Investigation of the Passivation of Semiconductor Surfaces Using Synchrotron X-ray Diffraction

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MURI review, Bozeman, Jan 2005

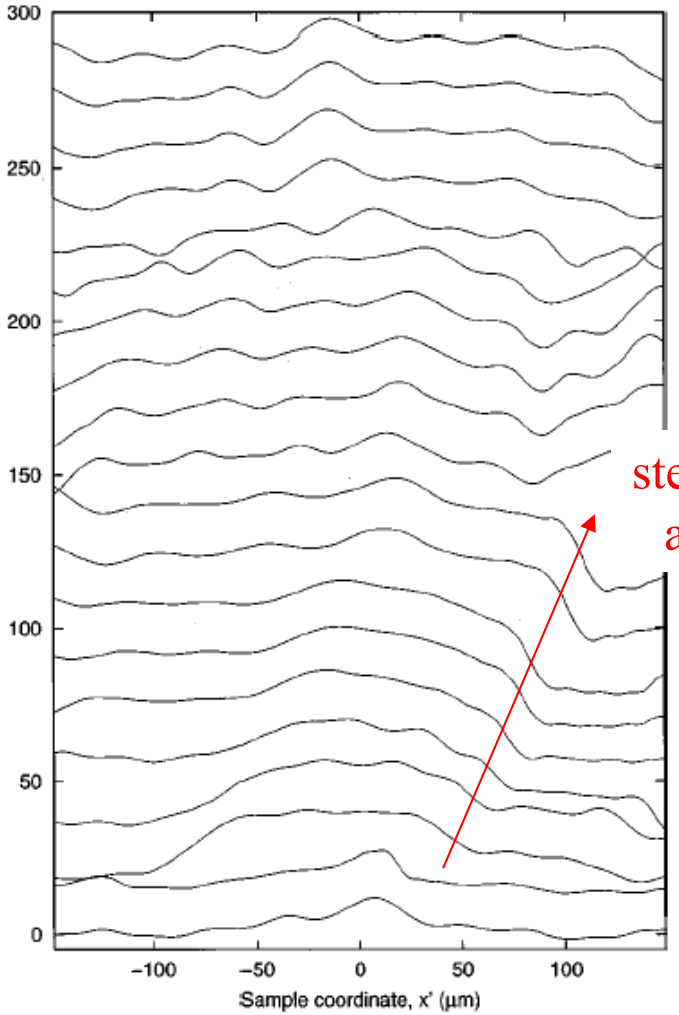
Outline

- Ambient Oxidation of Silicon
- Well-ordered structures of Au on Si(111)
- Passivation of Si by Au
- Future plans for AO source

In-situ Regrowth of Oxide on Si

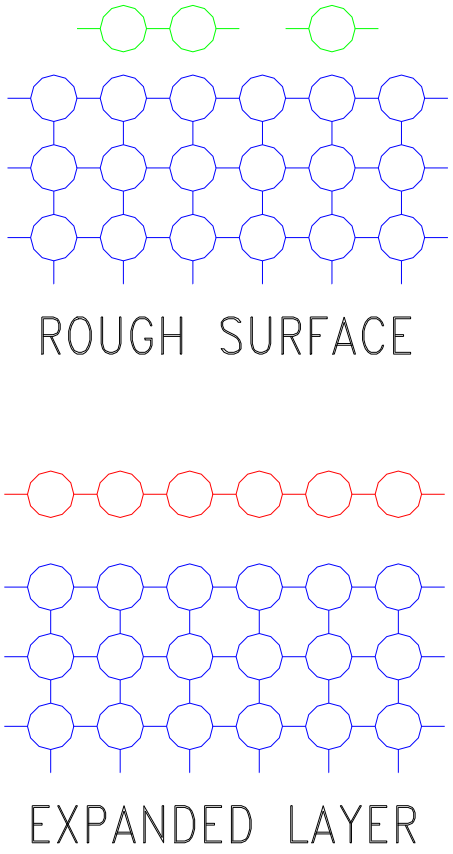
Phys. Rev. B **60** 9965 (1999)

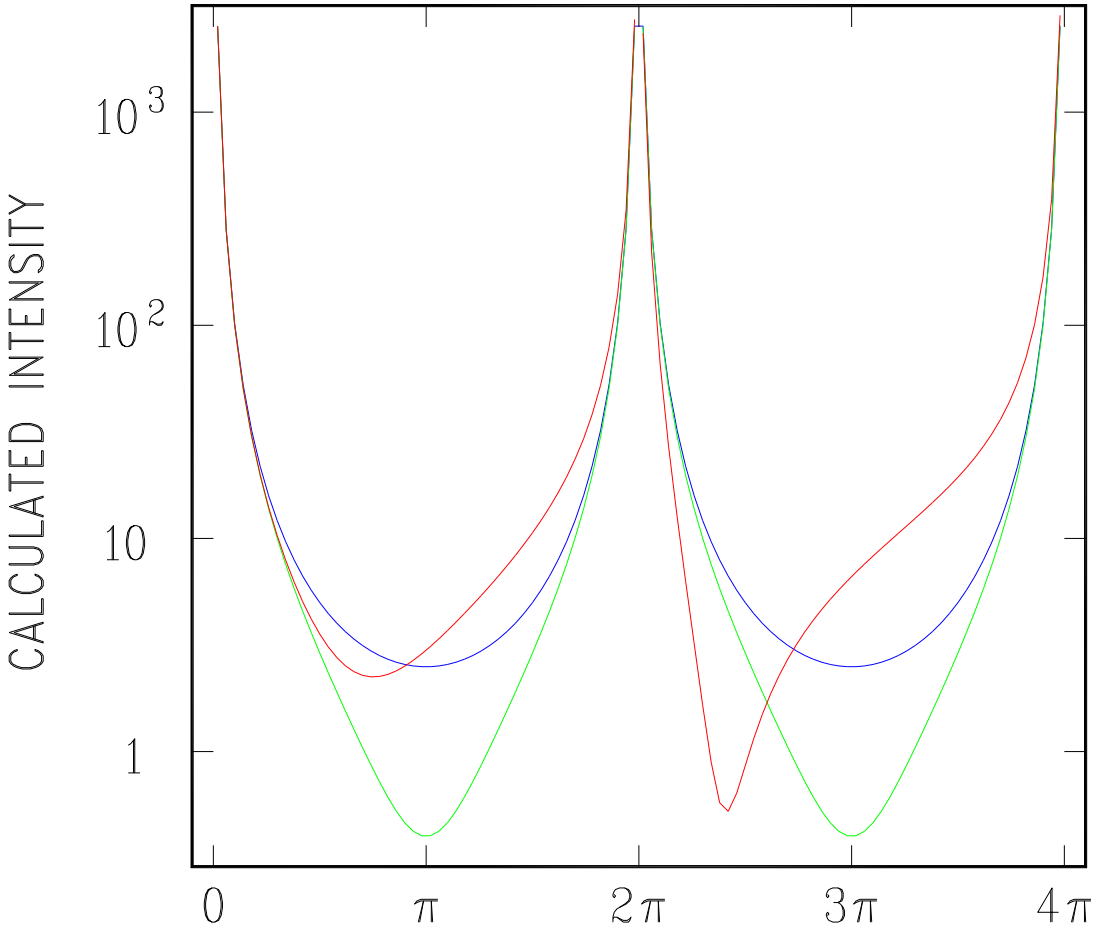
- Wafer stripped with HF at t=0
- CXD pattern measured every 180 sec
- Each profile reconstructed independently
- Random starting phase each time



