The Structure of Semiconductor Surfaces and Interfaces

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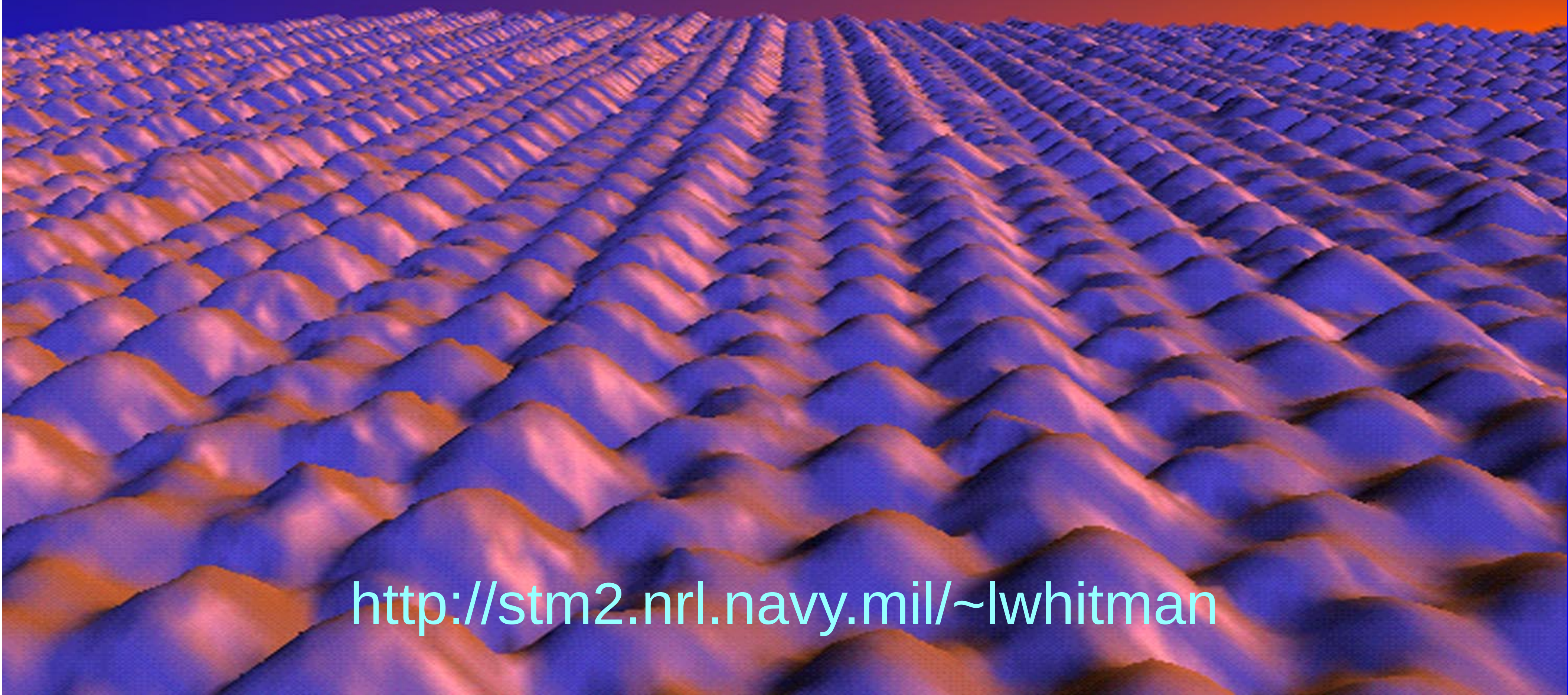

http://stm2.nrl.navy.mil/~lwhitman

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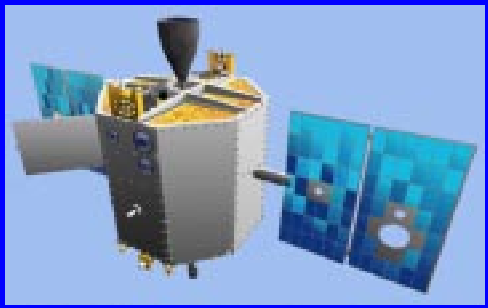
Why Study Semiconductor Surfaces?

We are studying surfaces and films important to the development of a variety of *advanced military electronics*, including:

- *Infra-red night vision sensors* fabricated on a single silicon chip



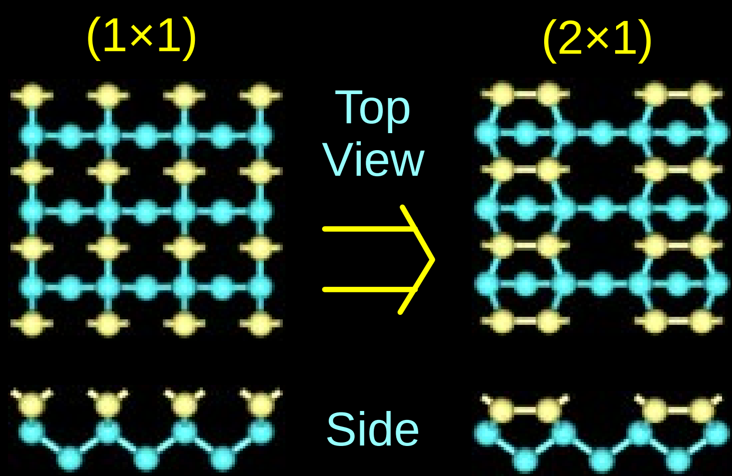
- Radiation-hard *solar cells for satellite* power
- Tunable *infra-red detectors* and infra-red *lasers*

- *High-frequency electronics* (1000 GHz) with ultra-low power consumption

We are working towards a fundamental, predictive understanding of the structure of semiconductor surfaces.

