

The Stability of Self-Interstitials on Si(113) and Ge(113)

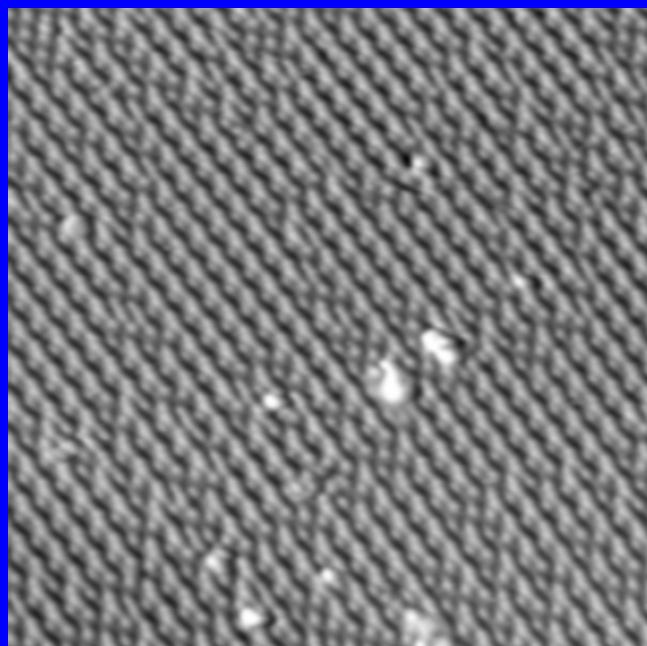
L.J. Whitman, A.R. Laracuente, S.C. Erwin

*Naval Research Laboratory
Washington, DC*



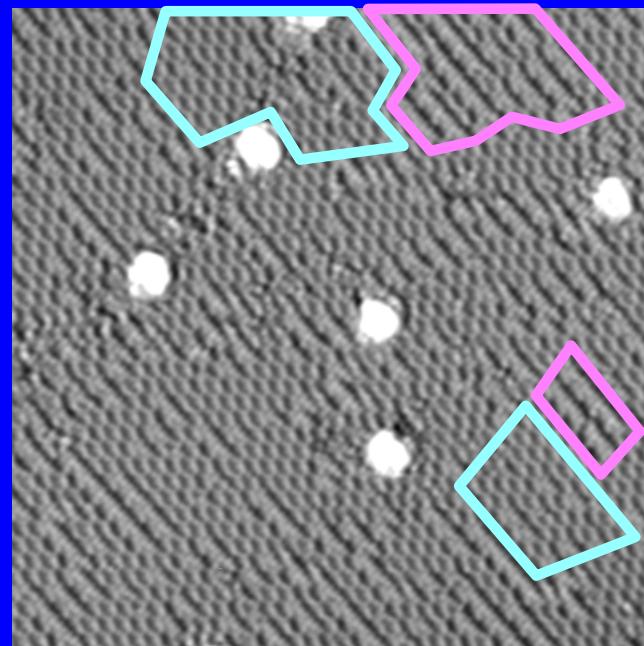
Morphology of Si(113) vs. Ge(113)

Si(113)-3x2



[$\bar{1}\bar{1}0$]
[$3\bar{3}\bar{2}$]

