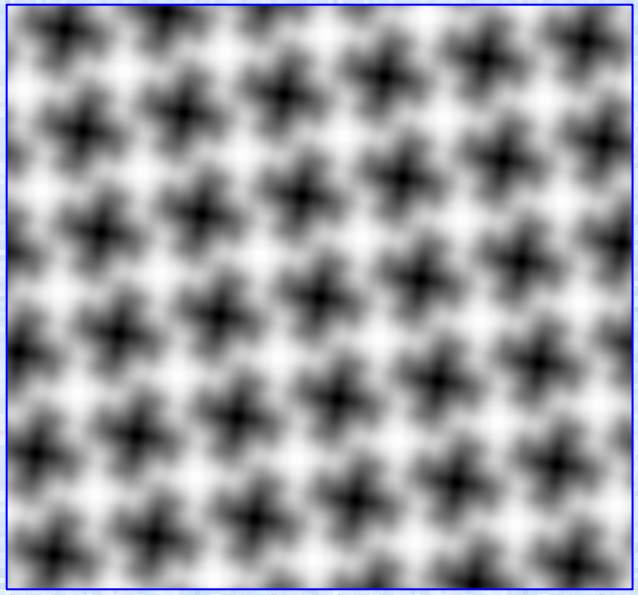




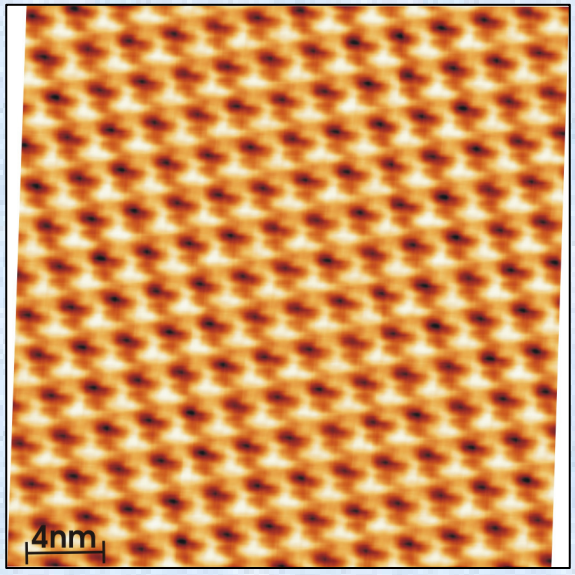
p2 symmetry enforced STM data. A two-fold axis is imposed. The lattice remains oblique. The motif acquires point symmetry 2 and the peculiar "overall image twist" is removed.

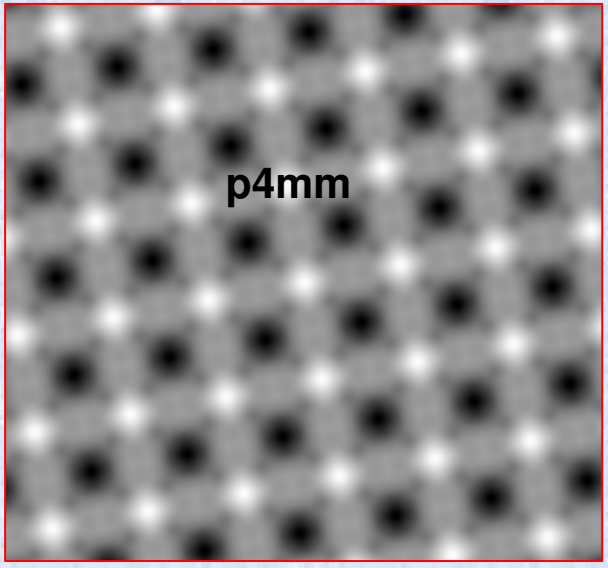


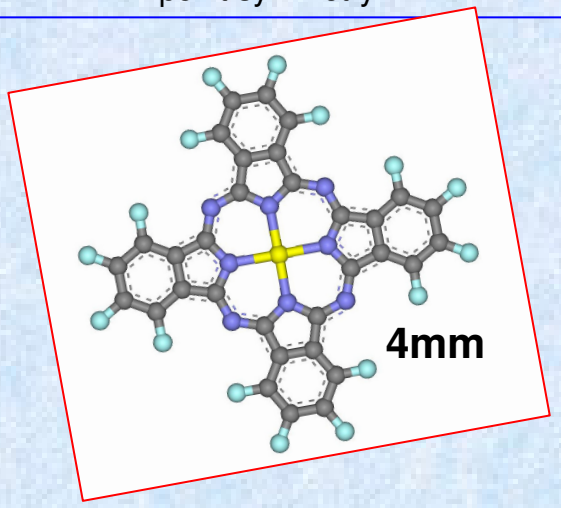
p2mm symmetry enforced STM data. A two-fold axis with a set of perpendicular mirrors is imposed. The lattice becomes rectangular. The motif acquires point symmetry 2mm



p4 symmetry enforced STM data. A four-fold axis is imposed. The lattice becomes quadratic and the motif acquires the point symmetry 4.

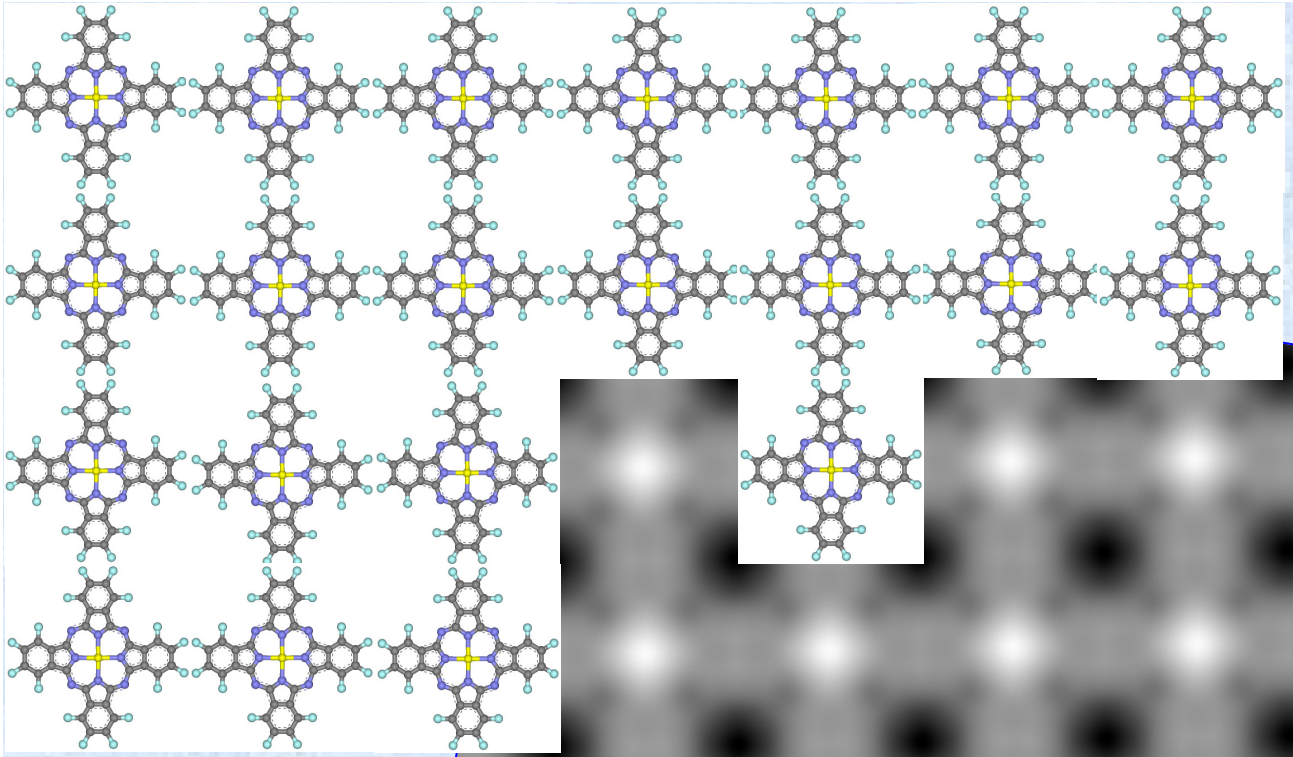




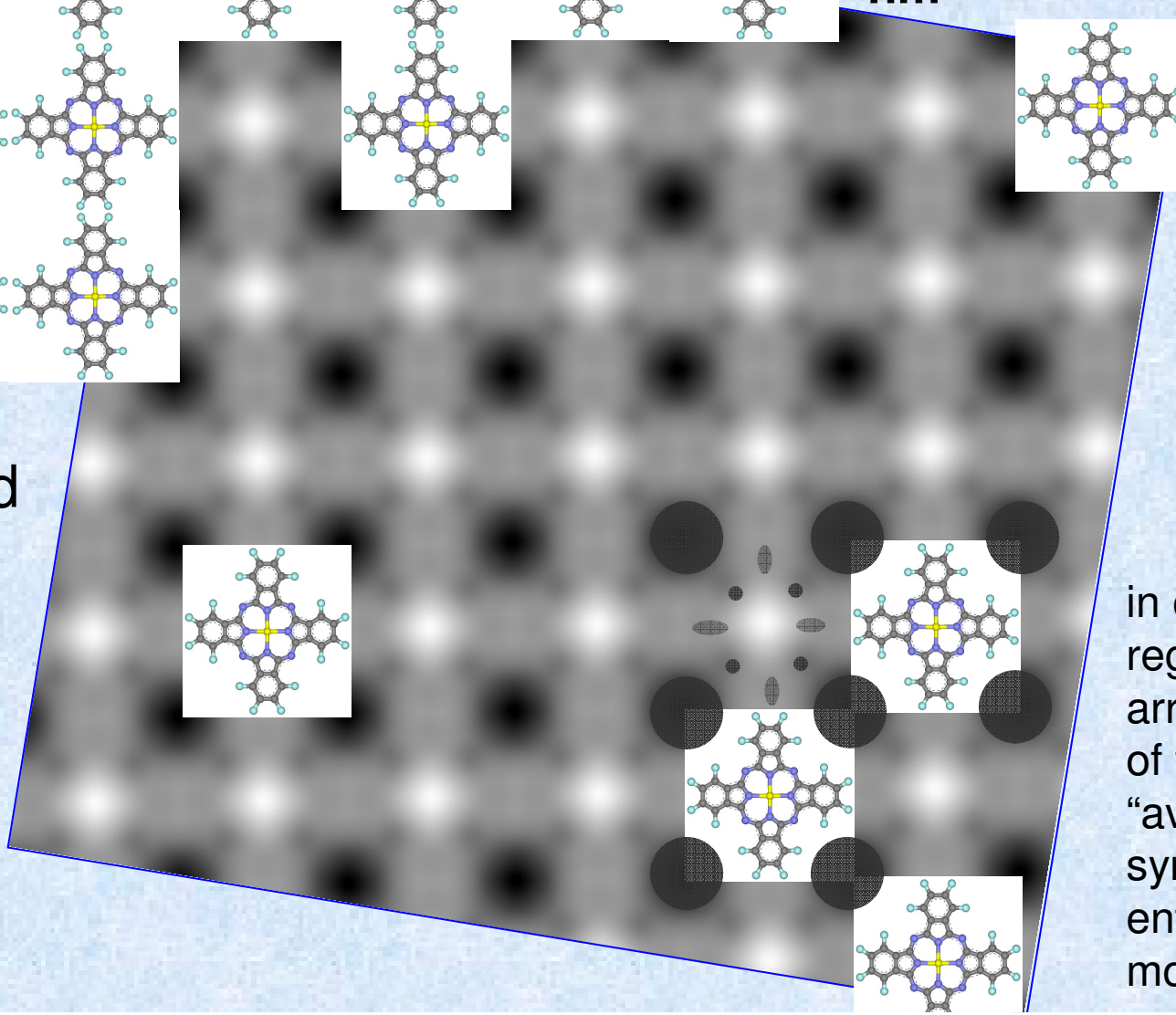


"Size" of molecule and basic periodicities in STM images approximately 1.5 – 2 nm

“Size” of molecule and basic 2D periodicities in STM images approximately 1.5 - 2 nm



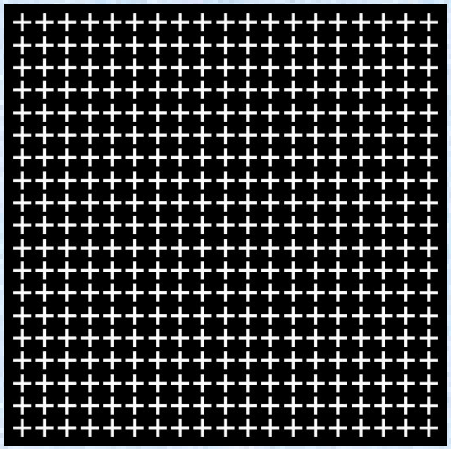
p4mm symmetrized version of STM data in comparison to a model array of $F_{16}CoPc$ molecules

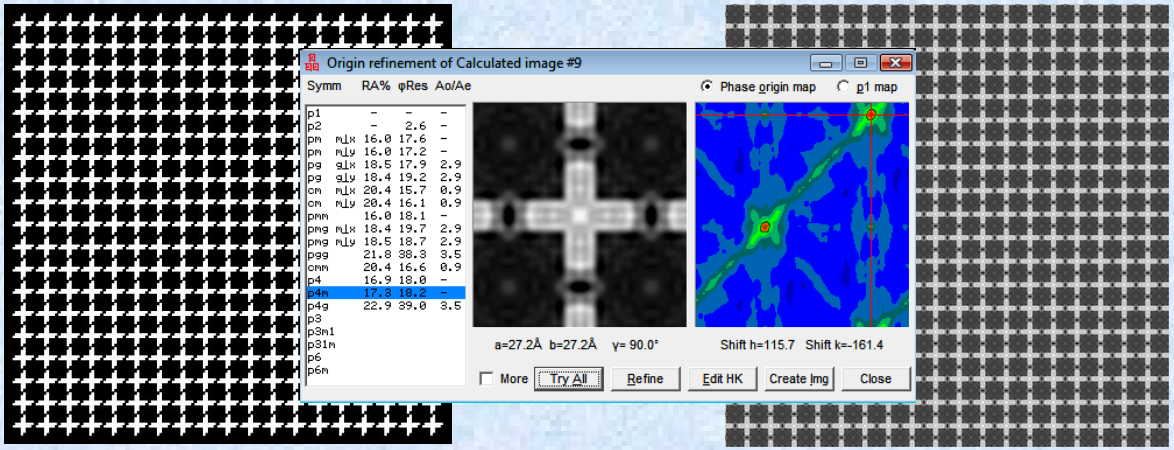


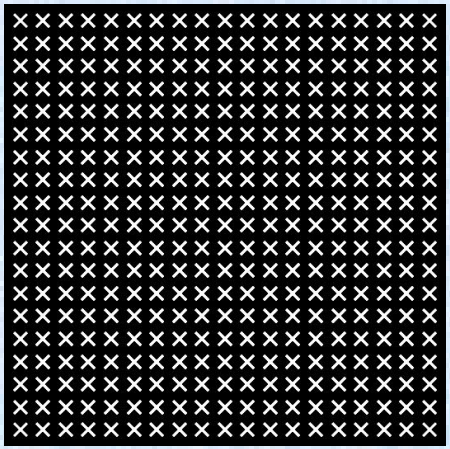
in essence regularly arrayed copies of the “average” and symmetry enforced molecule

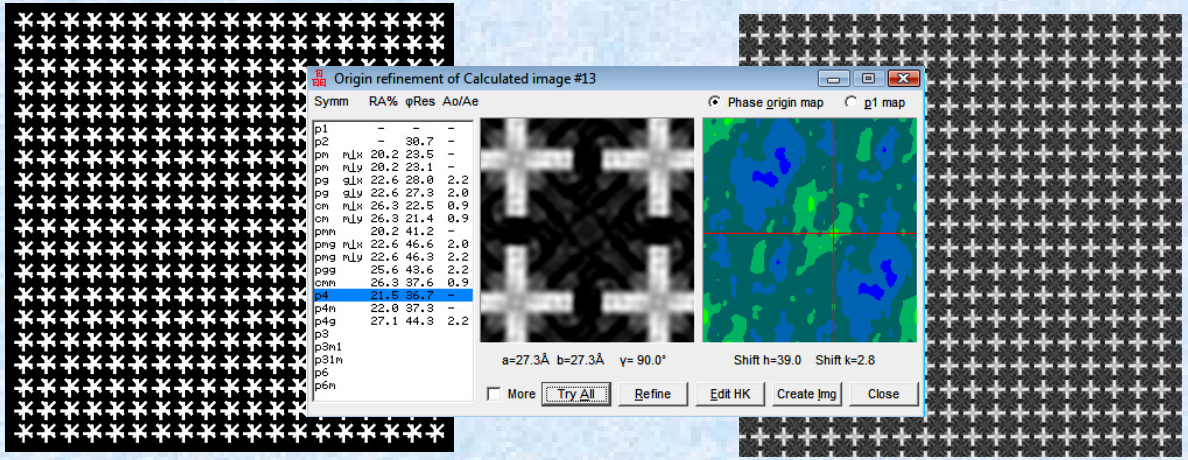
recovering one image of the original 2D array

two images of the "**same kind**" from the same 2D array
superimposed with translation