What is Interesting About Surfaces?

When a crystal is broken to create a surface, the exposed atoms have fewer neighbors than usual, leaving them with "dangling bonds." The surface atoms usually rebond to each other to reduce the number of dangling bonds, resulting in arrangements of atoms on the surface that are different than inside the crystal. This process is called *surface reconstruction*.



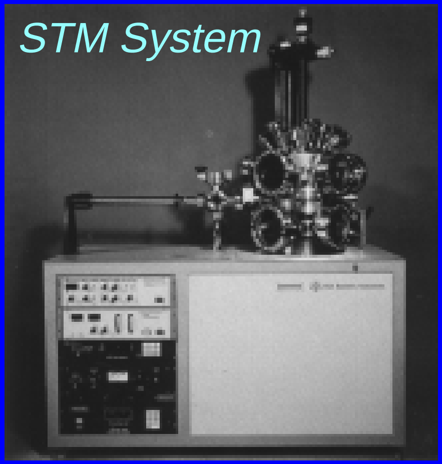
Example: Si(001)

The most studied surface of silicon is the "low index" (001) facet – the substrate for almost all electronic devices. On this surface the atoms pair up into rows of dimers. Because this pairing doubles the size of the periodic structural unit on the surface, it is denoted a "(2×1)" reconstruction.

We are trying to *discover how and why different semiconductor crystal surfaces reconstruct*, including surfaces of silicon (Si), germanium (Ge), and III-V compound semiconductors such as gallium antimonide (GaSb) and indium arsenide (InAs).

How Do We Study Surfaces?

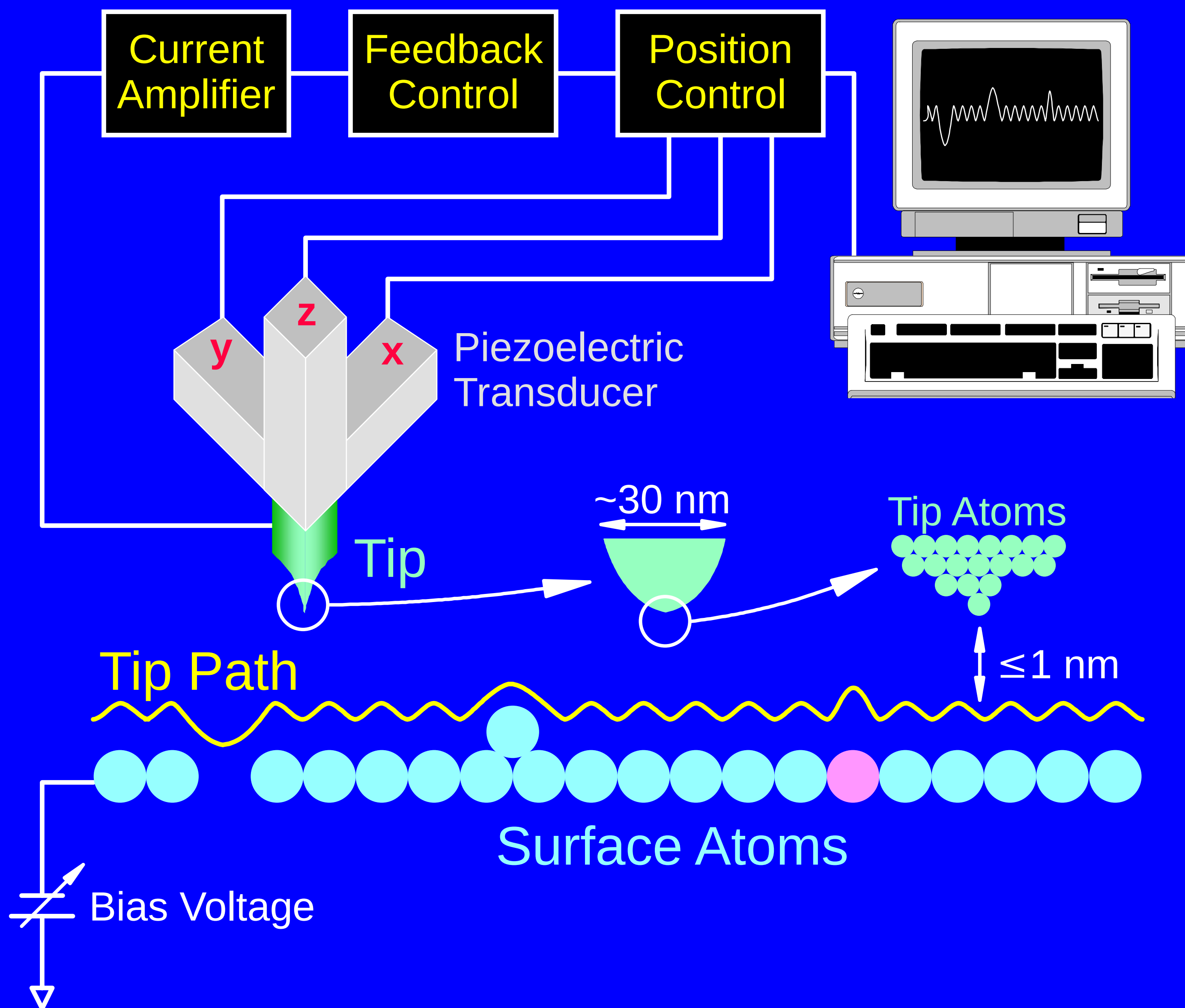
We use a complementary combination of experimental measurements and theoretical calculations.