I. K.

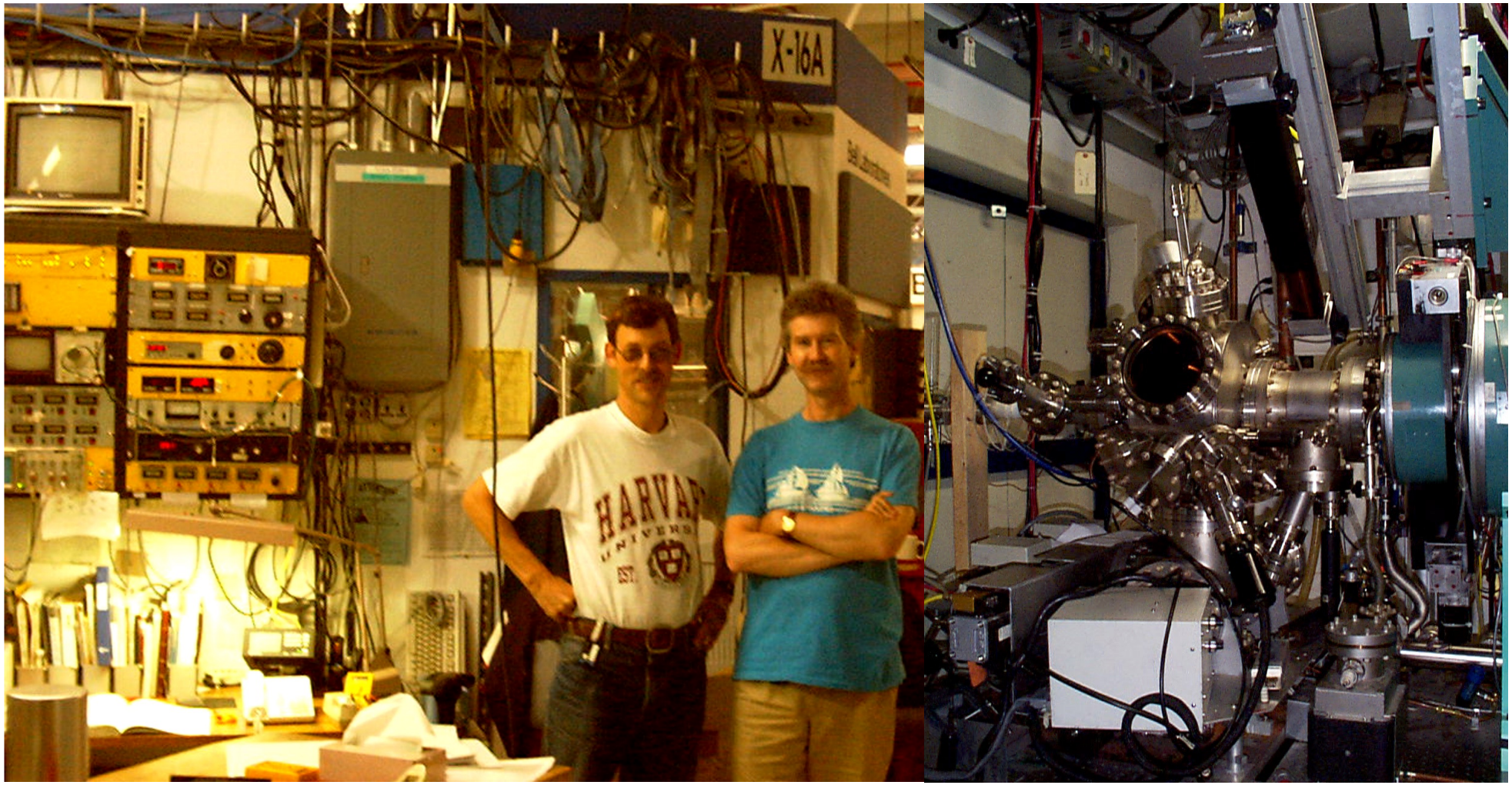
CTR is Sensitive to Surface Structure



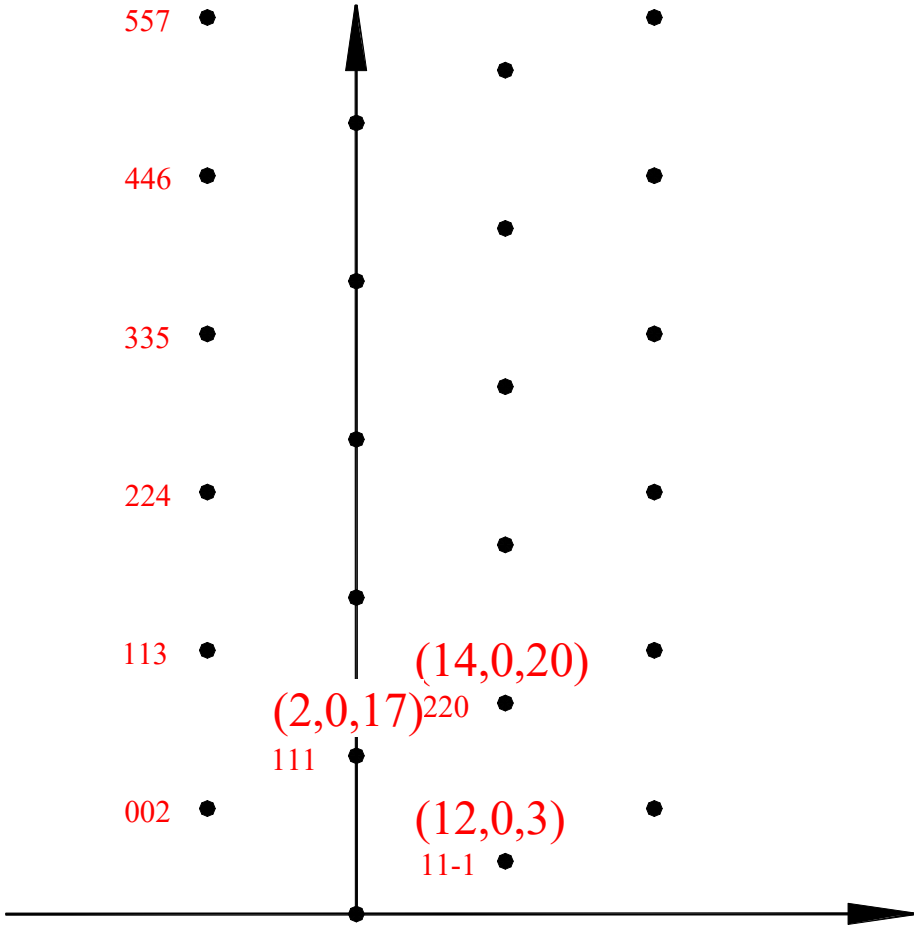


X16A Surface X-ray Diffraction

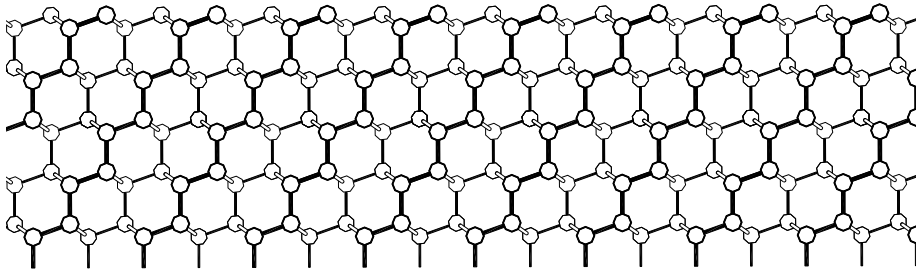
operating since 1987 ...