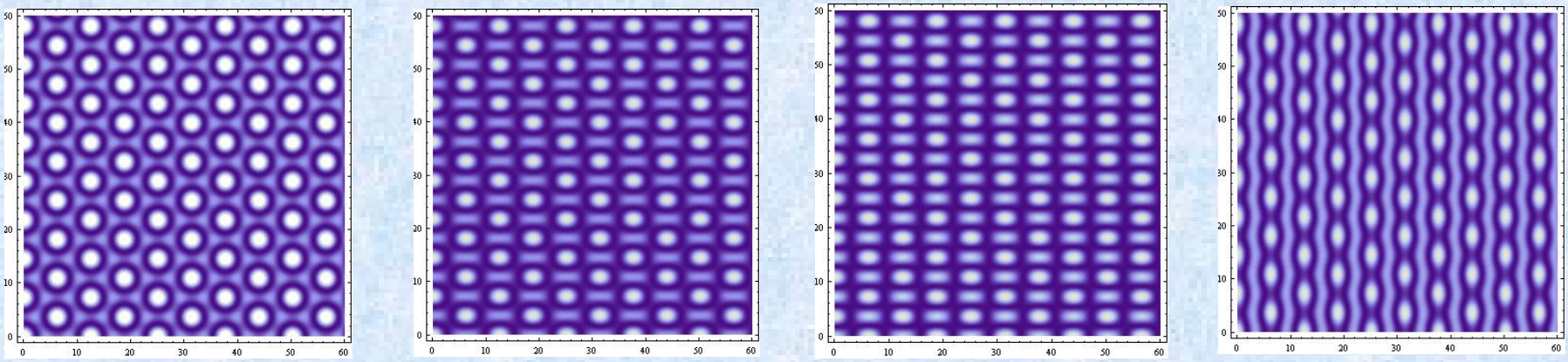




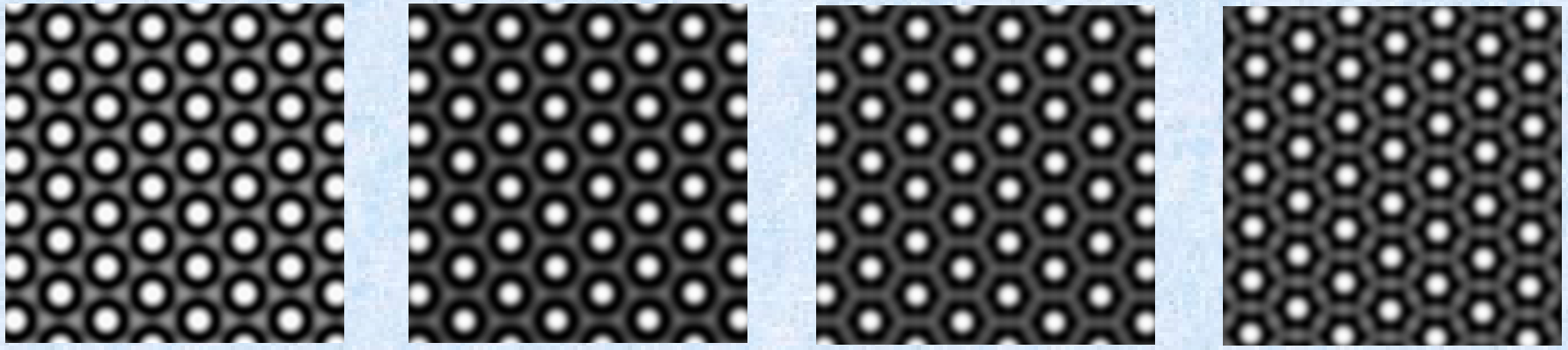


both p4mm

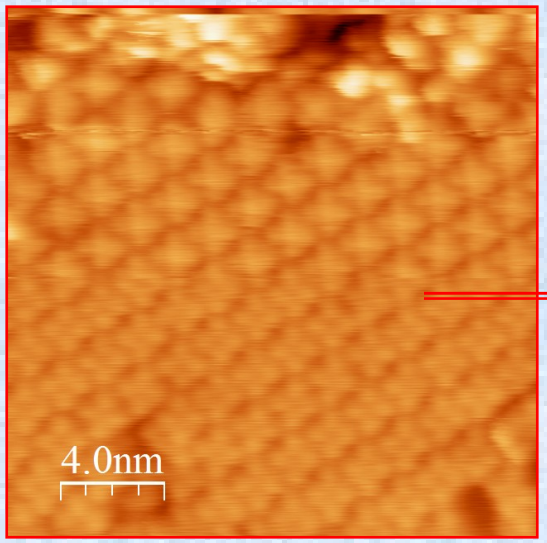
two images of "**each kind**" from the same 2D array
superimposed with translation

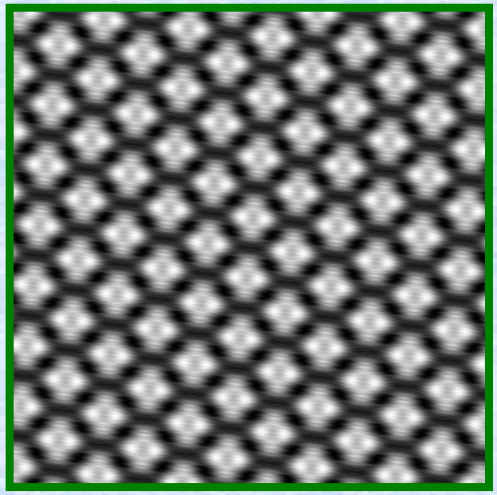


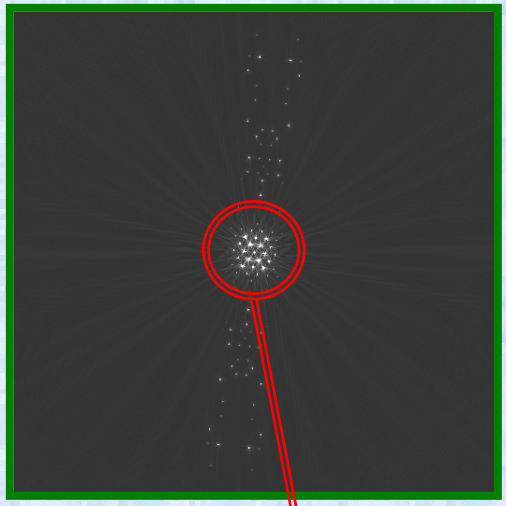
Simulated series of STM images of a sample surface with plane symmetry *p6mm*. The first image was simulated for a single tip. Two mini-tips (as a simple model of a blunt STM tip) were scanning from top to bottom in the other three simulations. The distance between the two mini-tips increases from left to right. Electron interference between the two tips was included in the simulations.



CIP processed STM images (of a sample surface with plane symmetry *p6mm*) as simulated in the figures above. Despite the two mini-tips and electron interference effects between these two tips in three of the simulated image, crystallographic image processing recovers in all cases the underlying plane symmetry of the sample surface reasonably well !

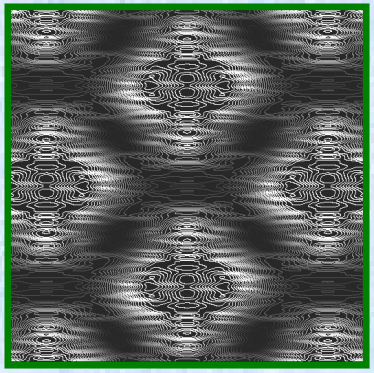


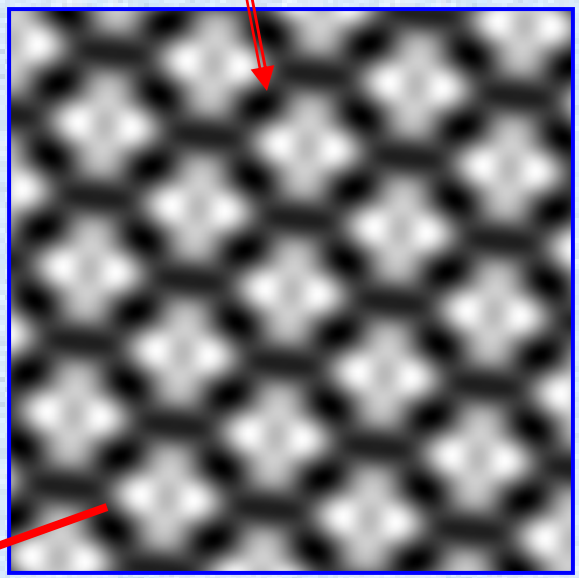




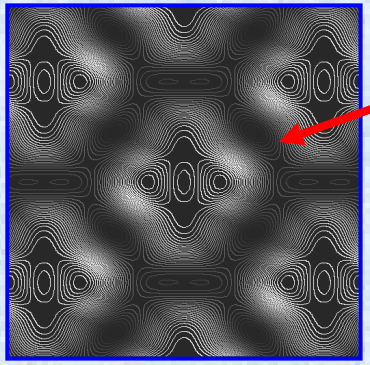
F_{16}CoPc on silver (110), UHV and 20 K, tungsten tip bias 1 V, constant 0.1 nA tunneling current

c2mm enforced





Working hypotheses: since the substrate has plane group *c2mm*, it is no coincidence that the monolayer also has this plane group (Curie's principle for strong epitaxial interaction), also directly above every 5th Ag atom, there is the central Co atom of every F_{16}CoPc molecule



Fourier filtered and contour map

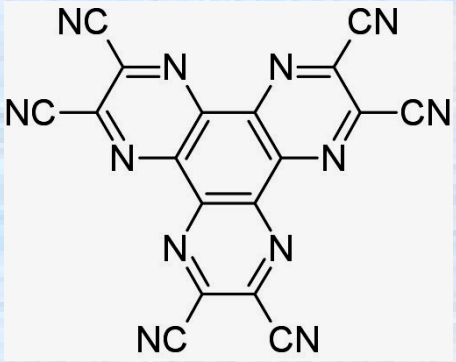
"Soft" Metallic Contact to Isolated C Molecules

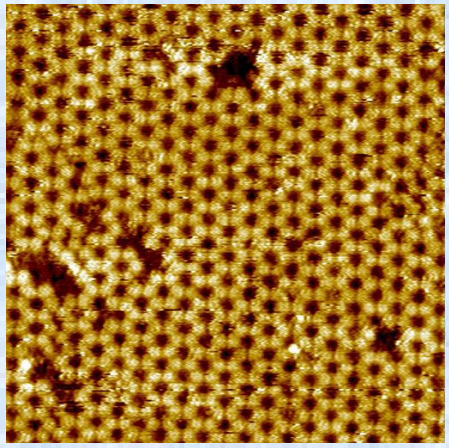
Hendrik Glowatzki, Benjamin Bro#ker, Ralf-Peter Blum, Oliver T. Hofmann, Antje Vollmer, Ralph Rieger, Klaus Mu#llen, Egbert Zojer, Ju#rgen P. Rabe, and Norbert Koch

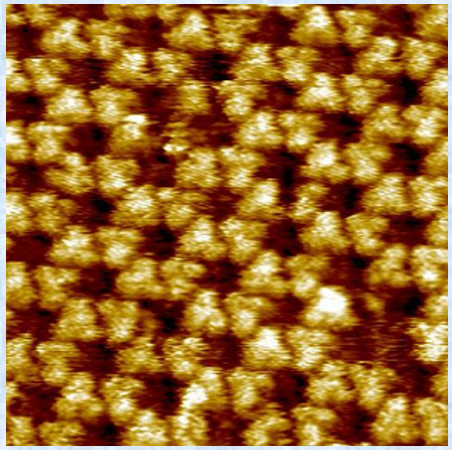
Nano Lett., **2008**, 8 (11), 3825-3829 • DOI: 10.1021/nl8021797 • Publication Date (Web): 28 October 2008

STM, UHV, 300 K, a genuine breakthrough

Ag (111), plane group p6mm +
hexaazatriphenylene -hexanitrile
HATCN

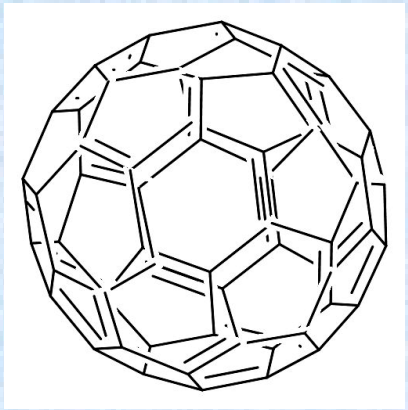


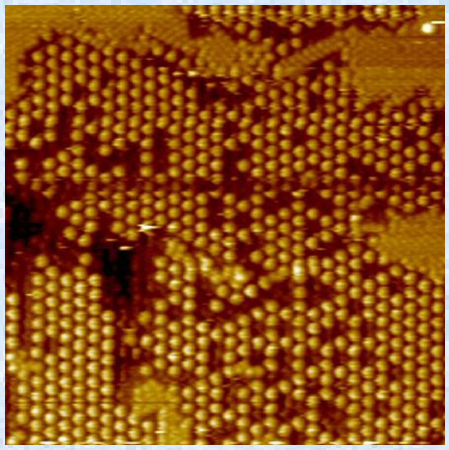


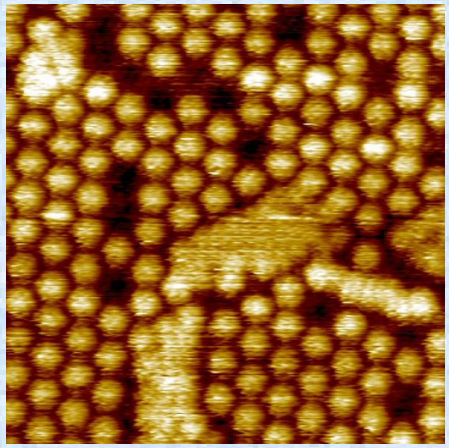


metallic when on Ag (111)

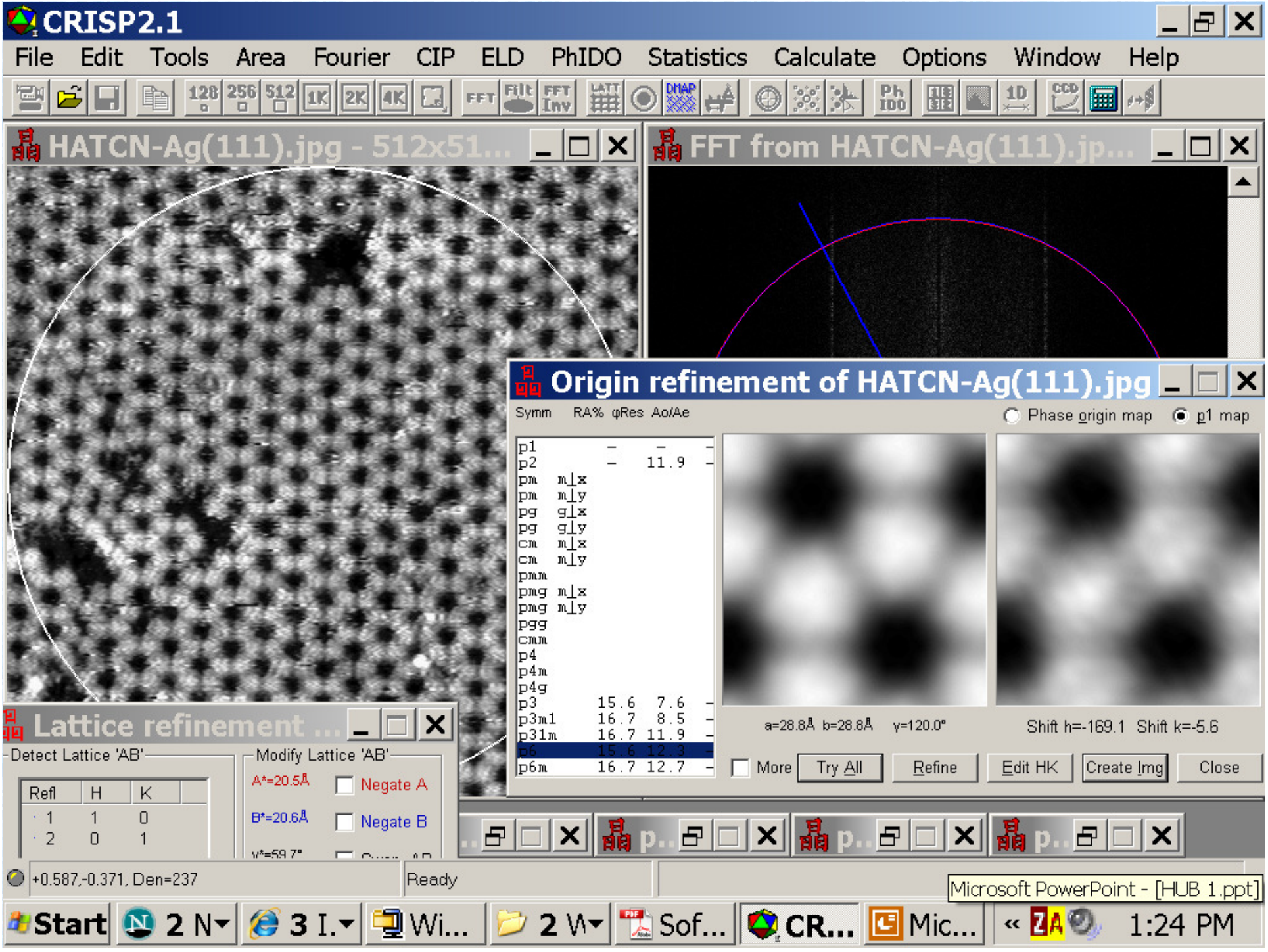
+ buckyballs in the centers of the molecules







electronic structure not modified by the soft metallic contact !