Experiments are performed on pristine surfaces prepared in an ultra-high vacuum chamber (where the absence of air keeps the surfaces clean). We use a *scanning tunneling microscope (STM)* to acquire images of the surface with atomic-scale resolution (~0.01 nm), allowing a magnification of about one billion times – enough to *see the individual surface atoms!*

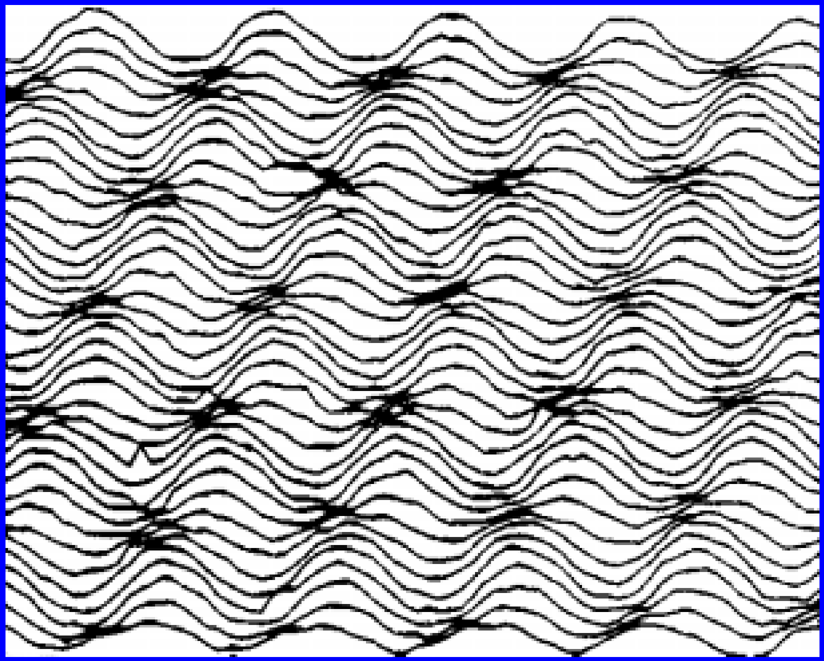
Starting with possible models derived from the STM images, calculations are then performed to find the correct surface structure. The *calculations are done on DoD supercomputers using state-of-the-art computational methods* based on quantum mechanics. The theoretical results also help us understand the basic physics causing the surface reconstruction.

Scanning Tunneling Microscopy

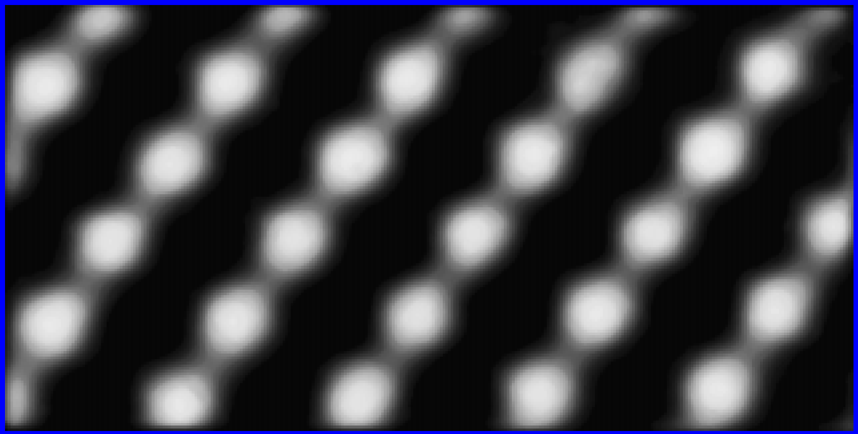


STM Image Presentation

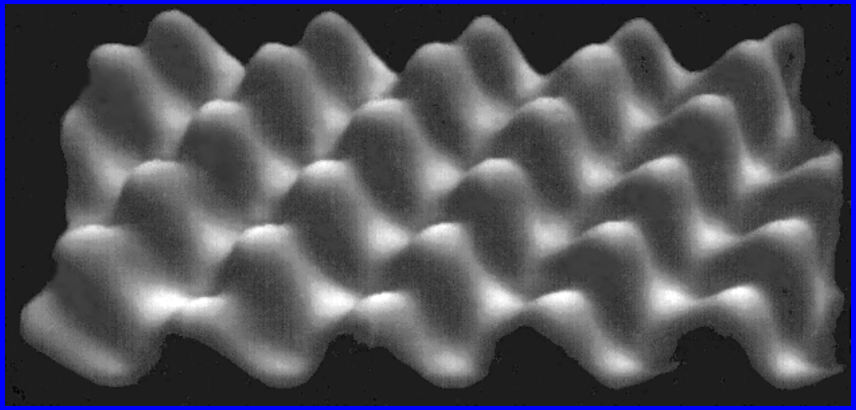
Line Scans (Raw Data)



Gray Scale



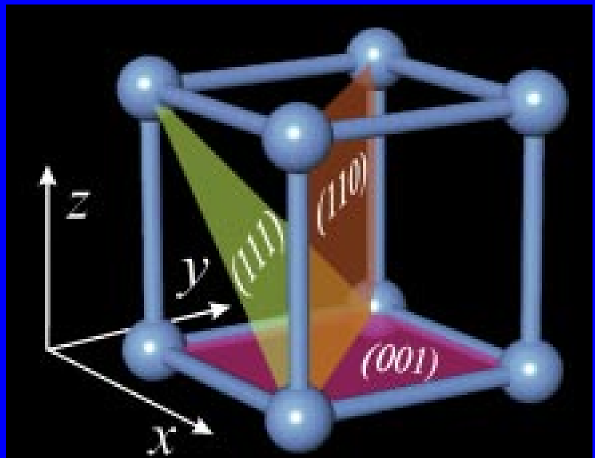
3-D Rendered



Example #1: High-Index Si Surfaces

Every different slice through a crystal exposes a *different facet*, described by a set of indices, ($h\ k\ l$). Each facet has a distinct periodic arrangement of atoms on it's surface, the "unit cell". Most studies of surfaces involve low-index facets with small unit cells and simple structures. We have studied a whole class of more *complex high-index surfaces*.

