

# The Structure and Electronic Properties of AlSb and GaSb (001) Surfaces\*

**L. J. Whitman**

P. M. Thibado,<sup>1</sup> S. C. Erwin,  
M. B. Weimer,<sup>2</sup> B. R. Bennett,  
and B. V. Shanabrook



*Naval Research Laboratory*  
*Washington, DC 20375*  
*USA*



- 1. Present address: Dept. of Physics, U. of Arkansas*
- 2. Permanent address: Dept. of Physics, Texas A&M U.*

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# InAs, GaSb, AlSb: "6.1 Å" Family of III-V's

- For high-speed and optoelectronic devices
  - Resonant tunneling diodes, IR detectors, IR lasers
- Interfaces critical in short-period superlattices, quantum-well structures
  - Make up large volume fraction of device
- Structure of growth surface critical
  - III/V  $\neq$  1 can lead to intermixing at interface
  - Growth morphology may depend on reconstruction

*To achieve atomic-level control of interfaces, must understand (001) surface reconstructions.*

# The Electron Counting Model for III-V Surface Structure

- Starting point for understanding III-V surface structure is *Electron Counting Model* (ECM)
  - Reconstruct so all III-dangling bonds (db's) empty, V-db's filled
- Commonly applied to III-V(001) surfaces
  - Works for III-As and III-P (001)-(2m×2n)
- Not discussed w.r.t. III-Sb(001) surfaces (??)
  - "Odd" reconstructions reported, e.g. (1×3)

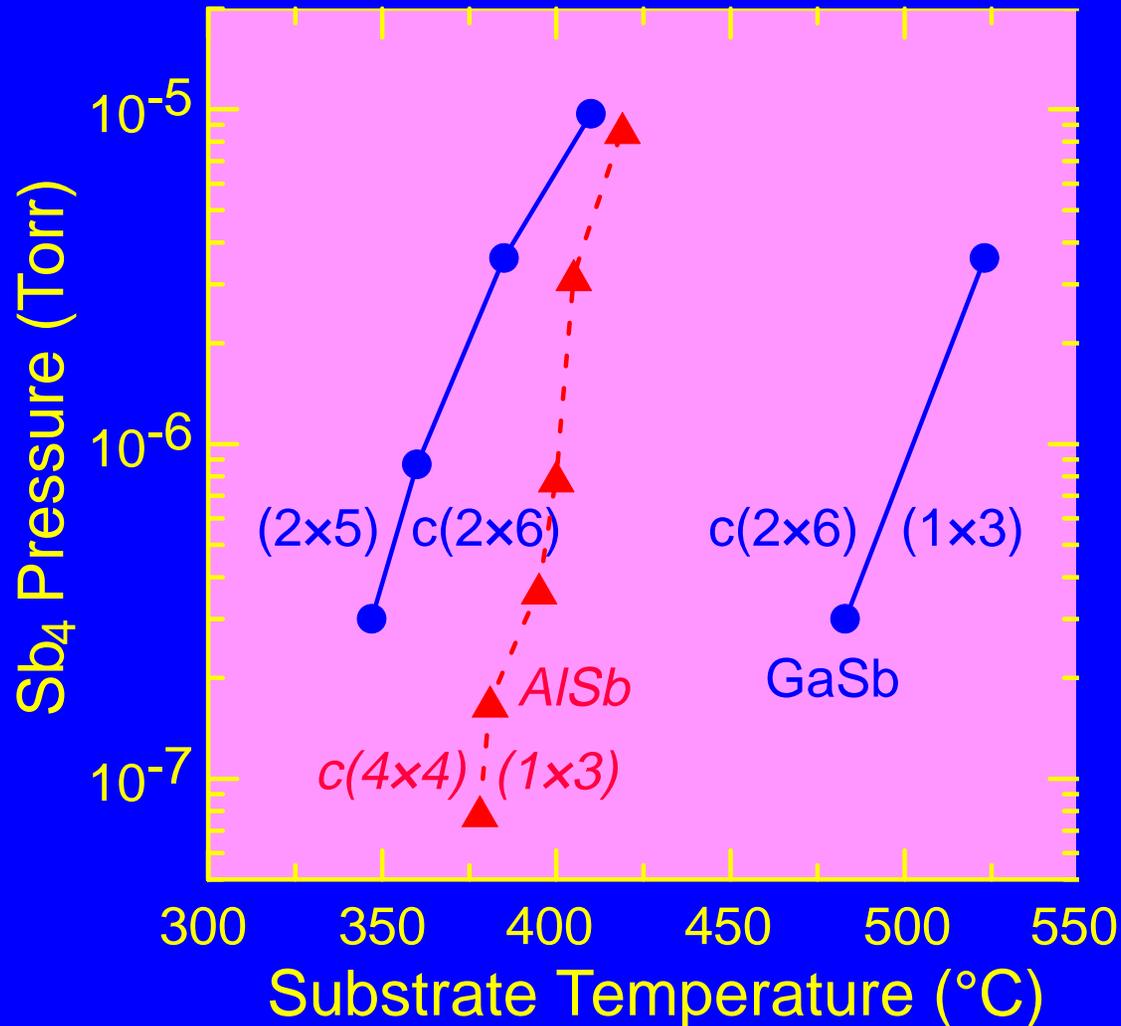
# Focus on AlSb and GaSb (001) Surfaces

- AlSb and GaSb almost lattice matched (AlSb 0.7% larger)
  - Highlight role of material properties vs. lattice constant
- Focus on device-growth conditions: ***Sb-rich***
- AlSb(001): only (1×3), c(2×6) RHEED reports
- GaSb: (1×3), c(2×6), (1×5), (2×5) by RHEED
  - STM of (1×3) only: (n×5) STRUCTURE?

