Face-to-Face With Silicon: Understanding The Structure From (001) to (111)

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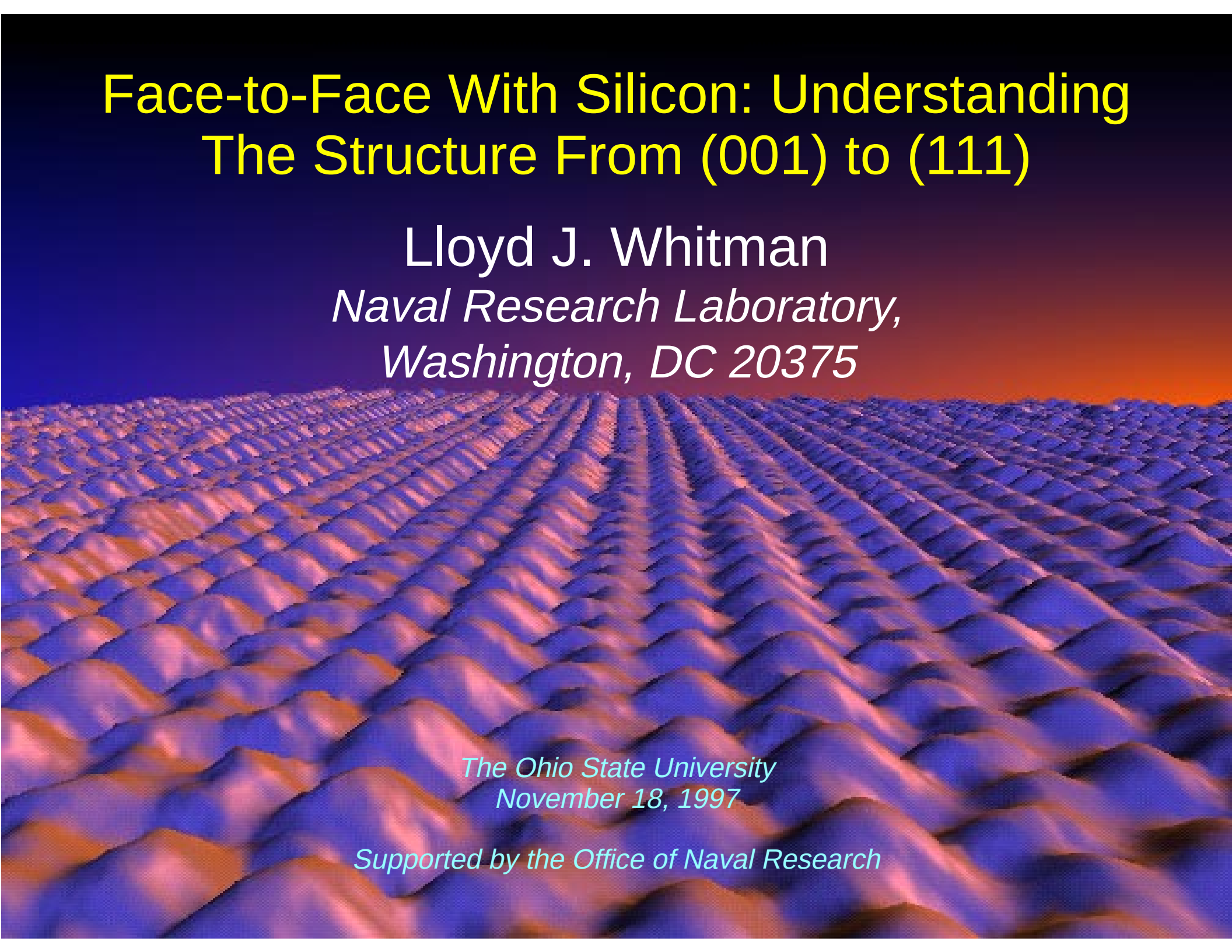


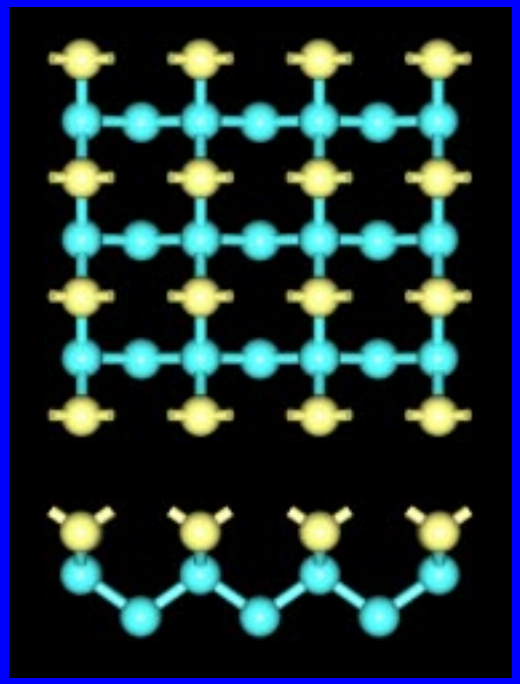
The Ohio State University
November 18, 1997

Supported by the Office of Naval Research

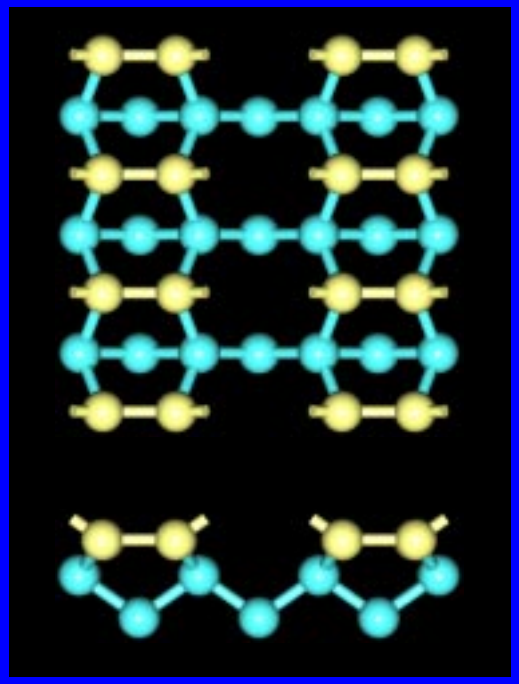
Semiconductor Surface Reconstruction: Dangling Bonds and Strain

Example: Si(001)

1x1



2x1



- 2 dbs/(1x1)
- Cubic

- 1 db/(1x1)
- Anisotropic stress (tensile along dimer bond)

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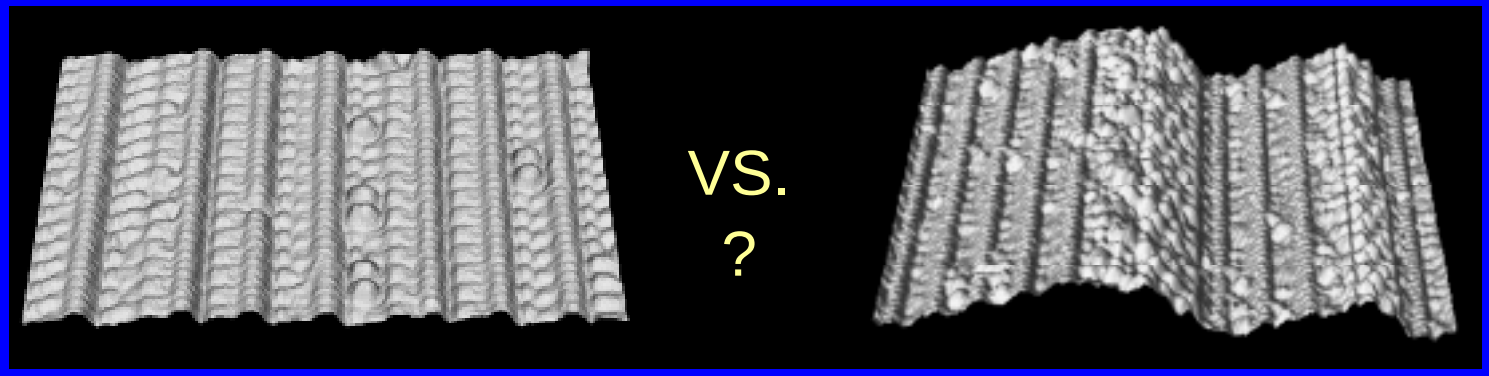
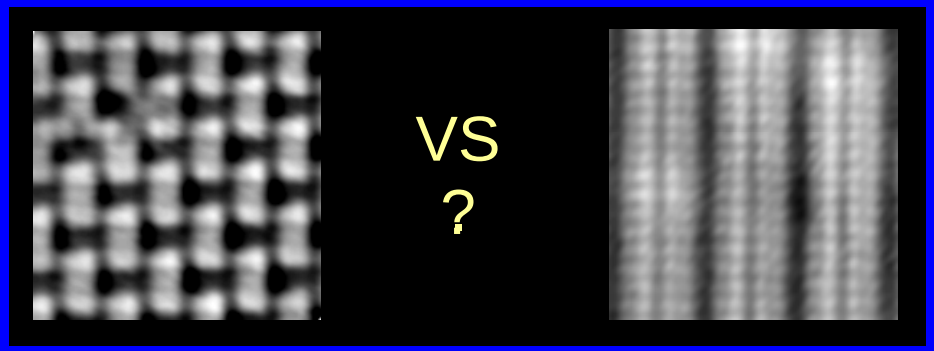
Dangling Bonds and Strain: Two Examples

- Structure, stability, and chemistry of Si surfaces
  - With A. A. Baski,* A. R. Laracuente, and S. C. Erwin (LDA)

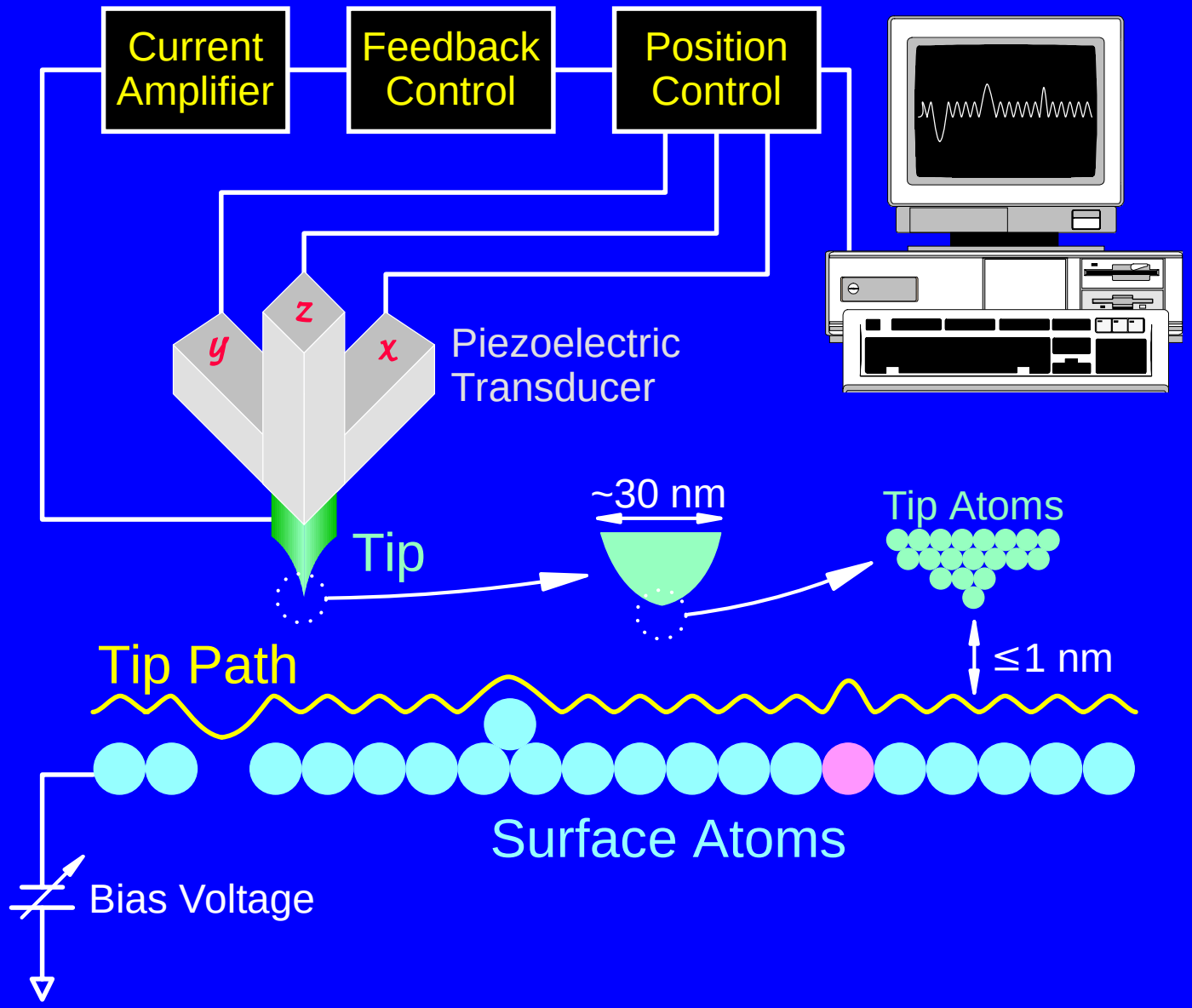


- Structure of AlSb(001)-c(4×4) vs. GaSb(001)-(1×5)
  - With P. M. Thibado*, B. R. Bennett, and B. V. Shanabrook



*Former NRL/NRC Postdocs

Scanning Tunneling Microscopy



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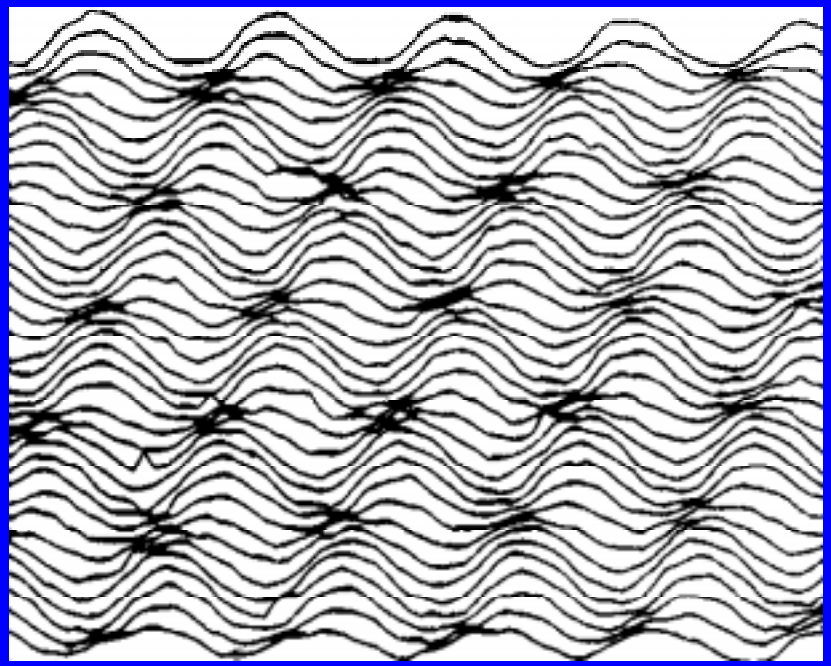
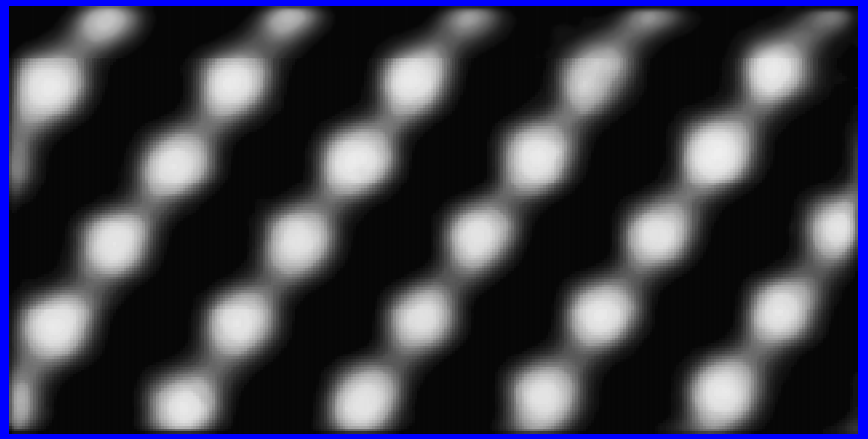
STM Image Presentation