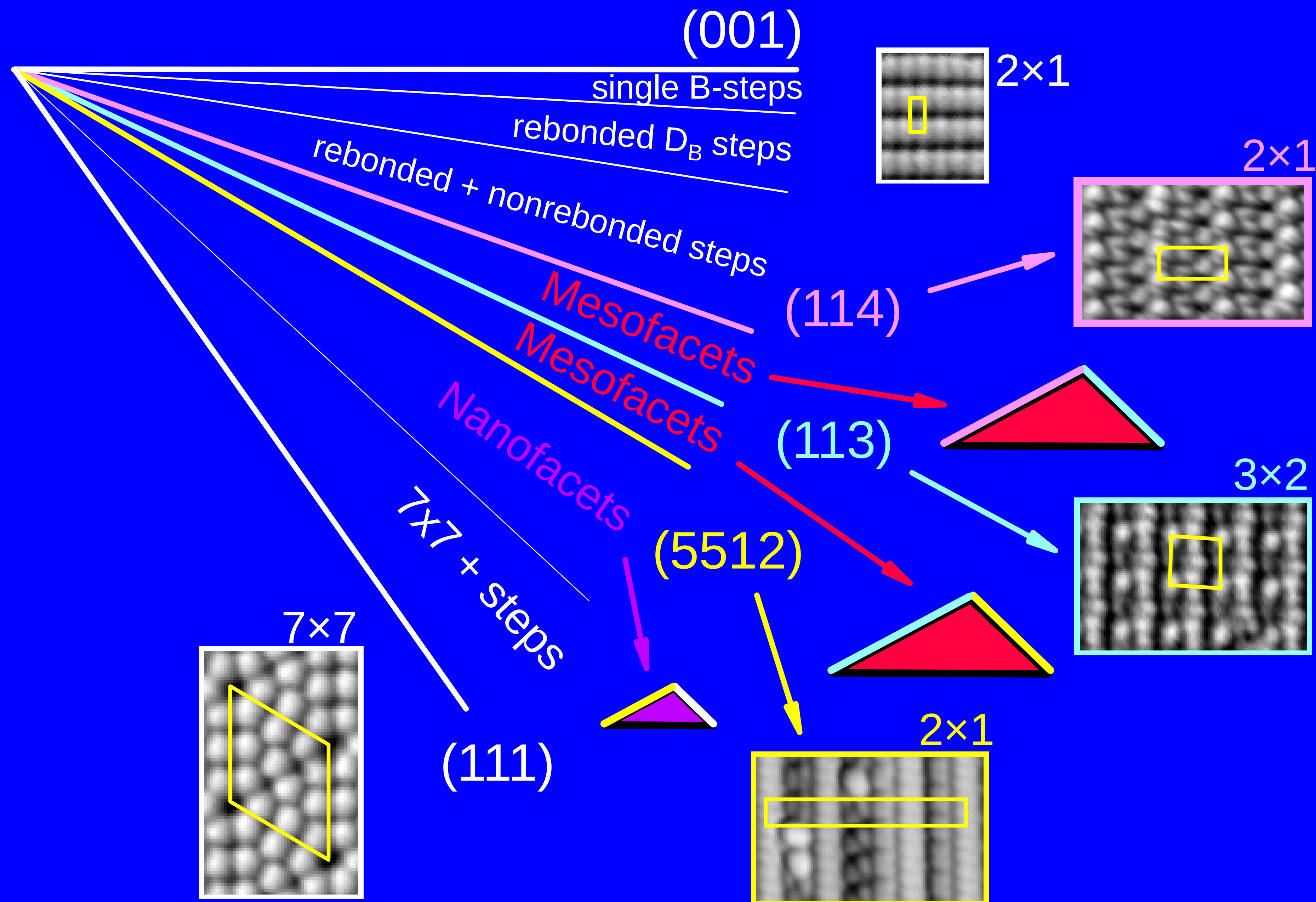
- What are the stable surfaces of silicon between (001) and (111)?
- Are there unknown surfaces that might be good substrates for electronic device fabrication?