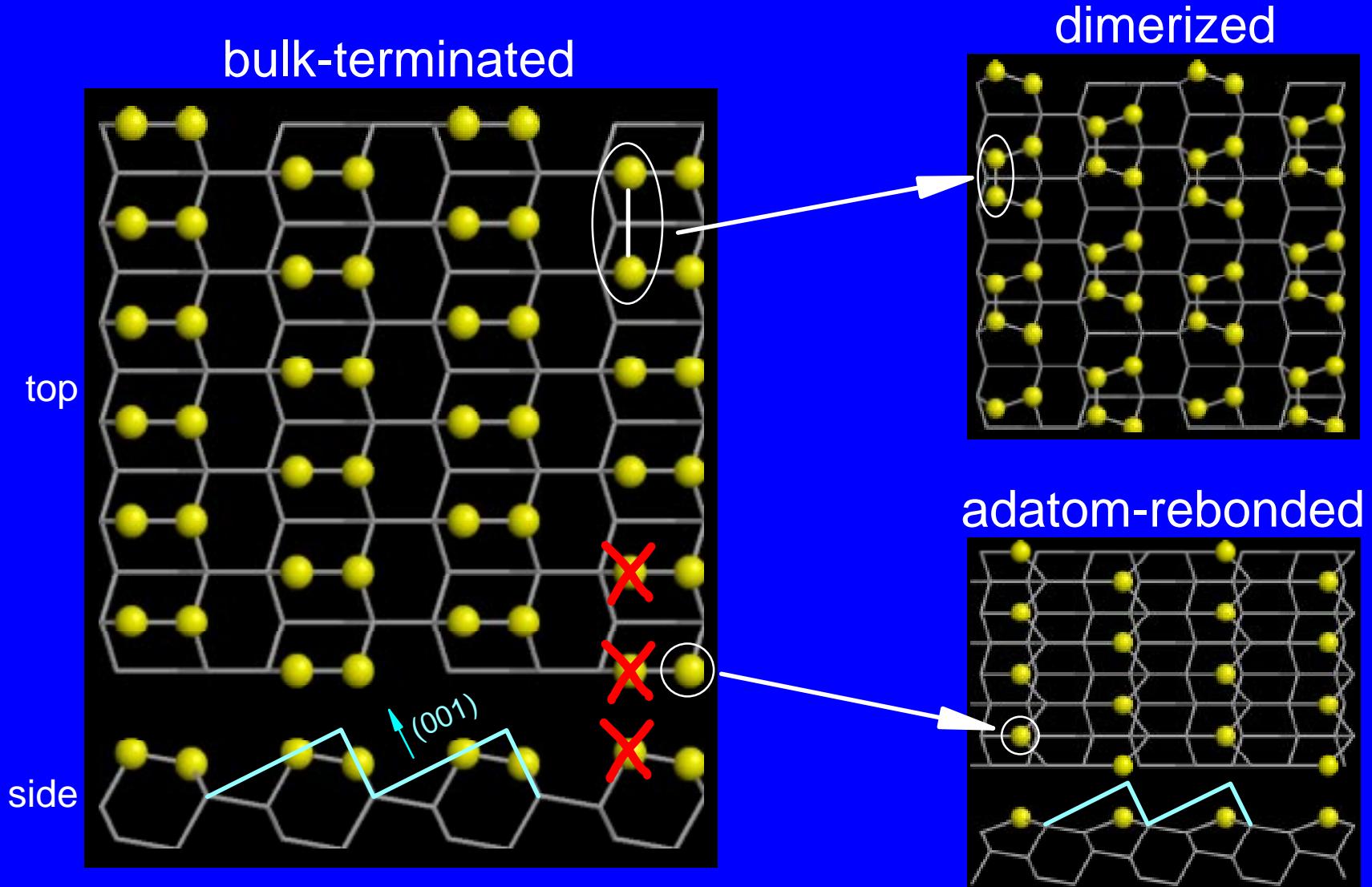
Ge(113)-3x1/3x2



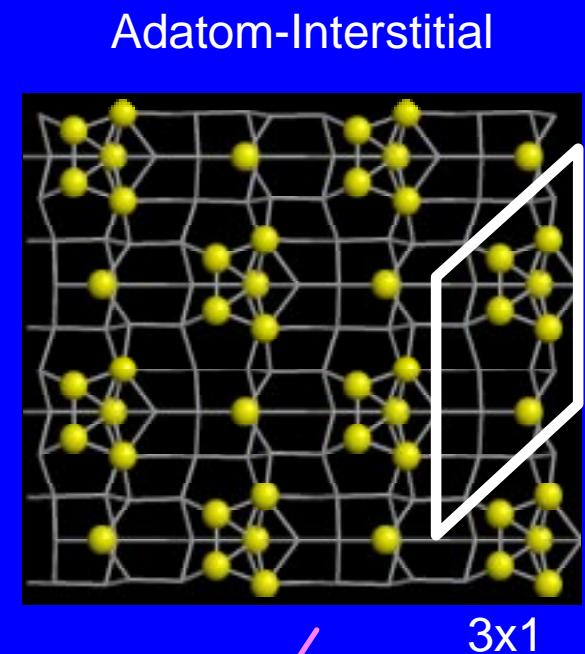
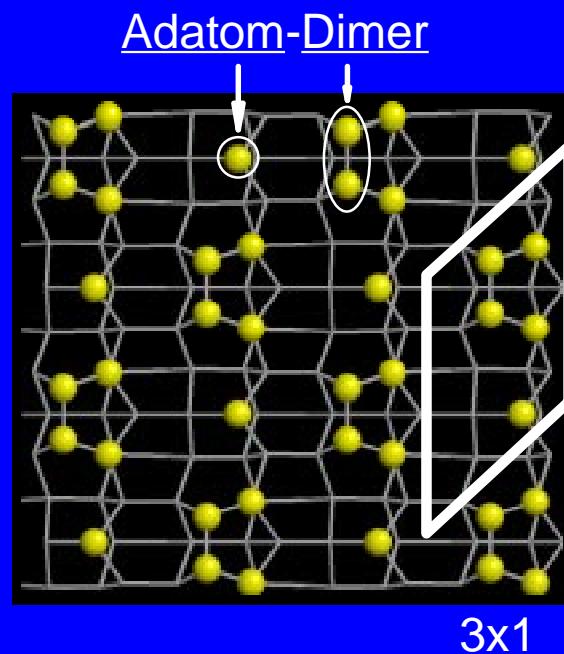
Filled States (2 V)
300 Å × 300 Å

About 50% 3x2

Reconstructing the (113) surface

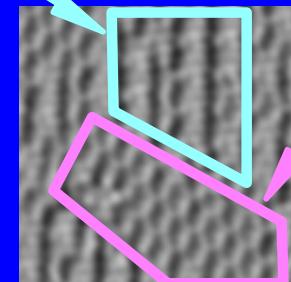
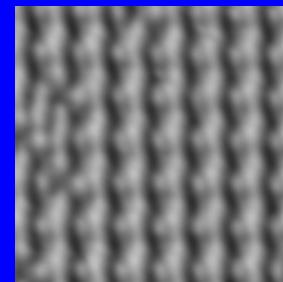


Reconstructed (113): "subsurface interstitials"