CRISP2.1
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HATCN-Ag(111).jpg - 512x51...
FFT from HATCN-Ag(111).jp...
Origin refinement of HATCN-Ag(111).jpg
Symm RA% φRes Ao/Ae
Phase origin map
p1 map
p1 - - -
p2 - 11.9 -
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pm m⊥y
pg g⊥x
pg g⊥y
cm m⊥x
cm m⊥y
pmm
pmg m⊥x
pmg m⊥y
pgg
cmm
p4
p4m
p4g
p3 15.6 7.6 -
p3m1 16.7 8.5 -
p31m 16.7 11.9 -
p6 15.6 12.3 -
p6m 16.7 12.7 -
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Shift h=-169.1 Shift k=-5.6
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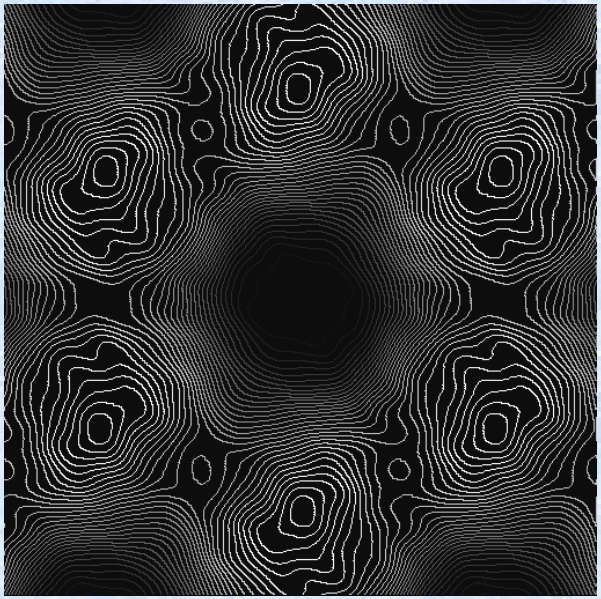
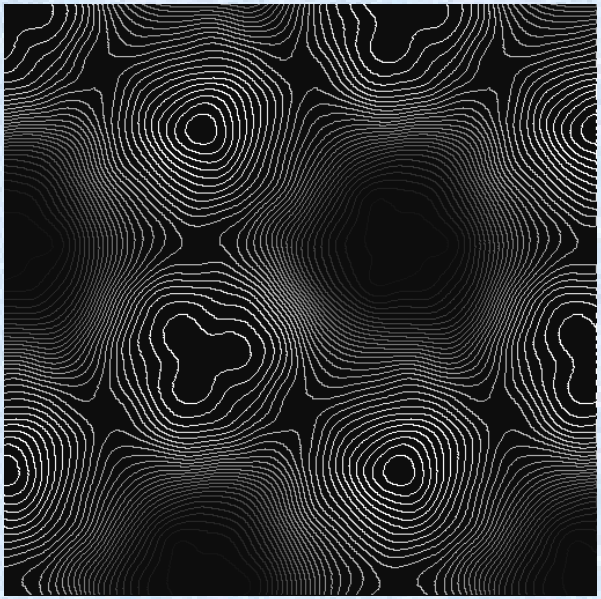
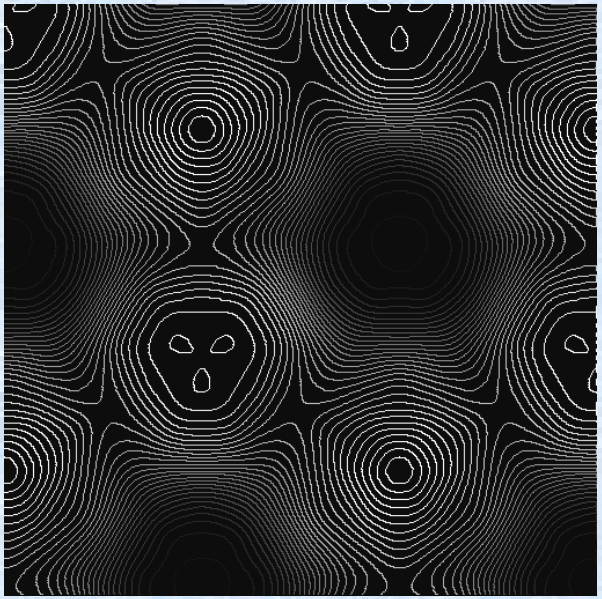
Try All
Refine
Edit HK
Create Img
Close
Lattice refinement ...
Detect Lattice 'AB'
Refl H K
1 1 0
2 0 1
Modify Lattice 'AB'
A*=20.5Å
Negate A
B*=20.6Å
Negate B
+0.587,-0.371, Den=237
Ready
Microsoft PowerPoint - [HUB 1.ppt]
Start
2 N
3 I.
Wi...
2 W
Sof...
CR...
Mic...
1:24 PM



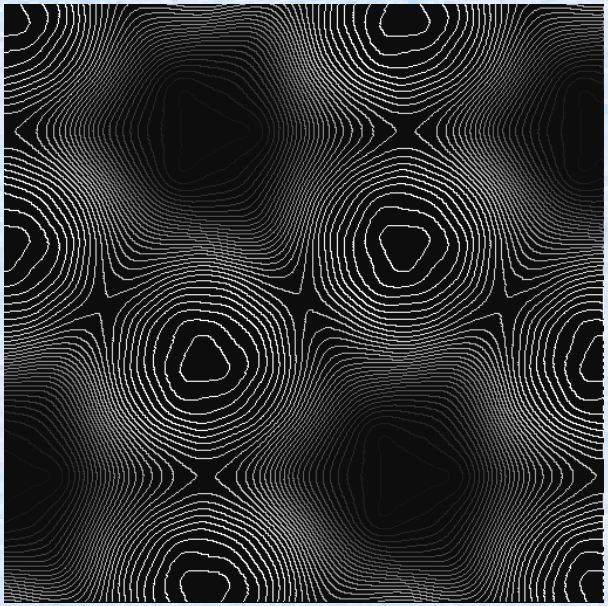
p2, α_{res}:11.9°



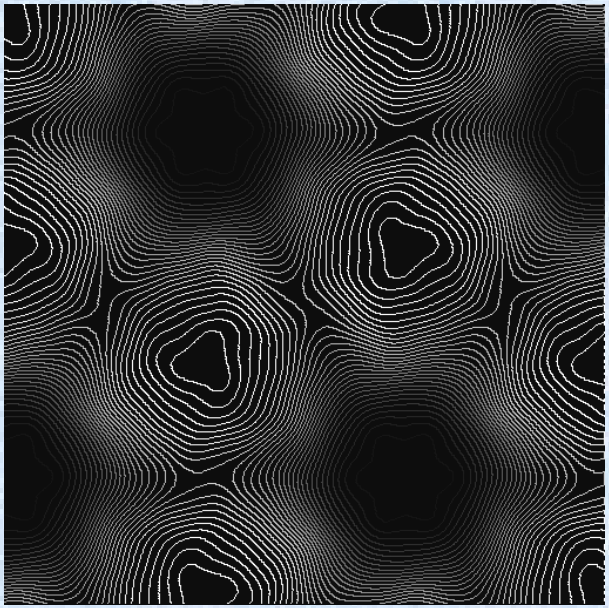
p3, F_{res}:15.6%, α_{res}:7.6°



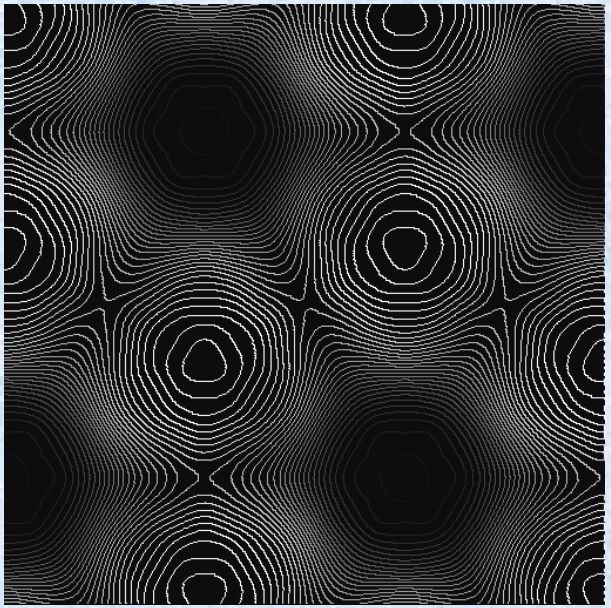
p3m1, F_{res}:16.7%, α_{res}:8.5°



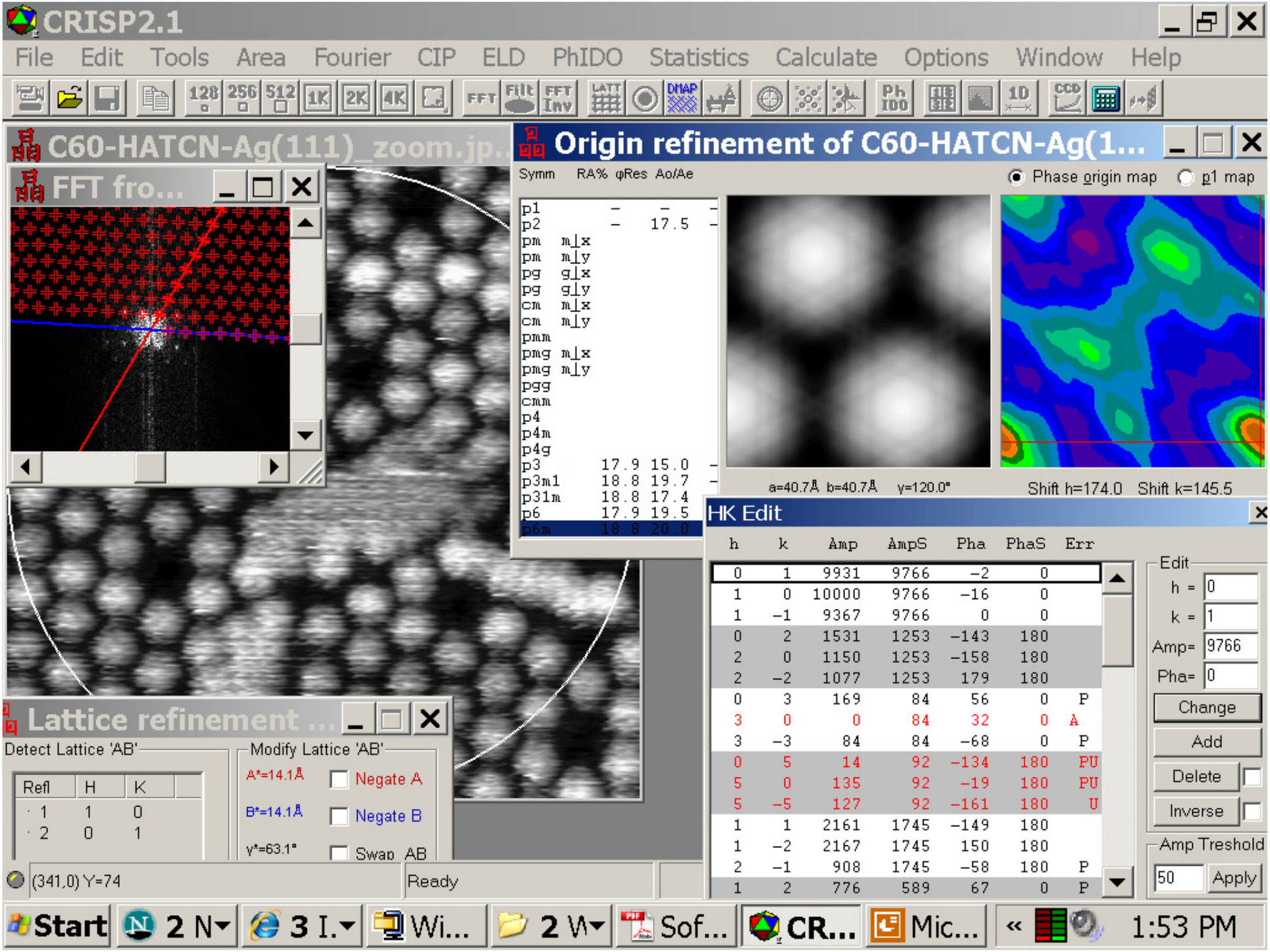
p31m, F_{res}:16.7%, α_{res}:11.9°

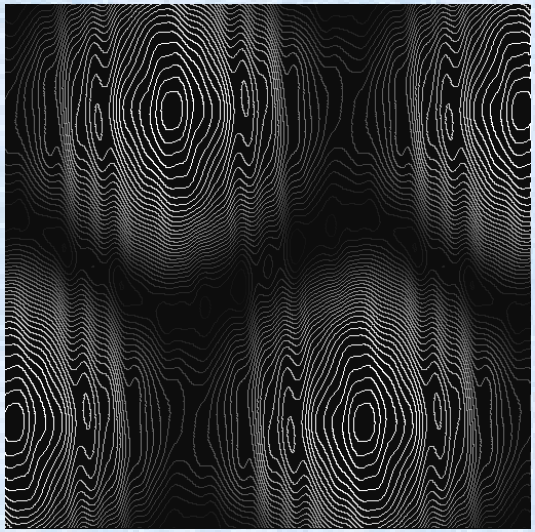


p6, F_{res}:15.6%, α_{res}:12.3°

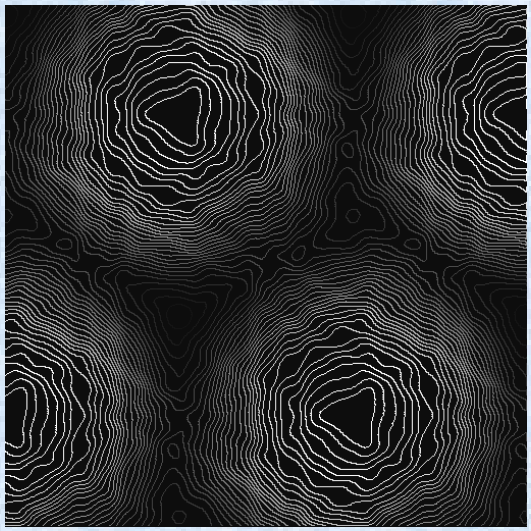


p6mm, F_{res}:16.7%, α_{res}:12.7°

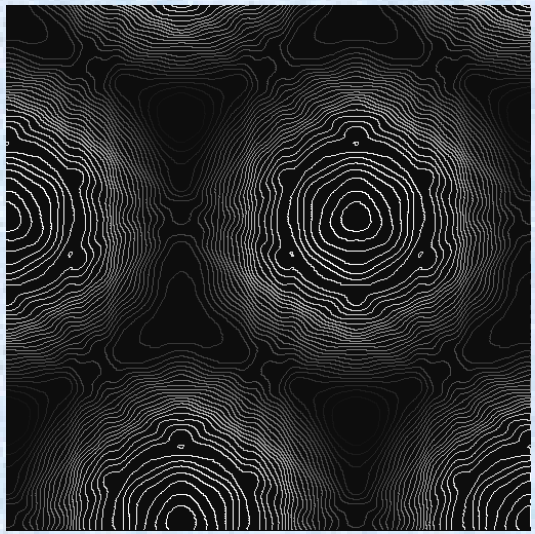

CRISP2.1
File Edit Tools Area Fourier CIP ELD PhIDO Statistics Calculate Options Window Help
C60-HATCN-Ag(111)_zoom.jp...
FFT fro...
Origin refinement of C60-HATCN-Ag(1...
Symm RA% φRes Ao/Ae
p1 – – –
p2 – 17.5 –
pm m|x
pm m|y
pg g|x
pg g|y
cm m|x
cm m|y
pmm
pmg m|x
pmg m|y
pgg
cmm
p4
p4m
p4g
p3 17.9 15.0 –
p3m1 18.8 19.7 –
p31m 18.8 17.4
p6 17.9 19.5
p6m 18.8 20.0
Phase origin map
p1 map
a=40.7Å b=40.7Å γ=120.0°
Shift h=174.0 Shift k=145.5
HK Edit
h k Amp AmpS Pha PhaS Err
0 1 9931 9766 −2 0
1 0 10000 9766 −16 0
1 −1 9367 9766 0 0
0 2 1531 1253 −143 180
2 0 1150 1253 −158 180
2 −2 1077 1253 179 180
0 3 169 84 56 0 P
3 0 0 84 32 0 A
3 −3 84 84 −68 0 P
0 5 14 92 −134 180 PU
5 0 135 92 −19 180 PU
5 −5 127 92 −161 180 U
1 1 2161 1745 −149 180
1 −2 2167 1745 150 180
2 −1 908 1745 −58 180 P
1 2 776 589 67 0 P
Edit
h = 0
k = 1
Amp= 9766
Pha= 0
Change
Add
Delete
Inverse
Amp Treshold
50 Apply
Lattice refinement ...
Detect Lattice 'AB'
Refl H K
1 1 0
2 0 1
Modify Lattice 'AB'
A*=14.1Å Negate A
B*=14.1Å Negate B
γ*=63.1° Swap AB
(341,0) Y=74
Ready
Start
2 N
3 I.
Wi...
2 W
Sof...
CR...
Mic...
1:53 PM