*Do "odd" structures violate ECM?*

*Prepare by MBE, study w/ in-situ RHEED and STM.*

# RHEED Structure Diagram



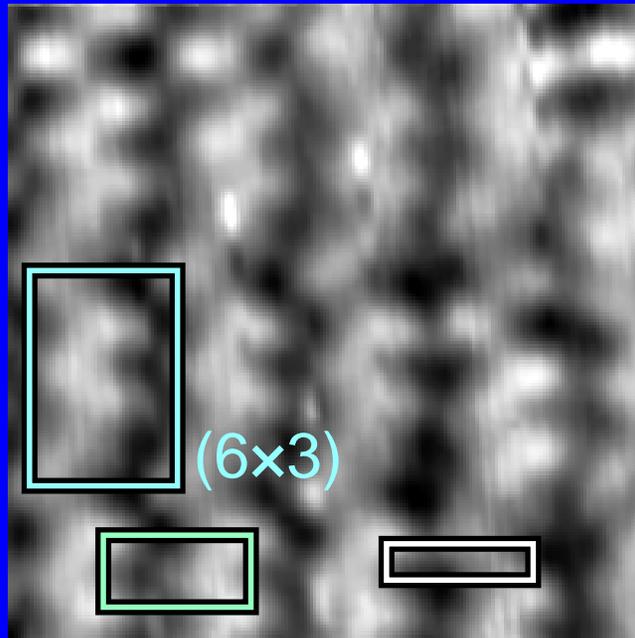
- GaSb: (1×3) - c(2×6) - (2×5): under optimal conditions no (1×5)
- AlSb: (1×3) - c(4×4), no c(2×6) observed
- AlSb(001)-c(4×4) for first time

*What are structures, what makes them different?*

# AlSb(001) Reconstructions: STM

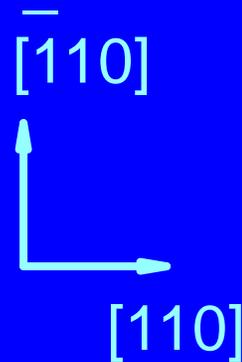
RHEED "(1×3)"

Empty-State Image (3.0 V)



(2×3)

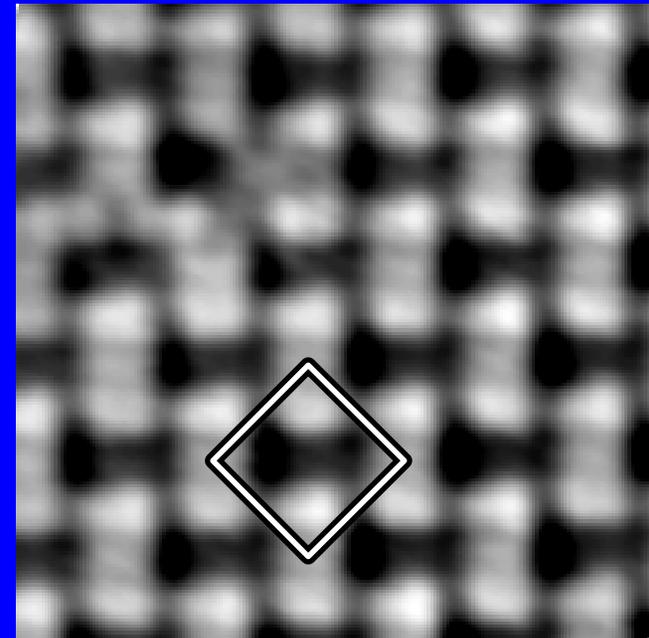
(1×3)?



10 Å

RHEED c(4×4)

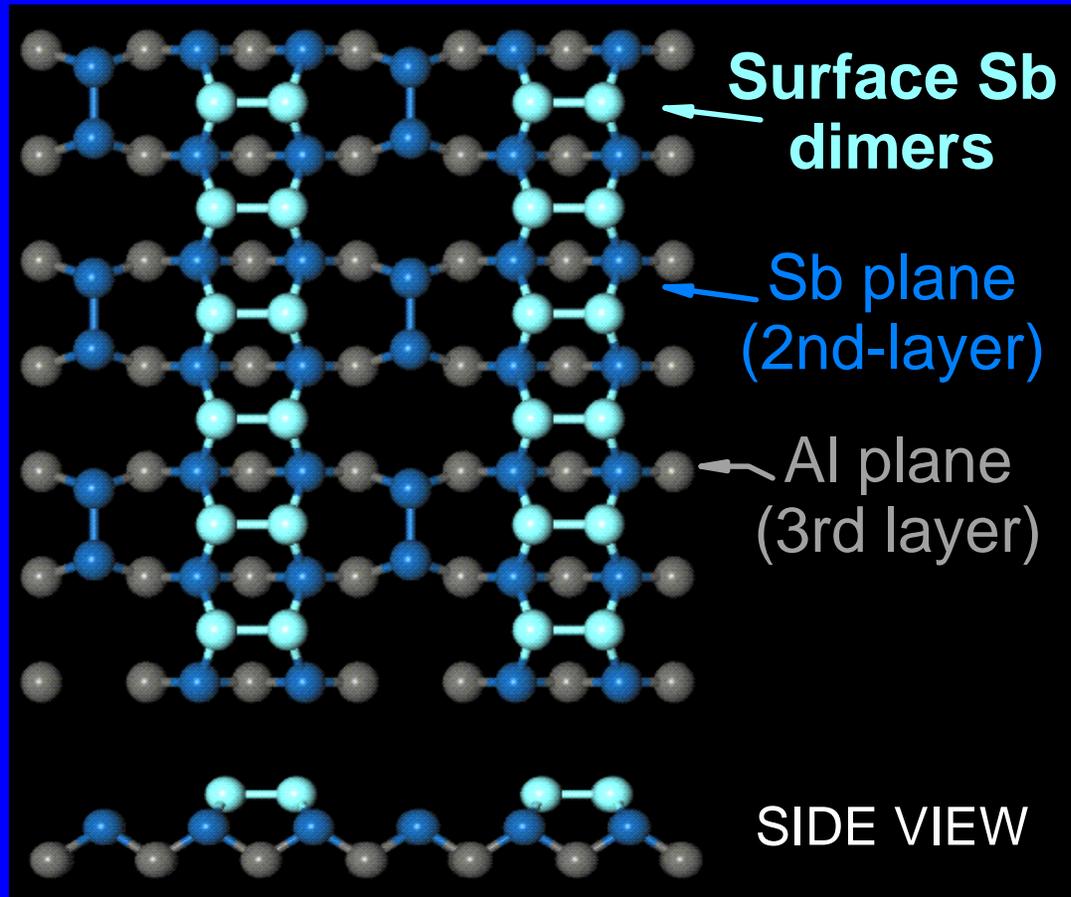
Filled-State Image (3.3 V)