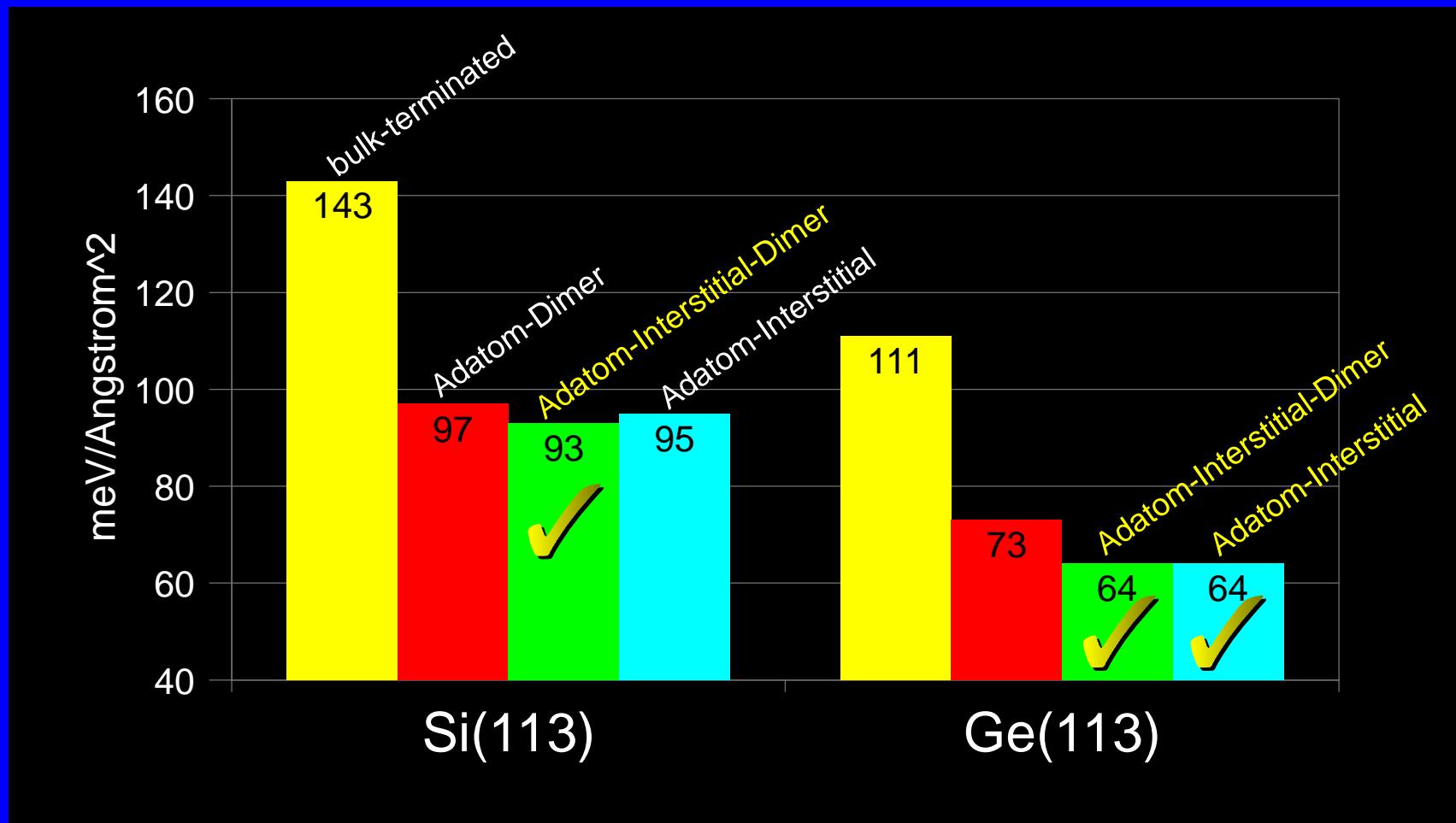


Brief history of Si(113)

- ◆ LEED: 3x1, 3x2 (Olshanetsky '81)
- ◆ STM & models (Ranke '90; ...)
- ◆ 3x2 reconstruction (Knall '94)
- ◆ Theory & AID model (Dabrowski '94)