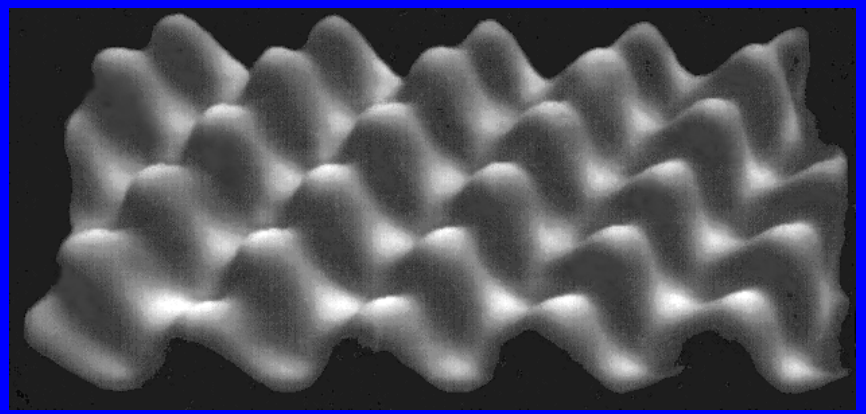
Line Scans



Gray Scale



3-D Rendered



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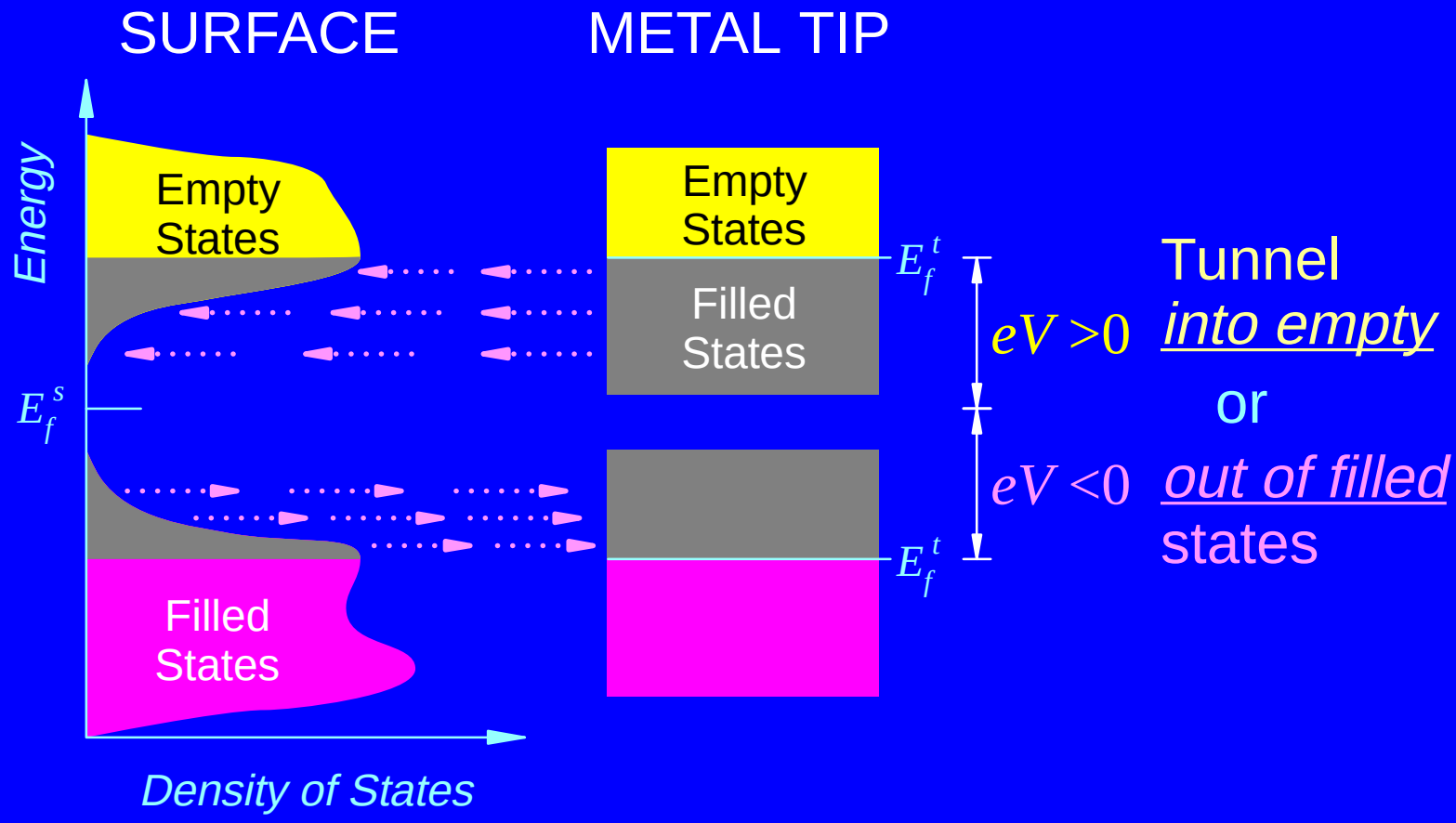
The Physics of STM



$$I \propto \int_{-eV}^{0} \rho_t(E)\rho_s(eV+E)\exp\left\{-2d\left[\frac{2m}{\hbar^2}\left(\overline{\phi}-E-\frac{eV}{2}\right)\right]^{\frac{1}{2}}\right\}dE$$

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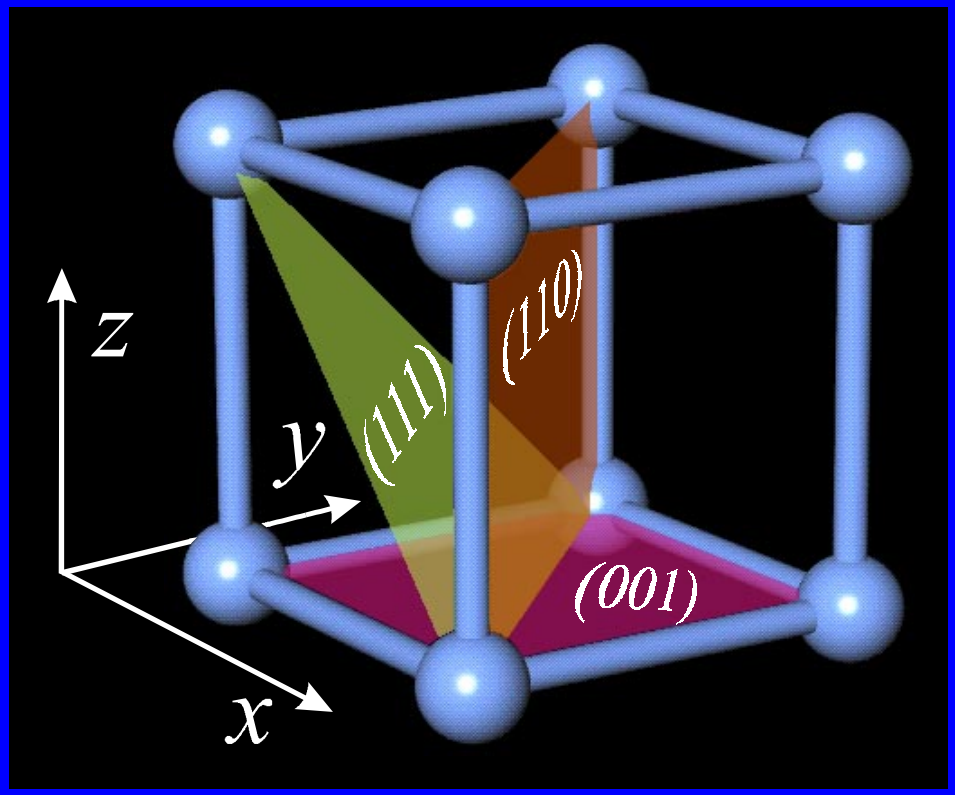
Single Crystal Surfaces in UHV

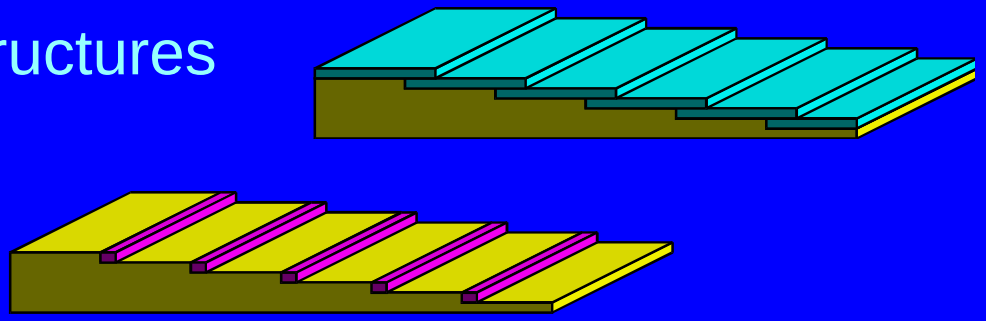


- Miller Indices, (hkl), describe vector normal to surface: $h\hat{\mathbf{x}} + k\hat{\mathbf{y}} + l\hat{\mathbf{z}}$

- Si: heat to ~1200 °C, cool slowly to room temp.
- Ge: sputter with 1 keV Ar^+, anneal at 800 °C

Why Study High-Index Silicon Surfaces?

- No Wulff plot for Si: what are stable surfaces?
- Substrates for specialized applications:
  - Heteroepitaxial structures
  - Quantum wires