Looks like InSb,  
GaSb(001)-(1×3):  
*Complicated structure(??)*

Like all other III-V's  
(except GaSb):  
*Simple dimer-row structure*

# AlSb(001)-"(1×3)" Model: 1.66 ML Sb

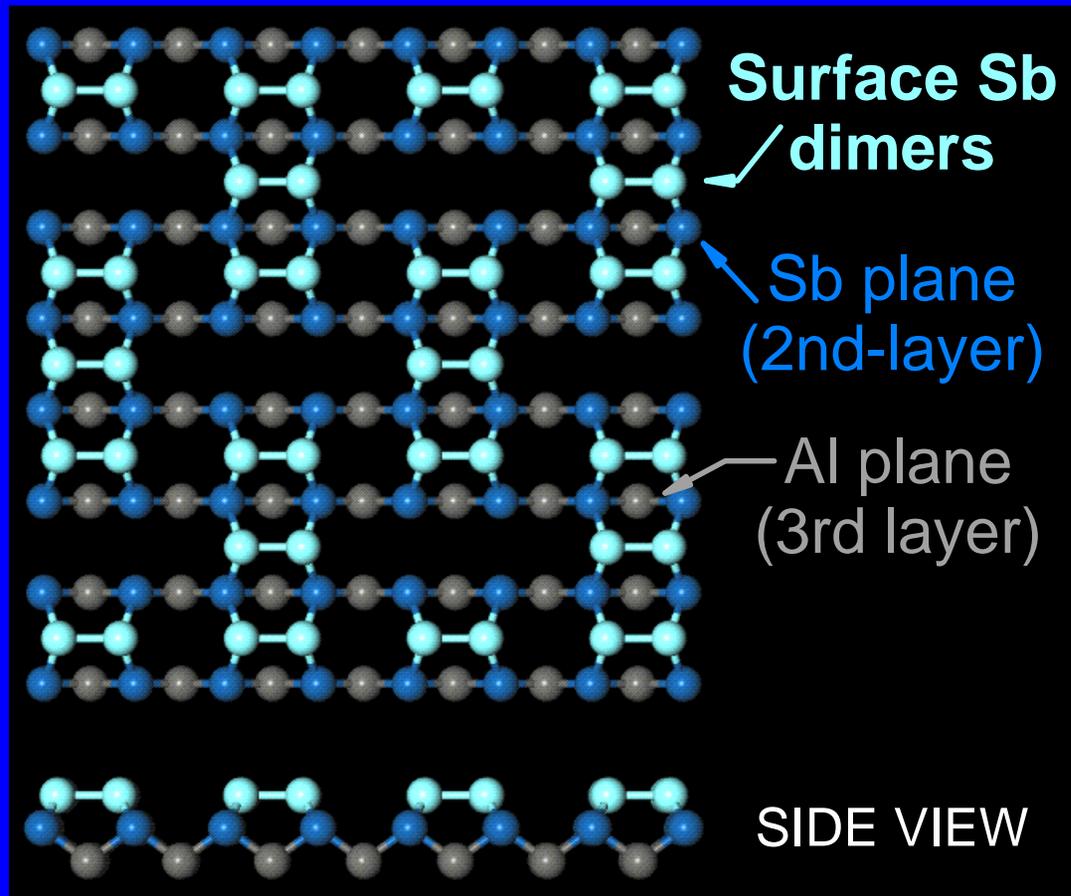


- Similar to model proposed for InSb and GaSb
- (2×3) as shown, could be c(2×6)
- Actual structure more complex: dimer buckling and/or kinking?

- 1 extra electron/(2×3)