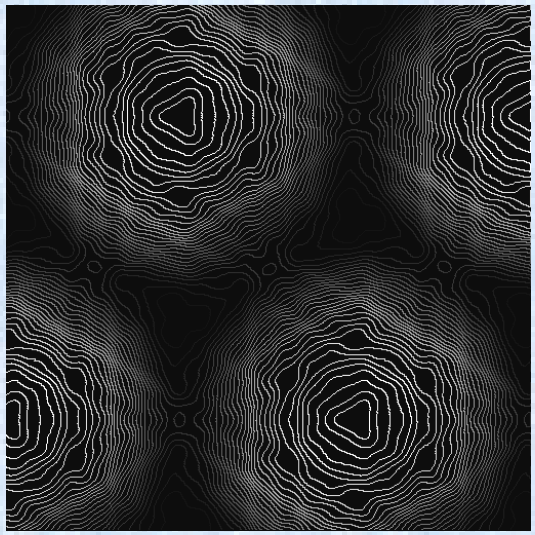
p2, α_{res}:17.5°



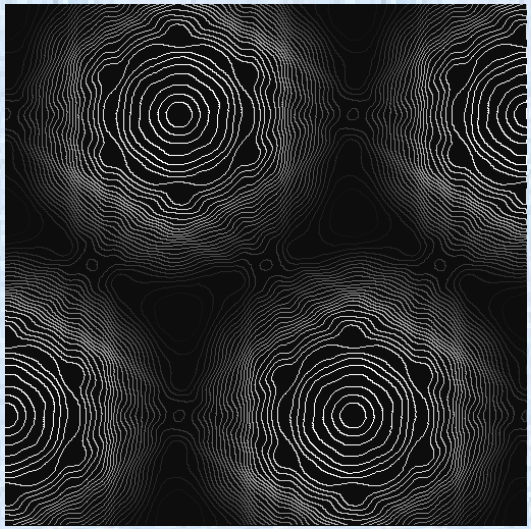
p3, F_{res}:17.9%, α_{res}:15.0°



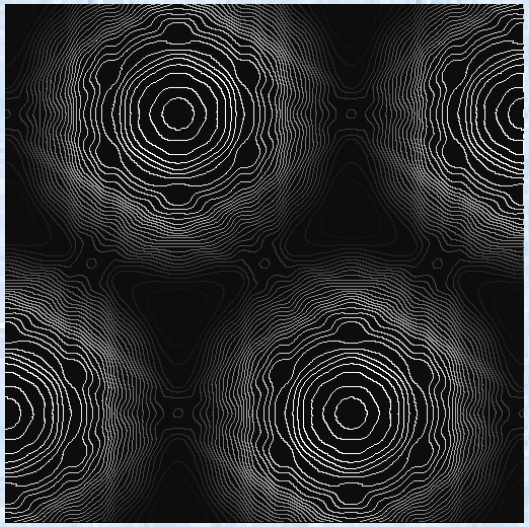
p3m1, F_{res}:18.8%, α_{res}:19.7°



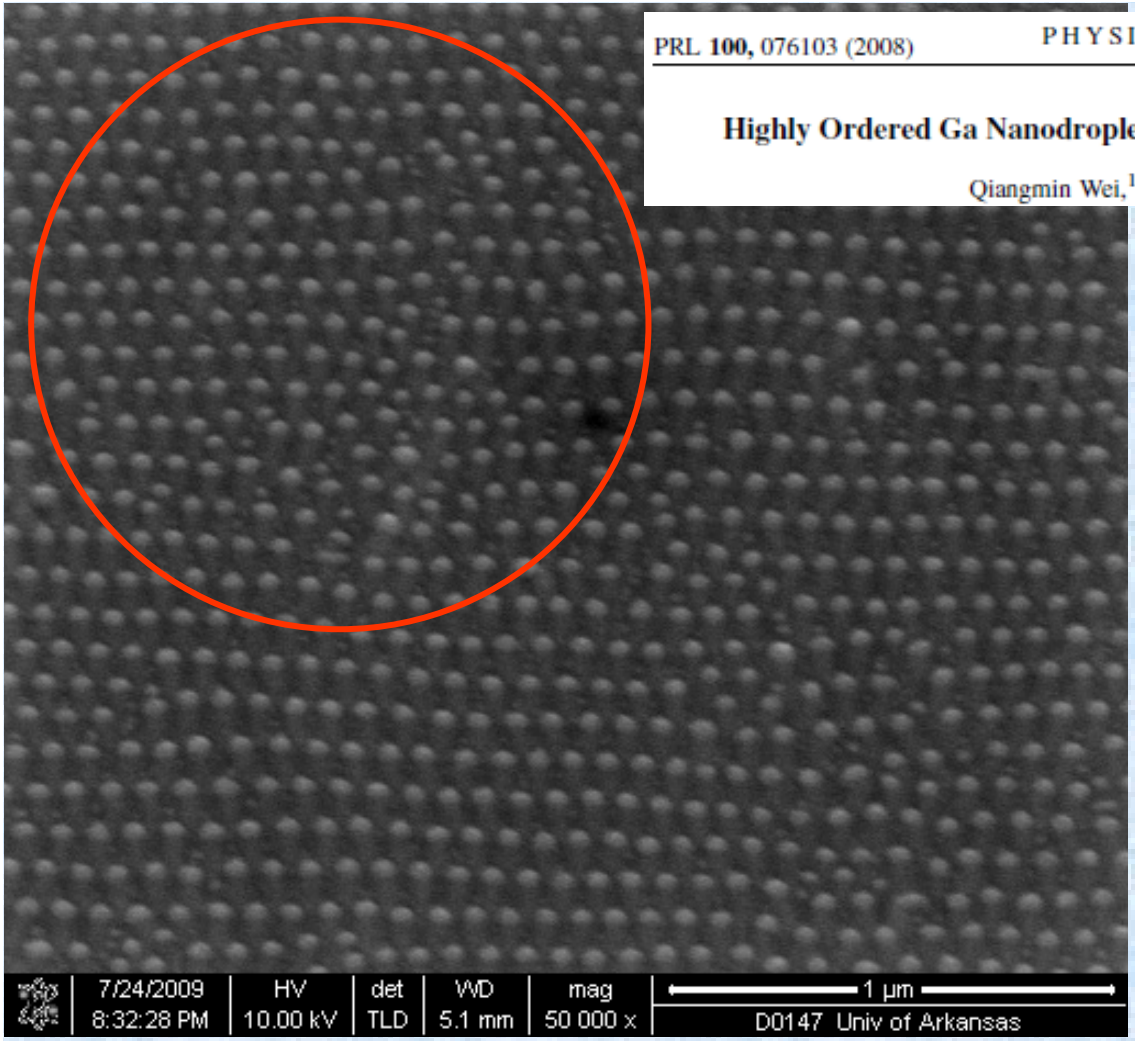
p31m, F_{res}:18.8%, α_{res}:17.4°



p6, F_{res}:17.9%, α_{res}:19.5°



p6mm, F_{res}:18.8%, α_{res}:20.0°



PRL 100, 076103 (2008) PHYSICAL REVIEW LETTERS week ending 22 FEBRUARY 2008

Highly Ordered Ga Nanodroplets on a GaAs Surface Formed by a Focused Ion Beam

Qiangmin Wei,[1] Jie Lian,[2,3] Wei Lu,[4] and Lumin Wang[1,5,*]

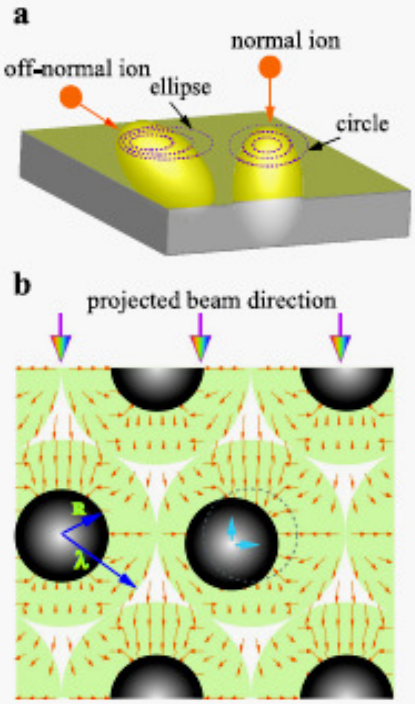
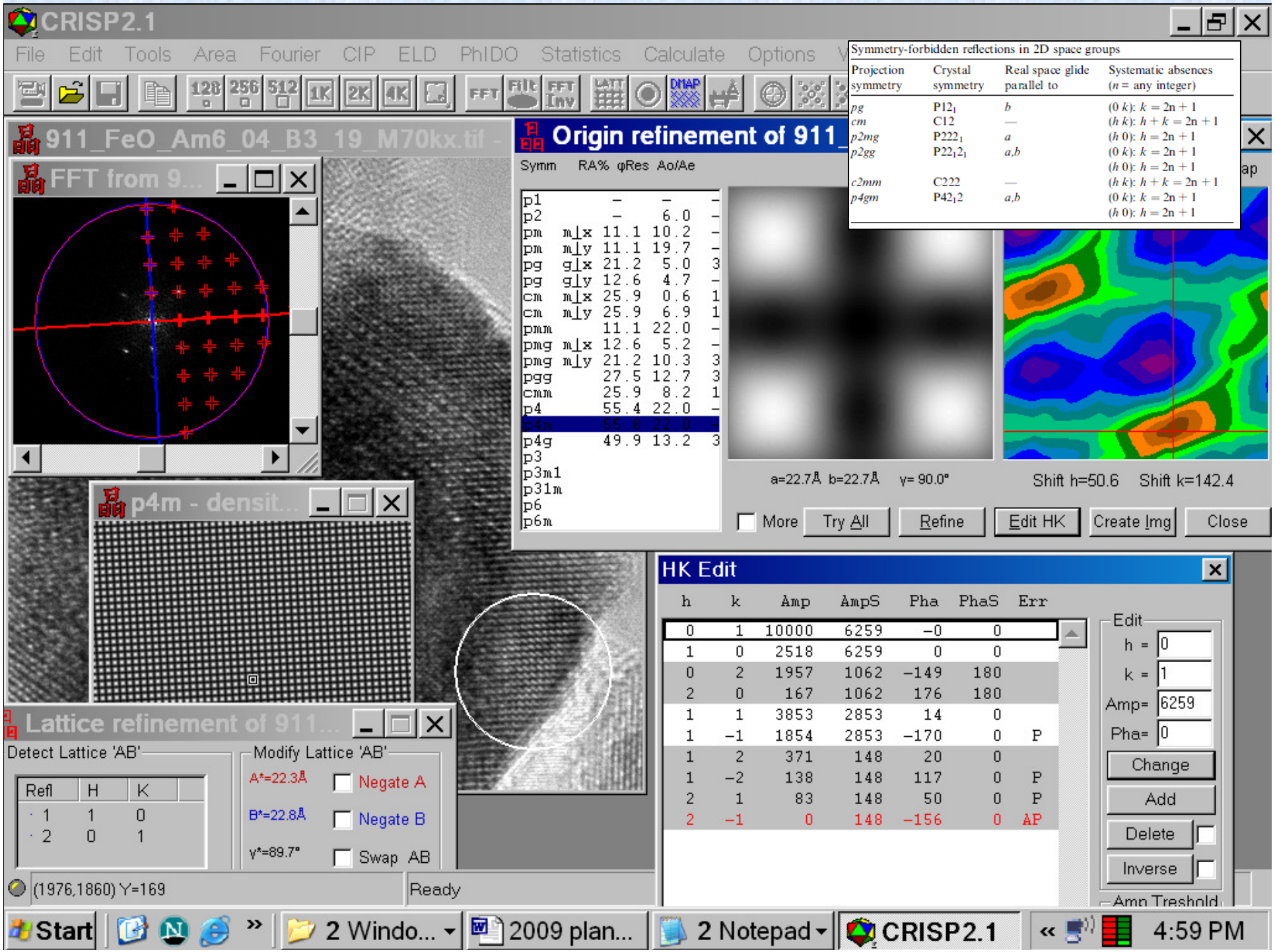
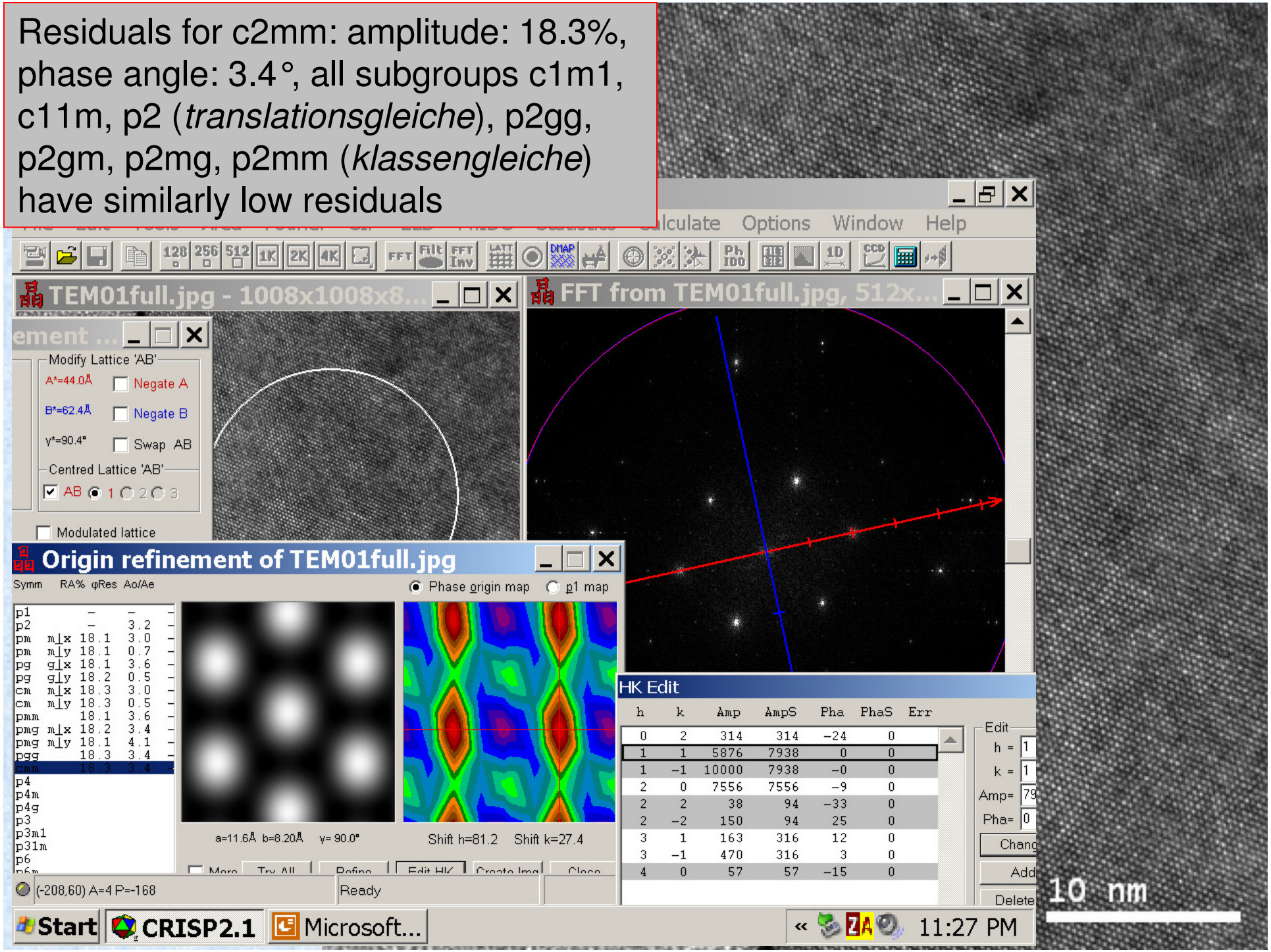


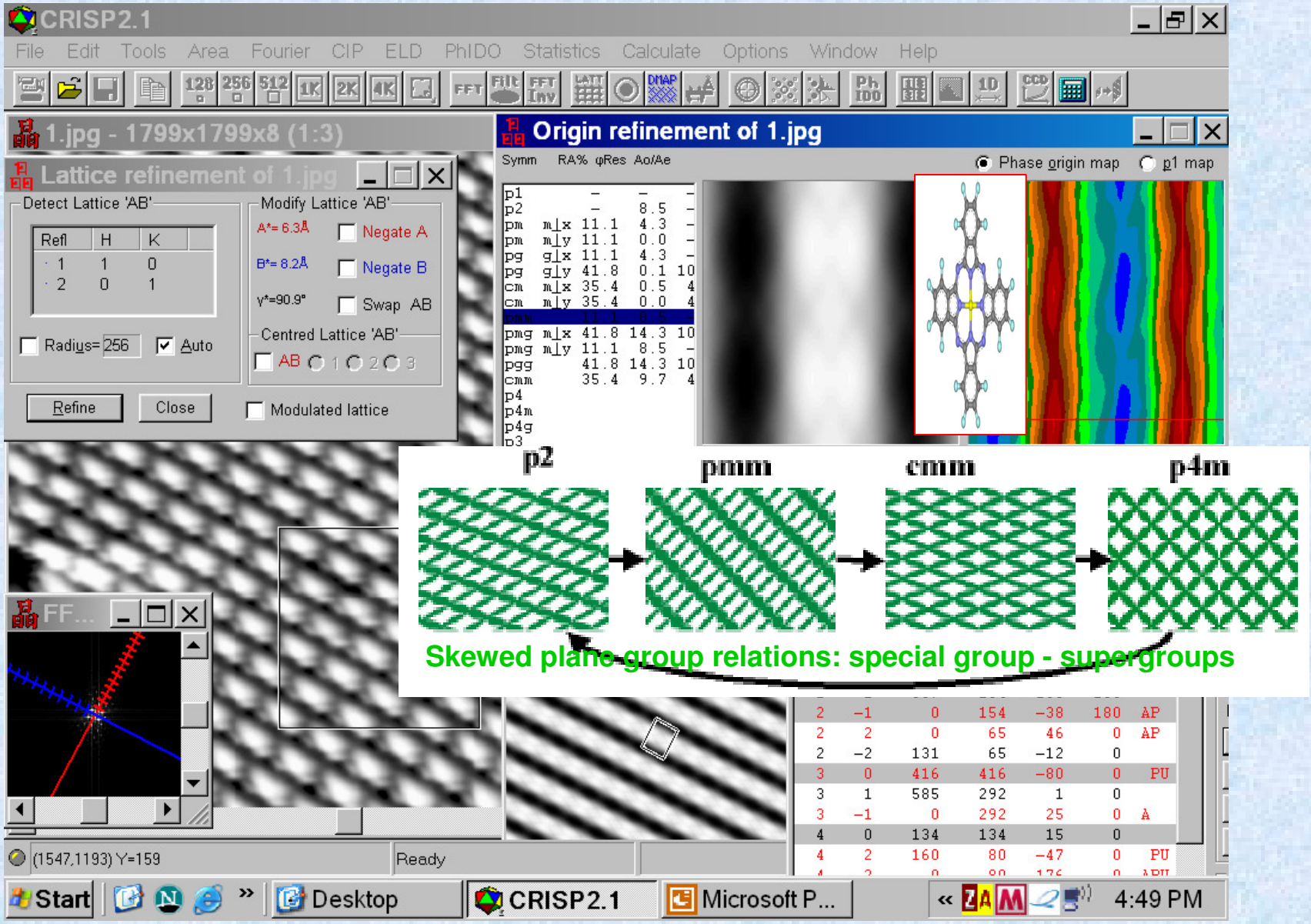
FIG. 4 (color online). Schematic illustration of a model for the formation of ordered droplet patterns. (a) Average energy distribution for ion bombardment. For normal bombardment, the deposited energy on the surface is circular, while for off-normal bombardment, it is elliptical where the energy contour along the projected beam direction is longer than other directions. The dashed curves represent the equal energy contours. (b) Atom supply and movement directions that cause an off-center particle to move to the center of nanoparticle lattice. Small arrows represent the direction and magnitude of local Ga atom migration induced by the ion beam on the substrate surface, radial dark shaded circle denotes the droplet, the light circle with radius λ is the exclusive zone for Ga, arrows inside droplet indicate the movement direction of droplets, and dashed circle shows the final position of partially aligned droplets.