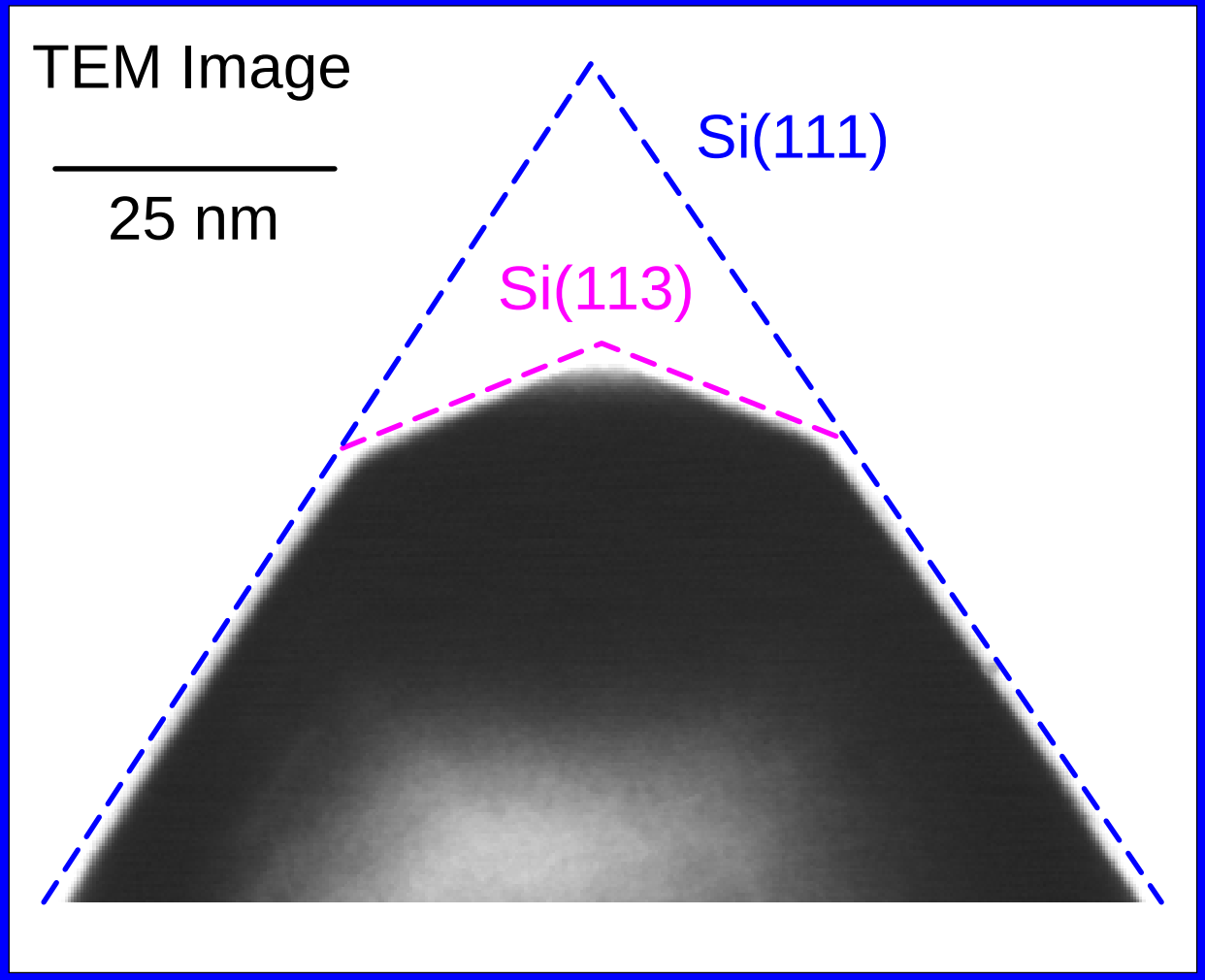


- Control of structure in Si MEMS

Pyramid

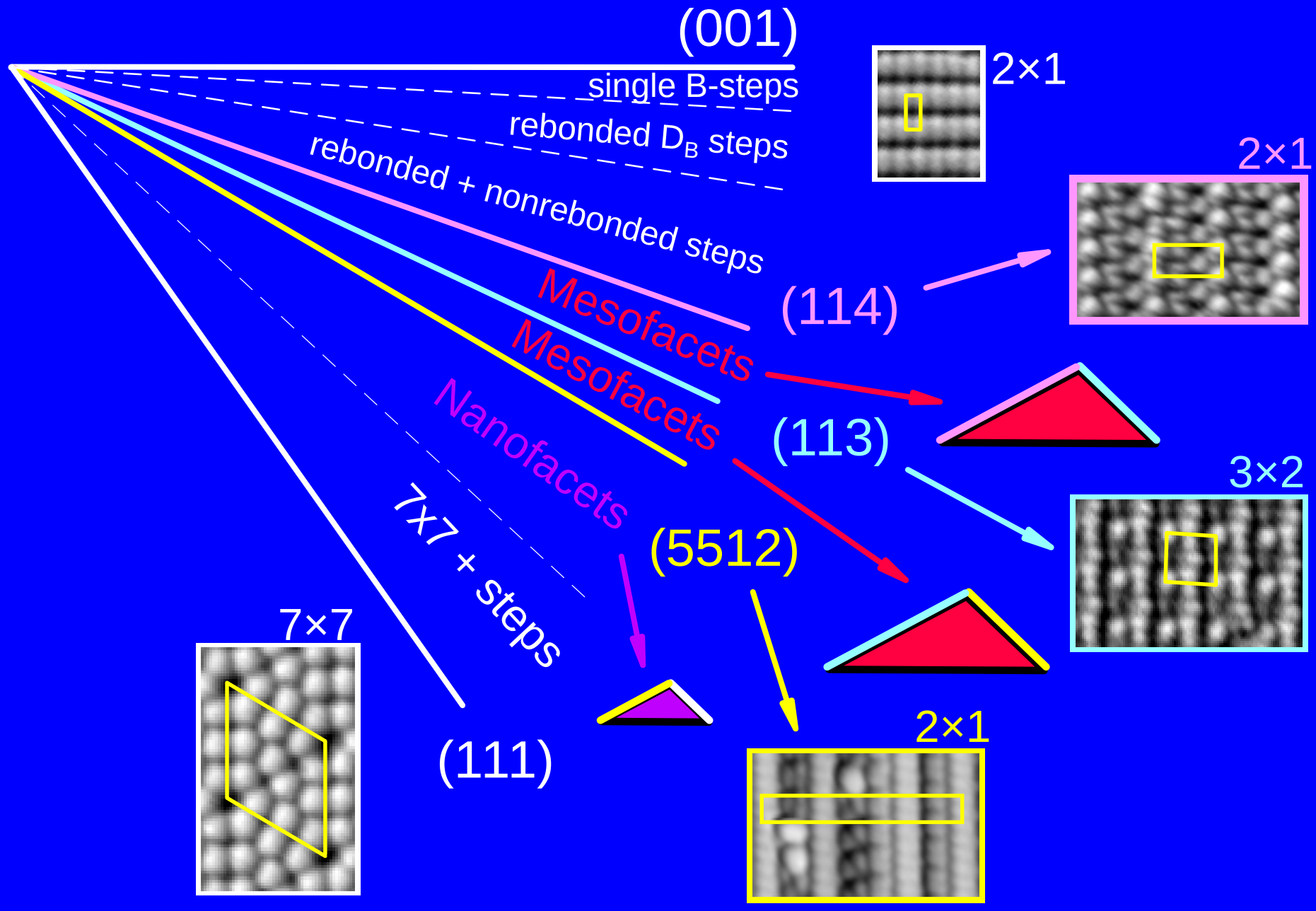
Trench

Si Field-Emitter Tip



Courtesy of K. Hobart and M. Twigg, Naval Research Laboratory

Si(001)-to-(111) Surface Structure



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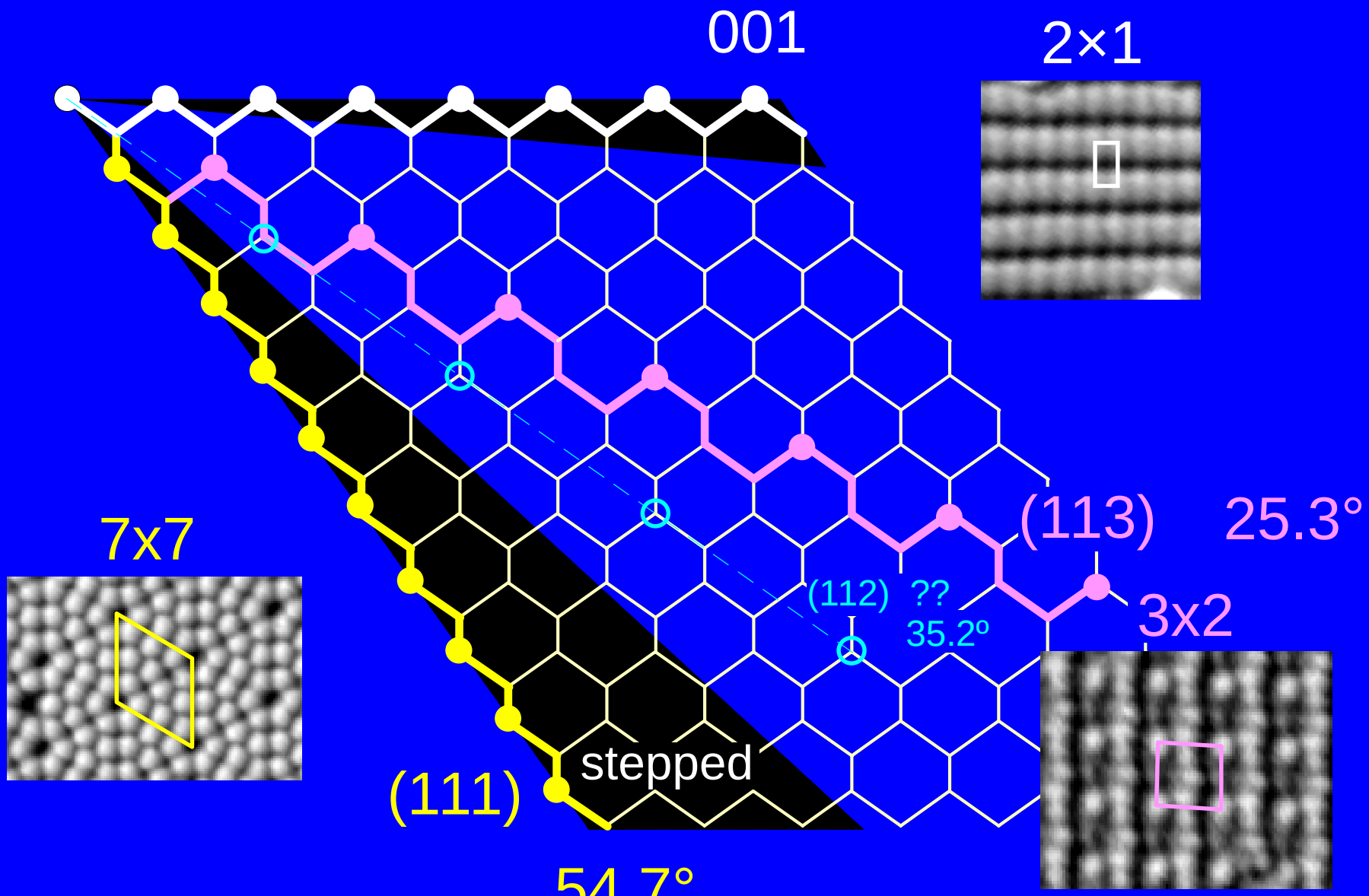
Si(001)-to-(111) Surfaces: (110) Projection



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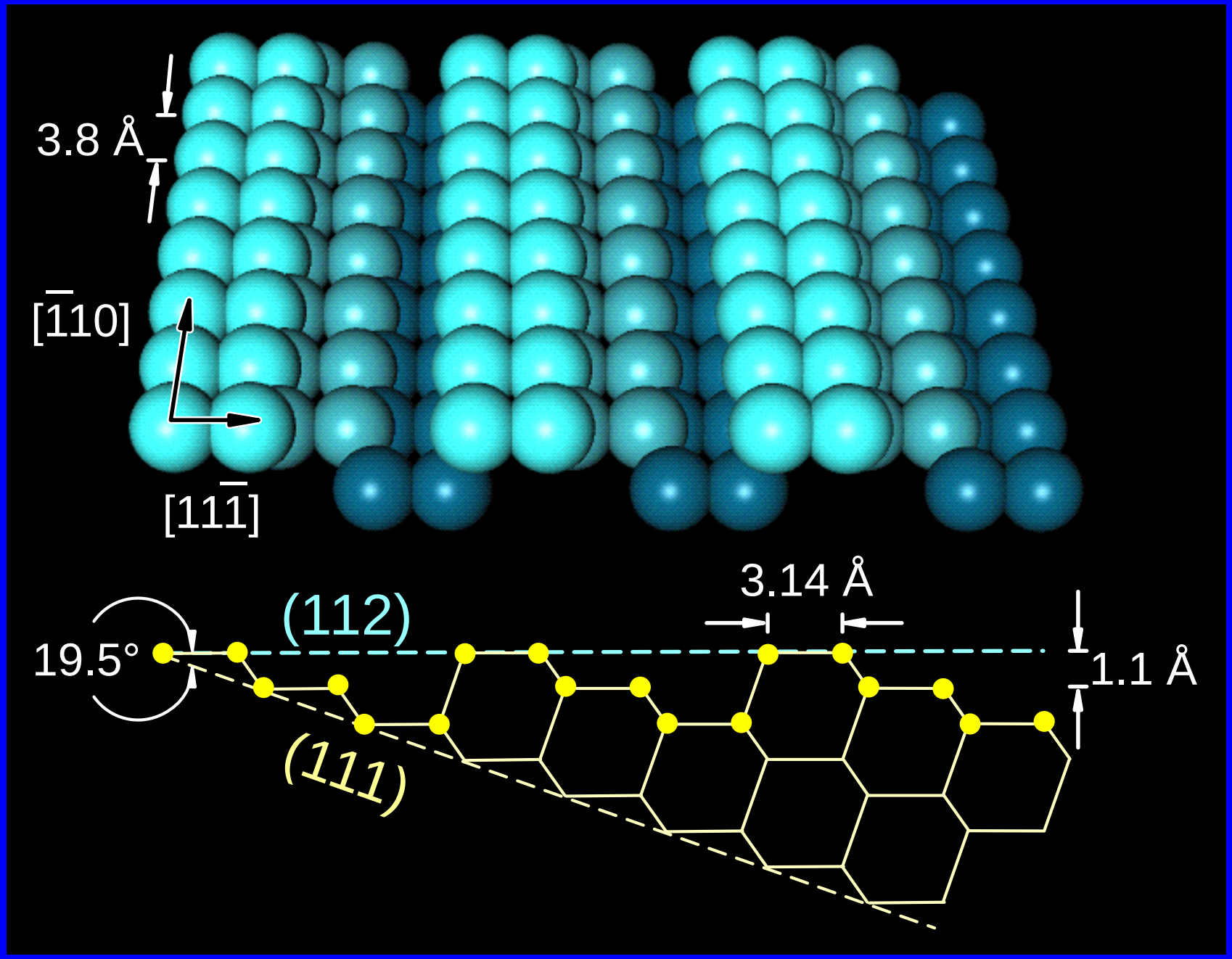
Bulk-Terminated Si(112)



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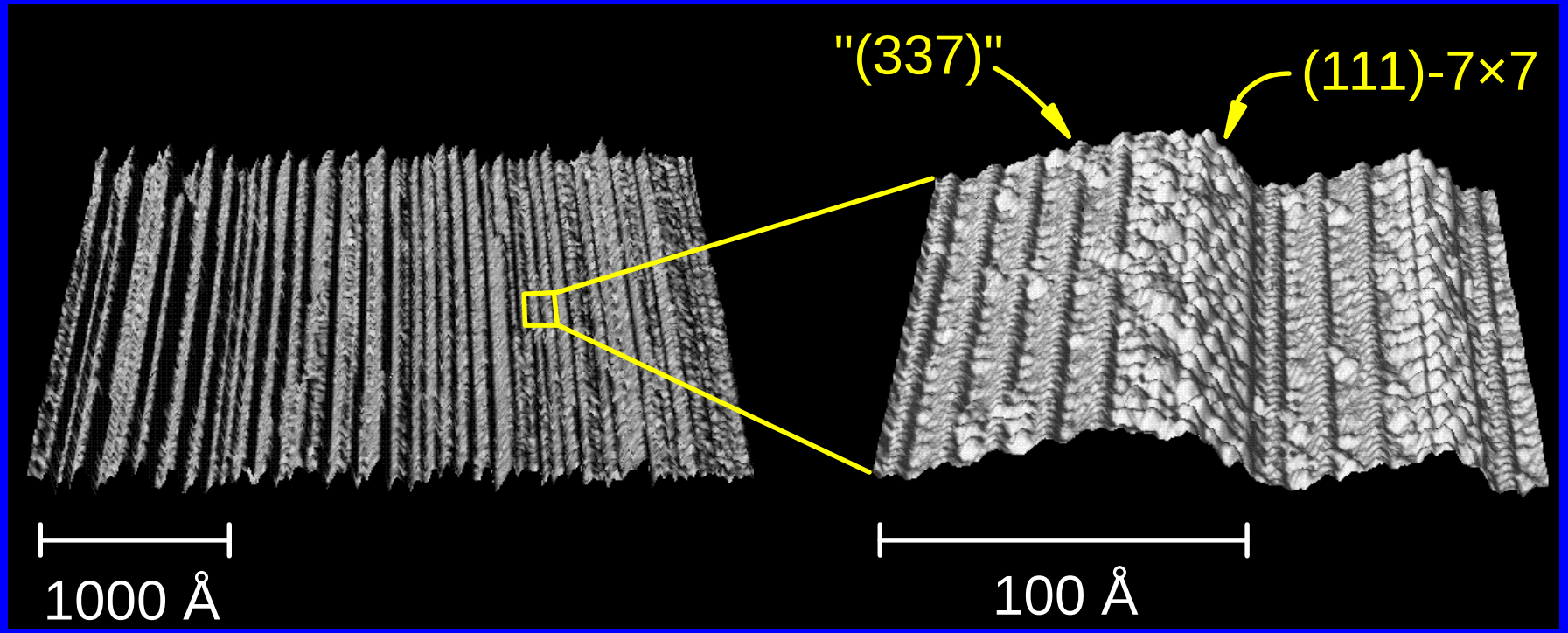
Clean Si(112): Nanofacets



- Unit cell-wide (111)-7×7 + "(3 3 7)" nanoterraces
  - (337) often interrupted by single units of (225)

(1 1 2.33) (1 1 2.5)

- Implication: ~(337) low energy surface.

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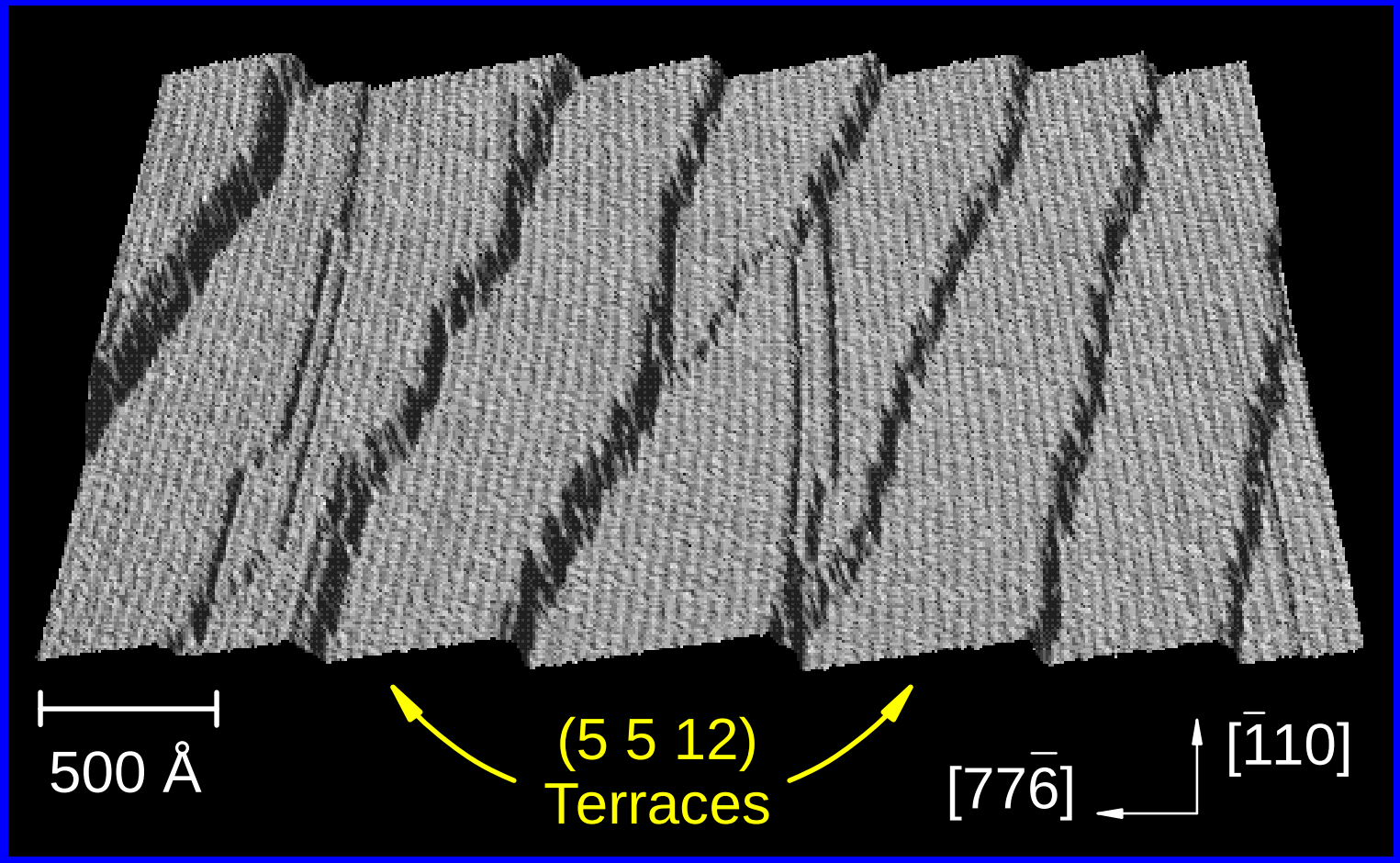
"Si(337)" Topography