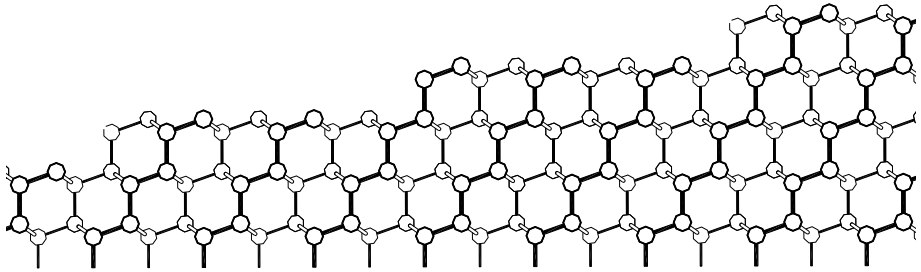


Crystallography of Stepped Surfaces

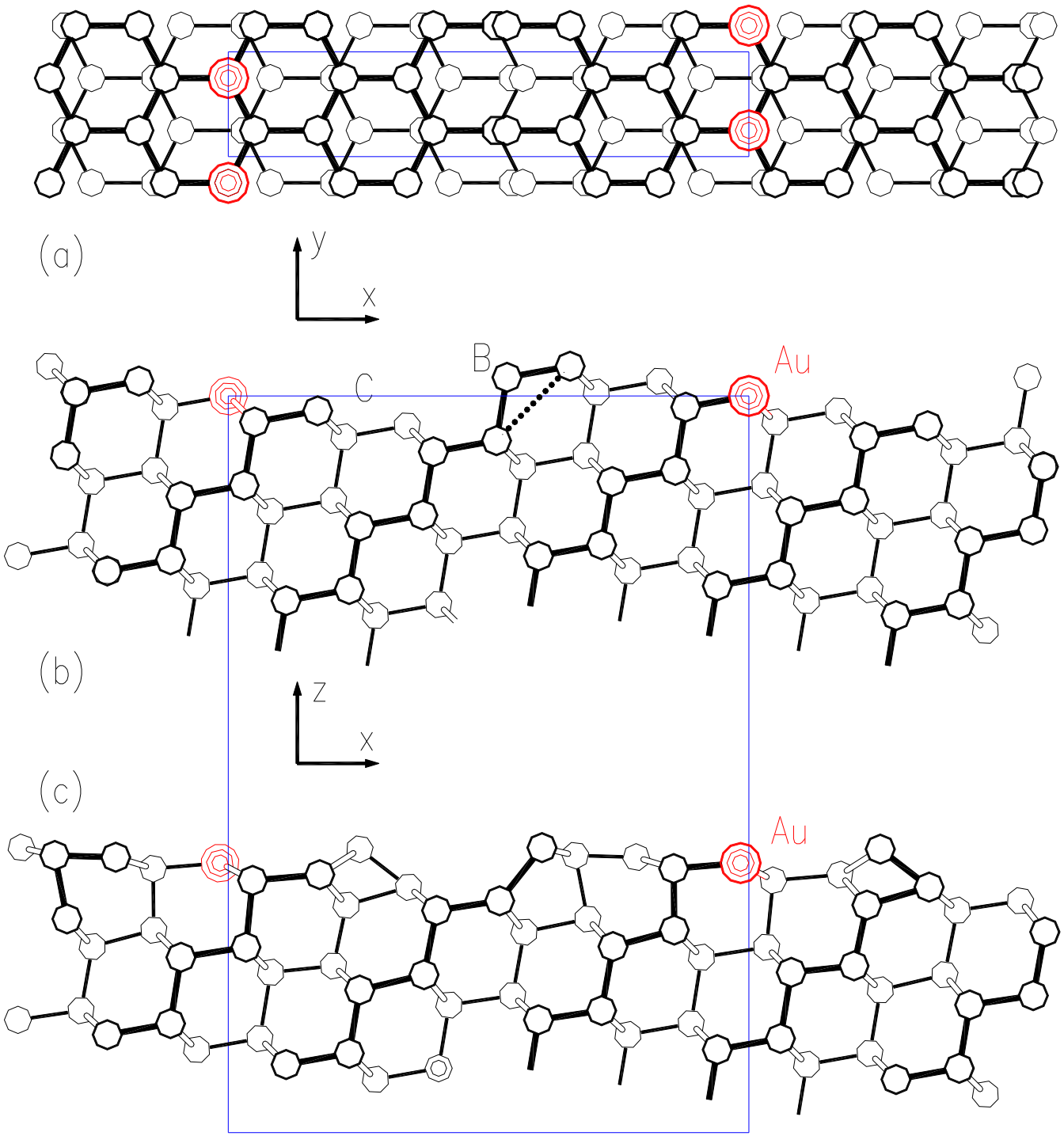


Silicon (111)

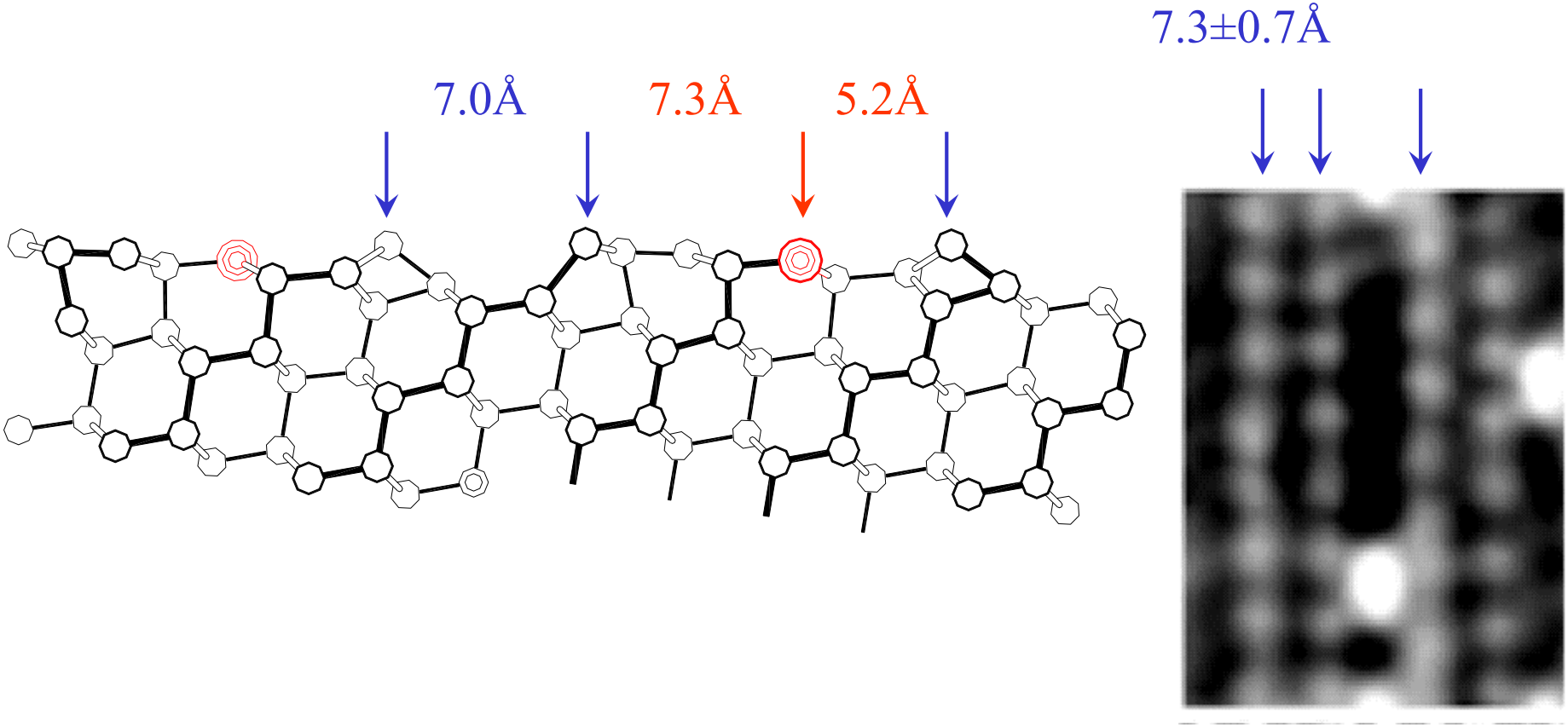




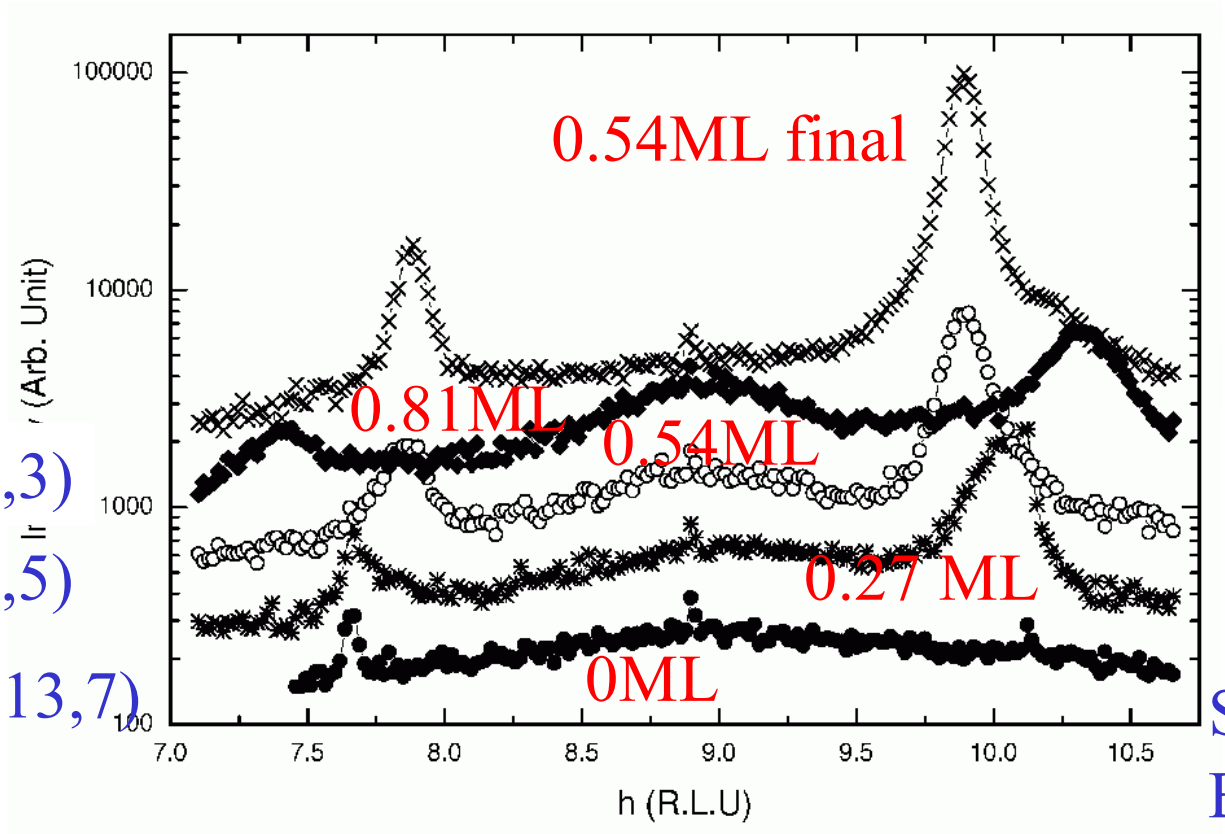
Si(557) surface


(a)
y
x
B
C
Au
(b)
z
x
(c)
Au

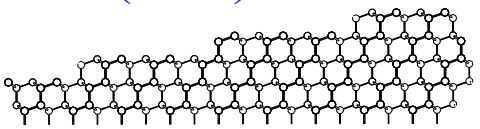
Comparison with STM



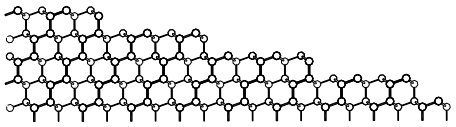
Au deposition on Si(13,13,7) at 650C



Si(557)