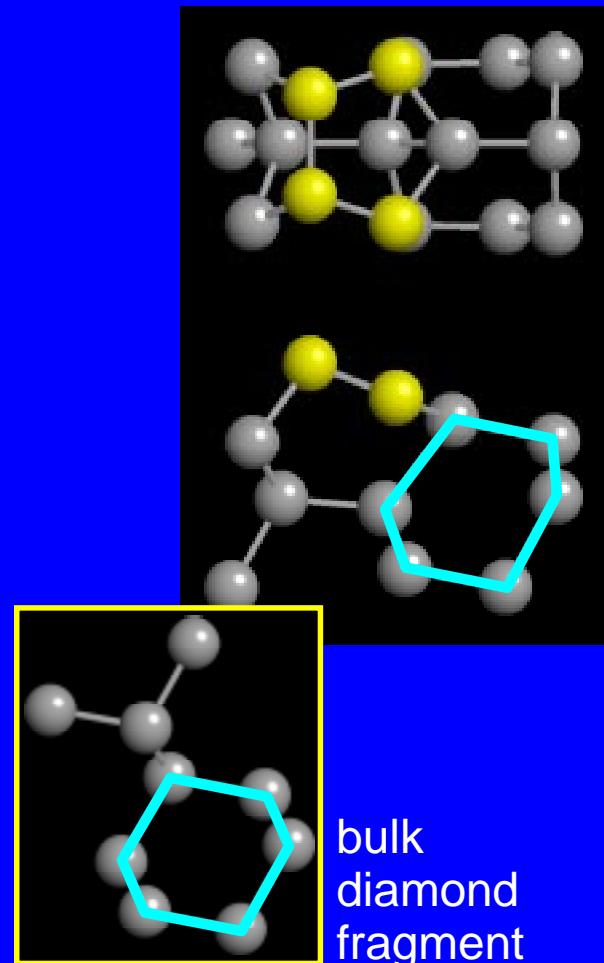


Theoretical (LDA) surface energies

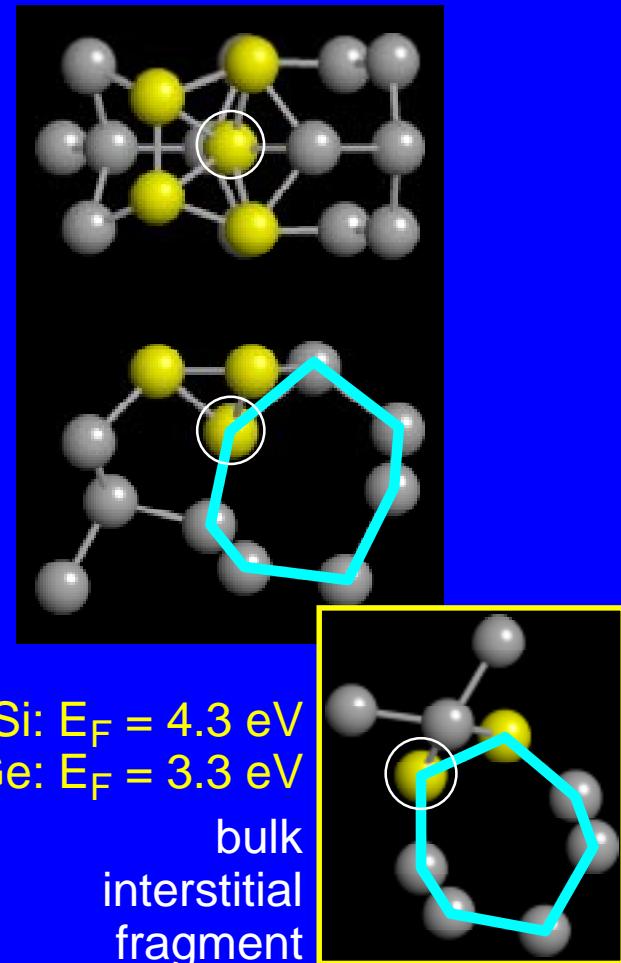