- (3 3 7) forms (5 5 12) terraces + step bunches

  (1 1 2.33) (1 1 2.4)

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Si(001)-to-(111) Unit Cells: (5 5 12)

(1 1 2.4)

(5 5 12) = (337) + (225) + (337)

(1 1 2.4) (1 1 2.33) (1 1 2.5) (1 1 2.33)

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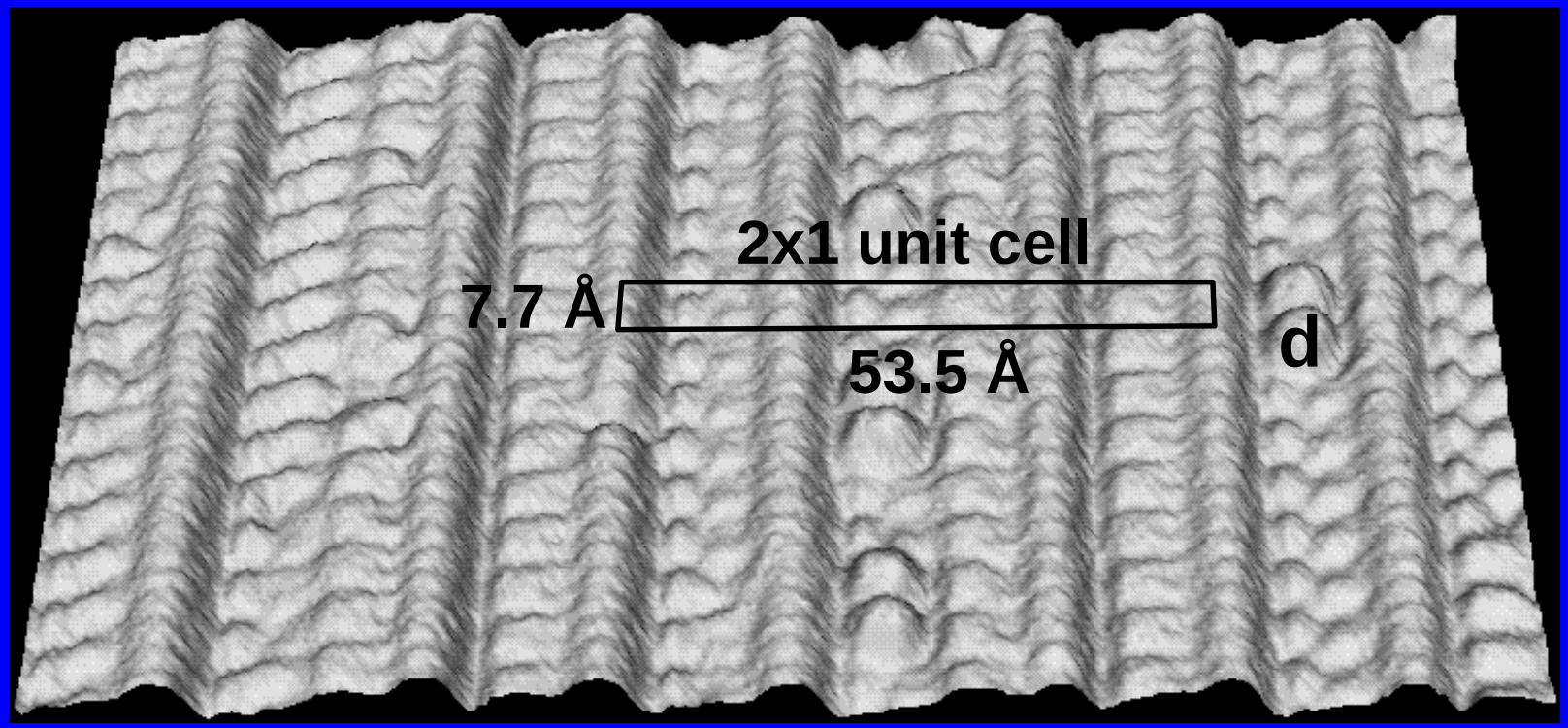
Si(5 5 12)-2x1 Reconstruction

(337) + (225) + (337) = (5 5 12)



1 3 1 3 2 1 2 1

$[\bar{1}10]$

$[66\bar{5}]$

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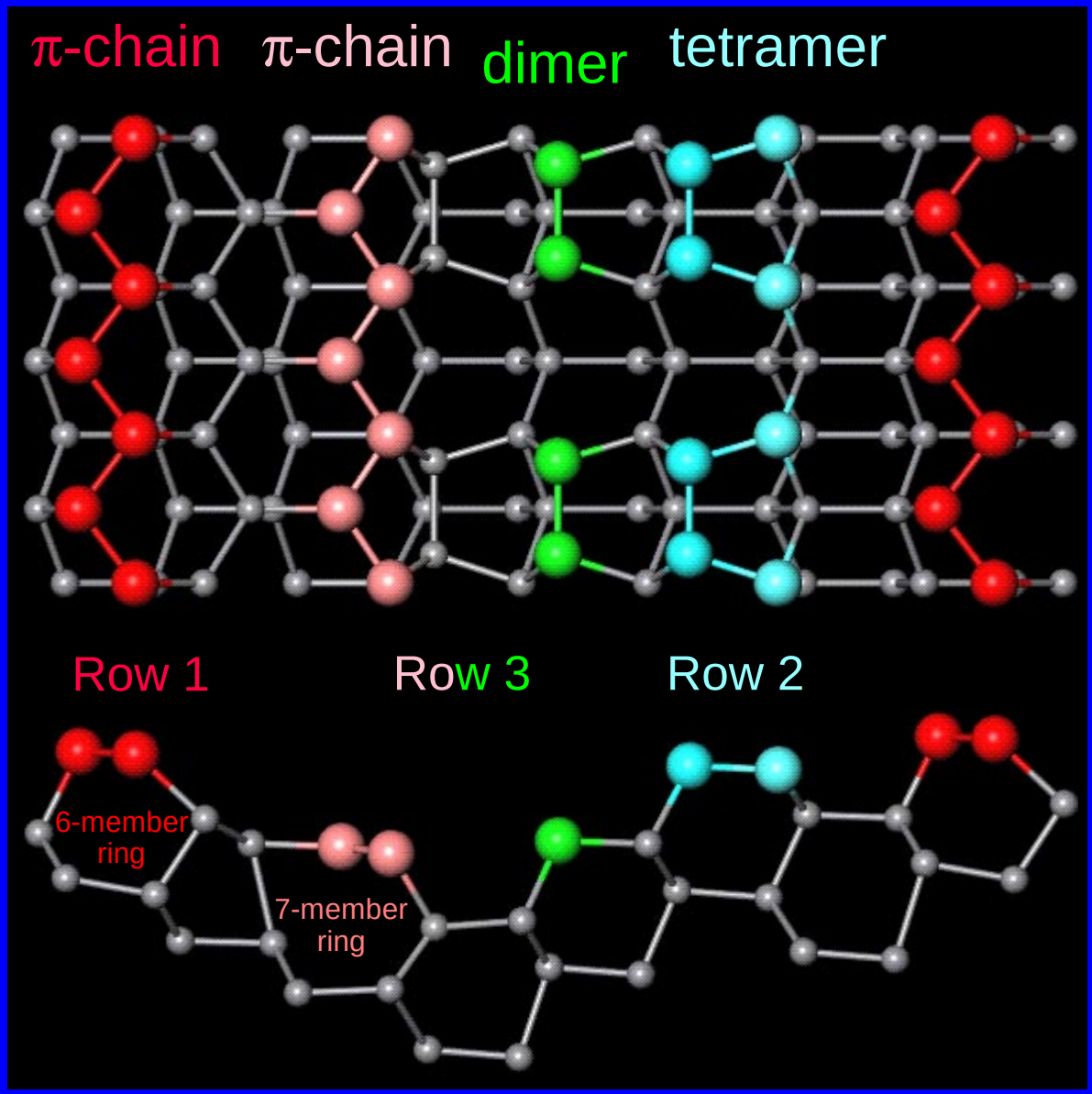
Model of (225) Subunit of Si(5 5 12)-2x1



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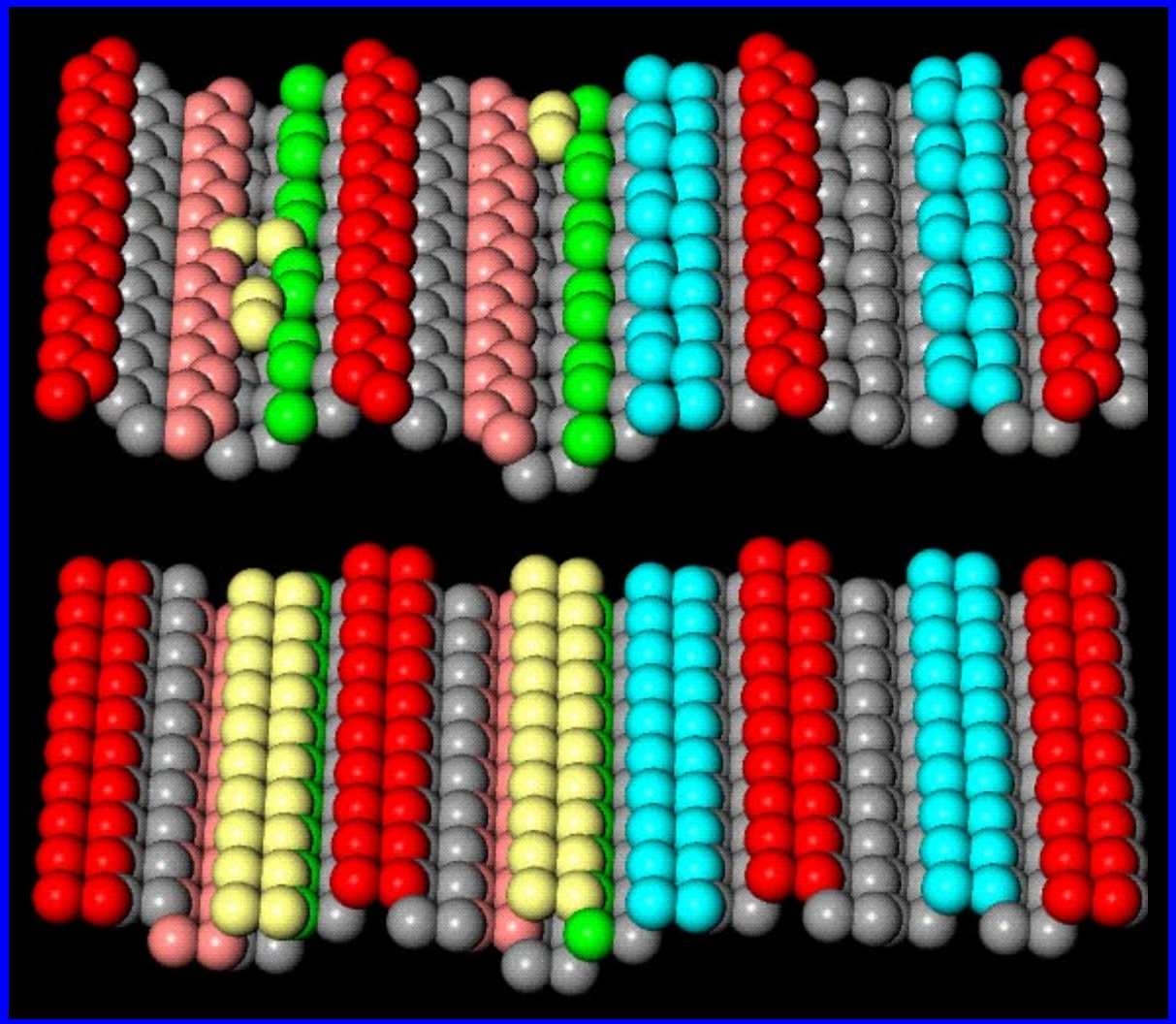
Bulk-Terminated vs. Reconstructed Si(5 5 12)

Proposed model

Bulk-terminated



π-chain (6)
π-chain (7)
dimer
tetramer
adsorbed dimer

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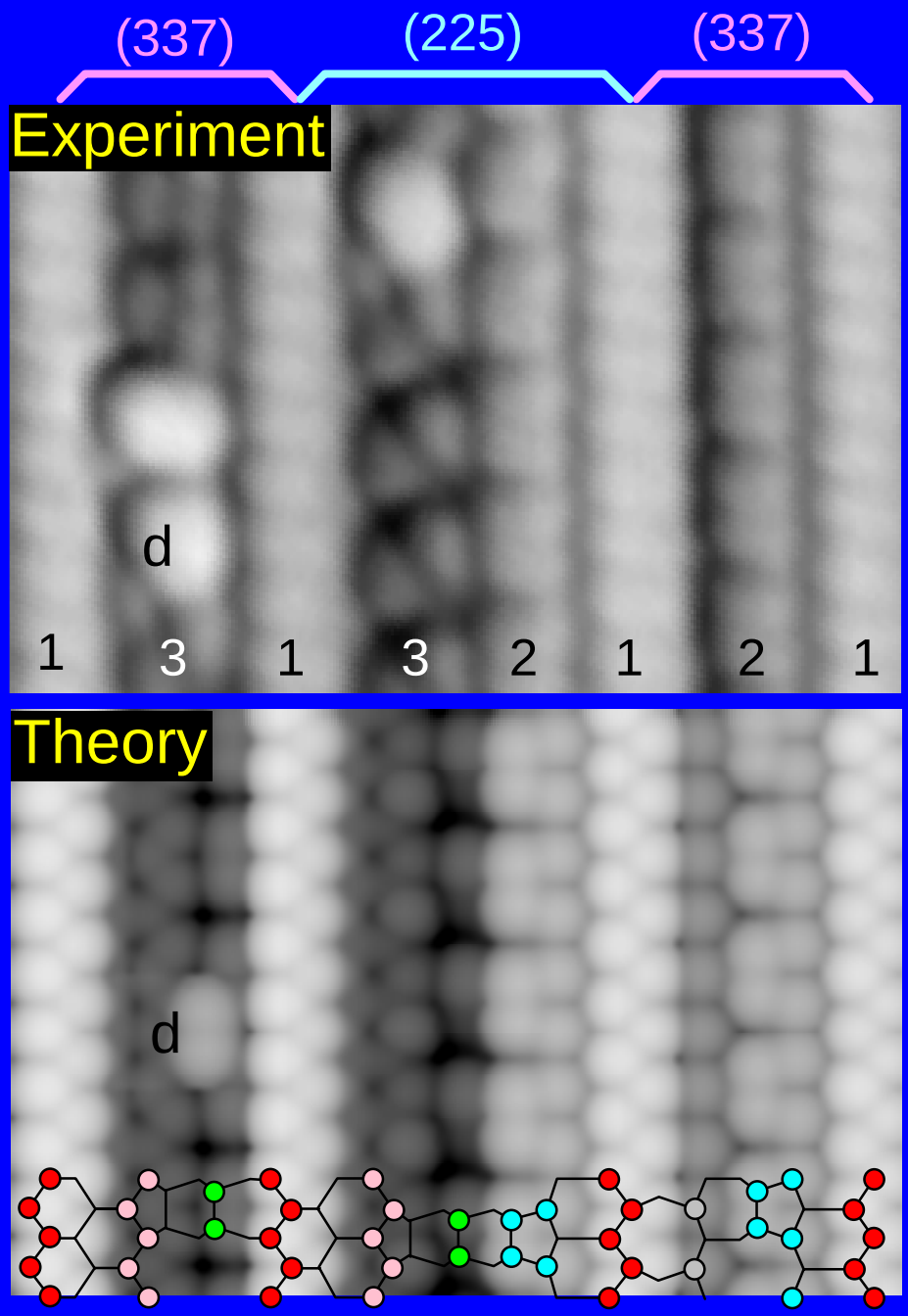
Theory: Simulated STM images

Work done by Steve Erwin.