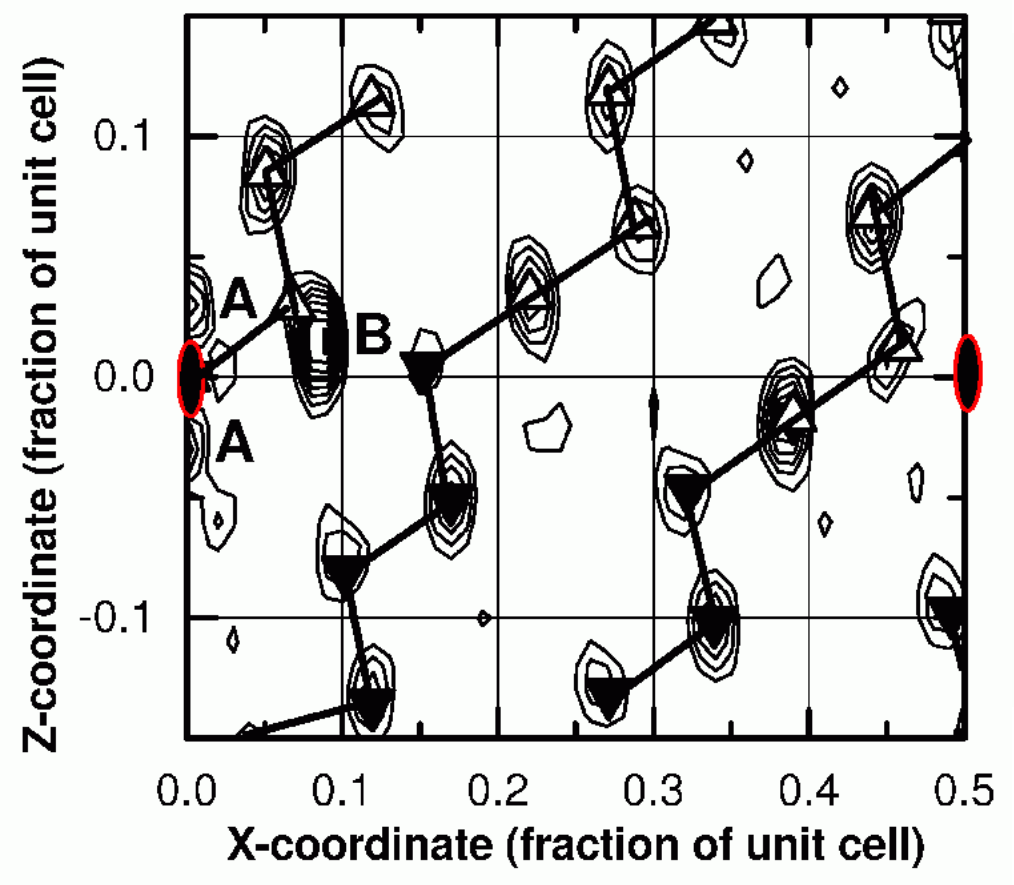


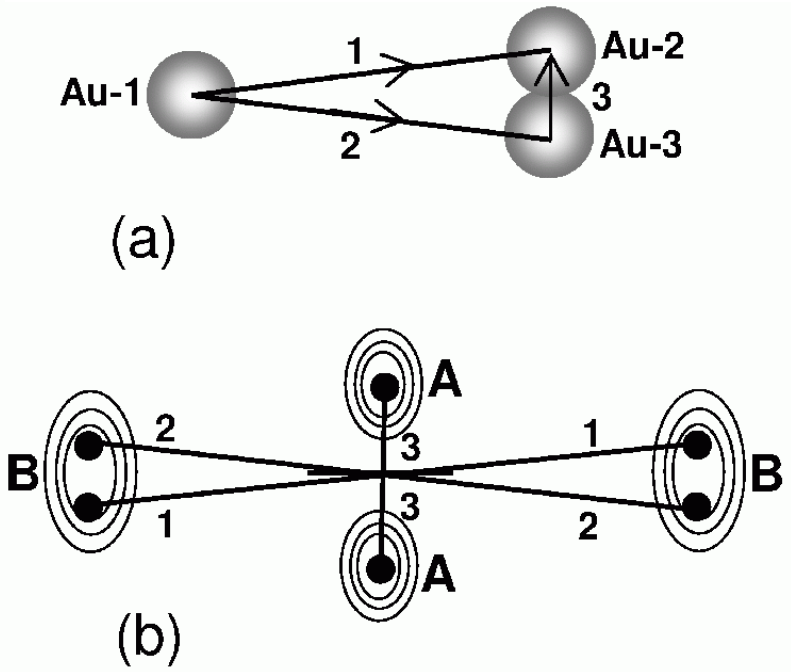
Si(553)



Scan along (h,0,11)
Bragg at (8,0,7)