***Violates electron counting model!***

# AlSb(001)-c(4x4) Model: 1.75 ML Sb

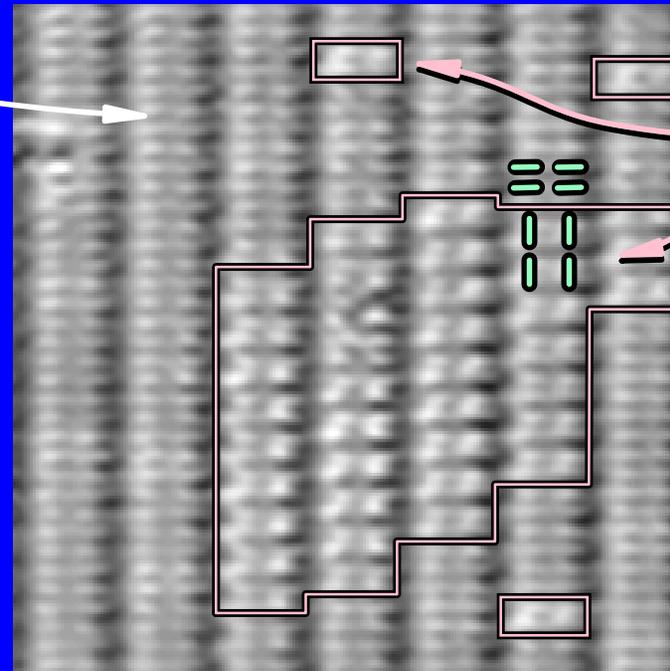


- Valence e's/unit cell = 2 x bonds
- No half-filled db's
- All Sb db's filled, (no Ga db's)
- Expect insulating surface

*Follows Electron Counting Model, like previous III-V(001) surfaces.*

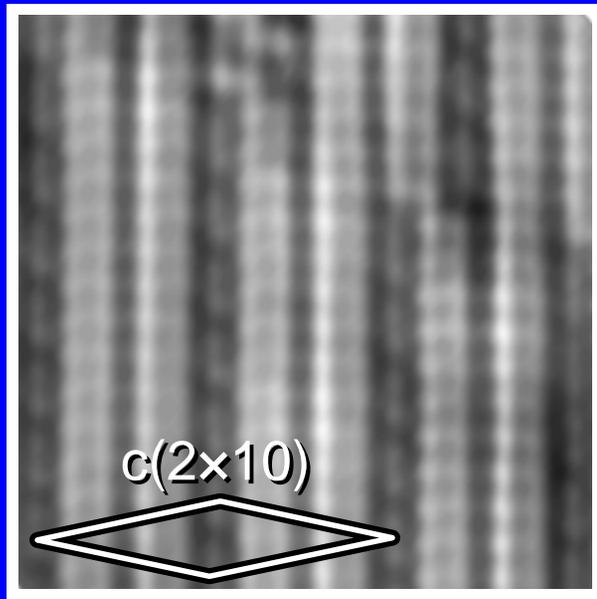
# GaSb(001)-"(2x5)" Reconstructions: STM

Two ( $n \times 5$ )-like structures  
(atypical mixed-phase shown)



At lower temp.'s,  
observe different  
( $2 \times 10$ ) phase:  
*features rotate,*  
*are  $\sim 1 \text{ \AA}$  higher*  
*than on  $c(2 \times 10)$*

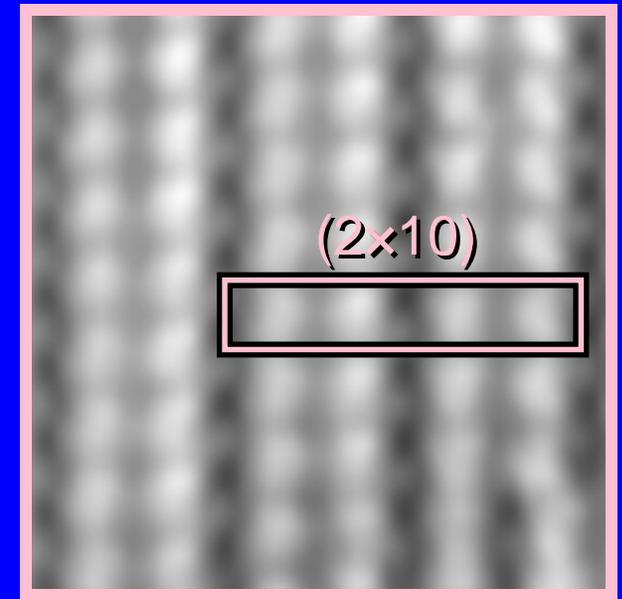
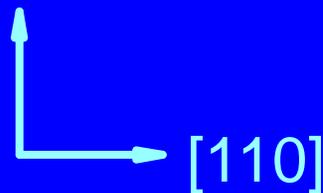
On high temp. side  
of "( $2 \times 5$ )" range, see  
 $c(2 \times 10)$  structure



65 Å: Filled States (1.8 V)

150 Å: Filled States (2.4 V)