- First-principles, electronic-structure calc. (LDA).
- Local-state density $\rho(r,\varepsilon)$ computed from wave functions.
- At each r, integrate $\rho(r,\varepsilon)$ over filled or empty states.
- Simulate constant current STM image by surface of constant integrated $\rho(r,\varepsilon)$.

Compare simulated images with STM images.

Si(5 5 12) Experiment vs. Theory



- 0.053 dbs/Å^2, lower than (001)-2×1.
- *Not* lowest db model!
- (337) compressive stress balanced by (225) tensile stress.

FILLED STATES

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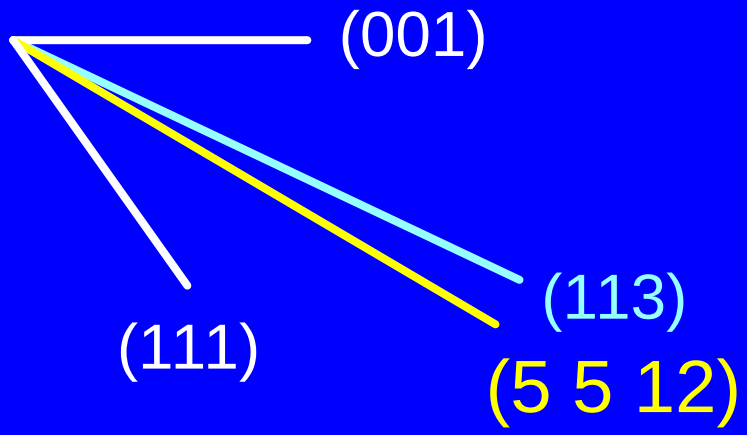
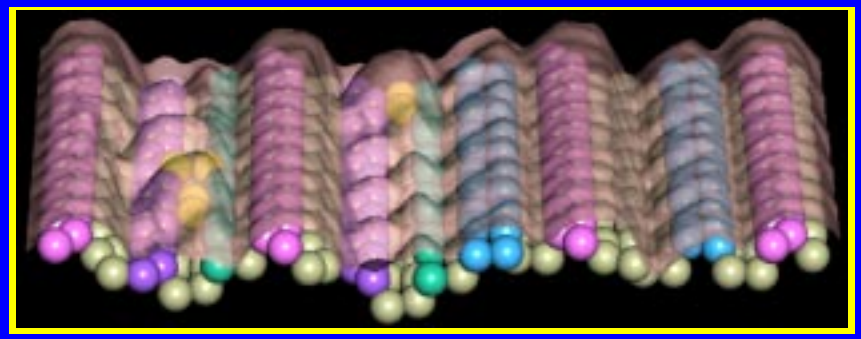
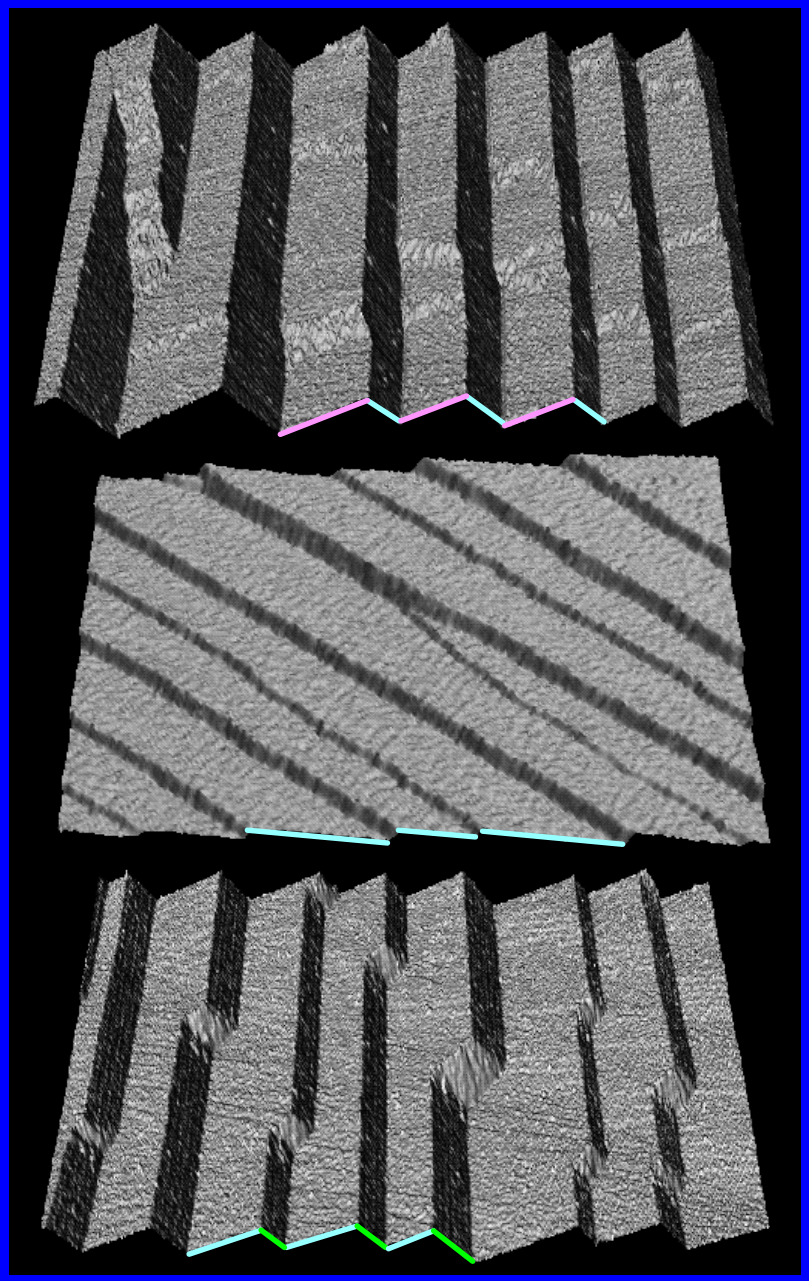
The Stable Si(5 5 12)-2×1 Surface

- One of the largest unit cells ever observed: 7.7 Å x 53.5 Å (68 atoms / unit cell).
- Consists of simple building blocks: π-bonded chains, dimers, and tetramers.
- Stable due to delicate balance between dangling bond reduction and stress relief.





Surfaces Around Si(113)



1000 Å

(113)+3.7°: Mesofacets

(001)

(114)
+
(113)

(111)

~(113): 3x2 Terraces

(001)

(113)

(111)

(113)-1.5°: Mesofacets

(001)

(113)
+
(5 5 12)

(111)

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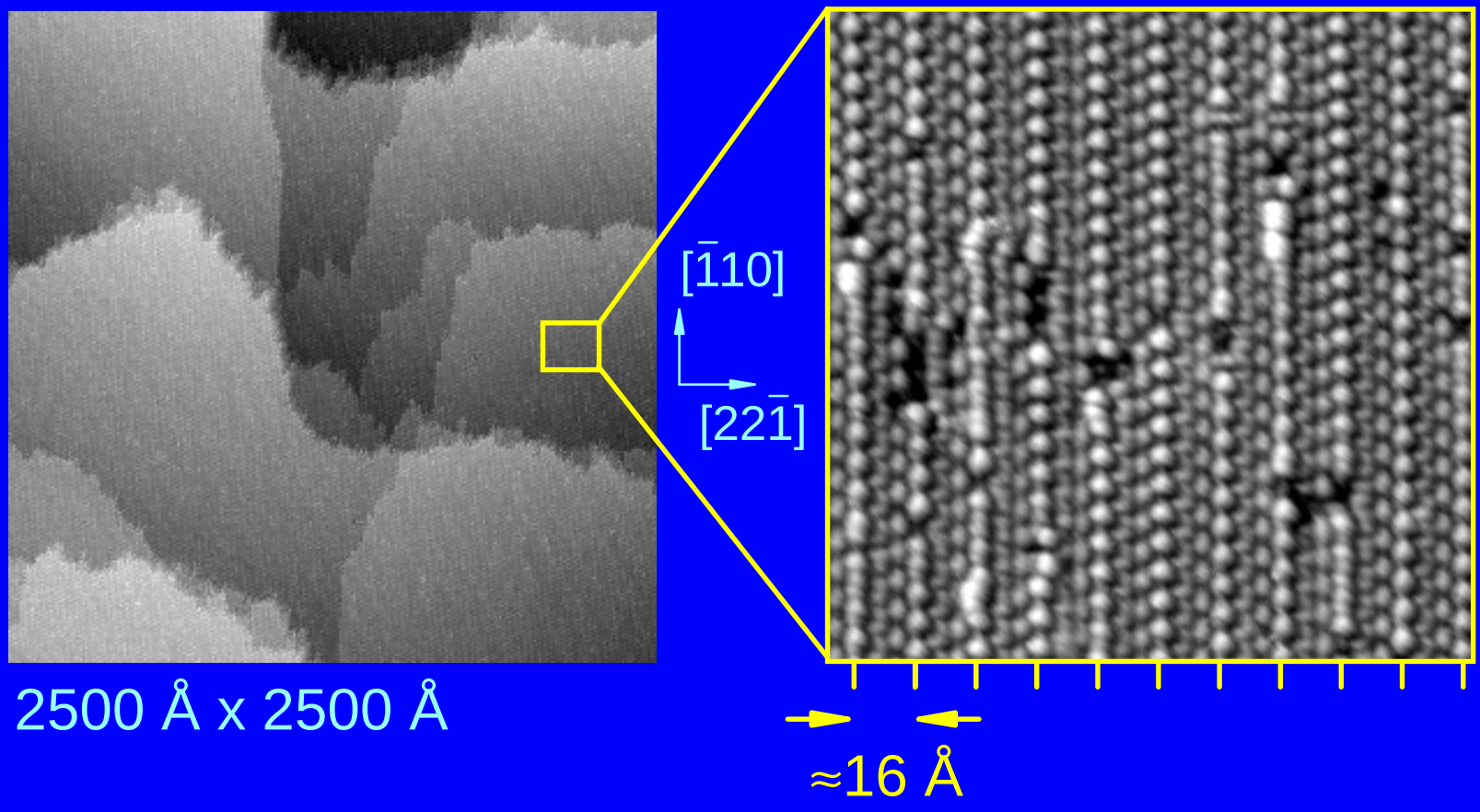
STM Images of Si(114) (19.5°)

Filled State Images



A stable planar surface with long-range order.

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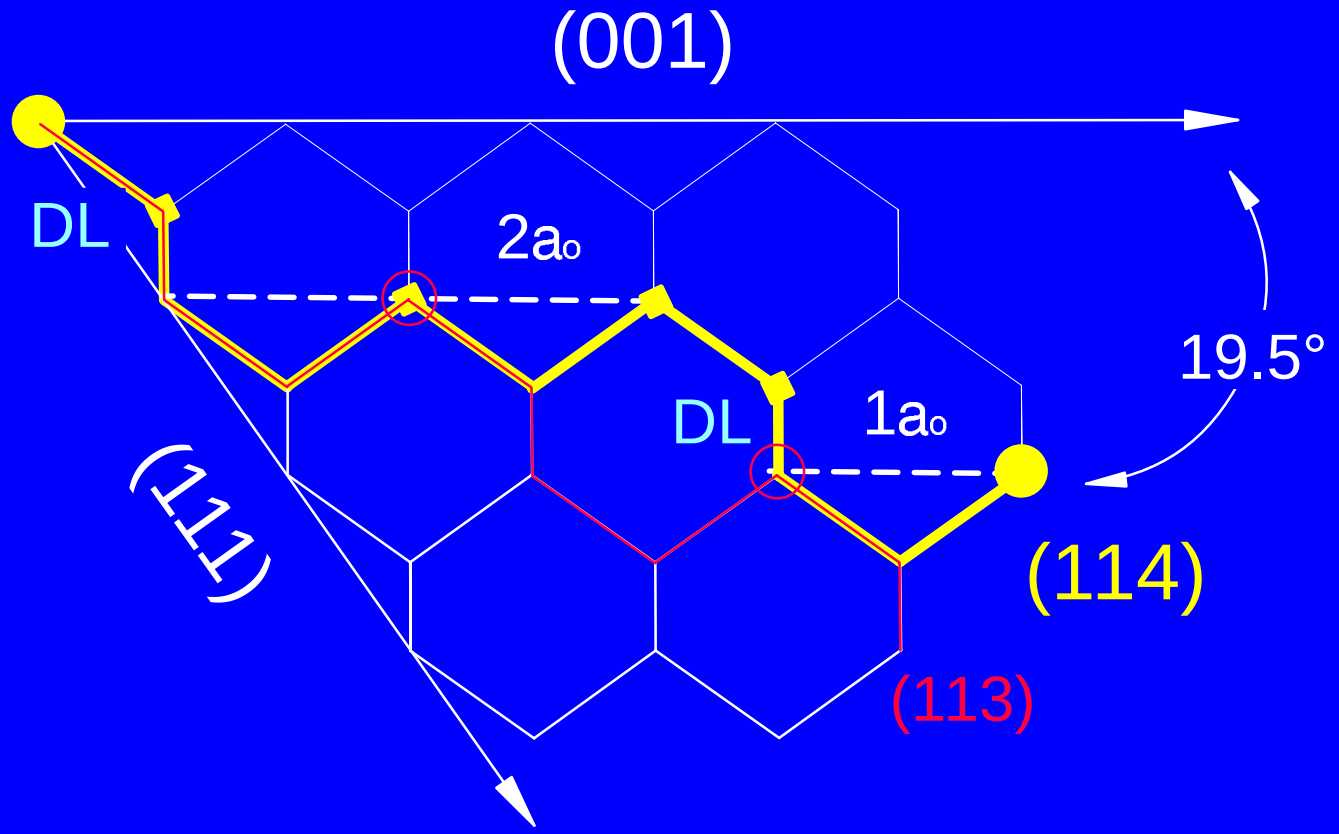
Bulk-Terminated Si(114)



Si(114) = 2 units (001) + DL
+ 1 unit (001) + DL

Alternating-width (001) terraces + double-layer steps.