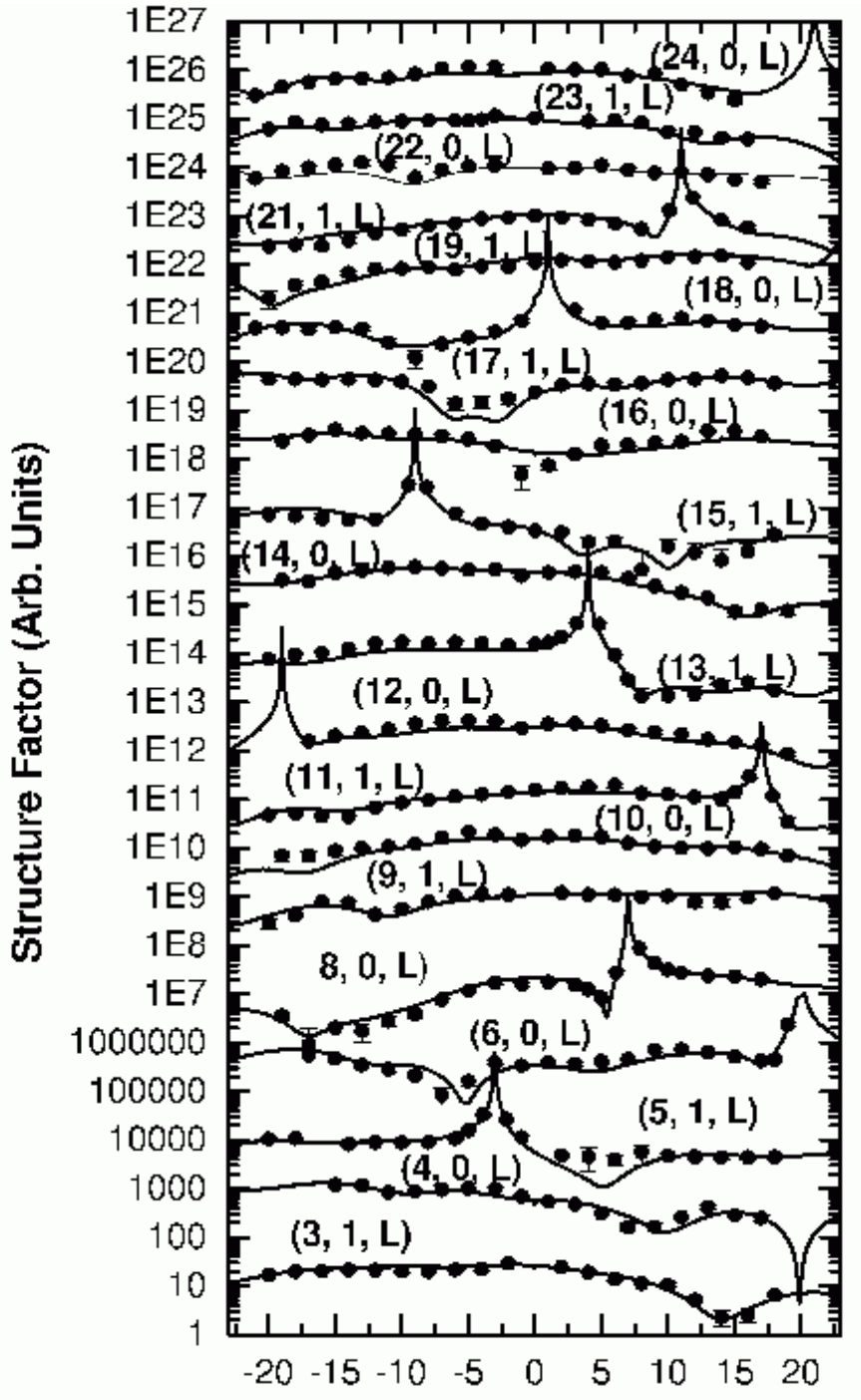
Patterson has extra peaks near origin



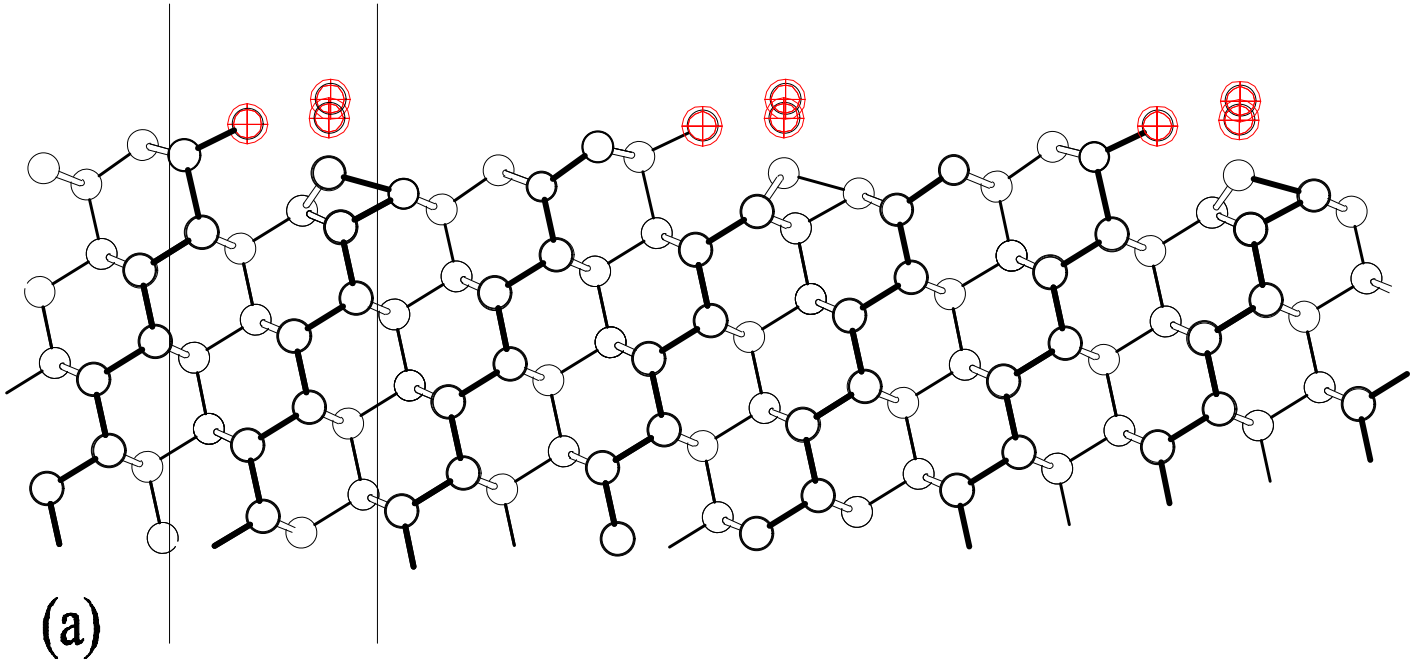


Fit to Data

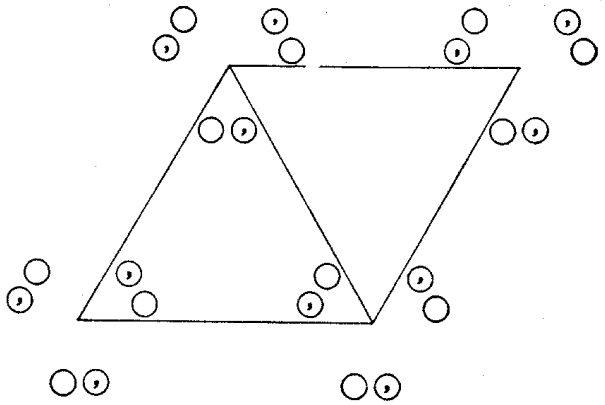
- Chisq = 6.5
- Au-1 at 70%
- Au-2,3 at 38% ea
- Extra Si at 50%
- Relaxations

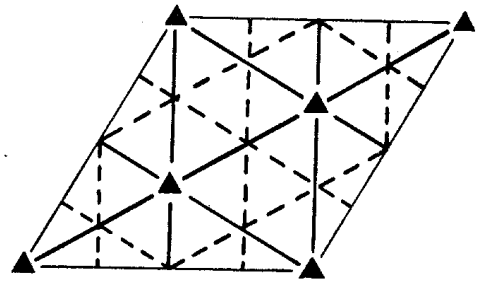


Final model of Au/Si(553)

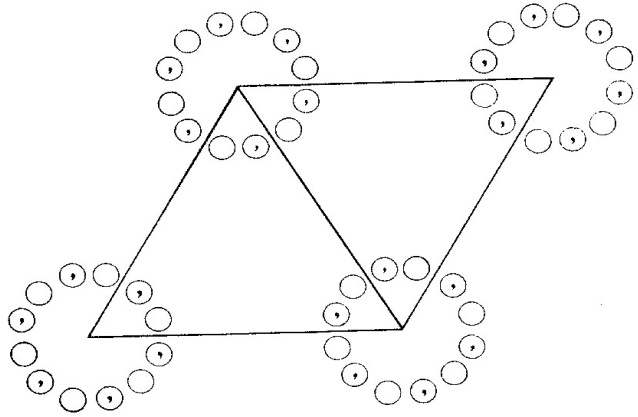


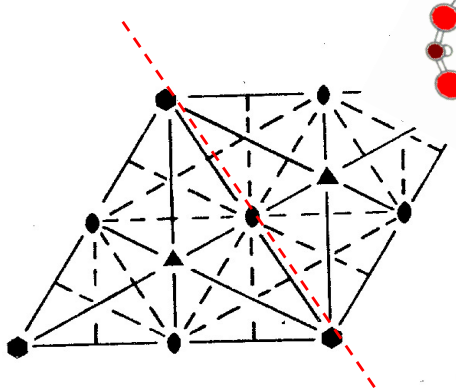
Importance of Symmetry in Si(111)7x7



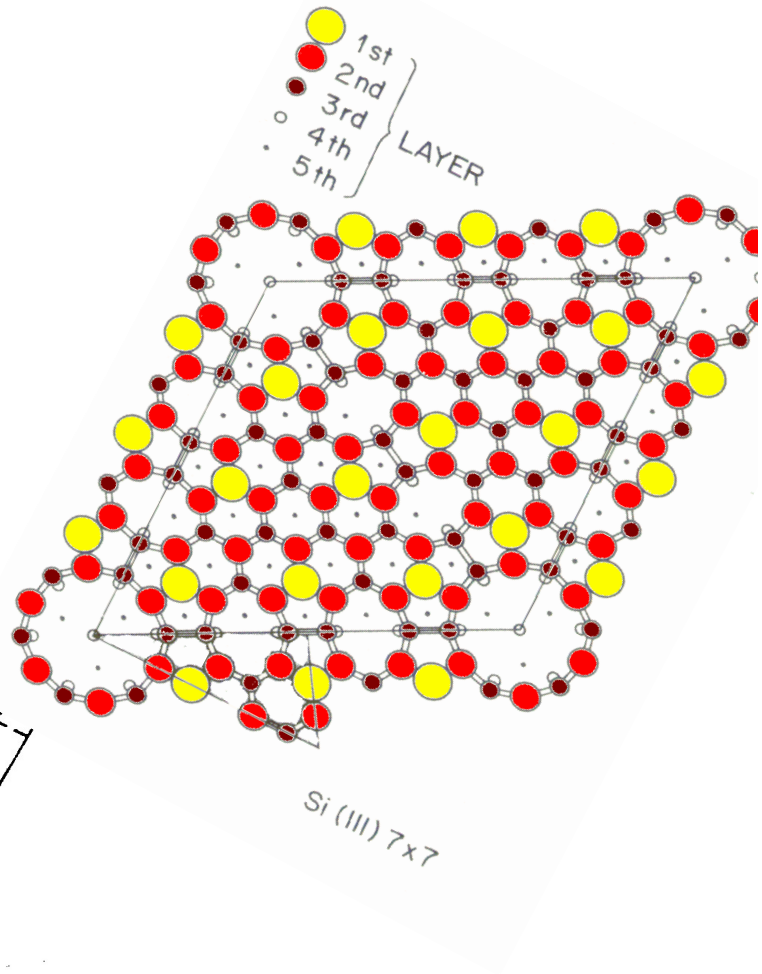


p3m1 → Bulk Symmetry





p6mm → Surface Symmetry



Au physisorption on Si(111)7x7?