The [110]-split self-interstitial

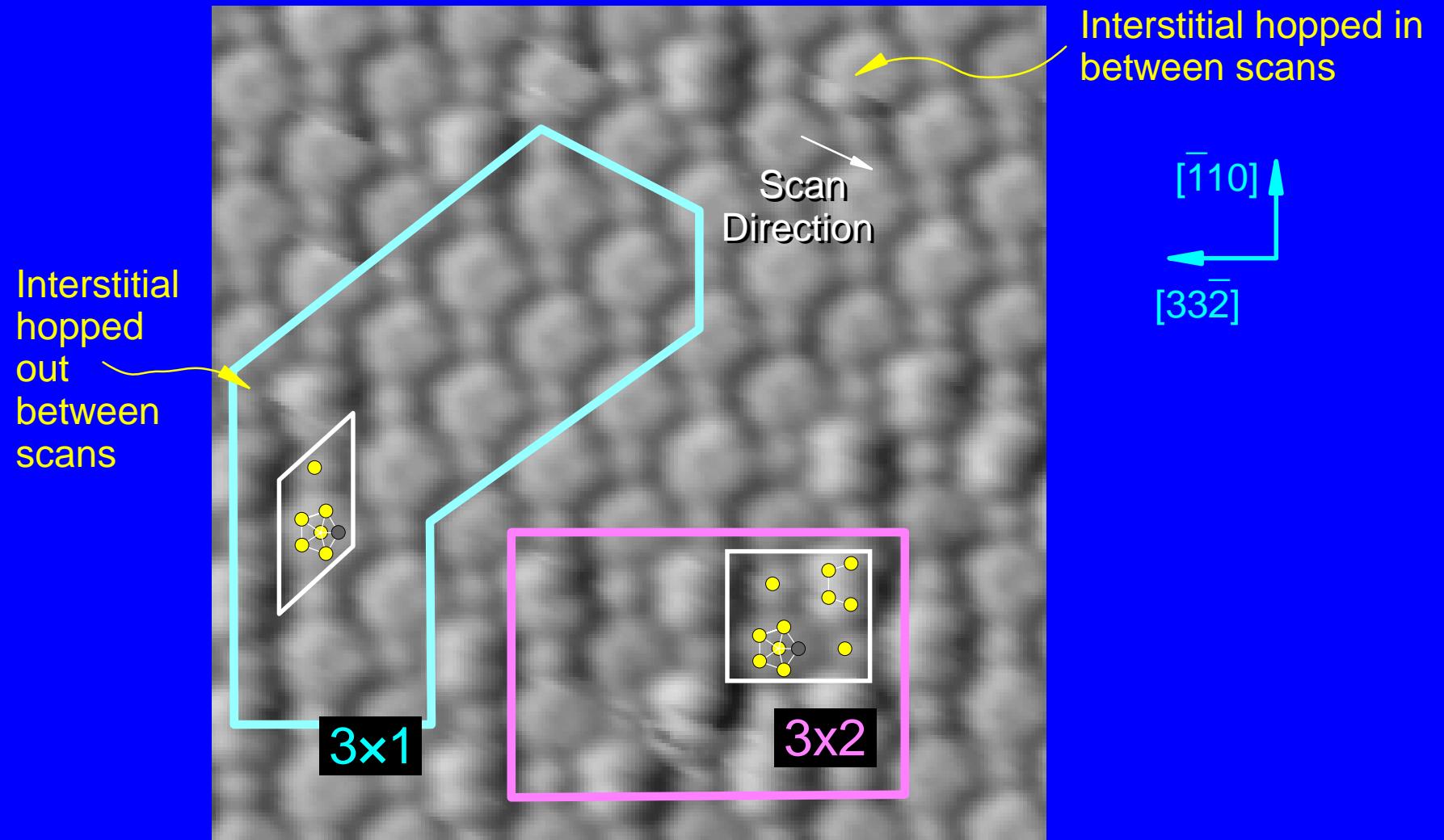
(113) surface dimer
without interstitial