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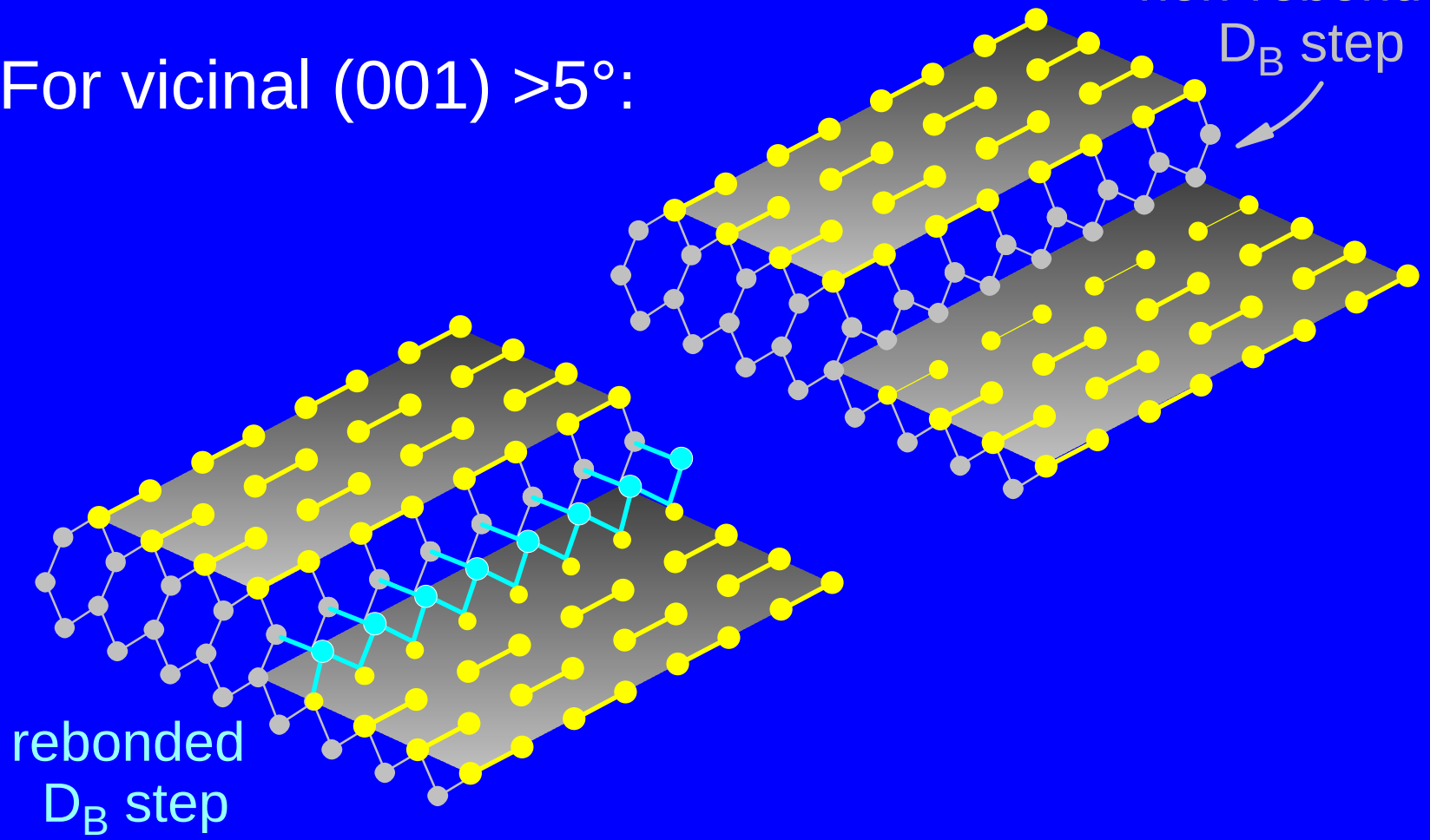
Rebonded vs. Non-rebonded D_B steps

For vicinal (001) >5°:



expect rebonded, double-layer, "B-type" steps.

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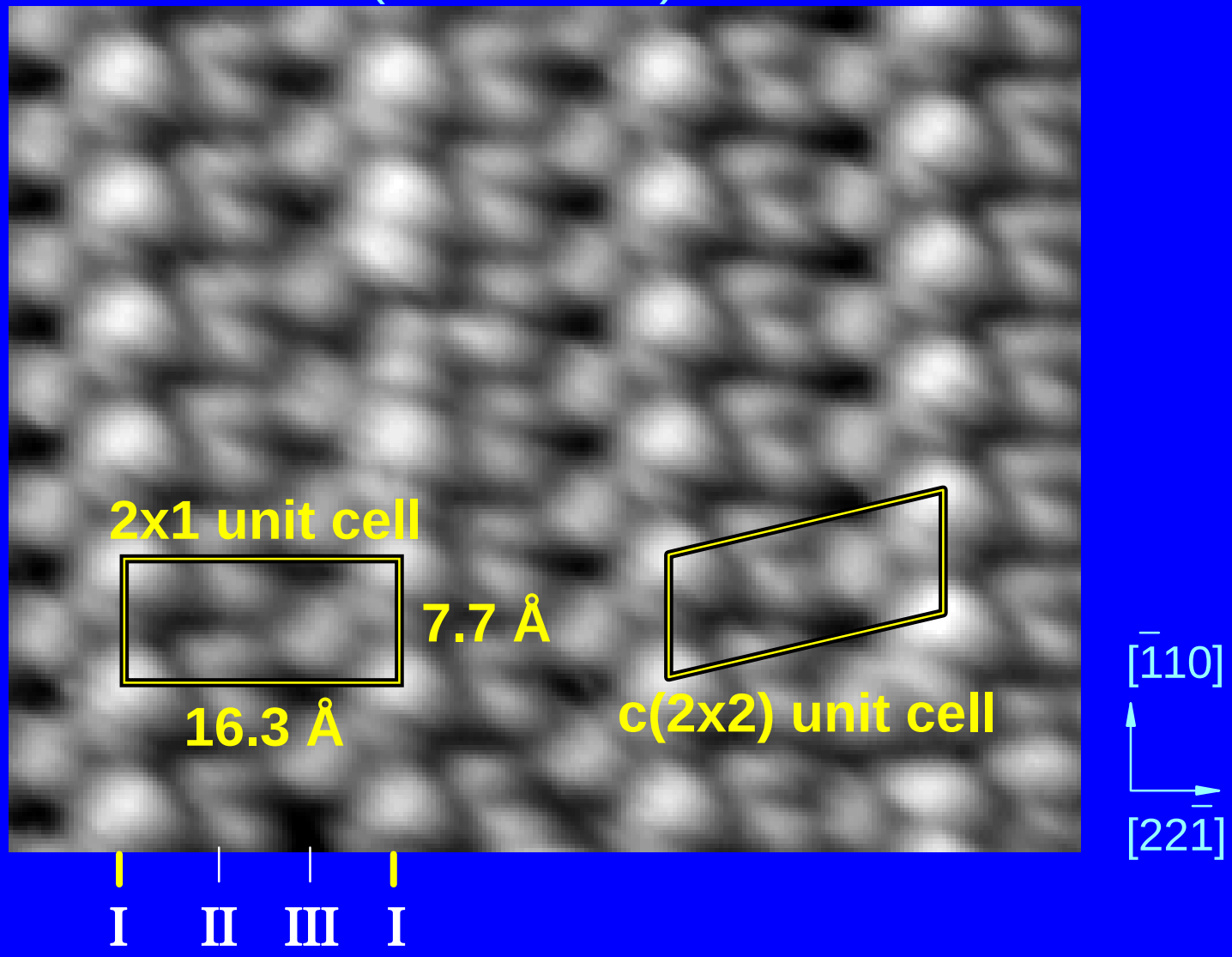
Si(114)-2x1 Reconstruction

210 Å x 180 Å (filled states)



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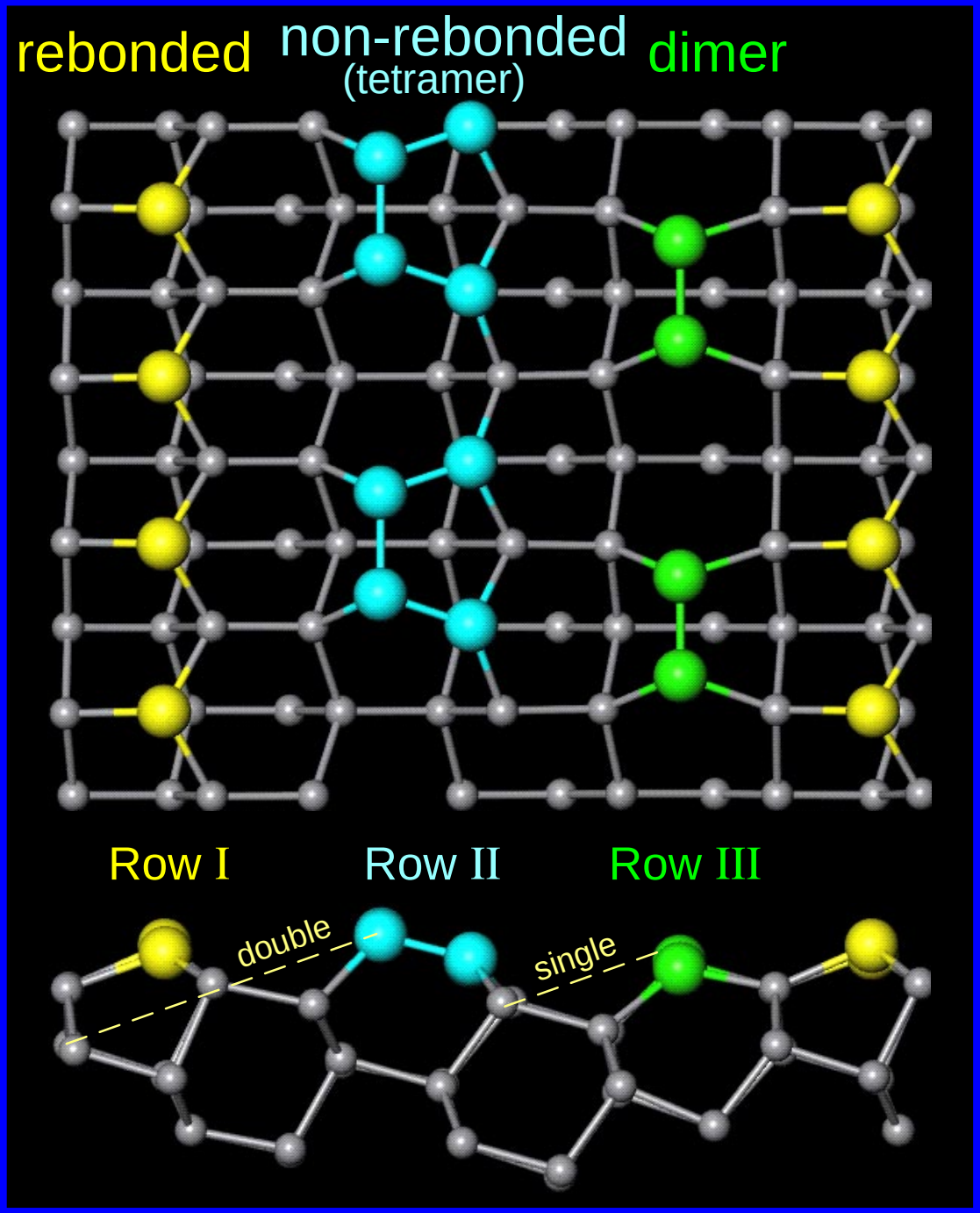

Model for Si(114)-2x1

Fully-relaxed LDA

Alternate rebonded, *non-rebonded* steps.

Not lowest db model: *both steps rebonded has two less dbs*.

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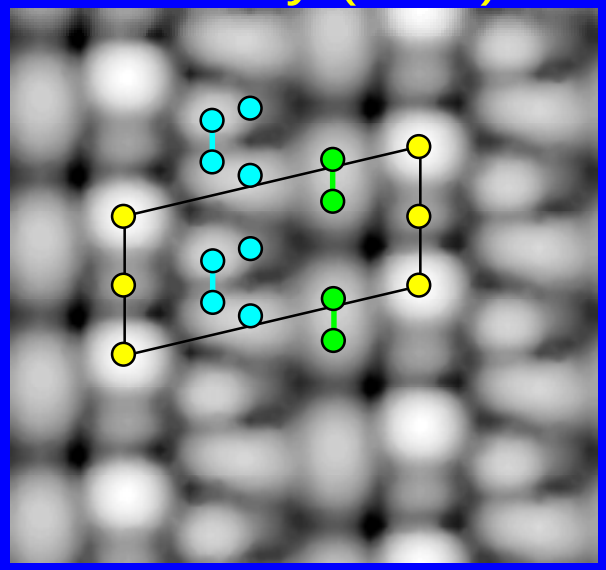
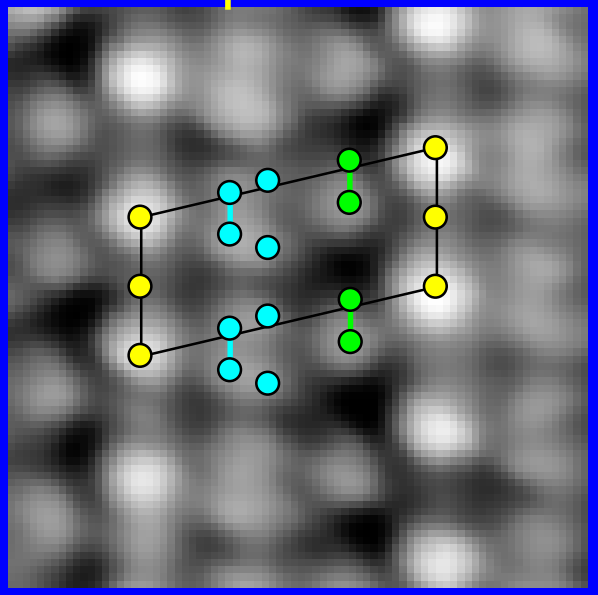
STM Images: Theory vs. Experiment

Filled States

Theory (LDA)



Experiment



I II III I

I II III I

Dimer row

Non-rebonded steps + dimer row

Rebonded D_B steps

All structures buckled along the rows.

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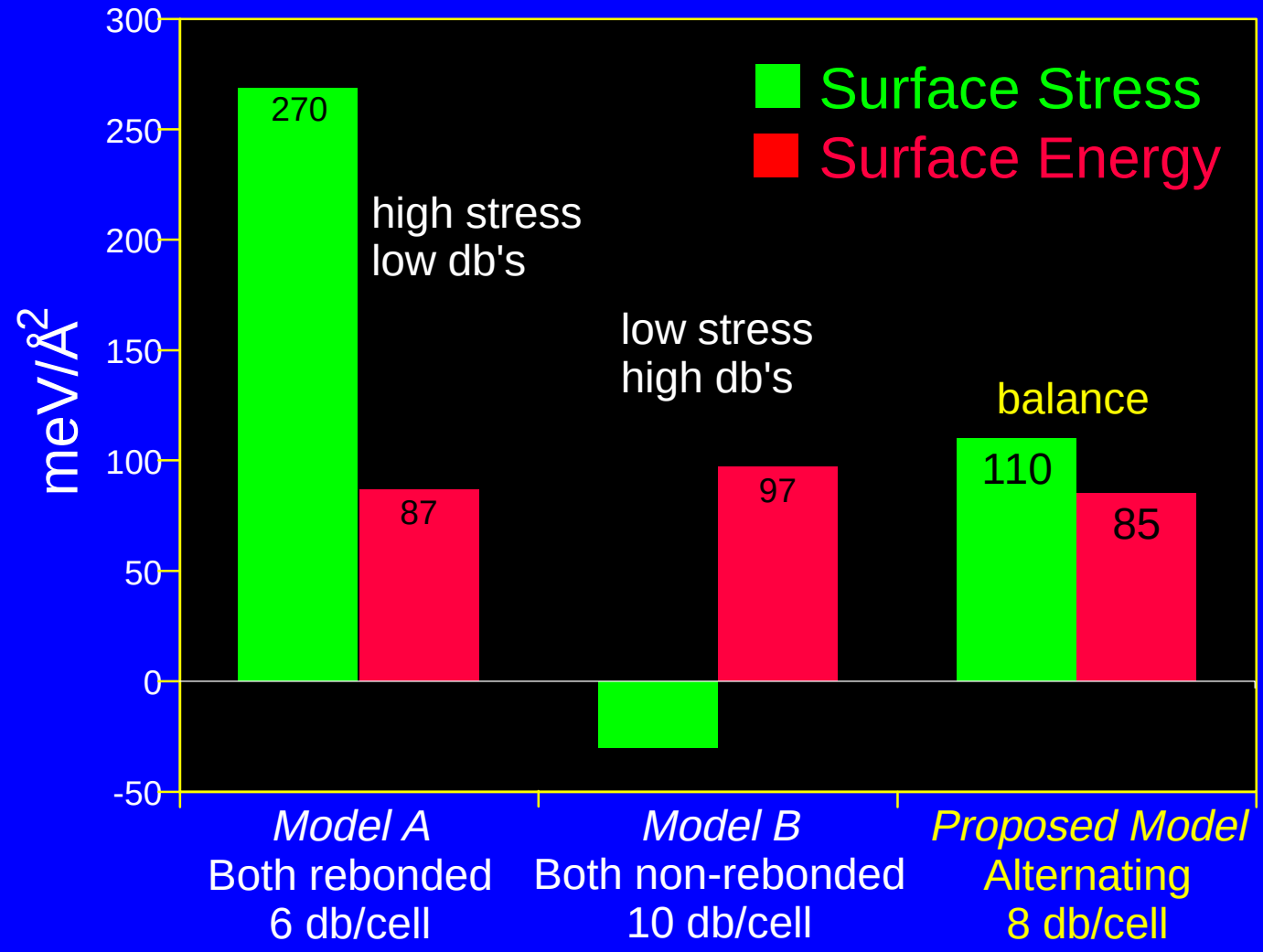
Why Rebonded *and* Non-rebonded Steps?