$[\bar{1}10]$

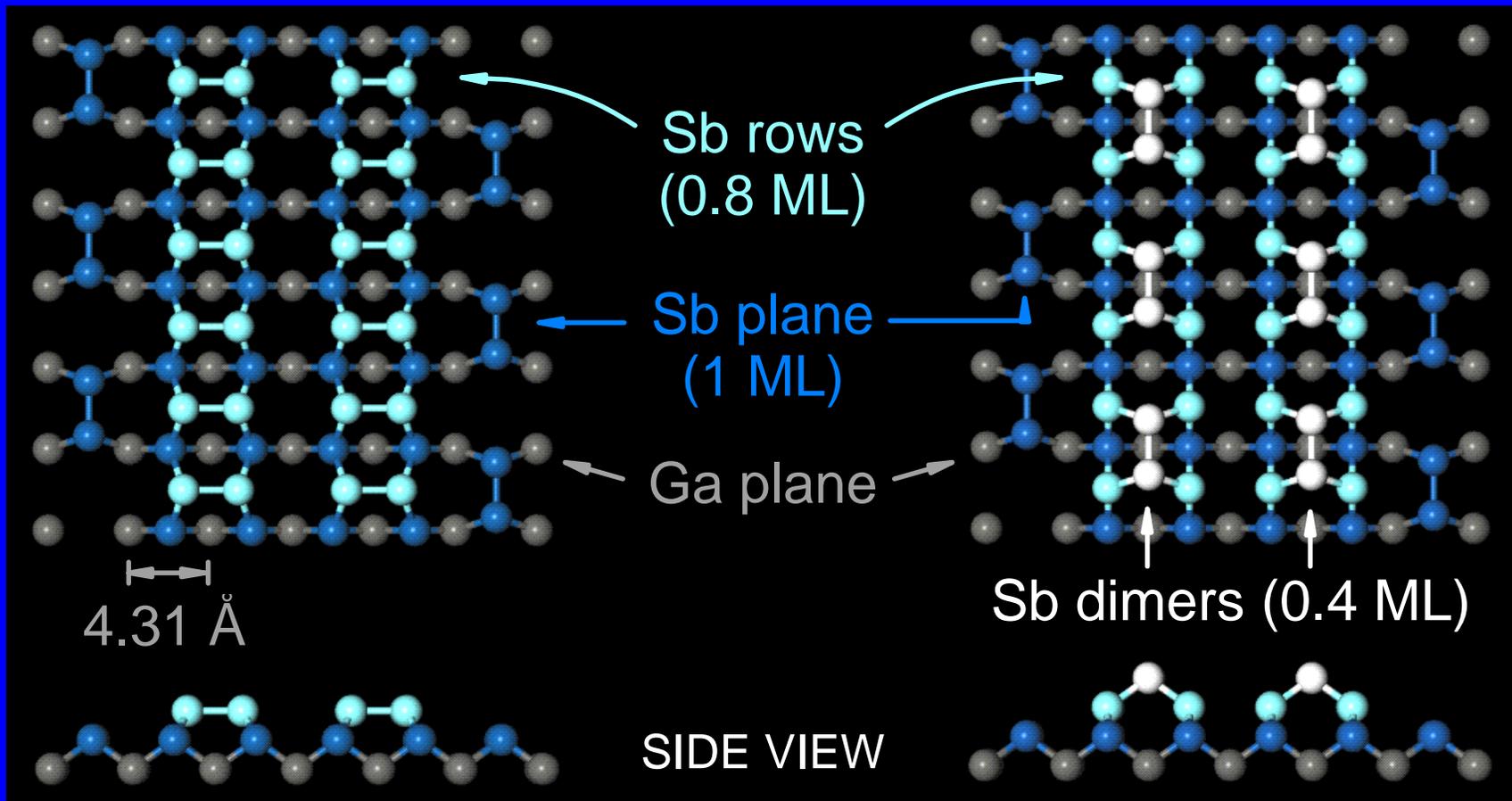


65 Å: Filled States (0.4 V)