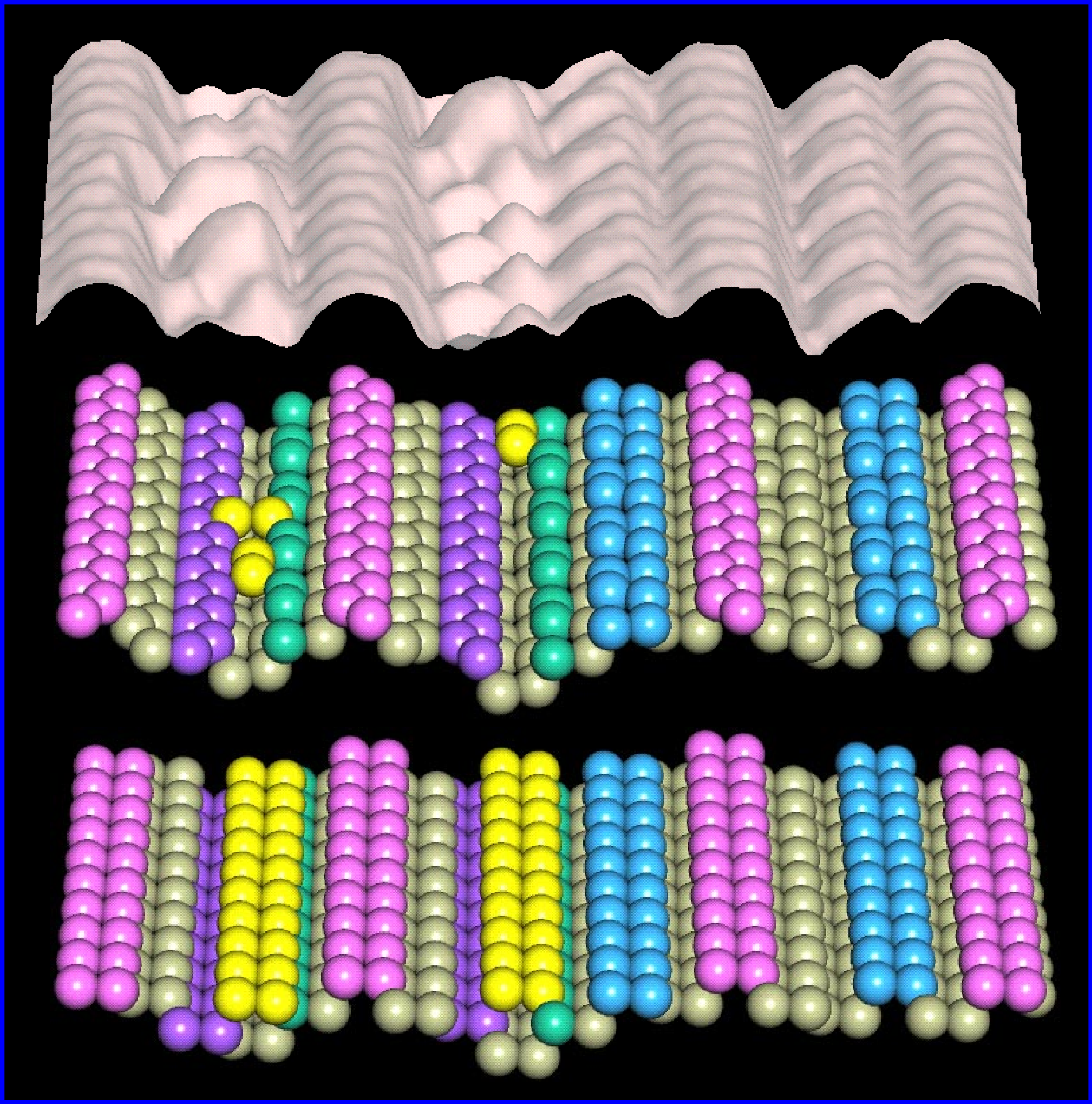
The indices ($h\ k\ l$) describe a vector normal to the surface, $h\hat{\mathbf{x}} + k\hat{\mathbf{y}} + l\hat{\mathbf{z}}$.

We have determined all the structures from (001) to (111), and discovered two new surfaces, Si(114) and Si(5 5 12).