(001) terraces too short for elastic strain relief.

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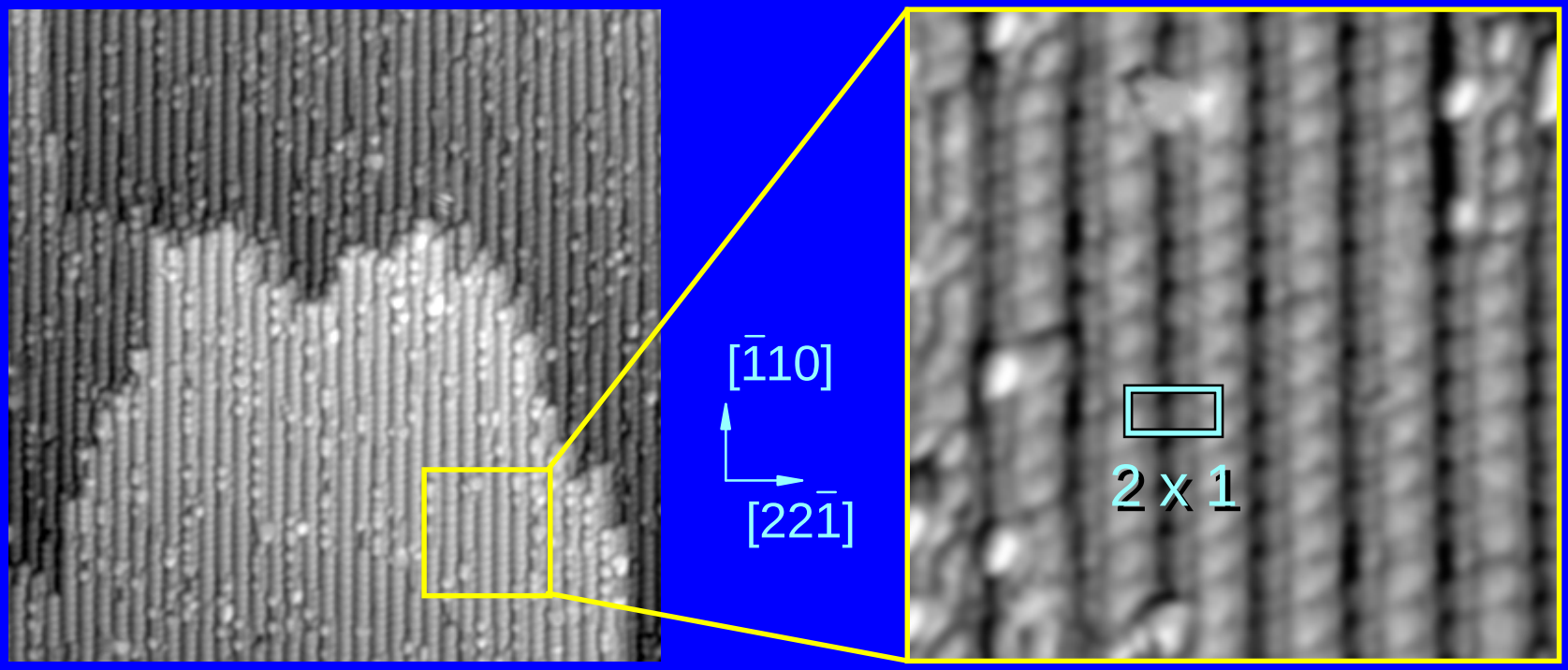
Hydrogen-Terminated Si(114)

- Surface can be passivated by atomic hydrogen
  - Use same conditions as for Si(001):H-(2×1) (T=400 °C + 500 L H_2 w/ hot filament)



610 Å x 610 Å

114 Å x 114 Å

A low-defect density, (2×1) monohydride surface.

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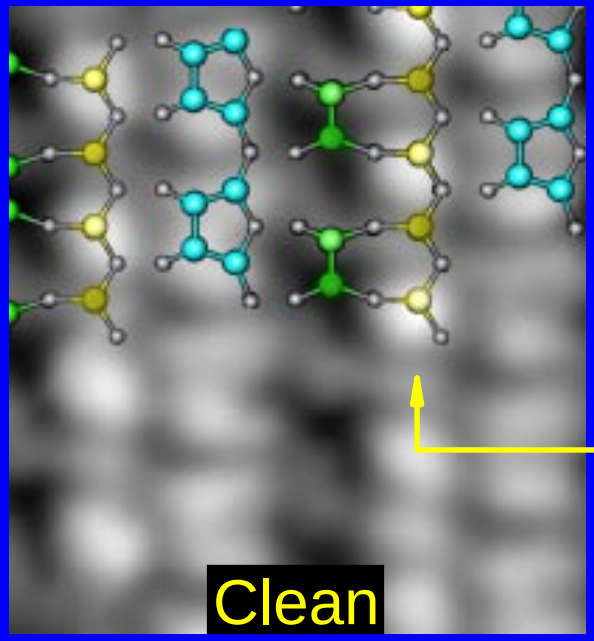
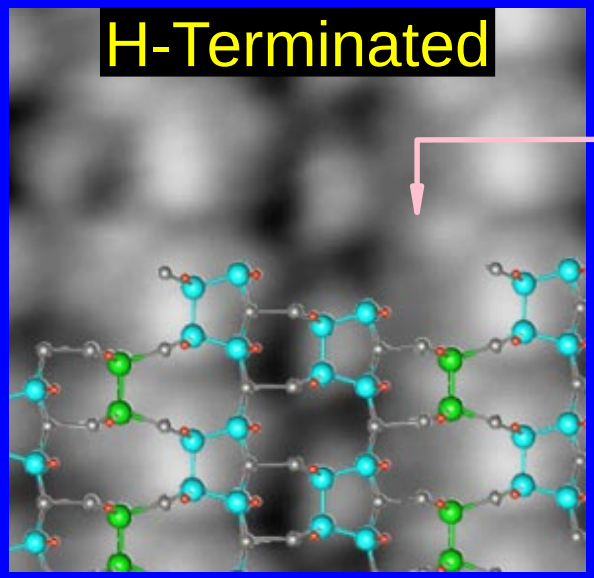
Si(114):H-(2×1): A Monohydride Surface



Rebonding atoms

- H saturates dbs, so don't "need" rebonding atoms



Rebonding atoms GONE

- Low-stress, monohydride surface; "bulk-like" (except for dimers)

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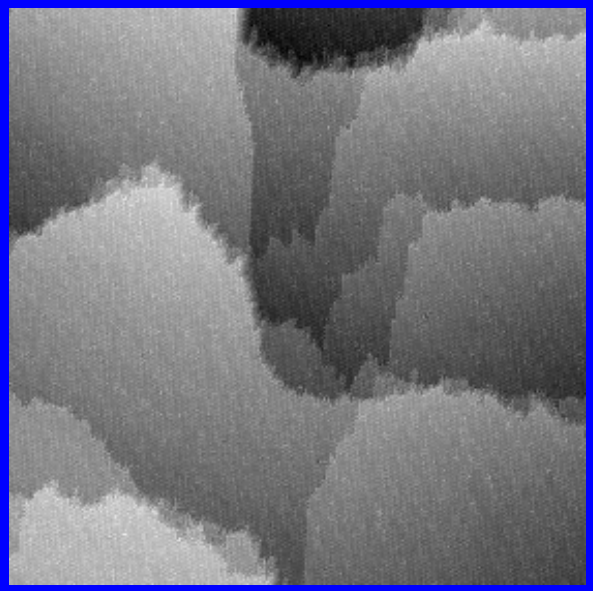
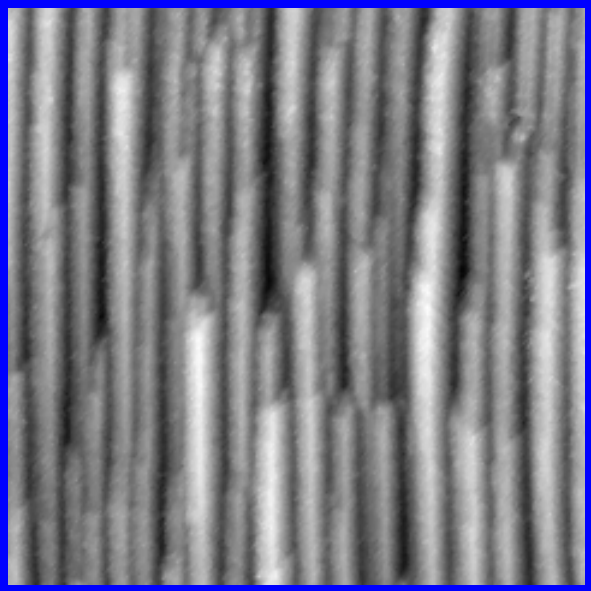
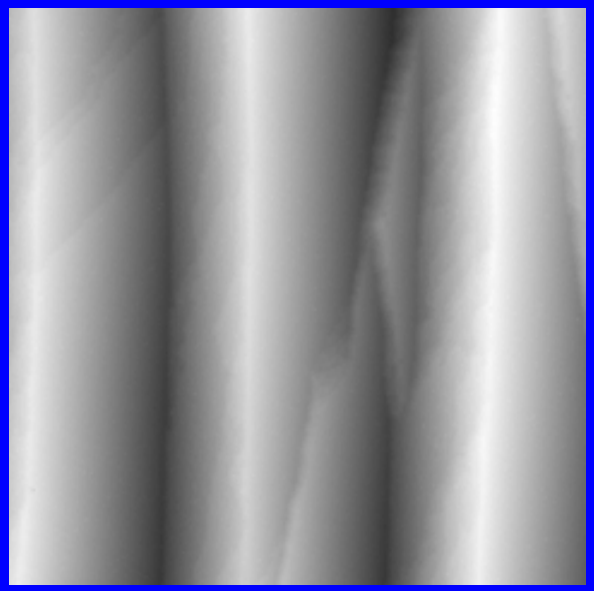
Si(114) vs. Ge/Si(114) vs. Ge(114)

Filled State Images: 2500 Å × 2500 Å

Clean Si(114)	~0.7 ML Ge/ Si(114)	Clean Ge(114)
		
(114) terraces	(117)/(113) facets, ~100 Å wide	(117)/(113) facets, ~1000 Å wide

Stability easily perturbed!

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The Stable Si(114)-2×1 Surface

- Low density of dangling bonds

Si(001)-2×1	=	0.068 dbs/Å^2
Si(114)-2×1	=	0.064 dbs/Å^2
Si(5 5 12)-2×1	=	0.053 dbs/Å^2
Si(111)-7×7	=	0.030 dbs/Å^2

- Like (5 5 12), balance between dangling bond reduction and stress relief
  - Tensile stress of rebonded steps relieved at non-rebonded steps.

Balance easily altered by removing dangling bonds or changing surface stress.

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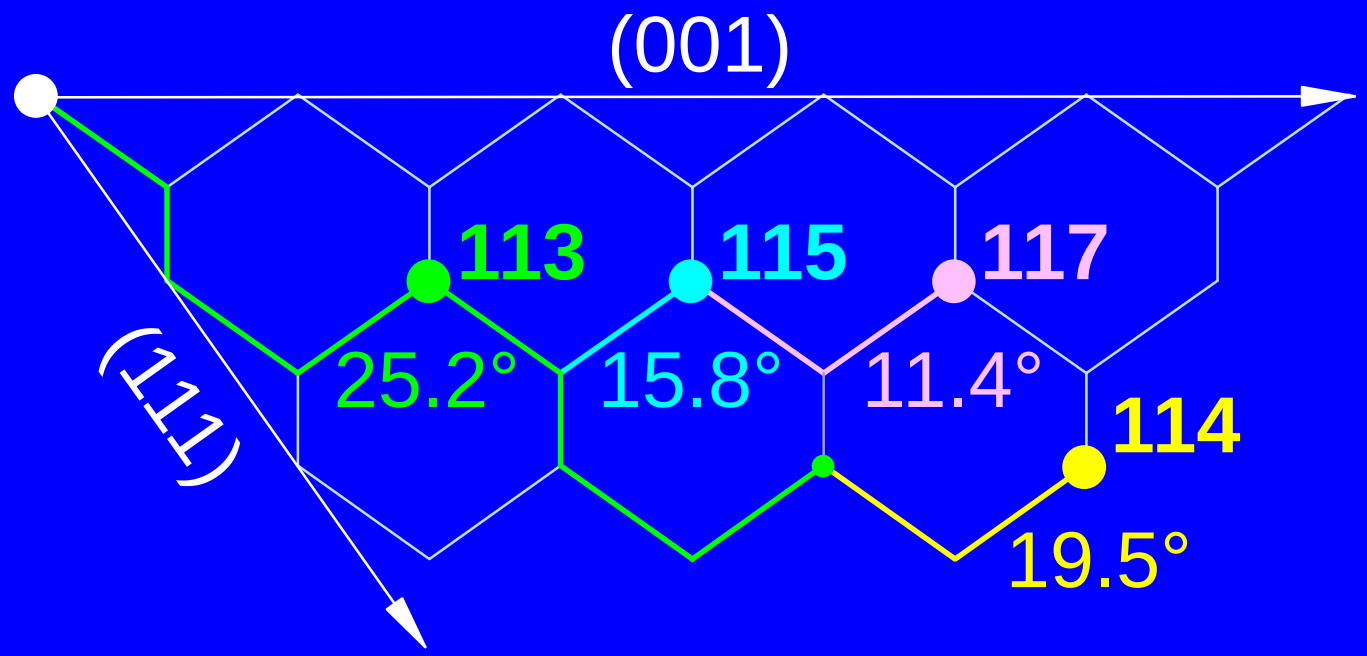
Lattice Orientations Near (001)



113: DL step + 1×(001)

114: DL step + 1×(001) + DL step + 2×(001)

115: DL step + 2×(001)

117: DL step + 3×(001)