# GaSb(001)-"(2x5)" Models

c(2x10): 1.8 ML Sb

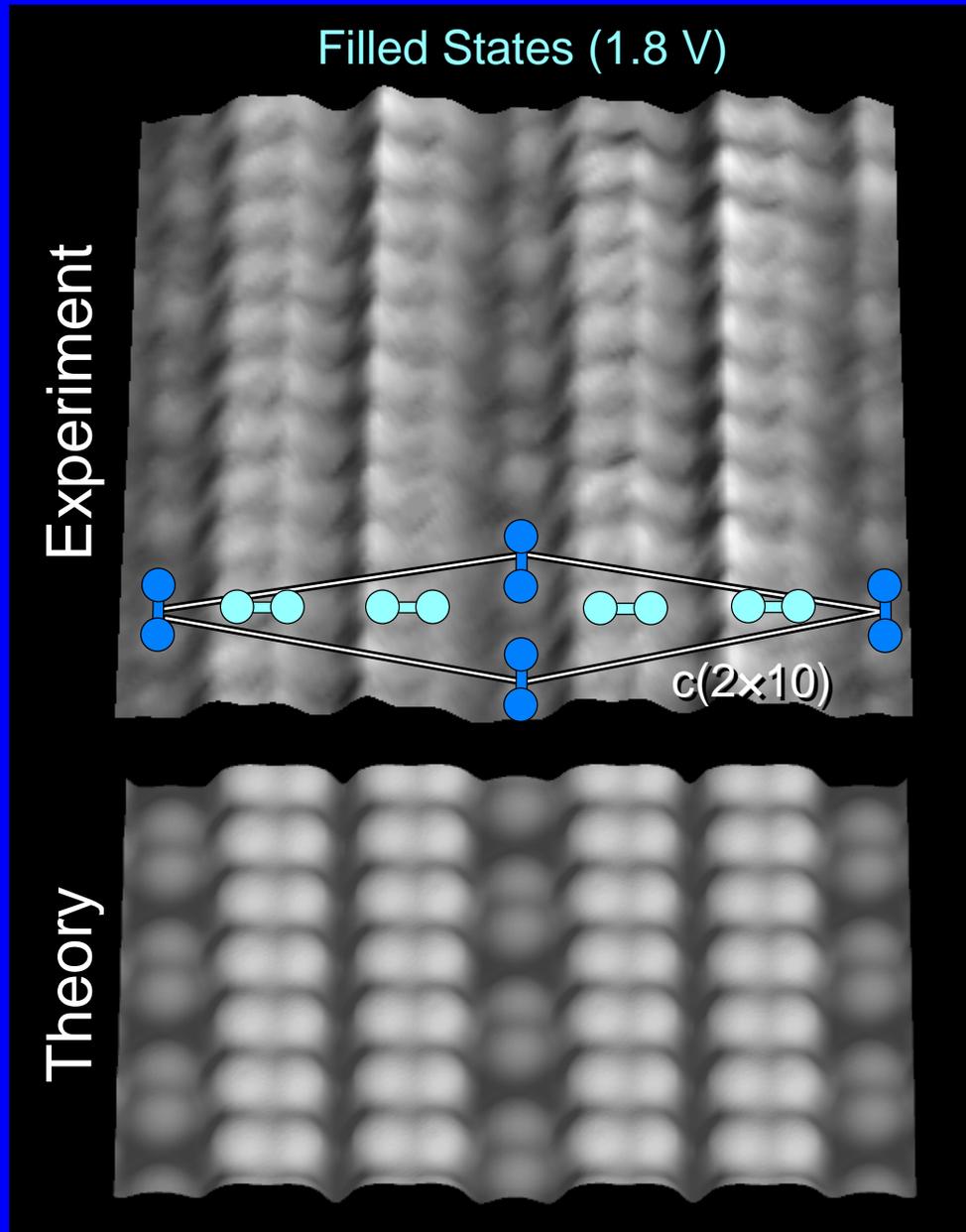
(2x10): 2.2 ML Sb



- 3 extra e's/(2x5): **expect metallic surfaces**

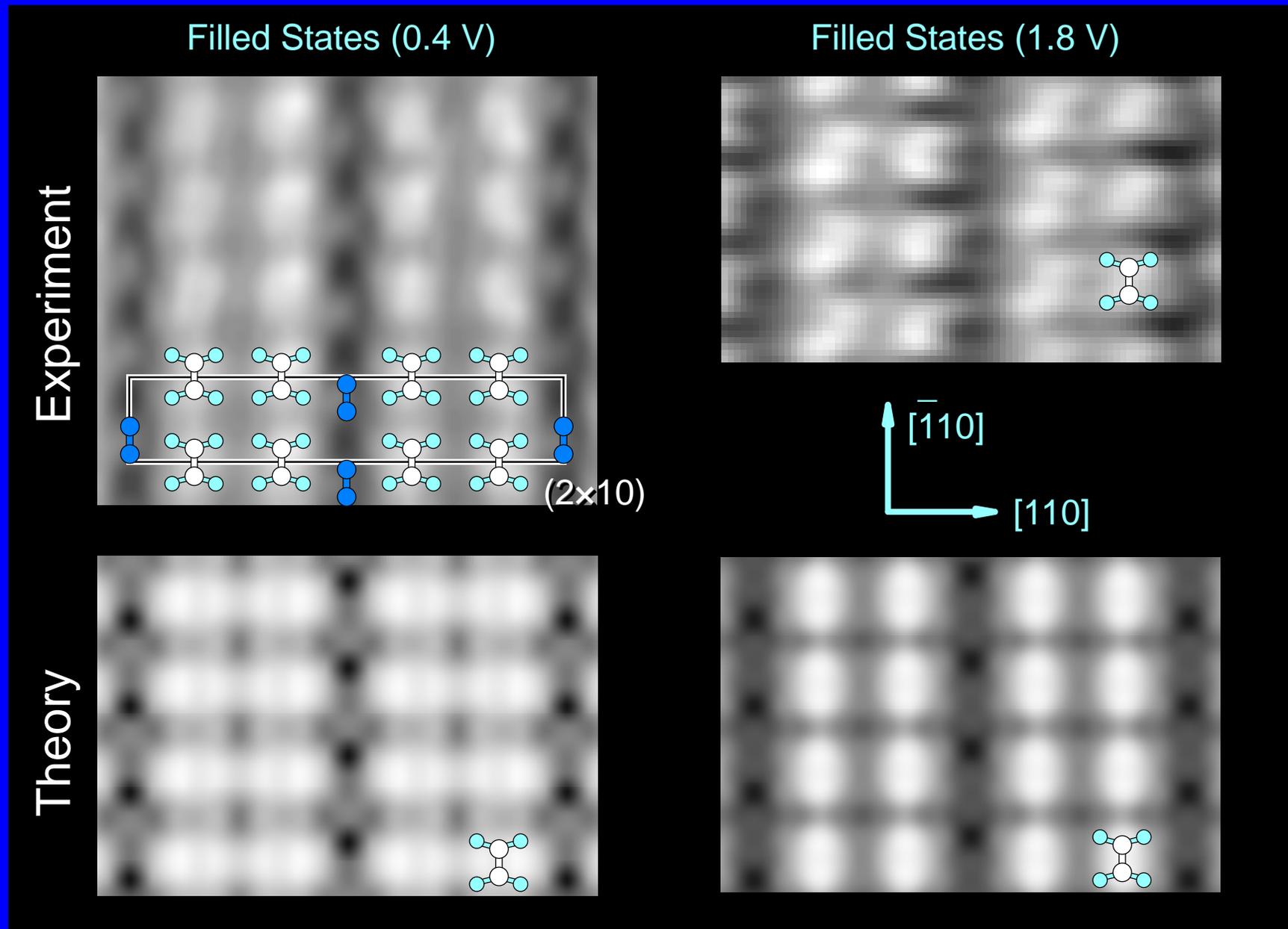
***Both models violate electron counting model!***