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



Si(5 5 12)-2×1 Reconstruction

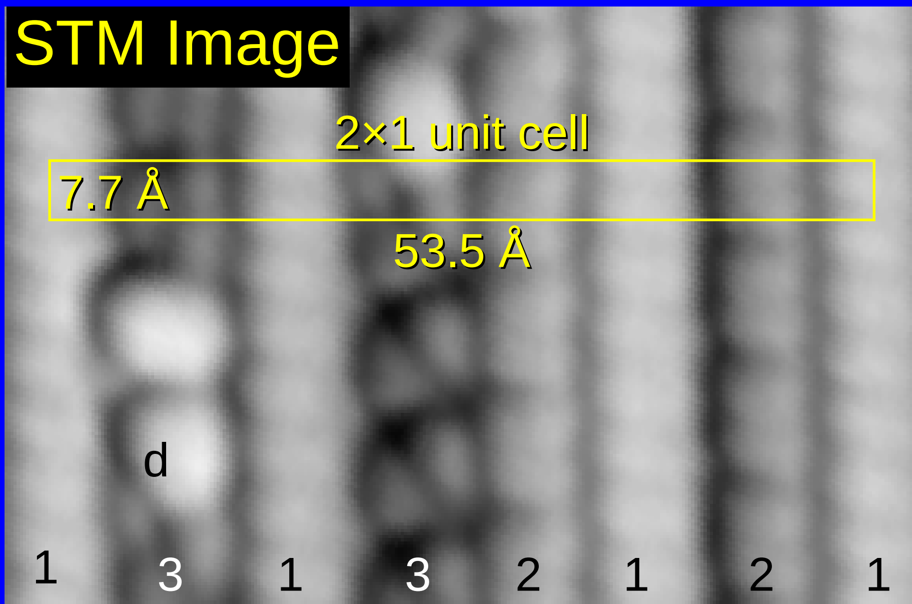


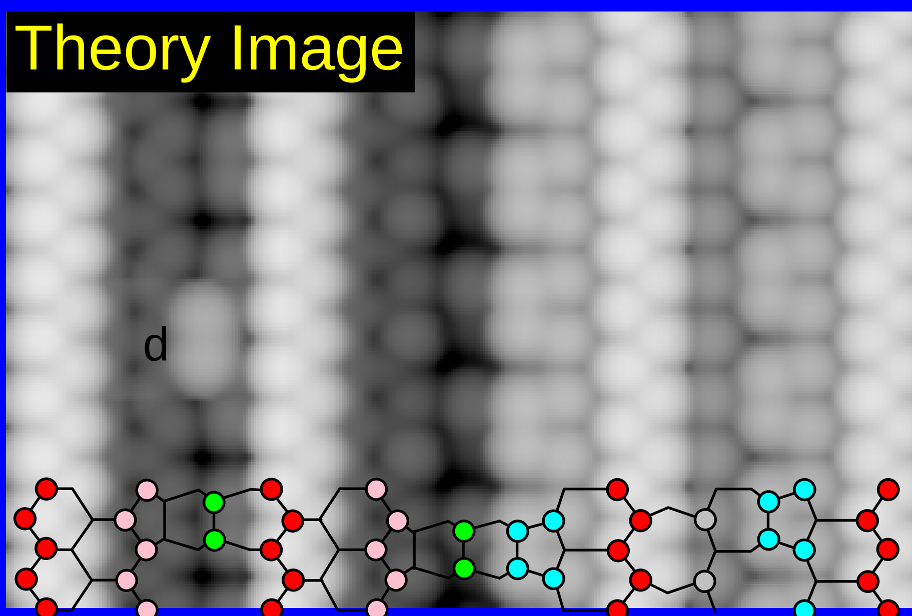
STM Image

Reconstructed Model

Bulk-Terminated Model

Si(5 5 12): Experiment and Theory





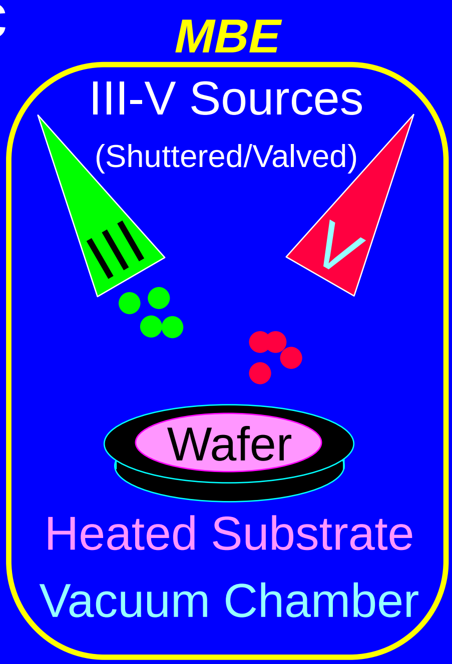
- *One of the largest unit cells* ever observed and modeled theoretically: 7.7 Å x 53.5 Å (68 atoms / unit cell).

- *Consists of simple building blocks* – π-bonded chains, dimers, and tetramers – stabilized by a delicate balance between dangling bond reduction and stress relief.

*Baski, Erwin, and Whitman, Science **269**, 1556 (1995)*

Example #2: III-V Semiconducter Surfaces

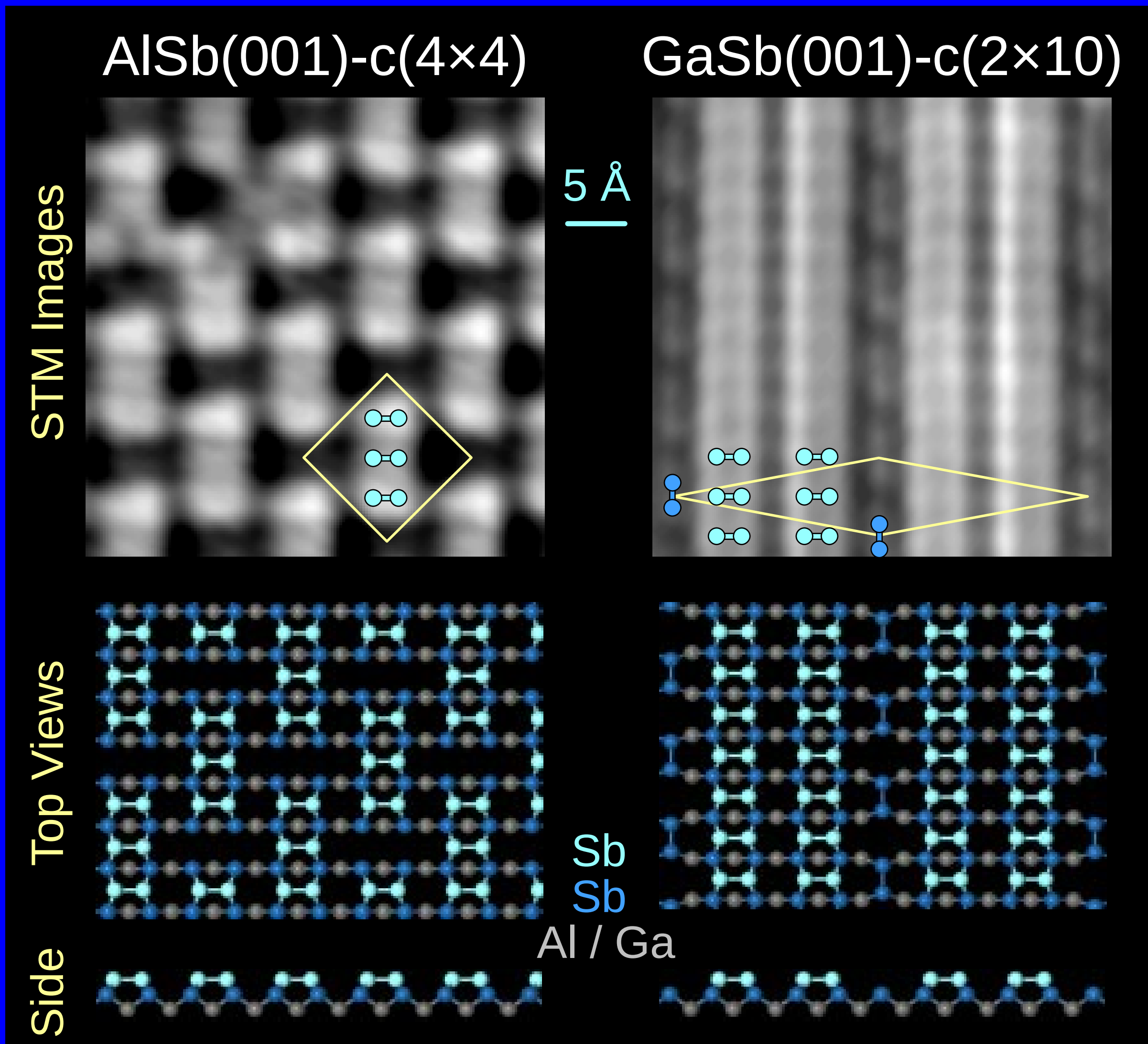
There is an extensive effort within the DoD to develop new high-frequency and optoelectronic devices using the *compound semiconductors InAs, GaSb, and AlSb*. The devices are made by *molecular beam epitaxy (MBE)* using thin alternating layers of the different semiconductors (layers only a few atomic planes thick). Because the surface of one layer becomes the interface to the next, *the surfaces are important to the final device performance*.