Motivation

To study the structure of self assembled metal nanostructures on Si(111)7x7 surface

Adsorption processes of Au on Si(111)7x7 surface

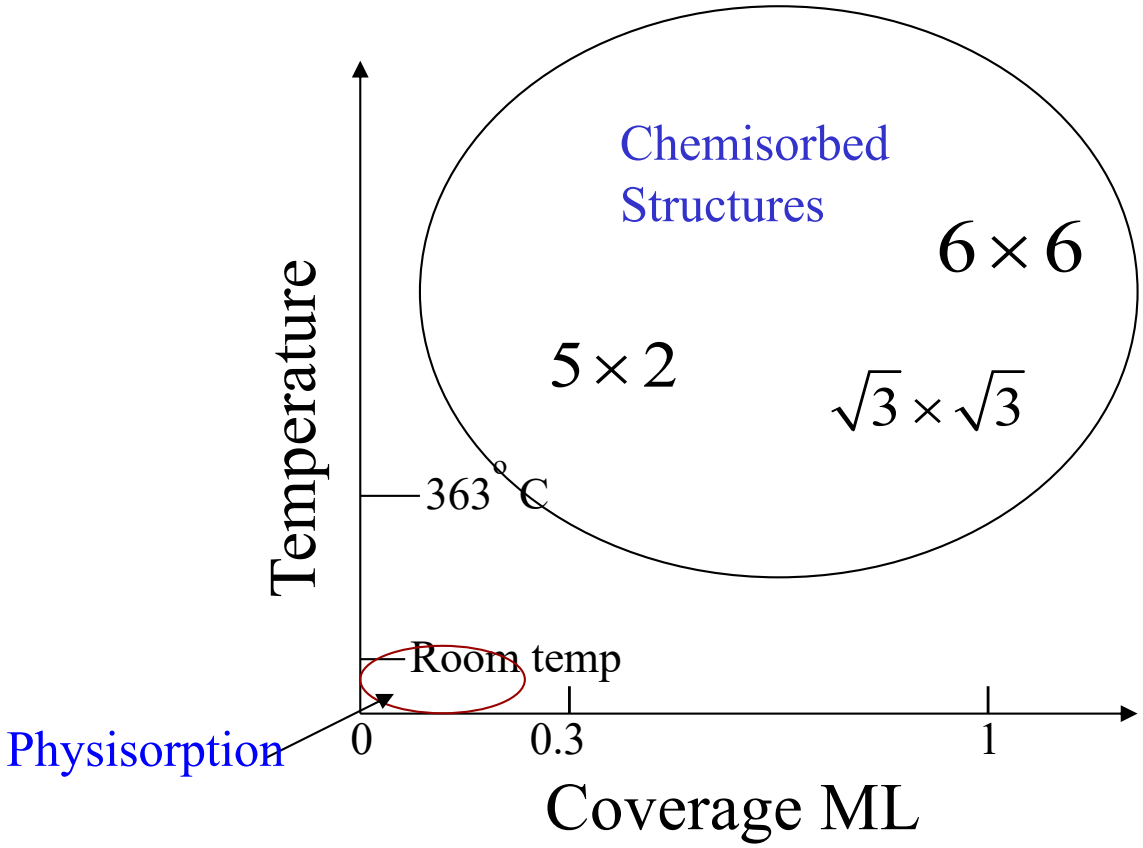
Physisorption (Physical absorption)

Adsorption in which the forces involved are inter-molecular (van der Waals forces), which do not involve a significant change in electronic orbital patterns of the species involved

Chemisorption (Chemical absorption)

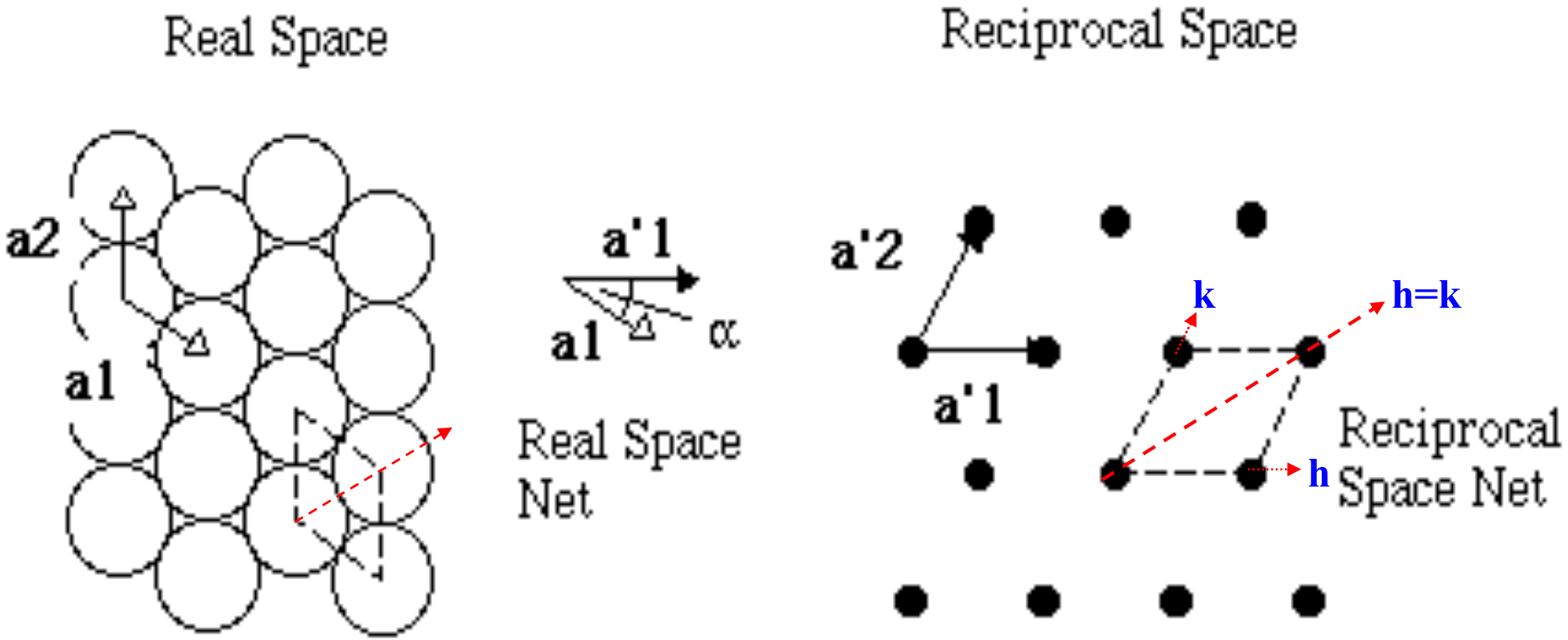
Adsorption in which the forces involved are electronic valence forces of the same kind as those operating in the formation of chemical compounds, i.e., ionic and covalent bonds

Au on Si(111) Phase Diagram



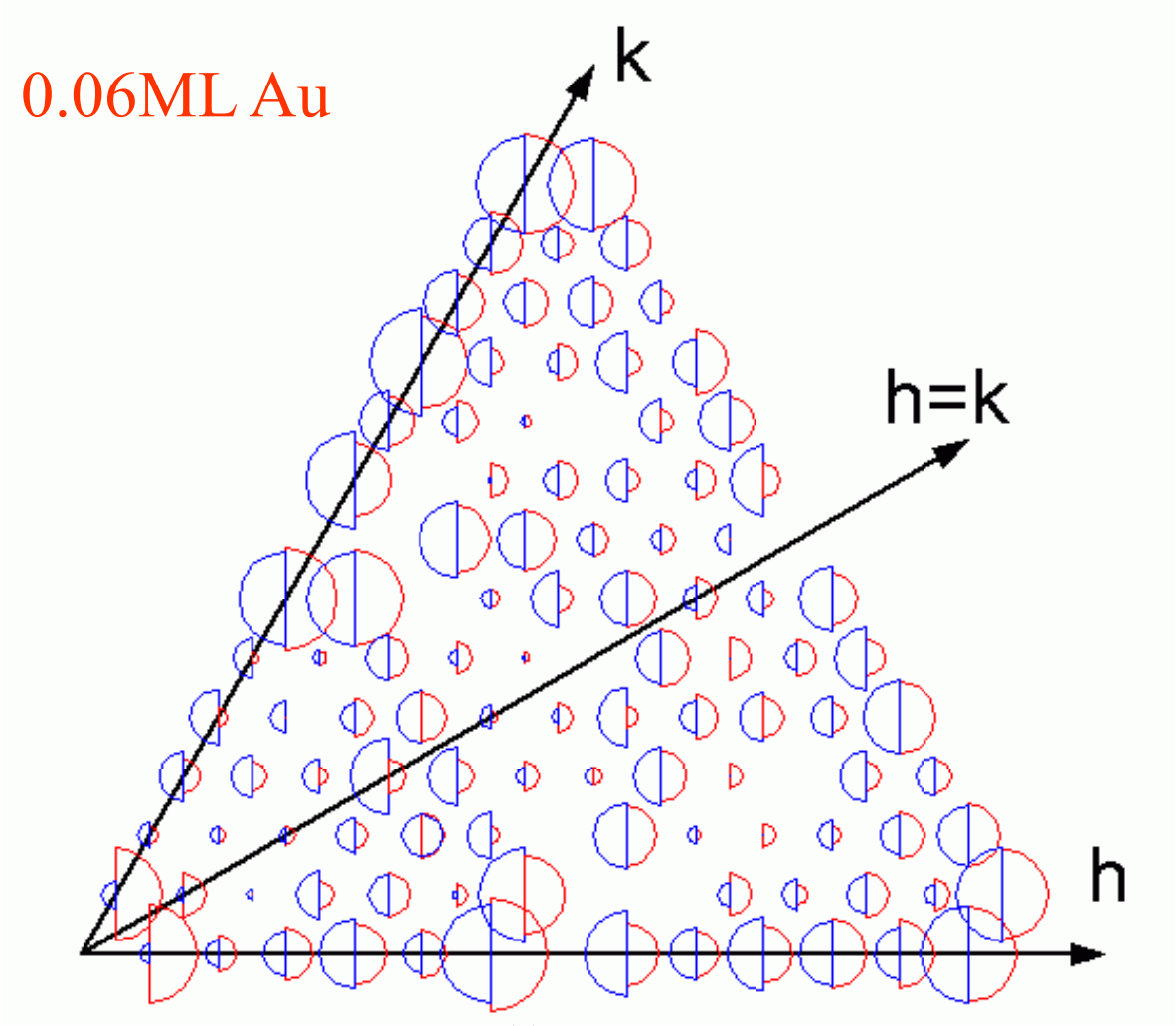
D. Grozea, E. Bengu and L. D. Marks, Surf.Sci. 461, 23(2000)