# GaSb(001)-c(2×10): Experiment vs. Theory

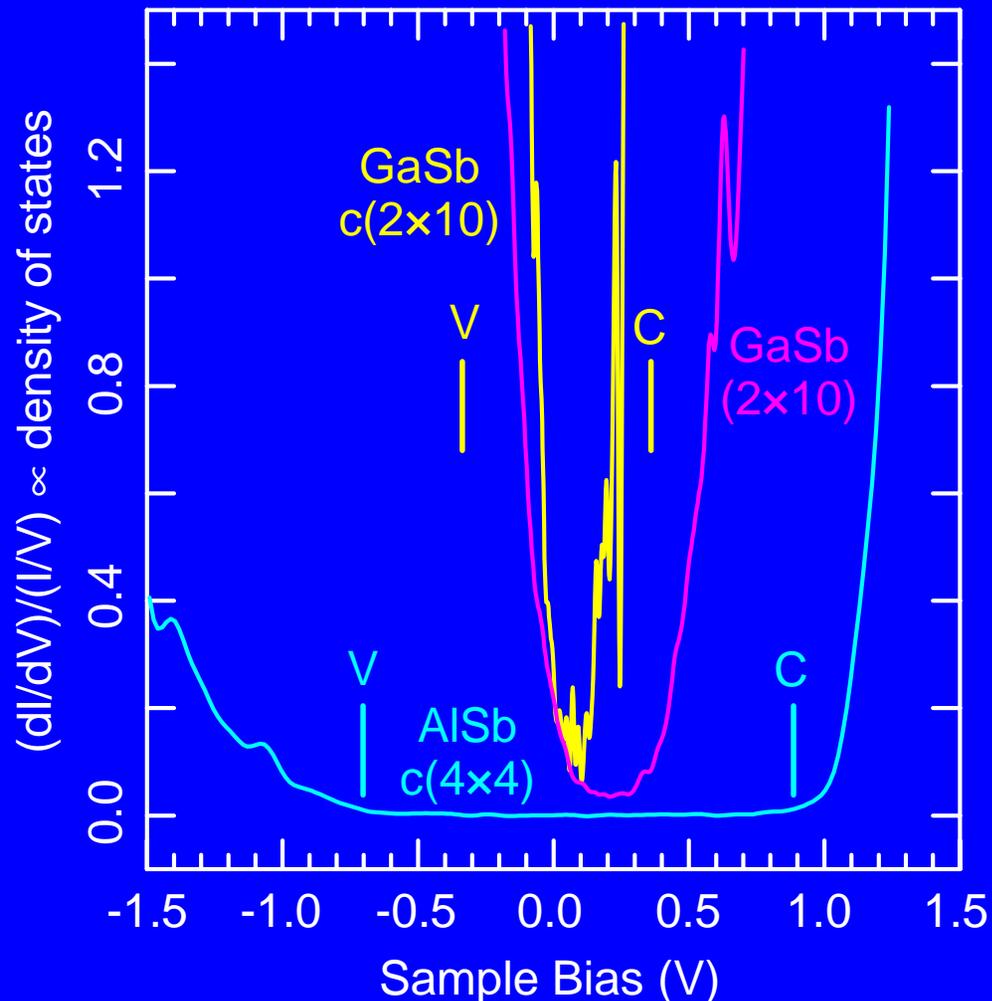


- **First-principles**, electronic-structure calculation (LDA)
- **Local-state density**  $\rho(r,\epsilon)$  computed from wave functions
- At each  $r$ , **integrate**  $\rho(r,\epsilon)$  over filled or empty states
- Simulate constant current **STM image** by surface of constant integrated  $\rho(r,\epsilon)$

# GaSb(001)-(2×10): Experiment vs. Theory



# AlSb and GaSb(001) Tunneling Spectroscopy



- AlSb insulating, as expected from ECM
- GaSb ***weakly metallic: non-zero conductivity at all bias voltages***
- Theory shows **occupied conduction band** states on GaSb

*Electron counting model violated on GaSb(001).*

# Strain Due to Sb Dimer Rows

Assume bulk-like Sb-Sb bonds (2.91 Å)



- Strain anisotropic: lower along dimer rows
- Displacements similar, but **GaSb 7% softer**:

*Strain energy lowest on GaSb => continuous rows.*

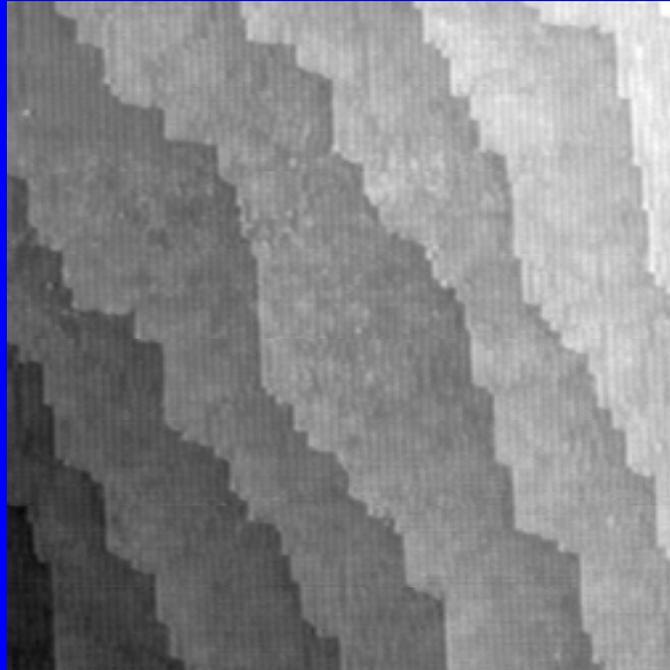
# Strain vs. Stiffness on III-V(001) Surfaces

- Multilayer structure with 3-fold Sb + filled db favored
  - Sb cohesive energy > than III-Sb = lower interface energy
  - Filled surface db's lower surface energy
- Resulting Sb dimers strain substrate:
  - Missing dimers relieve stress
- Strain **energy** depends on **substrate stiffness**:
  - AlSb 7% stiffer than GaSb: GaAs > AlSb > InAs > GaSb > InSb
- GaSb: good lattice match to Sb + low stiffness allows continuous dimer rows = **metallic** "(2×5)"