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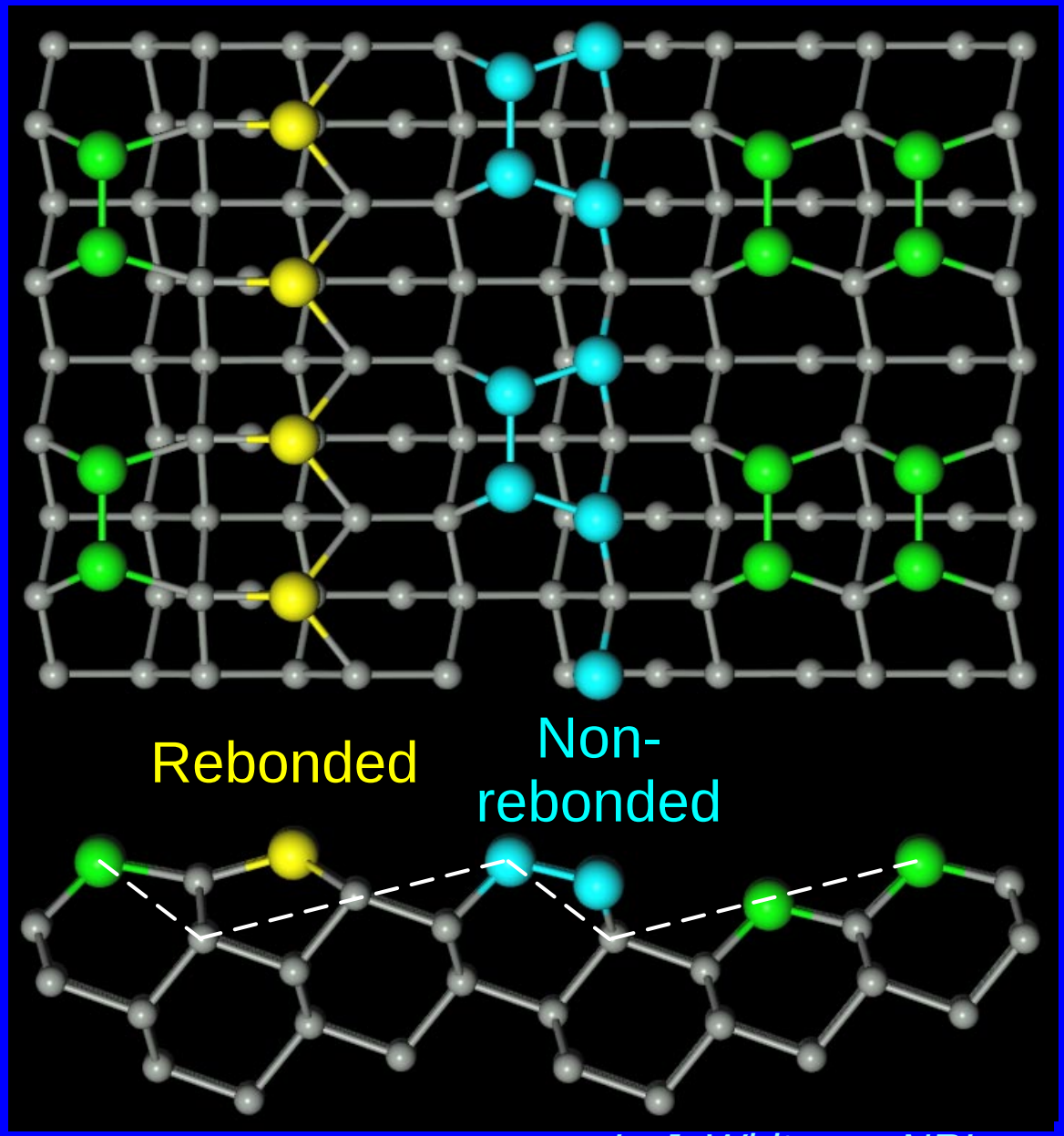
Si(115): Expected Structure



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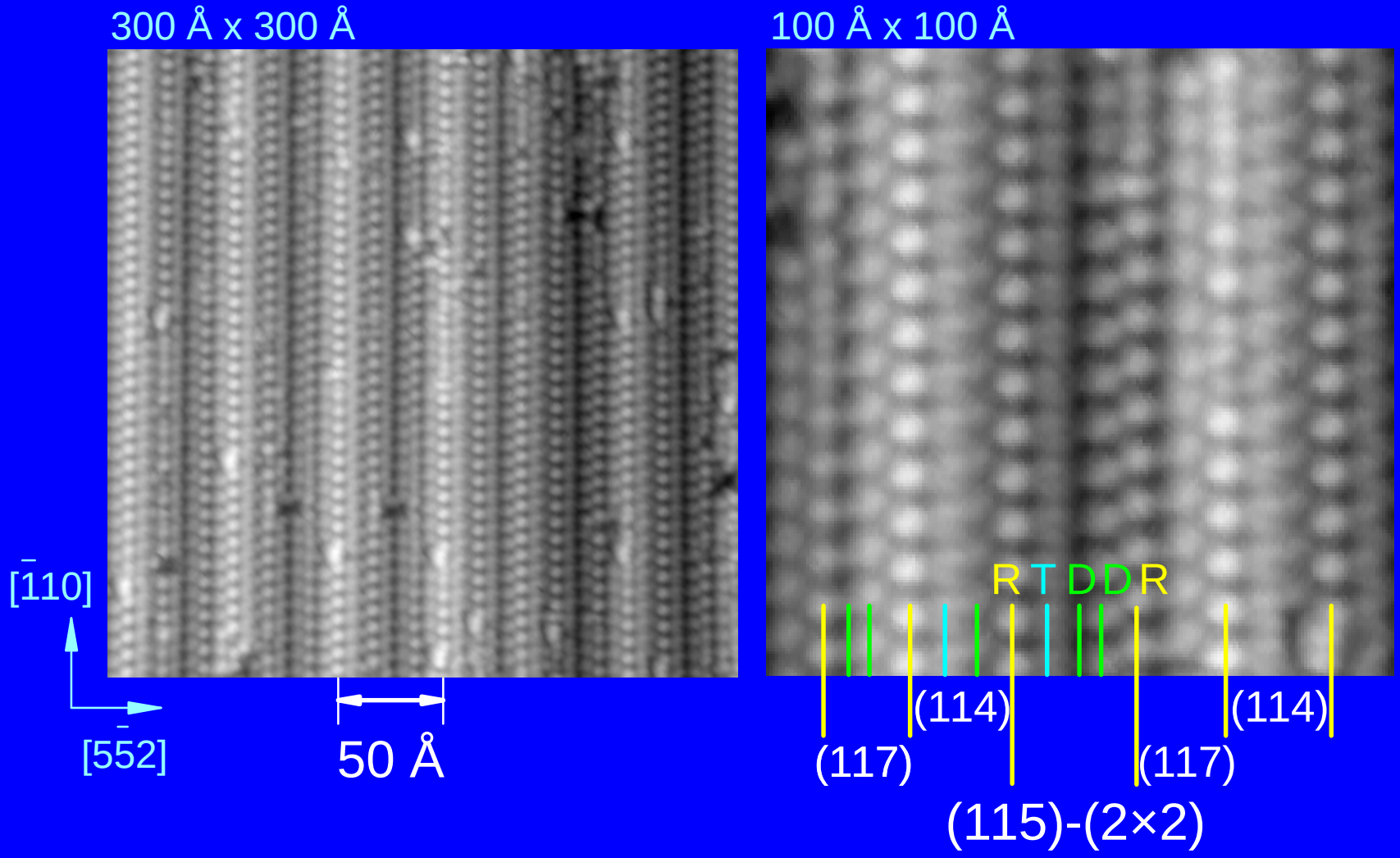
Based on (114), expect (2×2):

rebonded DL step
+
dimer
+
nonrebonded step
+
two dimers

Si(115): Filled-State STM Images



Complex sawtooth structure: (117)+(114)+(115).

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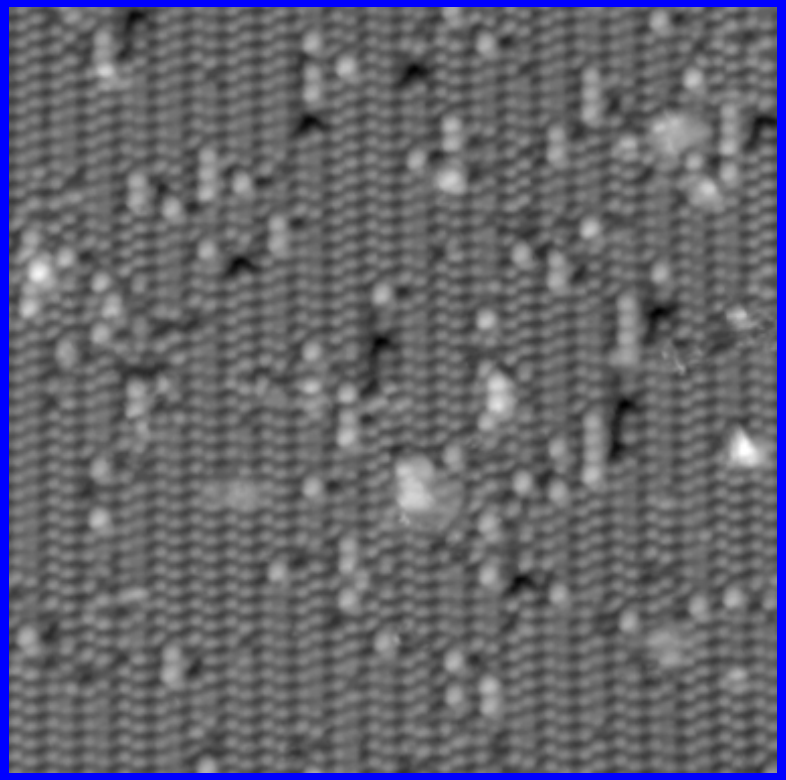
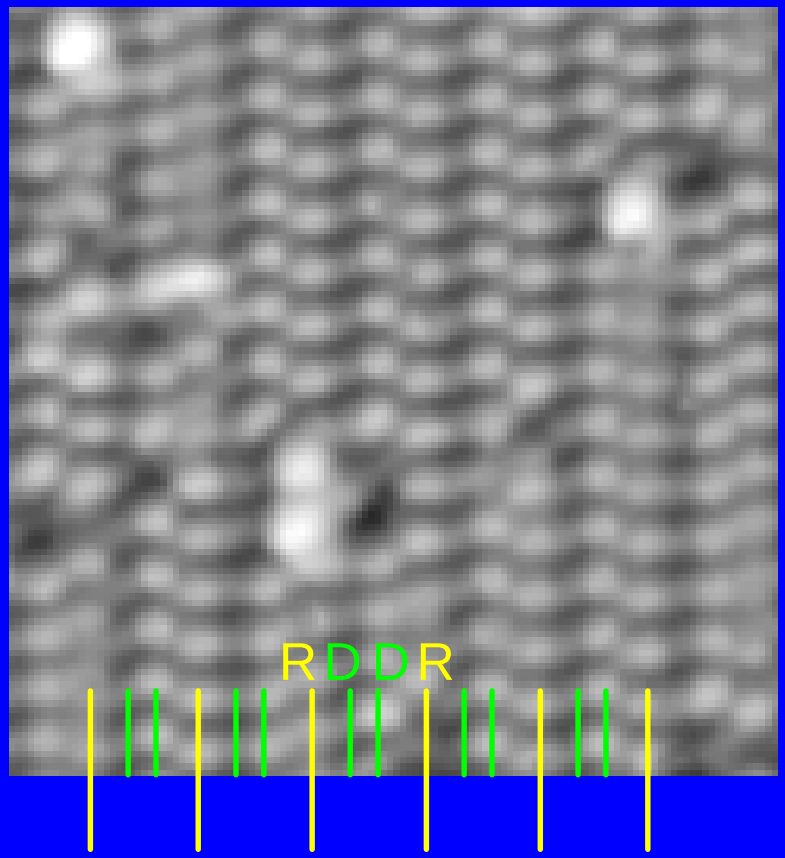
Si(117): θ = 11.4°

300 Å x 300 Å



100 Å x 100 Å



(117)-(2×1)

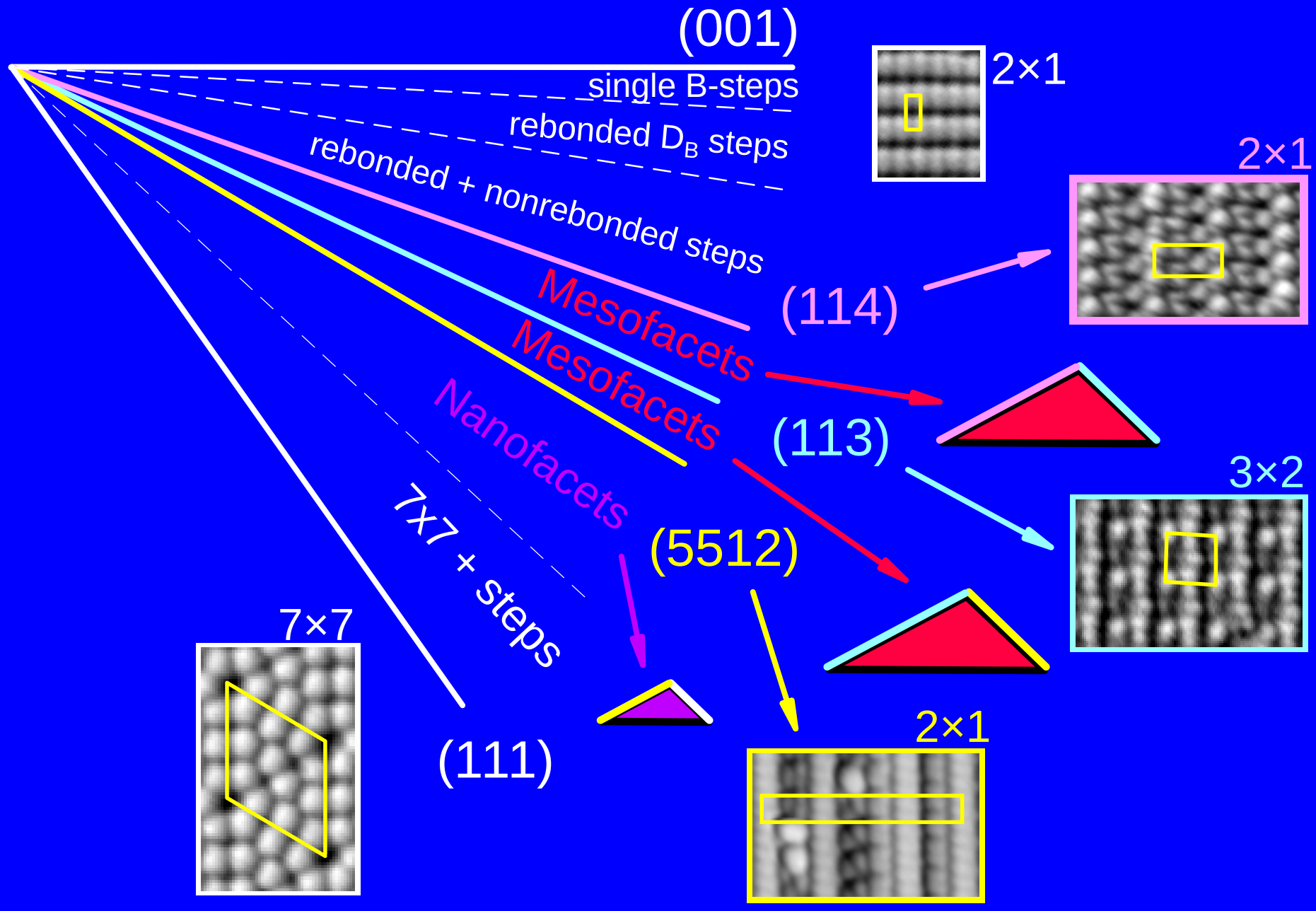
[$\bar{1}$10]

[$\bar{7}\bar{7}$2]

"Ideal" vicinal (001) structure: periodic rebonded DL steps + dimers.

L. J. Whitman, NRL

Si(001)-to-(111) Surface Structure



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The Atomic-Scale Structure and Stability of High-Index Si Surfaces

- New stable surfaces of Si: (5 5 12) and (114)
  - Basic building blocks that reduce dbs but balance stress
- Between stable planes, sawtooth-like structures
  - Alternating stable planes for lower surface energy

Structure/stability easily altered - Ge different!

Possible applications:

- High-index Si as substrates for heteroepitaxy
- Tailored self-assembled nanostructures?

L. J. Whitman, NRL


Visit "Planet Silicon" at:
http://stm2.nrl.navy.mil/~lwhitman