SEM of a “uniform” array of Ga droplets on crystalline GaAs obtained by simultaneous sputtering and low energy Ga-ion milling at a large inclination angle, residuals for p6mm, **amplitude: 37.2%, phase angle 23.6°**, i.e. the ideal closed packed hexagonal array of identical entities with a point symmetry higher than 6mm


CRISP2.1
File Edit Tools Area Fourier CIP ELD PhIDO Statistics Calculate Options
Symmetry-forbidden reflections in 2D space groups
Projection symmetry | Crystal symmetry | Real space glide parallel to | Systematic absences (n = any integer)
pg | P12₁ | b | (0 k): k = 2n + 1
cm | C12 | — | (h k): h + k = 2n + 1
p2mg | P222₁ | a | (h 0): h = 2n + 1
p2gg | P22₁2₁ | a,b | (0 k): k = 2n + 1
(h 0): h = 2n + 1
c2mm | C222 | — | (h k): h + k = 2n + 1
p4gm | P42₁2 | a,b | (0 k): k = 2n + 1
(h 0): h = 2n + 1
911_FeO_Am6_04_B3_19_M70kx.tif
FFT from 9...
Origin refinement of 911_
Symm RA% φRes Ao/Ae
p1 – – –
p2 – 6.0 –
pm m⊥x 11.1 10.2 –
pm m⊥y 11.1 19.7 –
pg g⊥x 21.2 5.0 3
pg g⊥y 12.6 4.7 –
cm m⊥x 25.9 0.6 1
cm m⊥y 25.9 6.9 1
pmm 11.1 22.0 –
pmg m⊥x 12.6 5.2 –
pmg m⊥y 21.2 10.3 3
pgg 27.5 12.7 3
cmm 25.9 8.2 1
p4 55.4 22.0 –
p4m 55.8 22.0 –
p4g 49.9 13.2 3
p3
p3m1
p31m
p6
p6m
a=22.7Å b=22.7Å γ= 90.0°
Shift h=50.6 Shift k=142.4
More Try All Refine Edit HK Create Img Close
p4m - densit...
Lattice refinement of 911...
Detect Lattice 'AB'
Refl H K
1 1 0
2 0 1
Modify Lattice 'AB'
A*=22.3Å Negate A
B*=22.8Å Negate B
γ*=89.7° Swap AB
(1976,1860) Y=169
Ready
HK Edit
h k Amp AmpS Pha PhaS Err
0 1 10000 6259 −0 0
1 0 2518 6259 0 0
0 2 1957 1062 −149 180
2 0 167 1062 176 180
1 1 3853 2853 14 0
1 −1 1854 2853 −170 0 P
1 2 371 148 20 0
1 −2 138 148 117 0 P
2 1 83 148 50 0 P
2 −1 0 148 −156 0 AP
Edit
h = 0
k = 1
Amp= 6259
Pha= 0
Change
Add
Delete
Inverse
Amp Treshold
Start
2 Windo...
2009 plan...
2 Notepad
CRISP2.1
4:59 PM

Residuals for c2mm: amplitude: 18.3%, phase angle: 3.4°, all subgroups c1m1, c11m, p2 (*translationsgleiche*), p2gg, p2gm, p2mg, p2mm (*klassengleiche*) have similarly low residuals



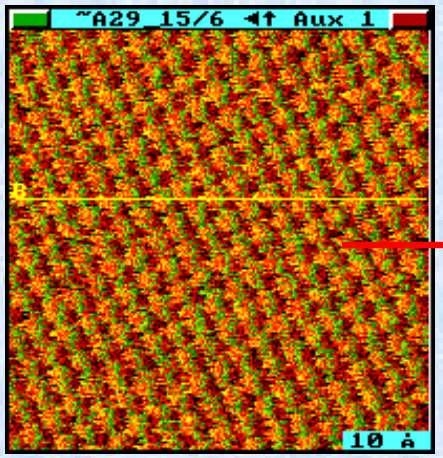


there are limits to detecting symmetries in STM images, but 2-fold axis and set of intersecting mirror lines, i.e. subgroup pmm at least identified correctly, skewed symmetry, due to affine transformation, different step sizes, non-orthogonality of fast and slow scan directions

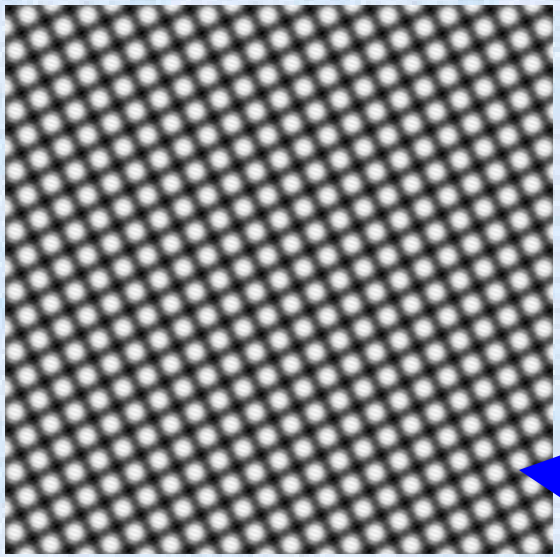
Limits of raw data quality for CIP procedure to work properly

Raw date courtesy Dr. Rachel Cannara, NIST

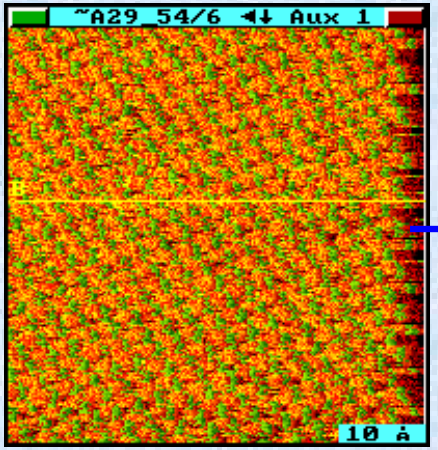
AFM images on LiF, only about 200 by 200 pixels, so "128 pixel masks" are necessary for FFT calculations



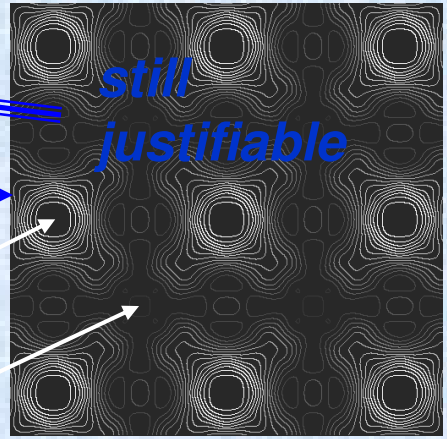
128 pixel diameter circular mask



only large F anions are clearly visible, H. Heinzelmann et al., Zeits. Physik B Condensed. Matter 79 (1990) 3-4

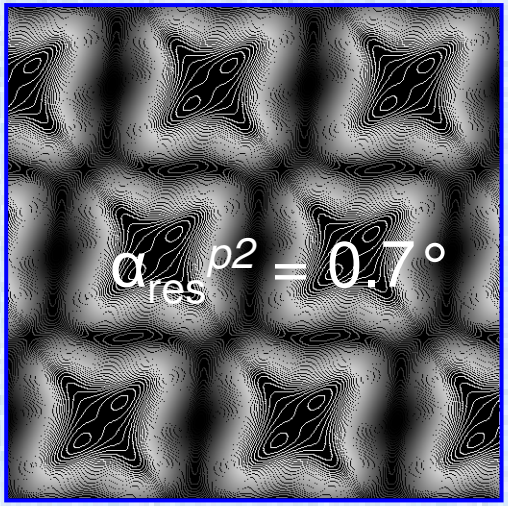


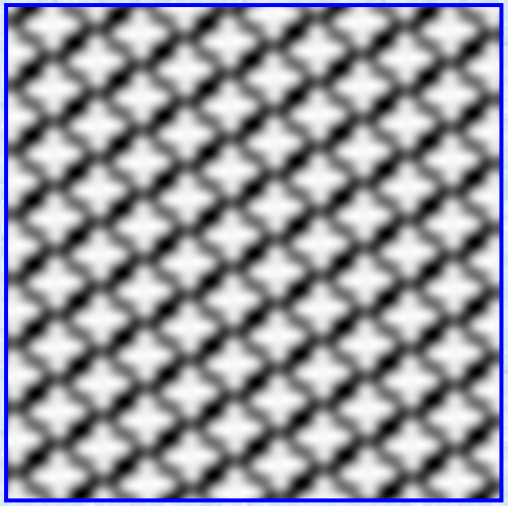
128^2 pixel square mask

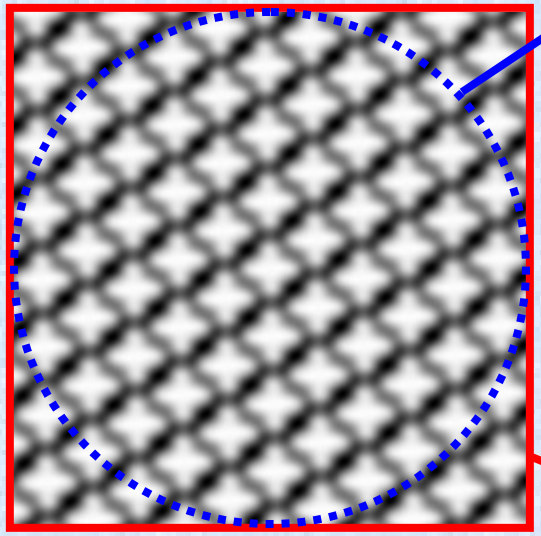


p4mm is detected and enforced for both raw images, but only for the square mask is 4mm enforced as site symmetry of (0,0) and (½,½) in the detailed counter map

Circular mask for calculation of fast Fourier transform, 256 pixel diameter



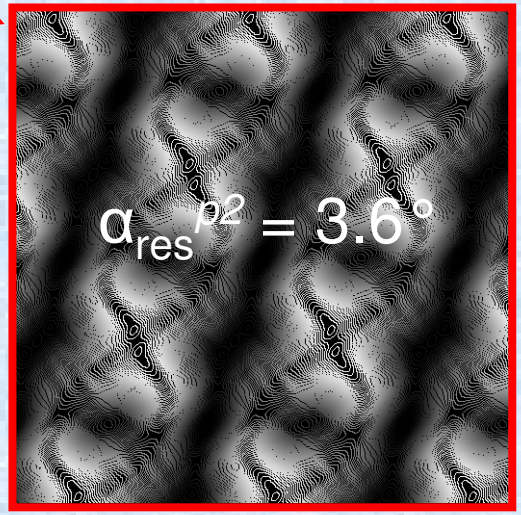


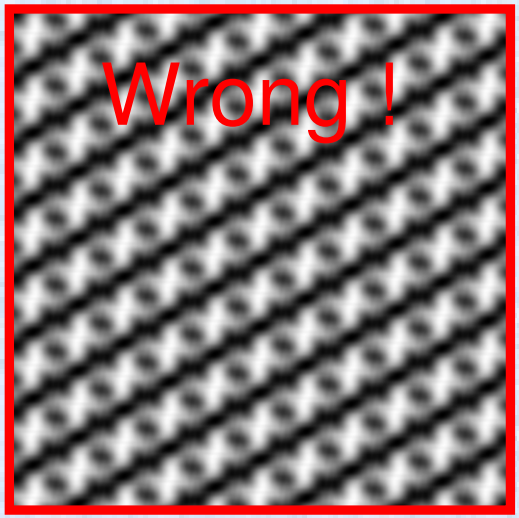


Avoid inclusion of image edges, example 256 by 256 pixel image

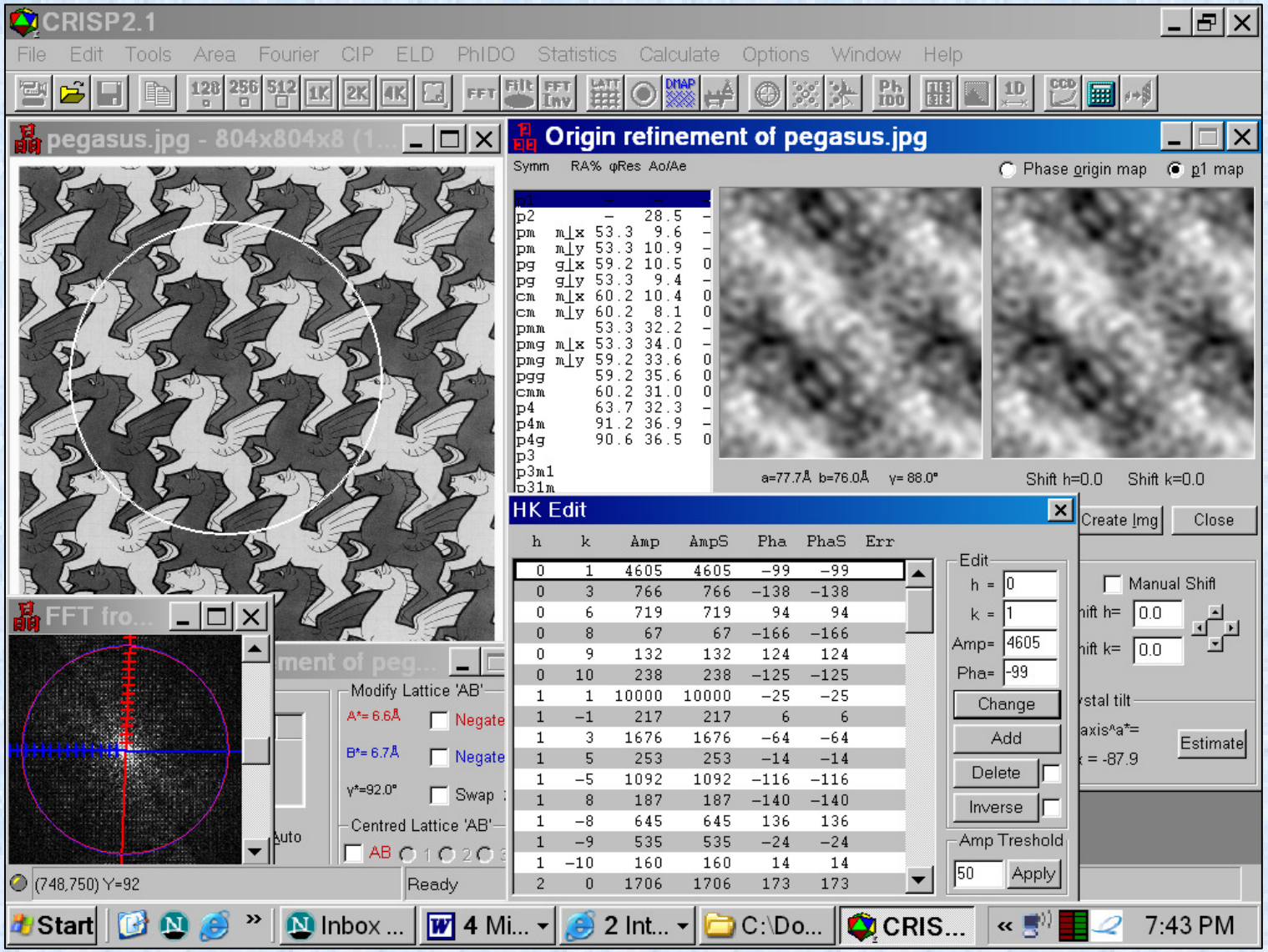
lattices are almost the same, but phase angles of a few “medium strong” Fourier coefficients flipped by about 180° due to convolution of image & mask