- What are the surfaces produced by MBE?
- How do the surface structures affect the device structures?

We have found a variety of novel structures on AlSb(001) and GaSb(001), including the first metallic (001) surfaces.

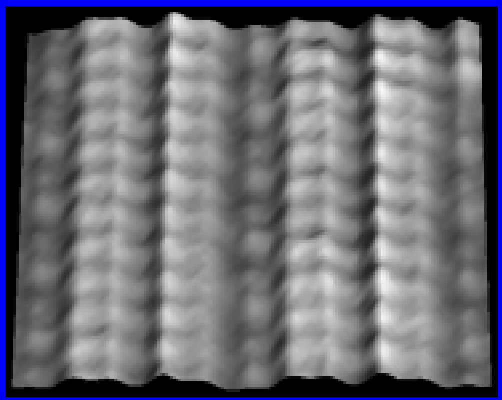
AlSb and GaSb (001) Sb-Rich Surface Reconstructions



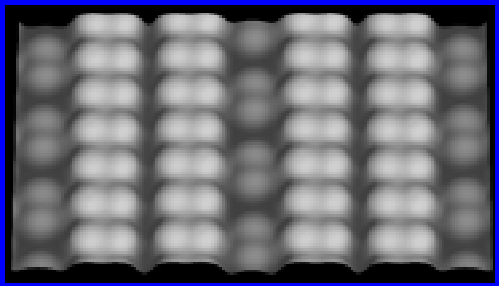
- Atomic *structures determined for the first time*.
- AlSb, GaSb have *similar lattices, but different surfaces*.
- AlSb is like all other III-V surfaces, *GaSb is different*.
- Novel GaSb surface should be metallic.