with subsurface interstitial

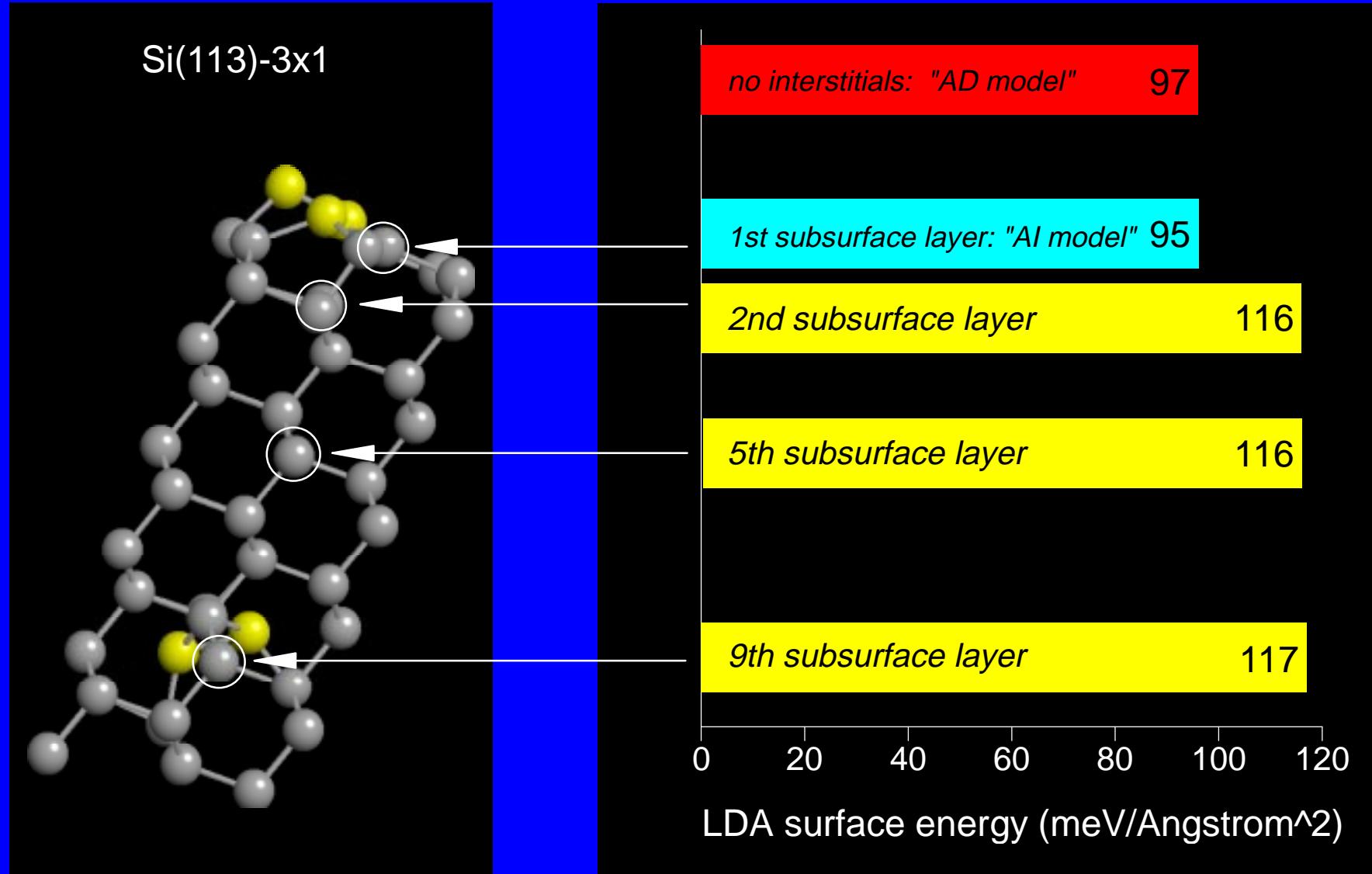


Ge(113)-3x1/3x2



Filled States (2 V)
70 Å × 70 Å

The cost of subsurface interstitials



Comments and conclusions

Why is the Si Adatom-Interstitial-Dimer reconstruction so stable?

- ◆ "Relief of tensile surface stress" (Dabrowski, PRL '94)
 - Calculated energies of deep interstitials: no supporting evidence
 - Calculated surface stresses: no supporting evidence

What is the nature of the Ge(113)-3x1/3x2 surface?

- ◆ "SXRD: random 50±10% distribution of subsurface interstitials" (Vogler, PRB '98)
 - STM: 50% coexistence of small AID and AI domains (\Rightarrow 75% interstitials)
- ◆ STM: interstitial migrations \Rightarrow 3x2 AID \leftrightarrow 3x1 AI (Gai, PRB '97)
 - Theory: migration into bulk unlikely \Rightarrow surface adsorbate gas?