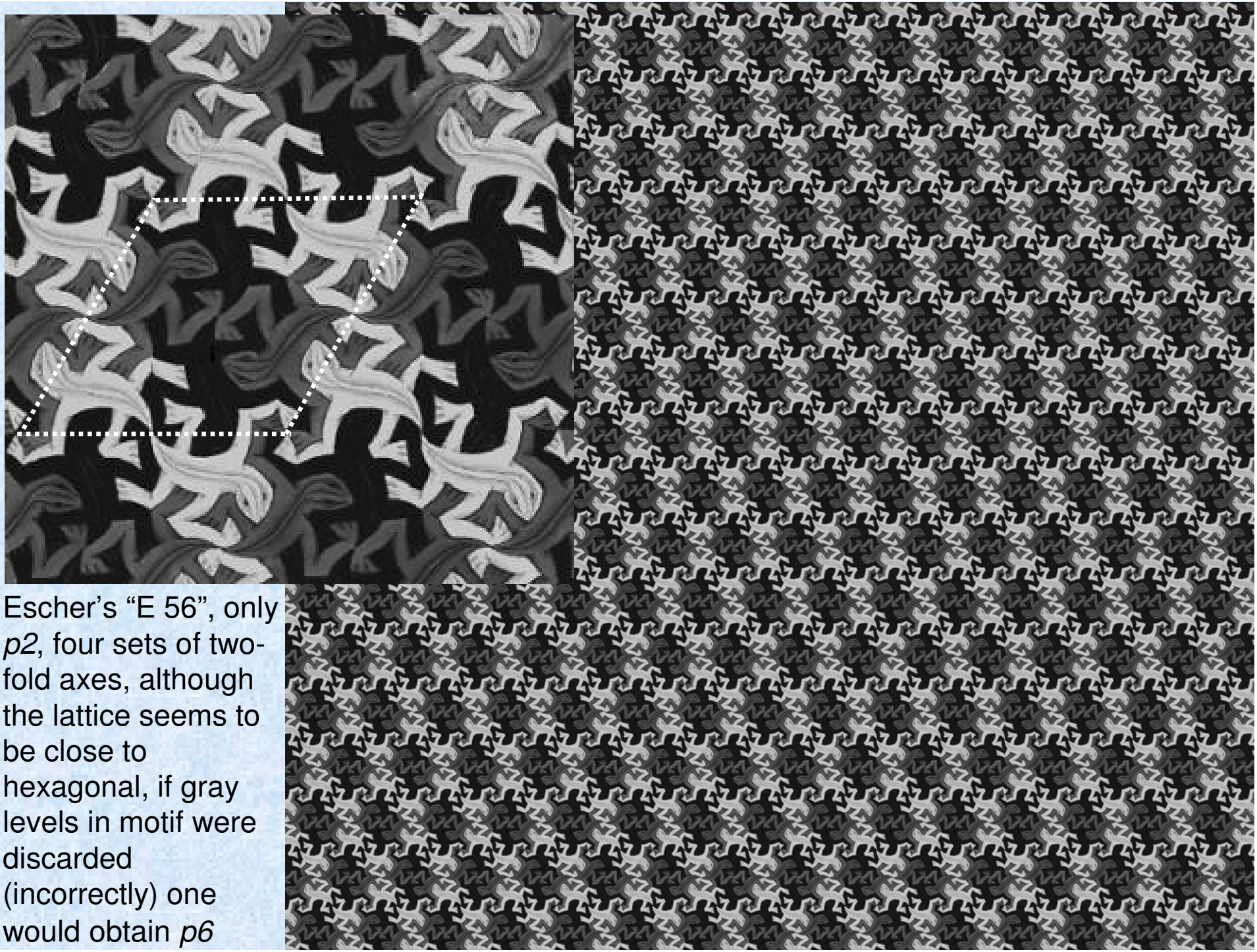
256 pixel square mask for calculation of fast Fourier transform



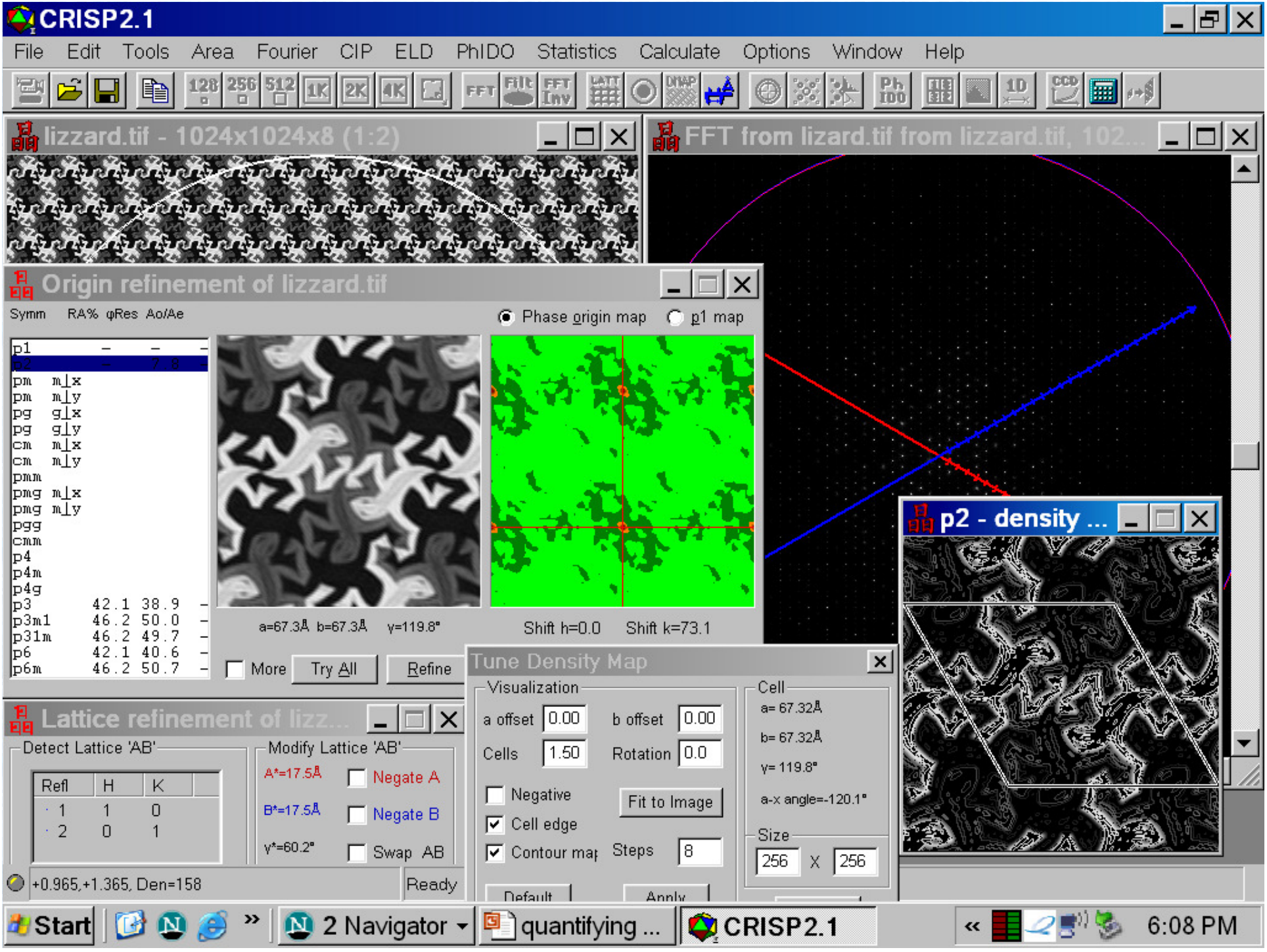


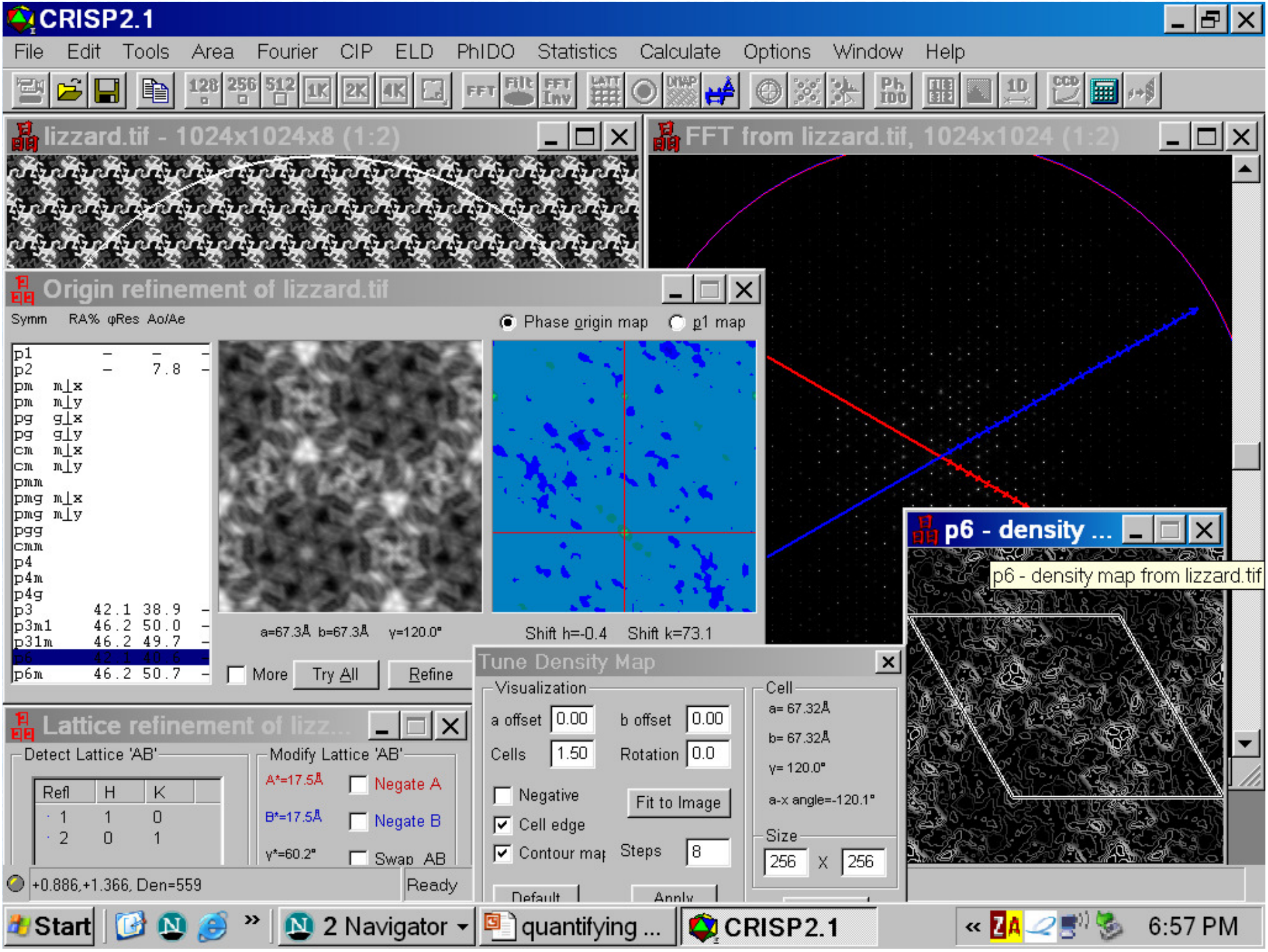
“Placebo Test”: Point symmetry 1 combined with oblique lattice = plane symmetry p1, note that all amplitude and phase residuals are very high, crystallographic image processing works well

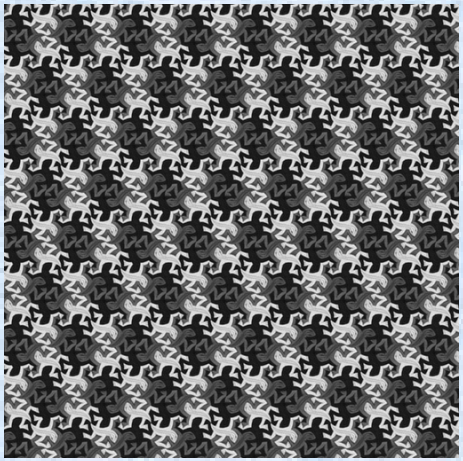


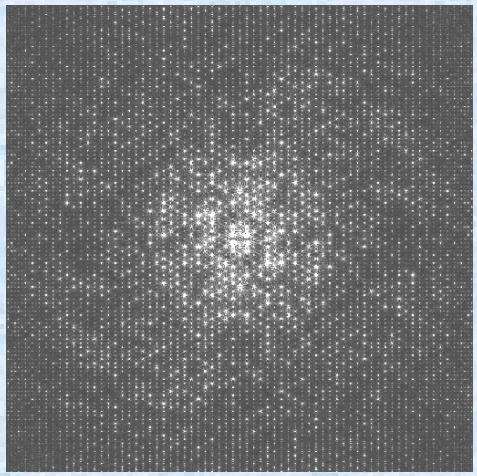


Escher's "E 56", only *p2*, four sets of two-fold axes, although the lattice seems to be close to hexagonal, if gray levels in motif were discarded (incorrectly) one would obtain *p6*

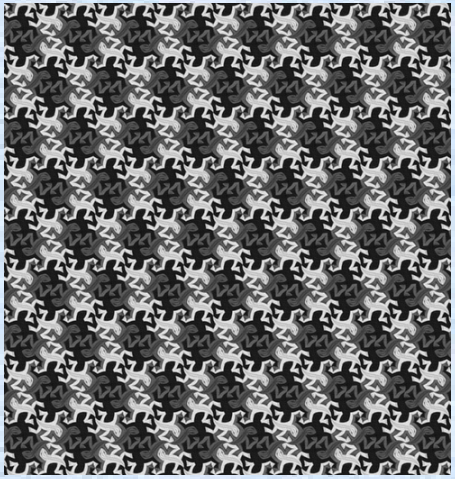

CRISP2.1
File Edit Tools Area Fourier CIP ELD PhIDO Statistics Calculate Options Window Help
lizzard.tif - 1024x1024x8 (1:2)
FFT from lizard.tif from lizzard.tif, 102...
Origin refinement of lizzard.tif
Symm RA% φRes Ao/Ae
Phase origin map
p1 map
p1 – – –
p2 – 7.8 –
pm m|x
pm m|y
pg g|x
pg g|y
cm m|x
cm m|y
pmm
pmg m|x
pmg m|y
pgg
cmm
p4
p4m
p4g
p3 42.1 38.9 –
p3m1 46.2 50.0 –
p31m 46.2 49.7 –
p6 42.1 40.6 –
p6m 46.2 50.7 –
a=67.3Å b=67.3Å γ=119.8°
Shift h=0.0 Shift k=73.1
More
Try All
Refine
p2 - density ...
Tune Density Map
Visualization
a offset 0.00
b offset 0.00
Cells 1.50
Rotation 0.0
Negative
Cell edge
Contour map
Steps 8
Fit to Image
Default
Apply
Cell
a= 67.32Å
b= 67.32Å
γ= 119.8°
a-x angle=-120.1°
Size
256 X 256
Lattice refinement of lizz...
Detect Lattice 'AB'
Refl H K
1 1 0
2 0 1
Modify Lattice 'AB'
A*=17.5Å
B*=17.5Å
γ*=60.2°
Negate A
Negate B
Swap AB
+0.965,+1.365, Den=158
Ready
Start
2 Navigator
quantifying ...
CRISP2.1
6:08 PM

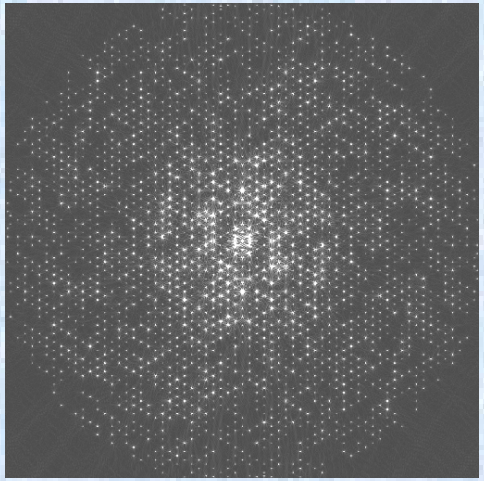

CRISP2.1
File Edit Tools Area Fourier CIP ELD PhIDO Statistics Calculate Options Window Help
lizzard.tif - 1024x1024x8 (1:2)
FFT from lizzard.tif, 1024x1024 (1:2)
Origin refinement of lizzard.tif
Symm RA% φRes Ao/Ae
Phase origin map
p1 map
p1 – – –
p2 – 7.8 –
pm m|x
pm m|y
pg g|x
pg g|y
cm m|x
cm m|y
pmm
pmg m|x
pmg m|y
pgg
cmm
p4
p4m
p4g
p3 42.1 38.9 –
p3m1 46.2 50.0 –
p31m 46.2 49.7 –
p6 42.1 40.6 –
p6m 46.2 50.7 –
a=67.3Å b=67.3Å γ=120.0°
Shift h=-0.4 Shift k=73.1
More
Try All
Refine
p6 - density ...
p6 - density map from lizzard.tif
Tune Density Map
Visualization
a offset 0.00
b offset 0.00
Cells 1.50
Rotation 0.0
Negative
Cell edge
Contour map
Steps 8
Fit to Image
Default
Apply
Cell
a= 67.32Å
b= 67.32Å
γ= 120.0°
a-x angle=-120.1°
Size
256 X 256
Lattice refinement of lizz...
Detect Lattice 'AB'
Refl H K
1 1 0
2 0 1
Modify Lattice 'AB'
A*=17.5Å
Negate A
B*=17.5Å
Negate B
γ*=60.2°
Swap AB
+0.886,+1.366, Den=559
Ready
Start
2 Navigator
quantifying ...
CRISP2.1
6:57 PM



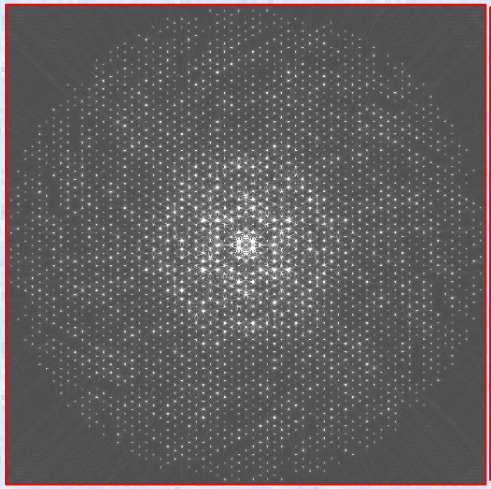


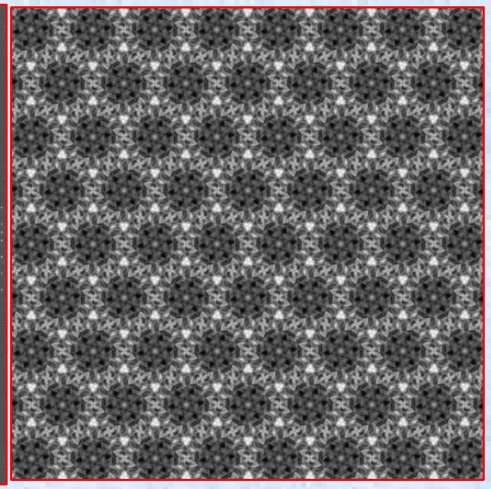
p1 version, no point symmetry elements besides 1, only translation symmetry of an oblique lattice, two-fold axis in reciprocal space for maps of amplitudes as property of Fourier transform