GaSb(001)-c(2×10): Theory and Spectroscopy

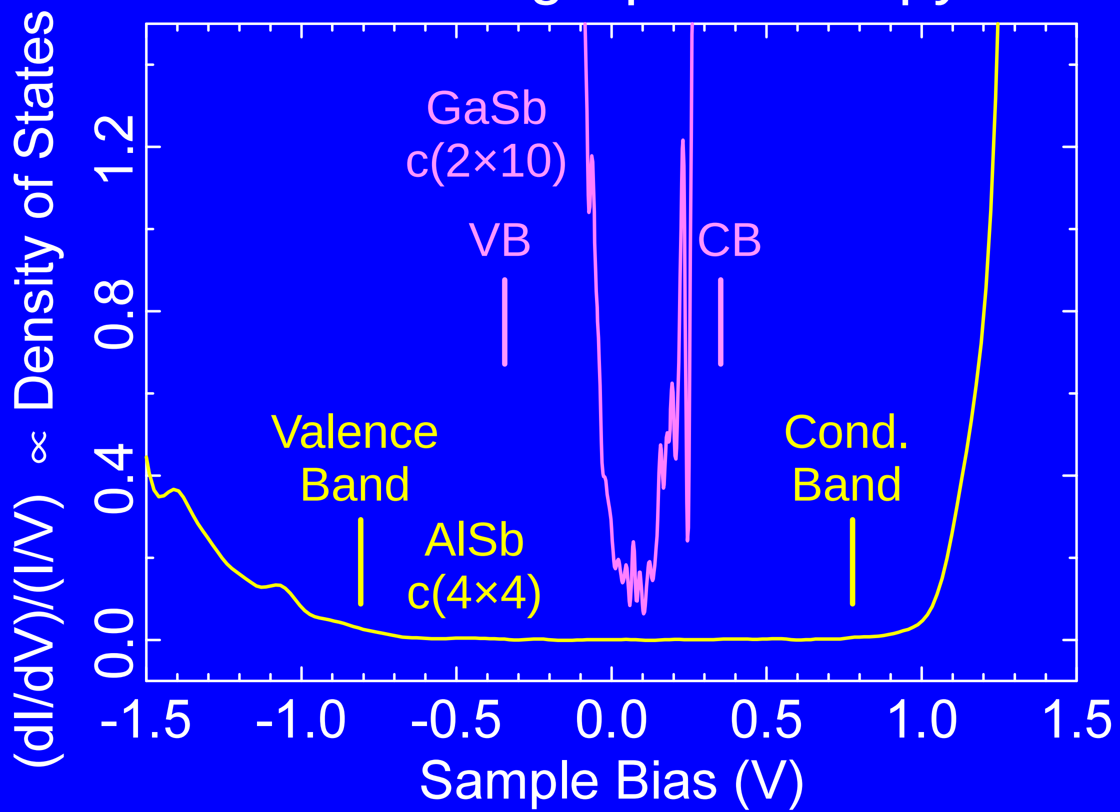
STM Image



Theoretical image



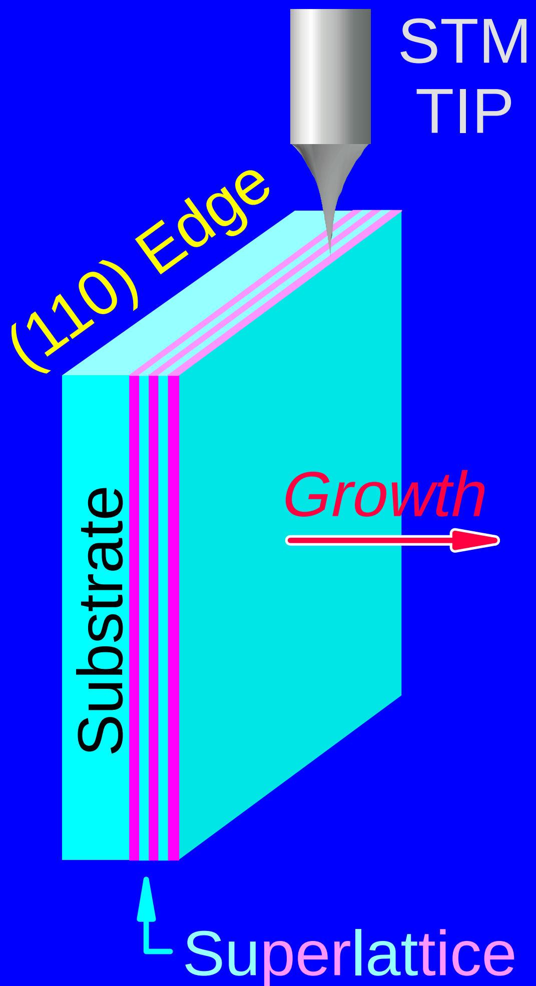
Tunneling Spectroscopy



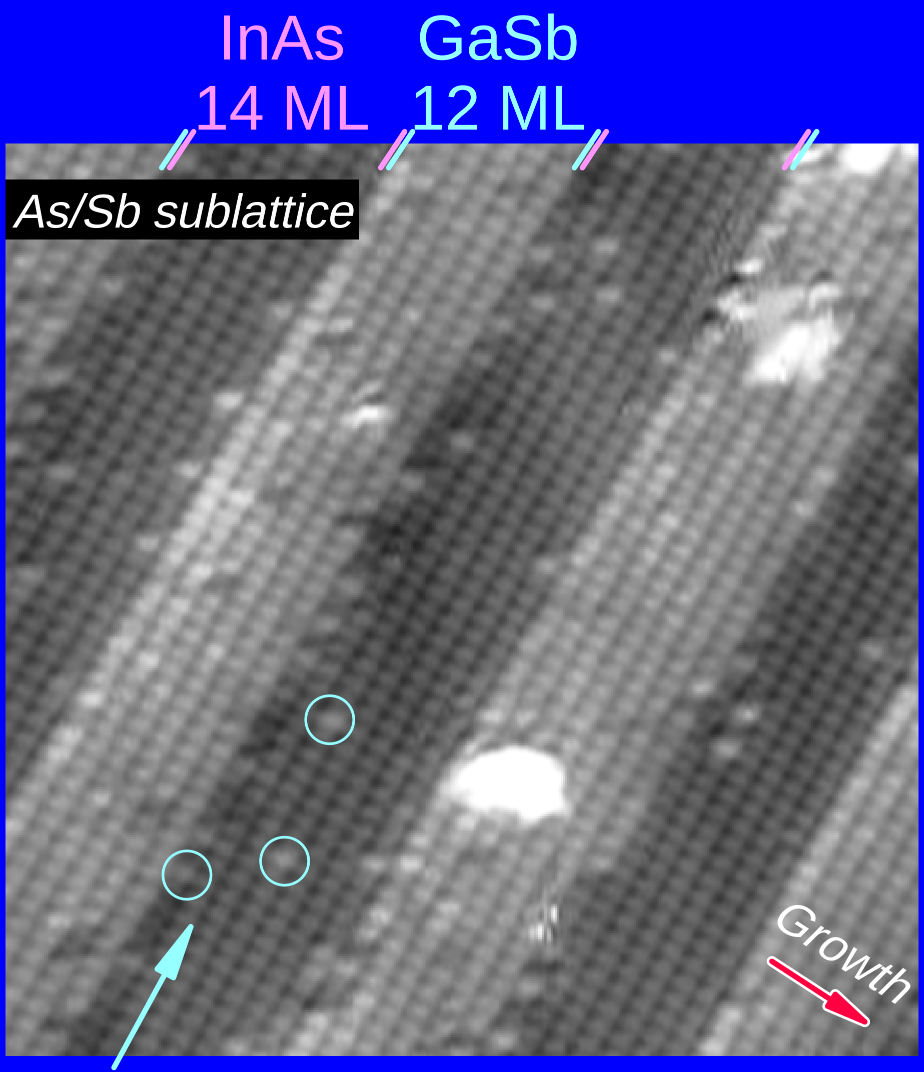
- Theory and experiment confirm *first metallic clean III-V surface*.
- Previously accepted "electron counting rule" violated.

Whitman, Thibado, Erwin, Bennett, and Shanabrook,
Phys. Rev. Lett. ***79****, 693 (1997)*

Cross-Sectional STM of GaSb/InAs Infra-red Detector



X-STM images **alternate** layers.



Excess Sb atoms in InAs from double-layer surface reconstruction

What Next?

Technology Transitions:

- High-index Si as substrates for:
  - HgCdTe sensors (with the Army Night Vision Lab, Fort Belvoir)
  - SiGe electronics (with NRL Electronics Science & Technology Div.)
- Ge solar-cell substrate optimization (with Eagle-Picher)
- III-V MBE device optimization
  - High-frequency diodes (~1000 GHz RTD's; with HRL, ONR/DARPA)
  - Infra-red lasers (with the Air Force Research Laboratory)

Further Basic Research:

- Chemical properties of high-index Si surfaces
  - Relevant to use as electronic device substrates
- Structure of high-index Ge surfaces
  - Important for satellite solar cell applications