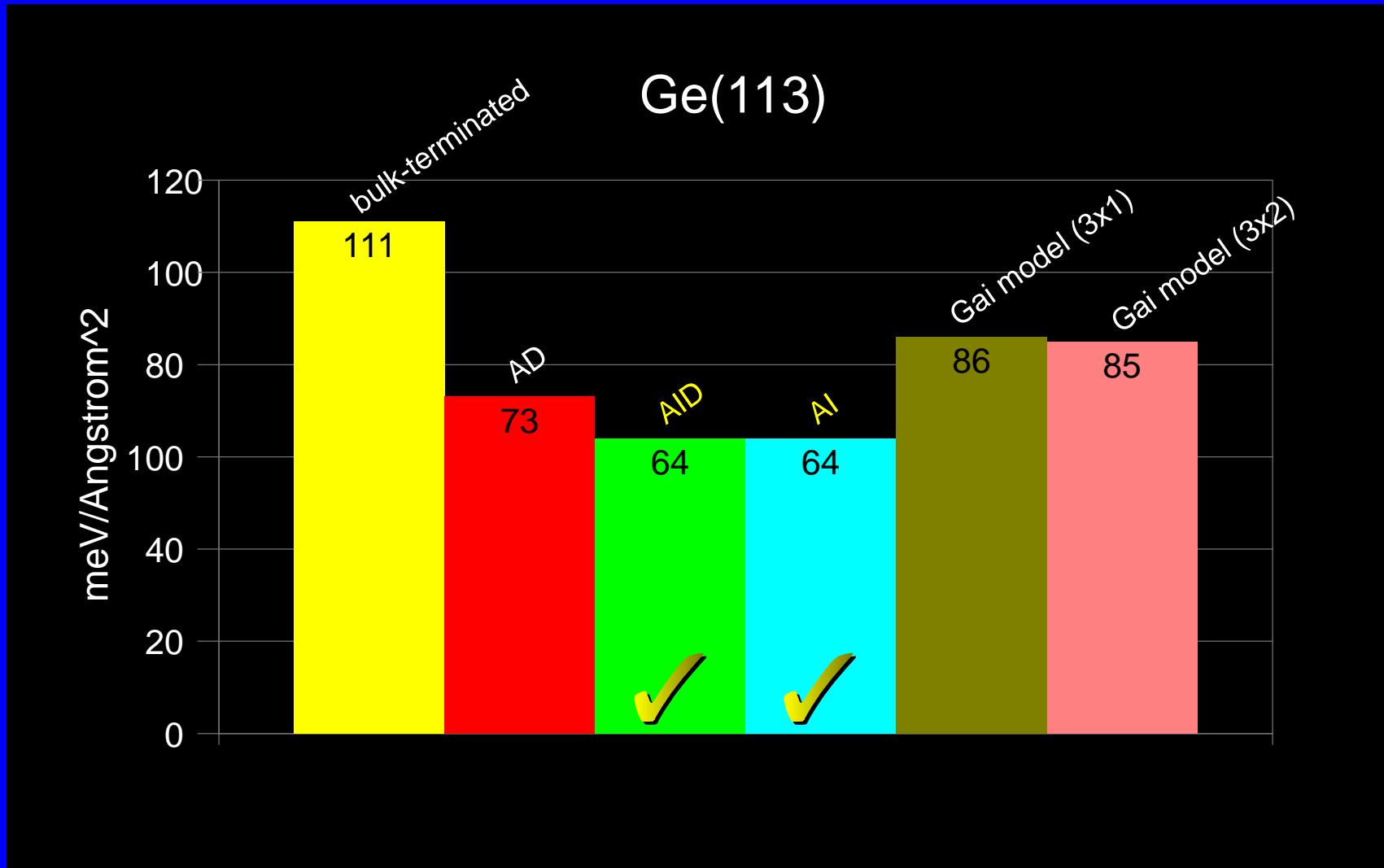
Why does Ge support both AID and AI reconstructions?

- ◆ "3x2 AID reconstruction \Rightarrow doubly occupied surface band" (Dabrowski)
 - Additional interstitial (3x2 AID \rightarrow 3x1 AI) dopes conduction bands
 - Si gap > Ge gap \Rightarrow Si-3x2 (AID), Ge-3x2/3x1 (AID/AI)

Computational details, etc.

Theoretical method	Local-Density Approximation
Electron-ion interaction	Troullier-Martins pseudopotentials
Supercell slab thickness	8 layers
Vacuum thickness	4 layers
Plane-wave energy cutoff	8 Ry (Si); 15 Ry (Ge)
Brillouin-zone sampling	4 k-points
Computer software	FHI96MD (Bockstedte, Kley, & Scheffler)
Computer hardware	Wright-Patterson DoD MSRC
Support	Office of Naval Research

Theoretical (LDA) surface energies



LDA surface energies & stresses