Surface Symmetry



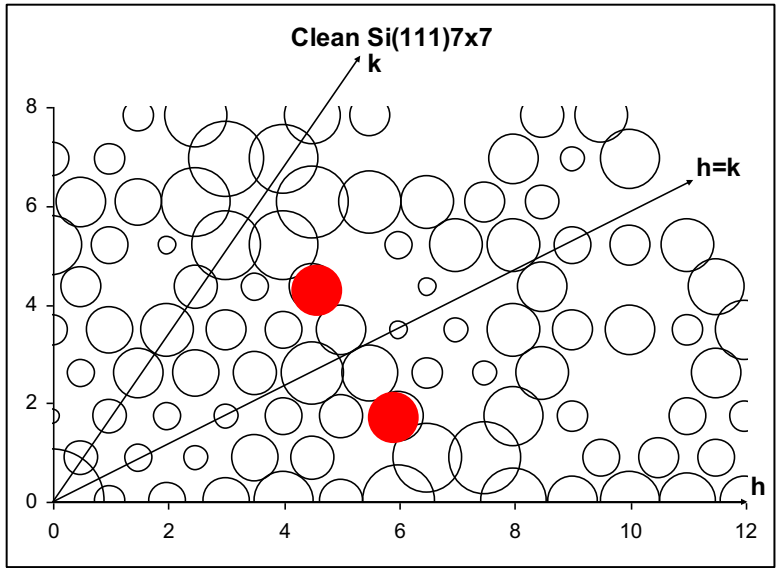
L=1.5 symmetry breaking

Clean | 0.06ML Au

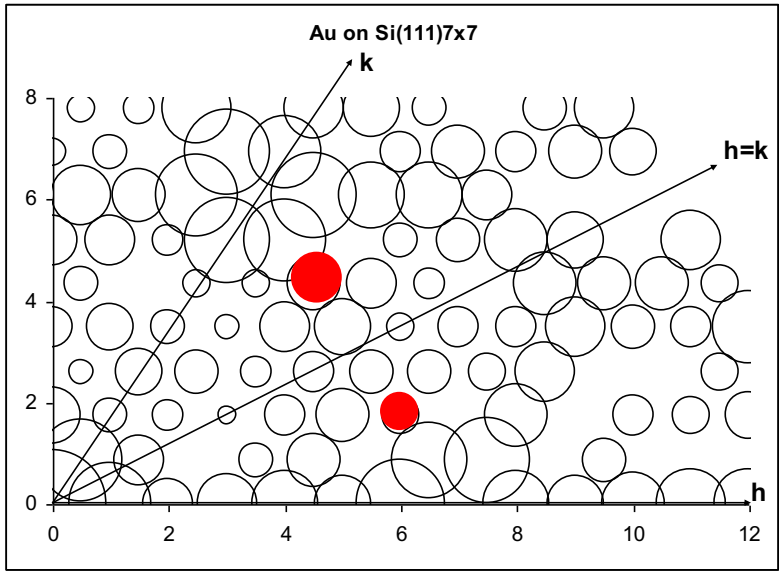


Structure factor data shows p6mm symmetry breaking

Clean Si(111)7x7



0.06 ML Au on -Si(111)7x7

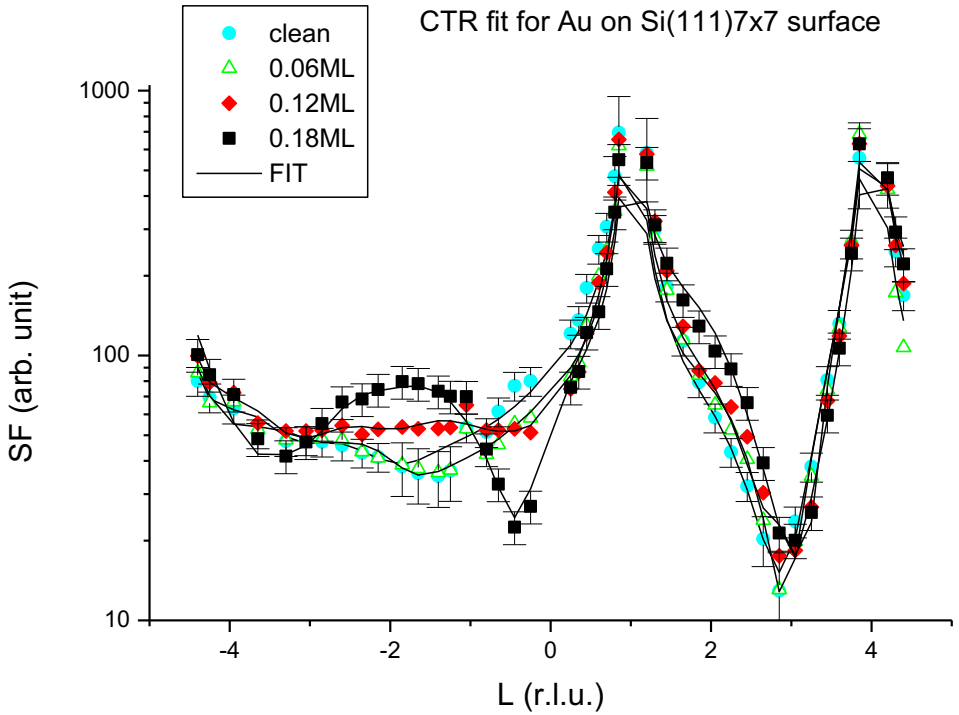


Agreement factor (□) between equivalent reflections (L = 1.5) averaged assuming P3m1 and P6mm symmetry

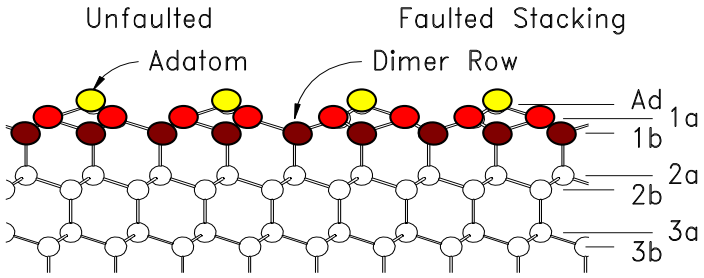
Sample Type	Agreement factor (□) P3m1	P6mm
clean	0.061	0.076
Au-0.06 ML	0.079	0.156
Au-0.12 ML	0.059	0.110
Au-0.18 ML	0.056	0.079

CTR's vs Au coverage

(10L) CTR for different coverage of Au

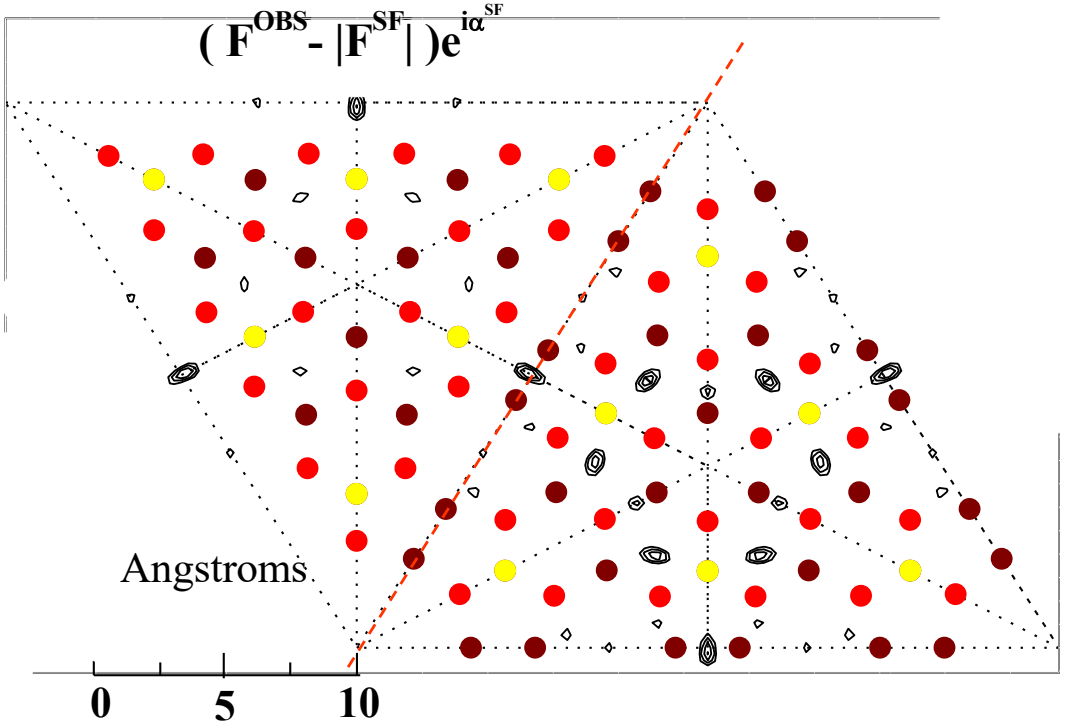


Model "1x1"