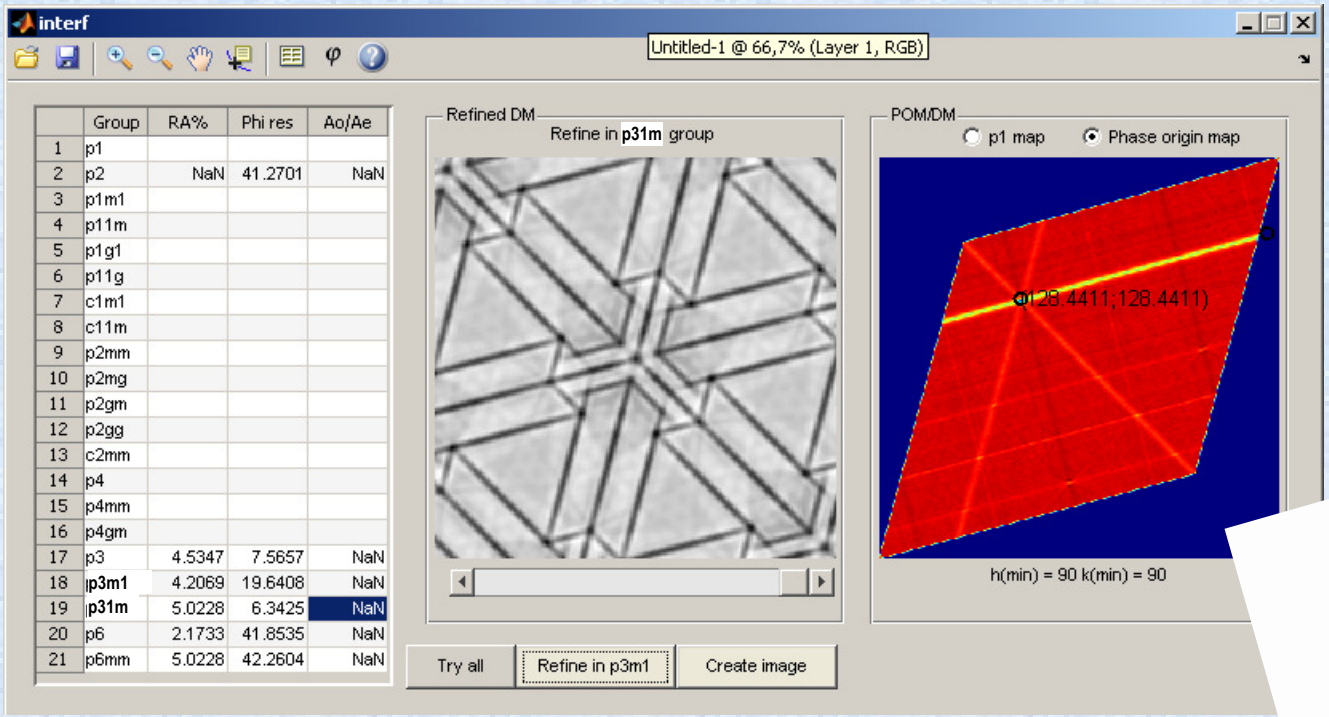


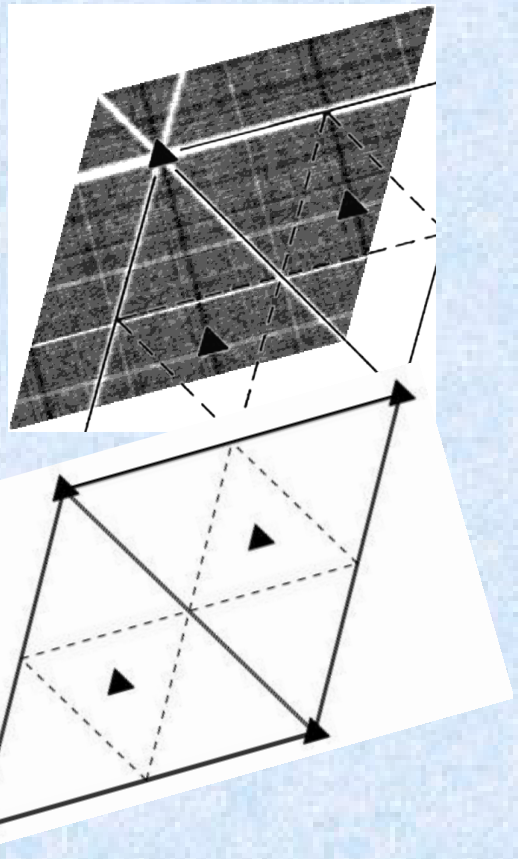
p2 enforced version, all phase angles 0 or 180 degrees, origin at the position of one set of these two-fold axes, one two-fold axis in maps of amplitudes, due to combined effect of symmetry in the *p2* image and Fourier transform



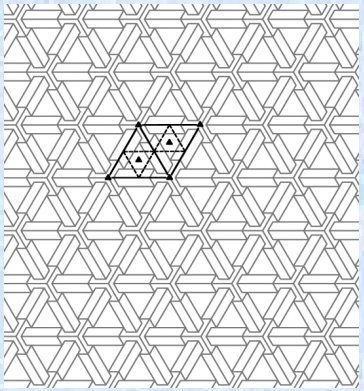


p6 enforced version, all phases 0 or 180 degrees, origin at the position of the six fold axis, almost same phase shift as for *p2*, three two-fold axes and two three-fold axes are also produced. Six-fold axis in map of Fourier coefficients amplitudes





development of a dedicated crystallographic image processing program for the scanning probe microscopy community

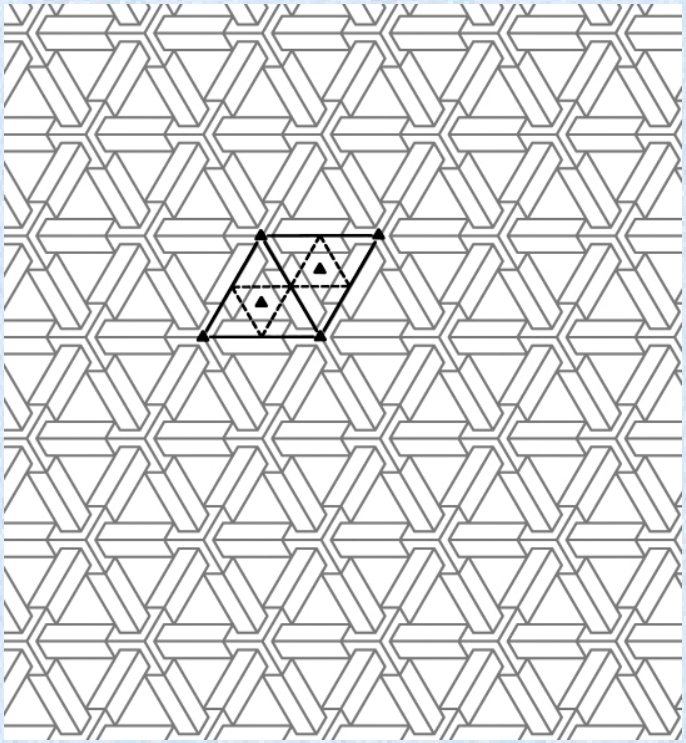


For “sufficiently” symmetric images without much distortion and noise, e.g. simulations or works of art, the map of the phase residuals indicates not only the correct origin, but also the location of the other symmetry elements,

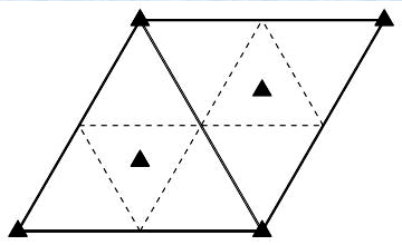
in case of *p31m*, the mirror lines, glide lines, and position of mirror equivalent three-fold rotation points at ($^1/_3$,$^2/_3$) and ($^2/_3$,$^1/_3$)

Cross correlation of a 2D periodic image with the symmetrized tile

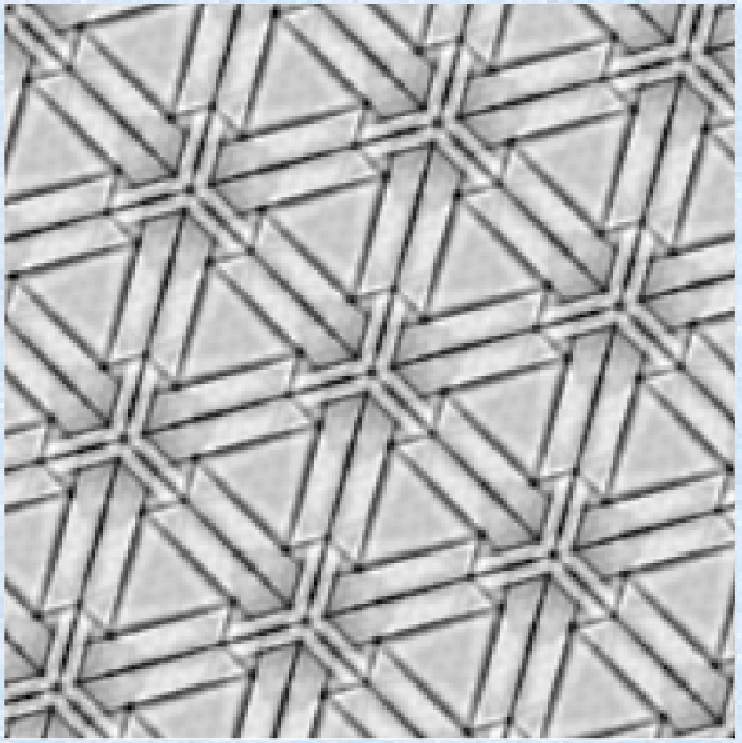
(that is Fourier back transformed after symmetrization of the Fourier coefficients of the image)



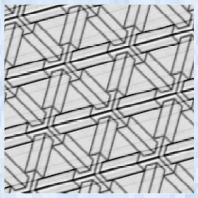
p31m



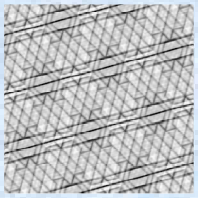
Idea: relative height of the central peak of CCF quantifies "similarity", *p1* value serves as a "baseline" of the FFT procedures



$$CCF(x,y)=\sum_{x'}\sum_{y'}[i(x',y')-<i(x',y')>]\cdot[t(x'-x,y'-y)-<t>] \Big/ \left(\sum_{x'}\sum_{y'}[i(x',y')-<i(x',y')>]^2\cdot\sum_{x'}\sum_{y'}[t(x'-x,y'-y)-<t>]^2\right)^{0.5}$$

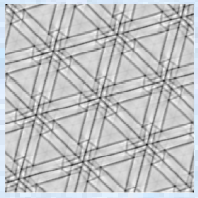


p1, 1.14

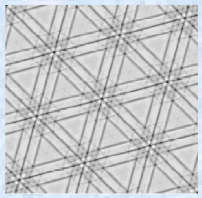


p2, 3.68

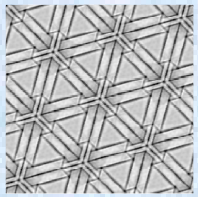
all site symmetries broken for p2



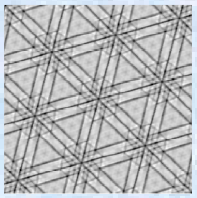
p3, 4.21



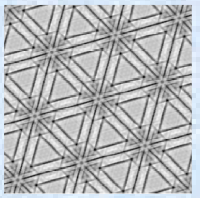
p3m1, 4.31



***p31m*, 4.48**

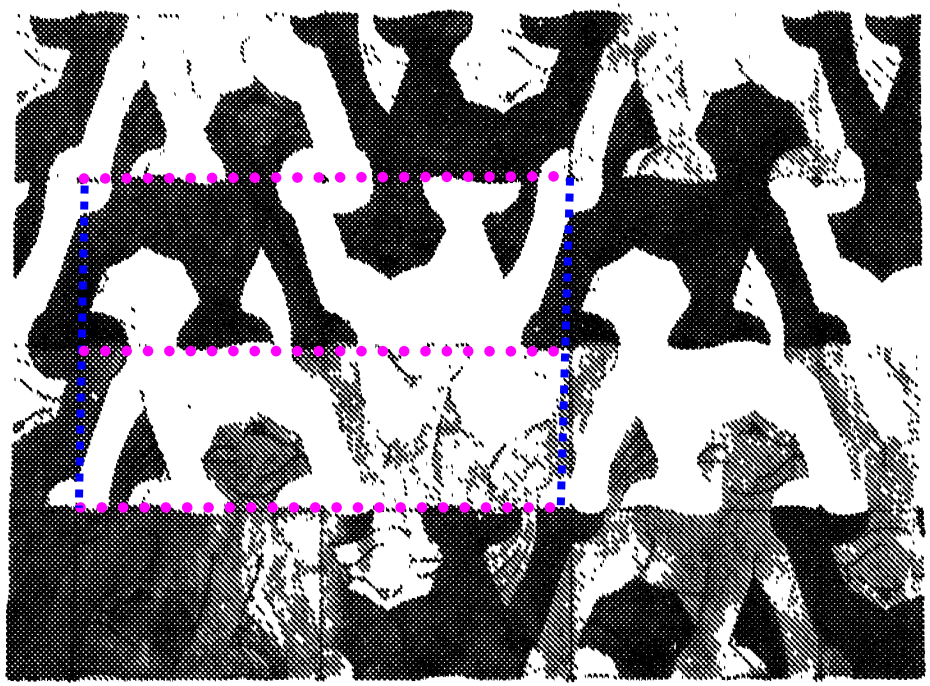


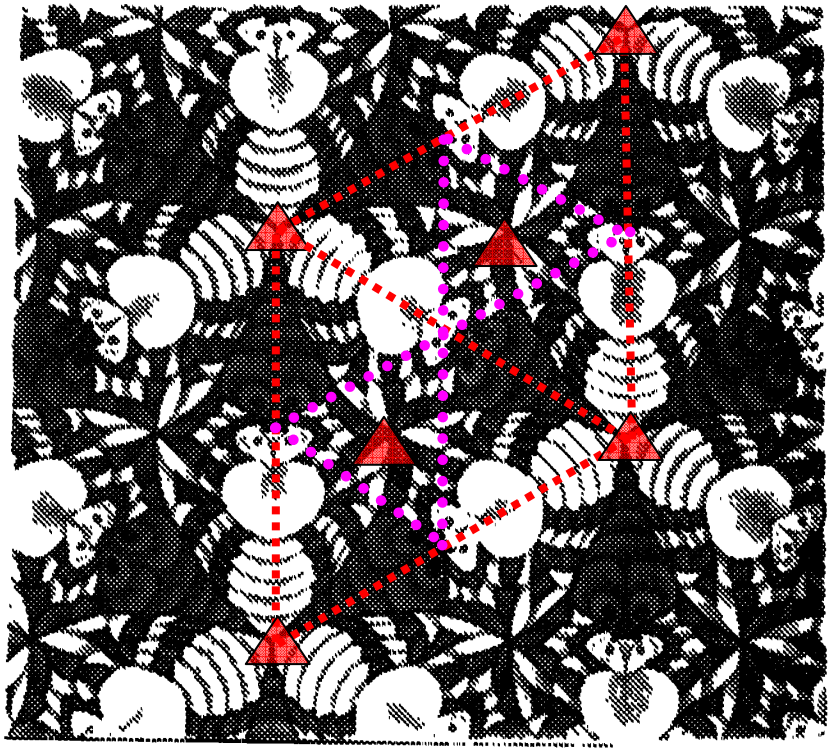
p6, 4.10



p6mm, 4.29

Exercise in mirror and glide lines plus three axes





pg unfinished

Escher Foundation, Haags Gemeentemuseum, The Hague.