*Many device implications.*

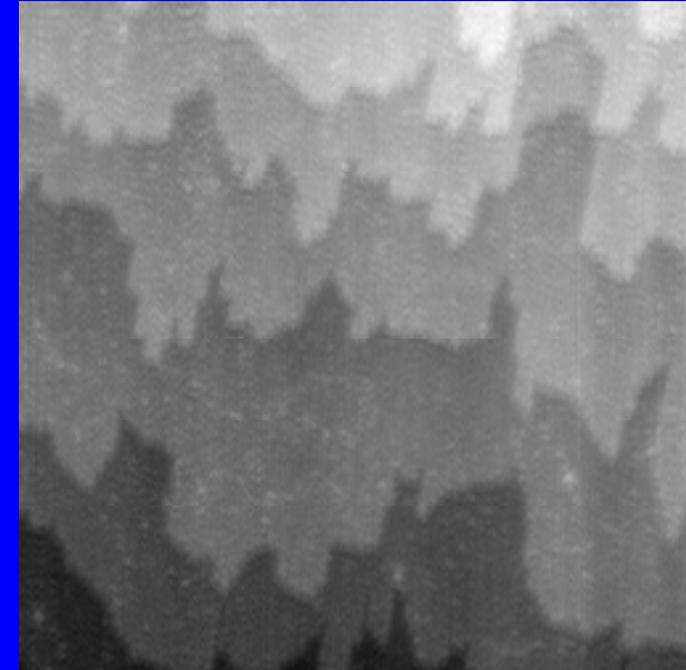
# Impact of Reconstruction on Step Structure

GaSb(001)-c(2×10)



Continuous double dimer rows  
=> high kink energy  
=> **straight steps along  $[\bar{1}10]$**

InAs(001)-(2×4)



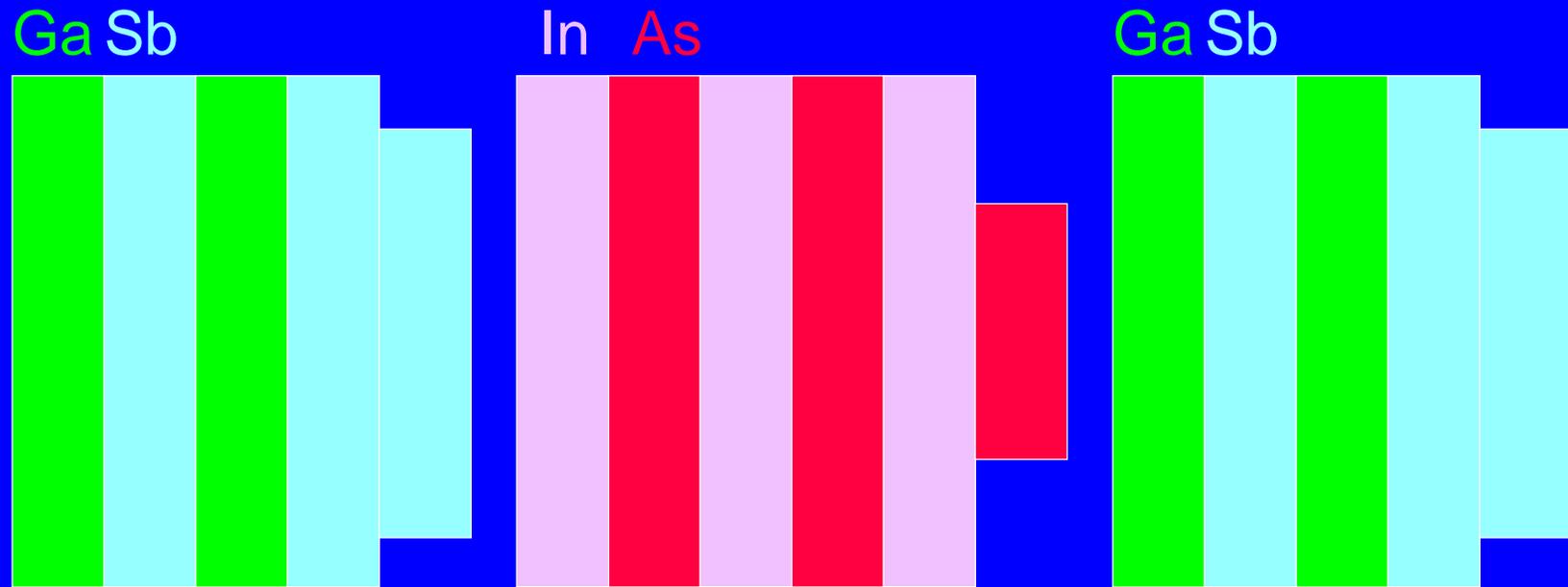
Different dimer row structure  
=> lower kink energy  
=> **rougher step edges**



*Implications for tilted superlattice and quantum wire growth.*

# Impact of Reconstruction on III-V Heterostructure Interfaces: GaSb/InAs

MBE Growth Direction  $\longrightarrow$



GaSb(001)-c(2x10)  
Excess Sb on growth  
surface (1.8 layers) =>  
*intermixing at interface?*

InAs(001)-(2x4)  
As deficient on growth  
surface (0.5 layers) =>  
*intermixing at interface?*

# Summary

- **AlSb(001)** forms a **c(4×4)** reconstruction, similar to GaAs, InAs, AlAs, and InSb, that **obeys the electron counting model**.
  - Spectroscopy reveals it is insulating, as expected.
- **GaSb(001)** forms **(2×5)-like** structures, c(2×10) and (2×10), that **violate the electron counting model**.
  - The structures are supported by LDA calculations.
- Spectroscopy reveals the GaSb (2×5)-like surfaces are (weakly) **metallic**, as predicted.
- GaSb unique (?) due to good **lattice match with Sb** combined with **softness of Ga-Sb bonds**.