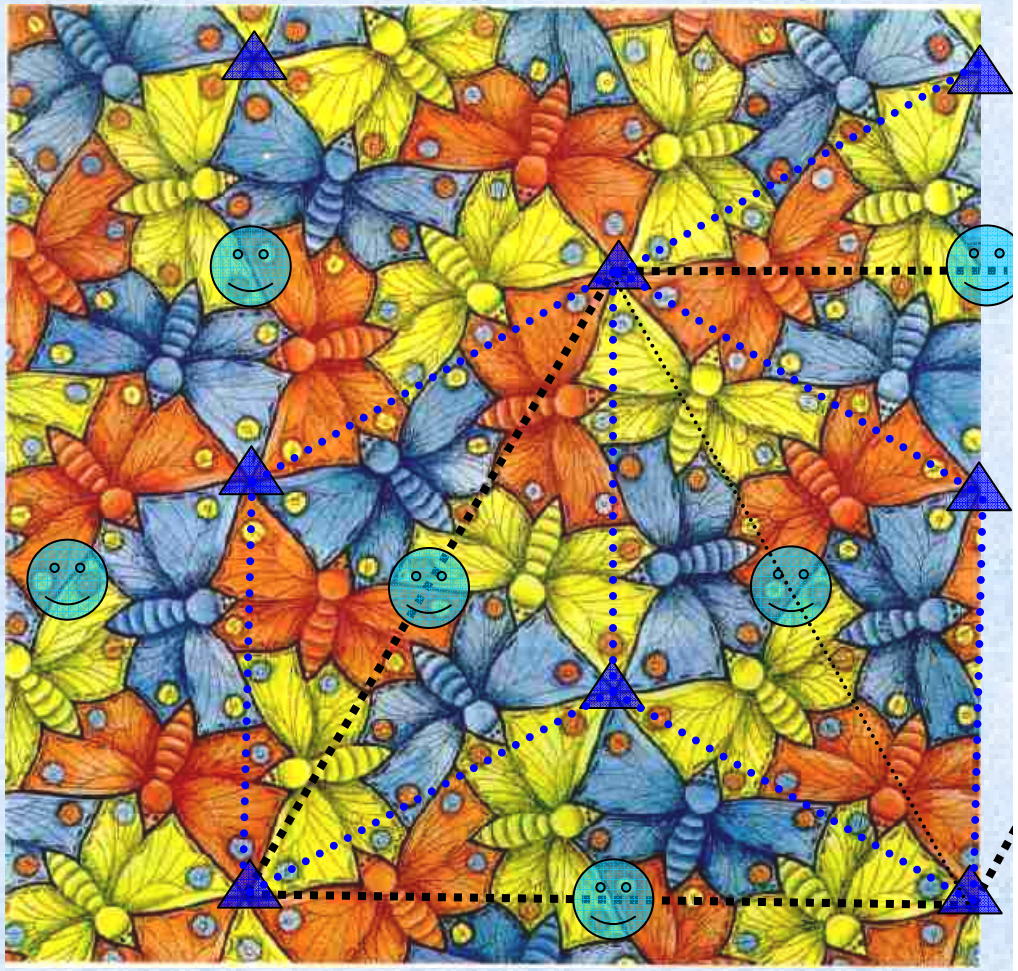
p31m

Two periodic drawings by M. C. Escher contrast his early effort at repeating design with his later masterful skill. The pattern of lions, dated "1926 or 1927," was done before he developed a system which grew out of his study of mathematical articles and periodic designs on the Alhambra. The pattern of bugs is dated 1942, one year after Escher recorded his codified system in notebooks.

G. Pólya, Über die Analogie der Kristallsymmetrie in der Ebene, *Zeits. Krist.* 60 (1924) 278-282;
P. Niggli, Die Flächensymmetrien homogener Diskontinuen, *Zeits. Krist.* 60 (1924) 283-298.

D. Schattschneider, *The American Mathematical Monthly* **85** (1978) 439-450

almost square lattice, but no point symmetries at all, ***very special case of p1***



p6 deliberately broken (removing two fold axes ☺ *) by coloring so that drawing becomes* ***special case of p3****,*

18 moths in total per unit cell, half of a unit cell – a triangle - clearly visible, so let's account for 9 moths, three are blue the, other six are red and yellow, asymmetric unit – dotted blue lines - contains two moth of each color

Summary and conclusions

All periodic 2D images can be classified to belong to one of only 17 plane symmetry groups

Deviation from each of these groups can be quantified, correct plane group can often be identified on basis of quantitative measures (plus some prior knowledge), i.e. the amplitude and phase angle residuals of the Fourier coefficients of the image intensity

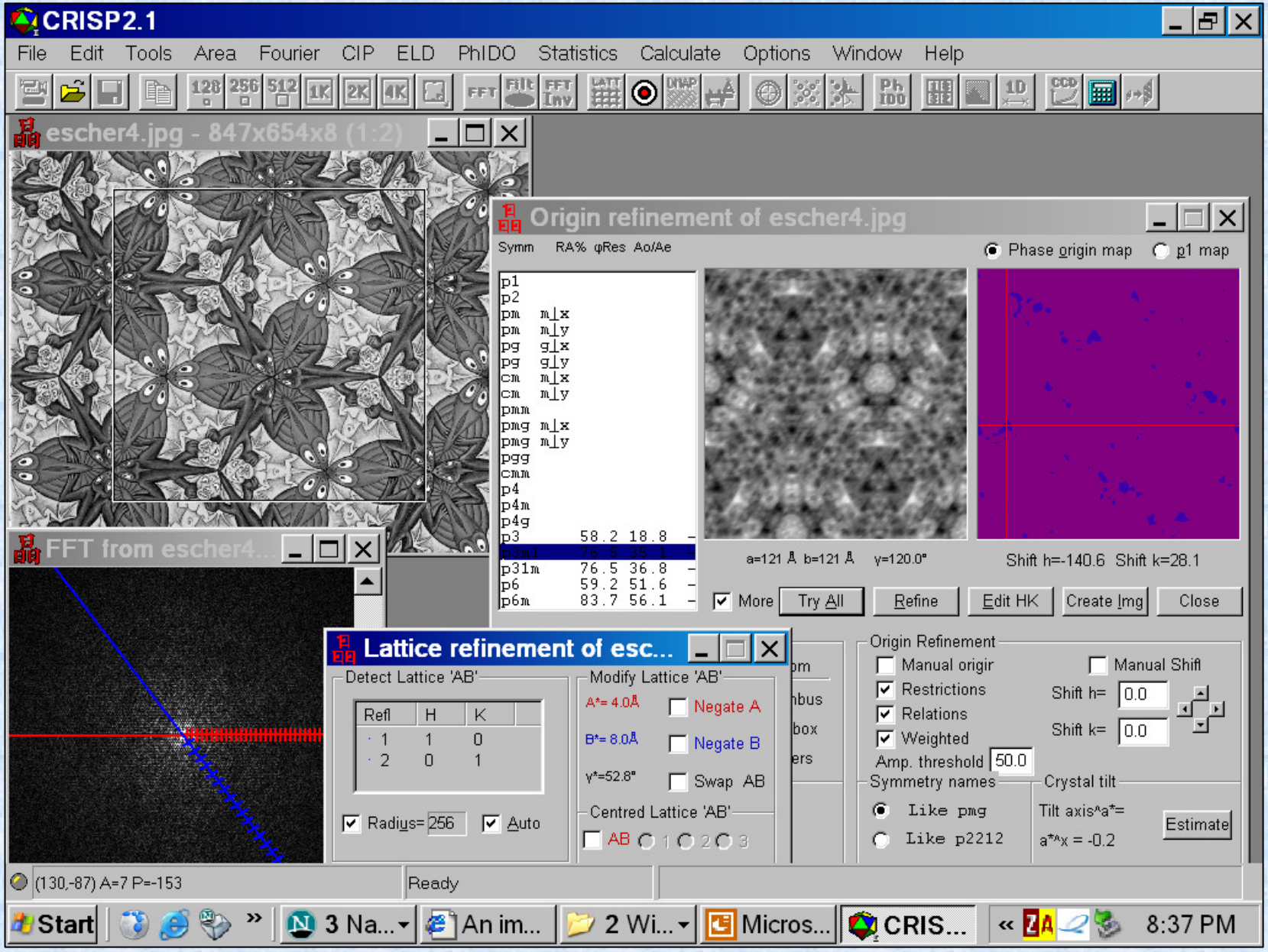
HOPG is a good calibration sample, one can determine the point spread function of the microscope on its basis, then the same function can be utilized to correct images from unknowns, allows for better measurements and surface science

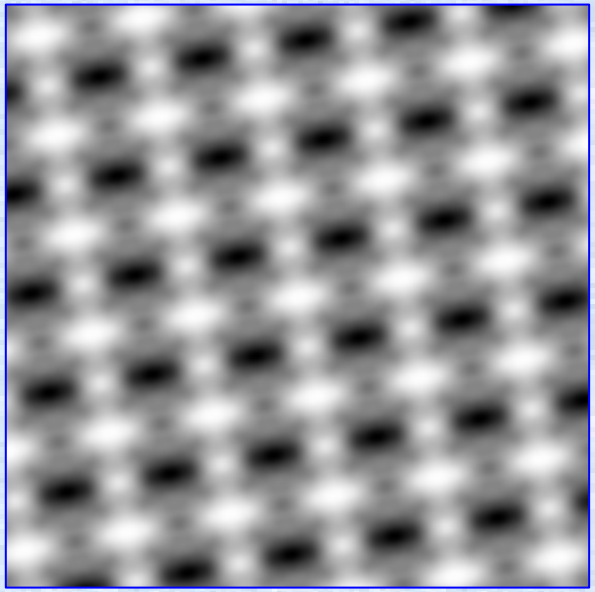
A blunt STM tip can be symmetrized

There are problems on how to decide on the correct plane group if there is no prior knowledge, some clever geometric AIC is needed

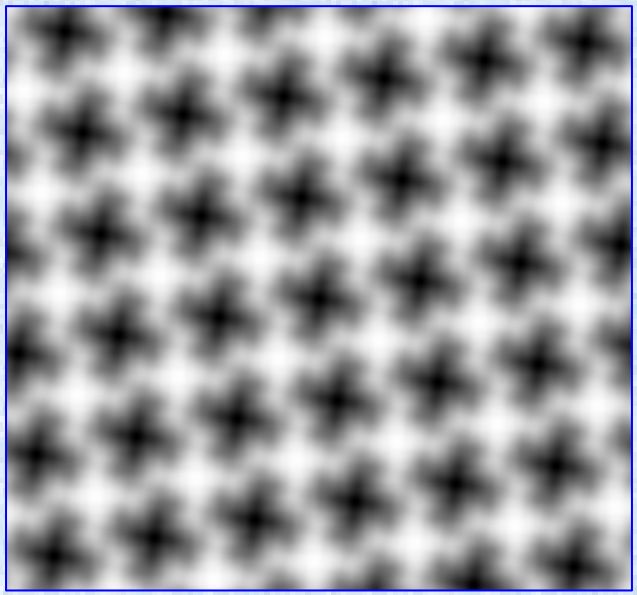
Knowledge of 2D symmetry made Maurits Cornelis Escher (17 June 1898 – 27 March 1972) a more sophisticated artists, it may also result in better surface- and nano-science

Crystallographic Image Processing works even for noisy Fourier transforms

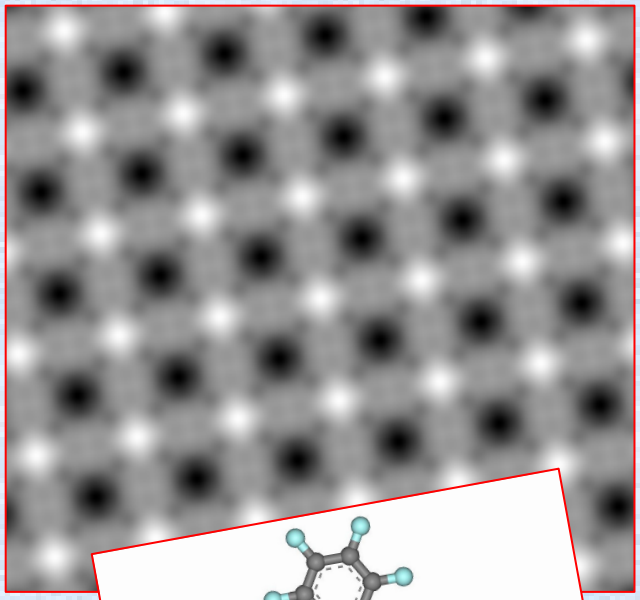


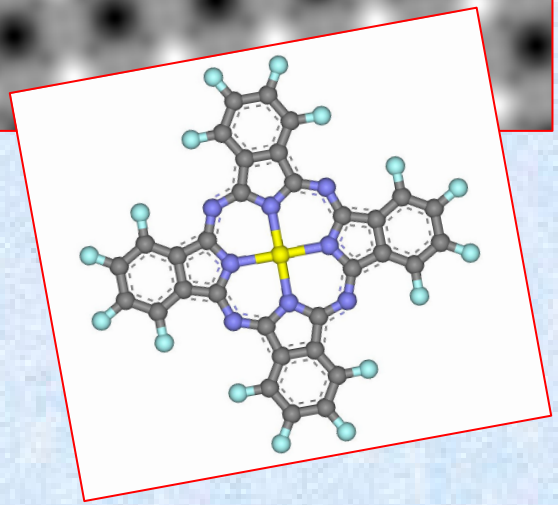


p2mm symmetry enforced STM data. A two-fold axis with a set of perpendicular mirrors is imposed. The lattice becomes rectangular. There is no 4, so the molecules 'line up" at two of the 2mm positions.



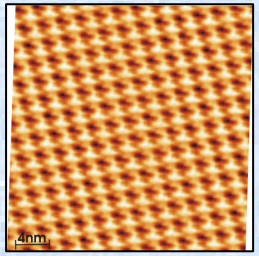
p4 symmetry enforced STM data. A four-fold axis is imposed. The lattice becomes quadratic. Because the "azimuthal orientations" of the molecules are not restricted, there is molecular mis-alignment and "washed out detail"



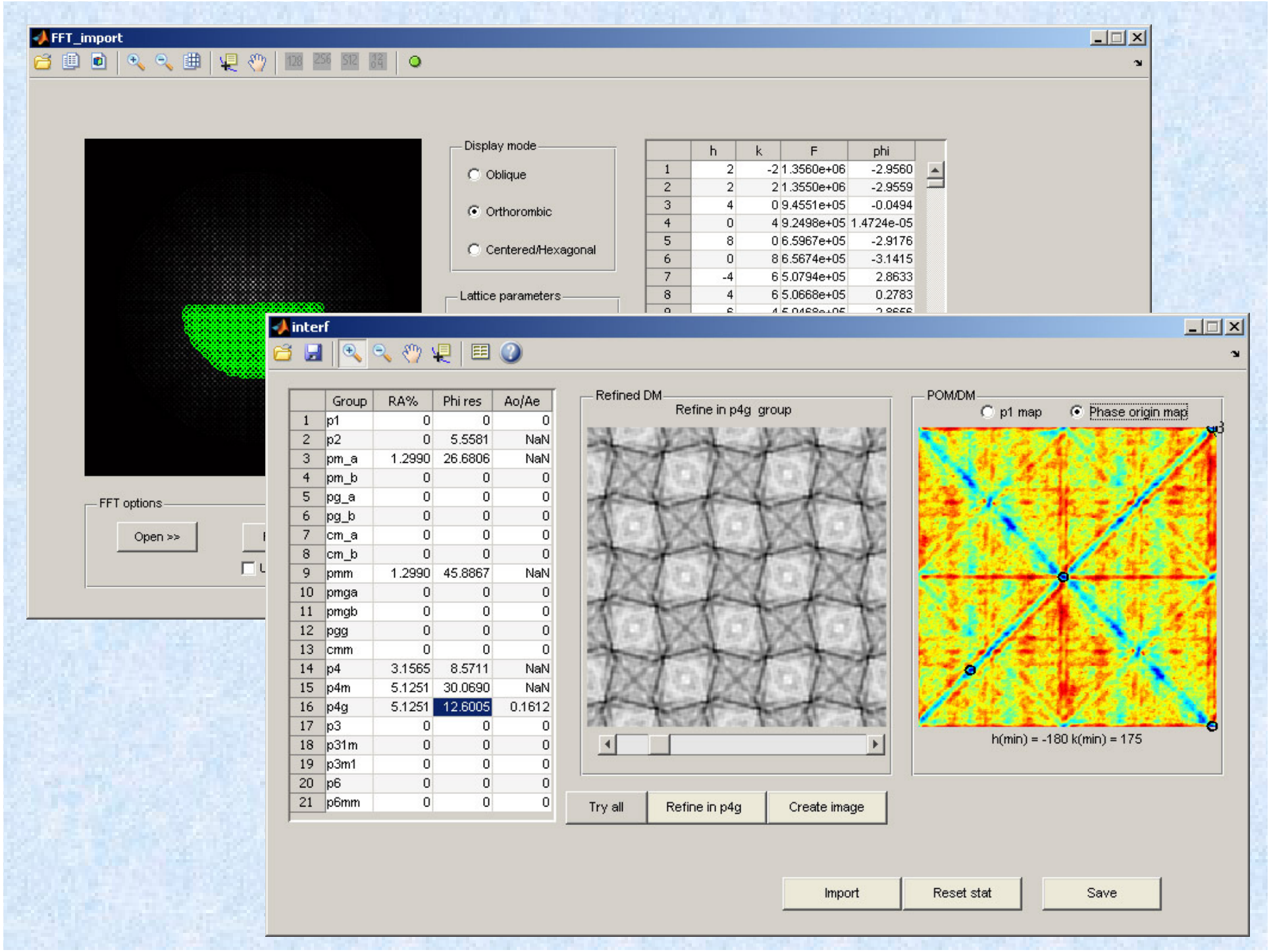


"Size" of molecule and basic periodicities in STM images approximately 1.5 – 2 nm

In effect, the "imperfections" of the scanning probe imaging process by a real microscope are removed from the data by imposing the most likely symmetry ! This is possible because all molecules are quantum mechanically identical and we may know the point group of a molecule in advance from quantum mechanics!



p4mm symmetry enforced STM data. Two additional sets of perpendicular mirror lines are imposed. The motif "rotates" counter clockwise and acquires the full point symmetry of the molecule.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Orthorombic
Centered/Hexagonal
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2 2 2 1.3550e+06 -2.9559
3 4 0 9.4551e+05 -0.0494
4 0 4 9.2498e+05 1.4724e-05
5 8 0 6.5967e+05 -2.9176
6 0 8 6.5674e+05 -3.1415
7 -4 6 5.0794e+05 2.8633
8 4 6 5.0668e+05 0.2783
FFT options
Open >>
interf
Group RA% Phi res Ao/Ae
1 p1 0 0 0
2 p2 0 5.5581 NaN
3 pm_a 1.2990 26.6806 NaN
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8 cm_b 0 0 0
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11 pmgb 0 0 0
12 pgg 0 0 0
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16 p4g 5.1251 12.6005 0.1612
17 p3 0 0 0
18 p31m 0 0 0
19 p3m1 0 0 0
20 p6 0 0 0
21 p6mm 0 0 0
Refined DM
Refine in p4g group
POM/DM
p1 map
Phase origin map
h(min) = -180 k(min) = 175
Try all
Refine in p4g
Create image
Import
Reset stat
Save