- Best fit obtained with two Au atoms positions
- Occupancy of Au atom increases for higher coverage Au
- CTR fit gives the z-positions of Au atoms

Real Space 3D-Density Difference Map



$$\rho_{xyz}^{obs} = \sum_{hkl} (|F_{hkl}^{obs}| - |F_{hkl}^{c}|) e^{i\alpha_{hkl}^{c}} \exp(-2\pi(hx + ky + lz))$$

z~ adatom height

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Cho & Kaxiras Surf. Sci. 396 L261 (1988)

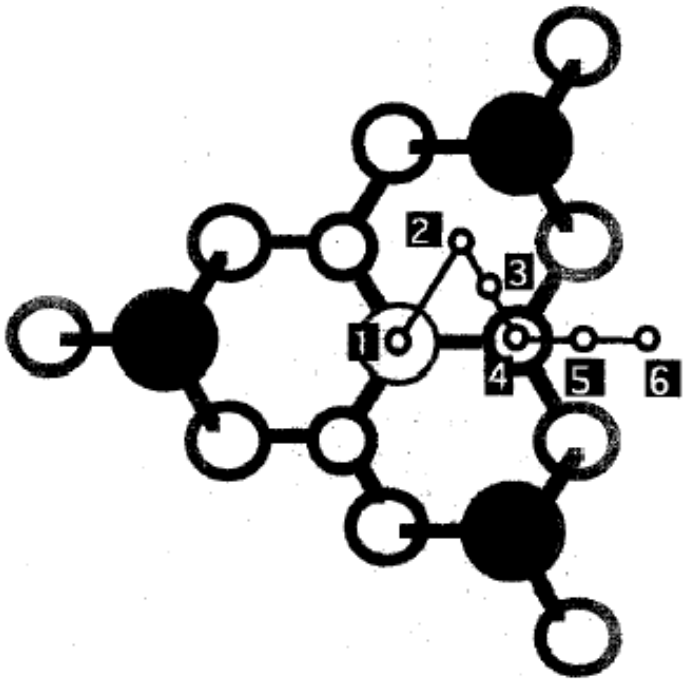


Fig. 1. Schematic top-view representation of a portion of the Si(111) reconstruction containing three Si adatoms (large black circles) and one rest-atom (grey circle) as well as the substrate atoms directly bonded to those (smaller open circles). The sites where the adsorbate atoms are placed are indicated by the numbers 1–6. These sites are used for the energy plots in Fig. 2.

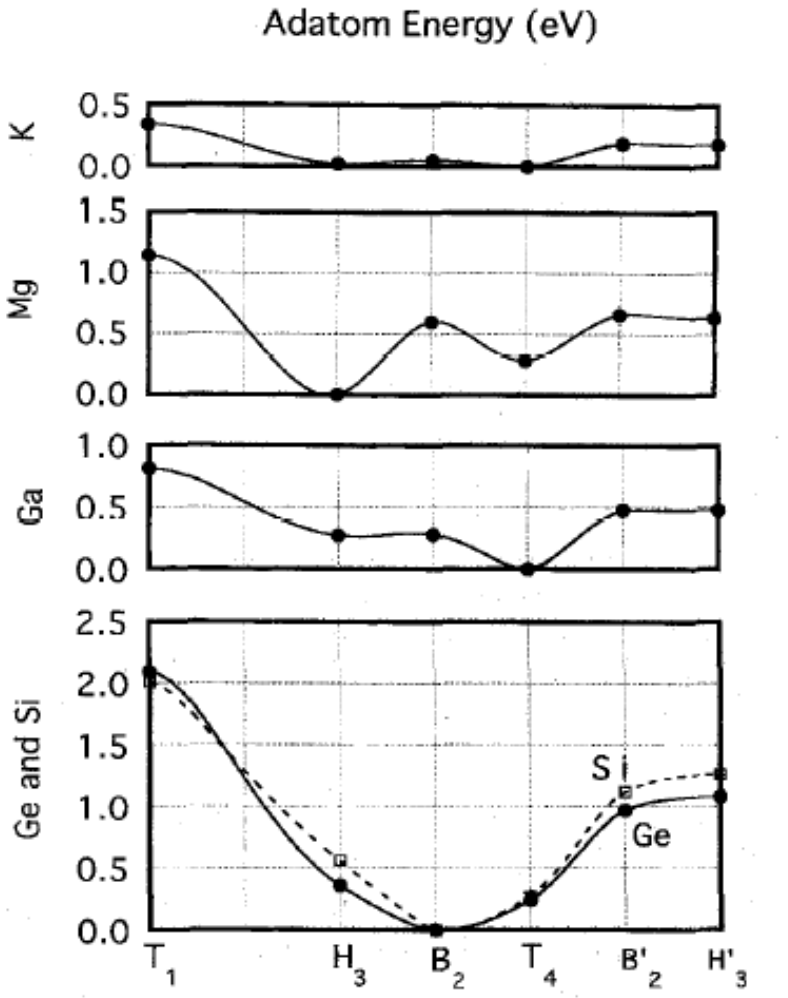
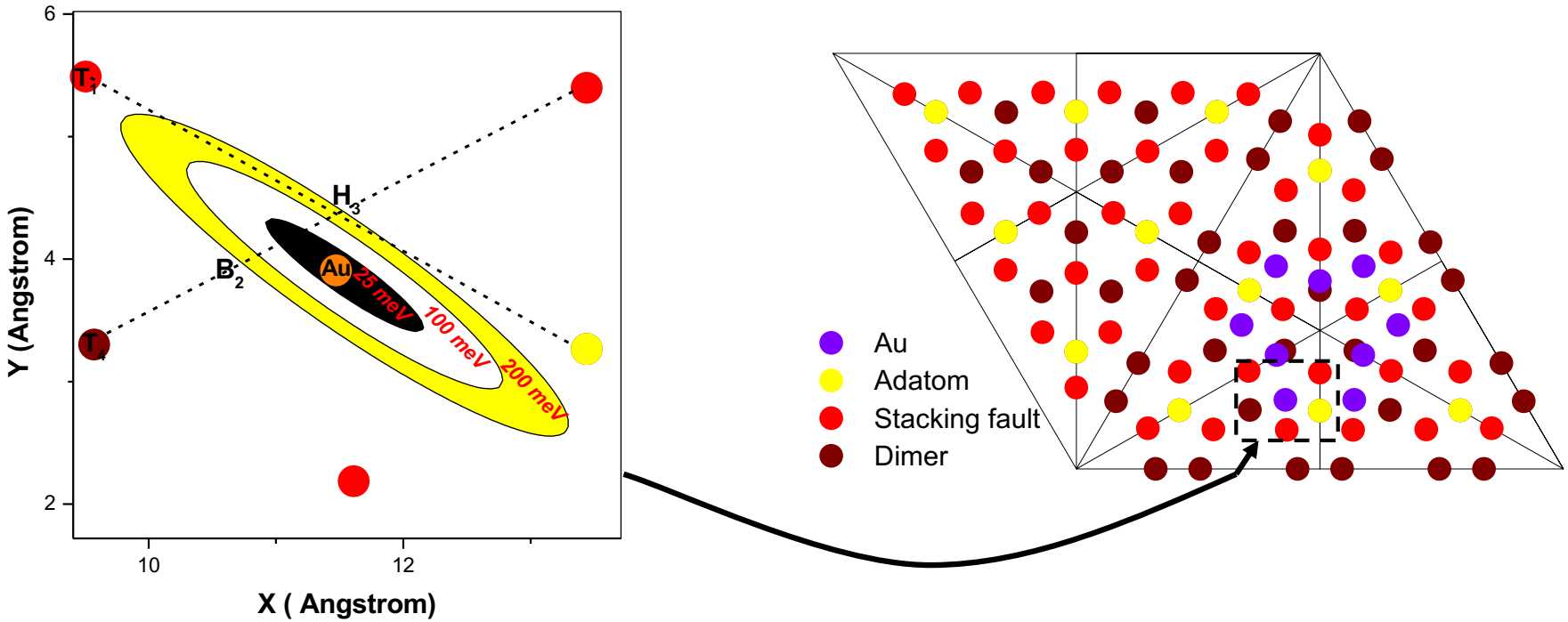


Fig. 2. Plots of the adsorbate atom energies along the six sites defined in Fig. 1 (from left to right the six sites are T_1, H_3-type, B_2-type, T_4-type, B_2'-type and H_3'-type). The energies are relative to the lowest energy sites for each adsorbate atom (see Table 1).

Potential from Anistropic DWF

One Particle Potential $V(x,y) = - k_B T [\text{Log} \{ \text{FT (DWF)} \}]$
$= -25.84 [\text{Log} \{ \text{FT (DWF)} \}]$ meV at 300 K

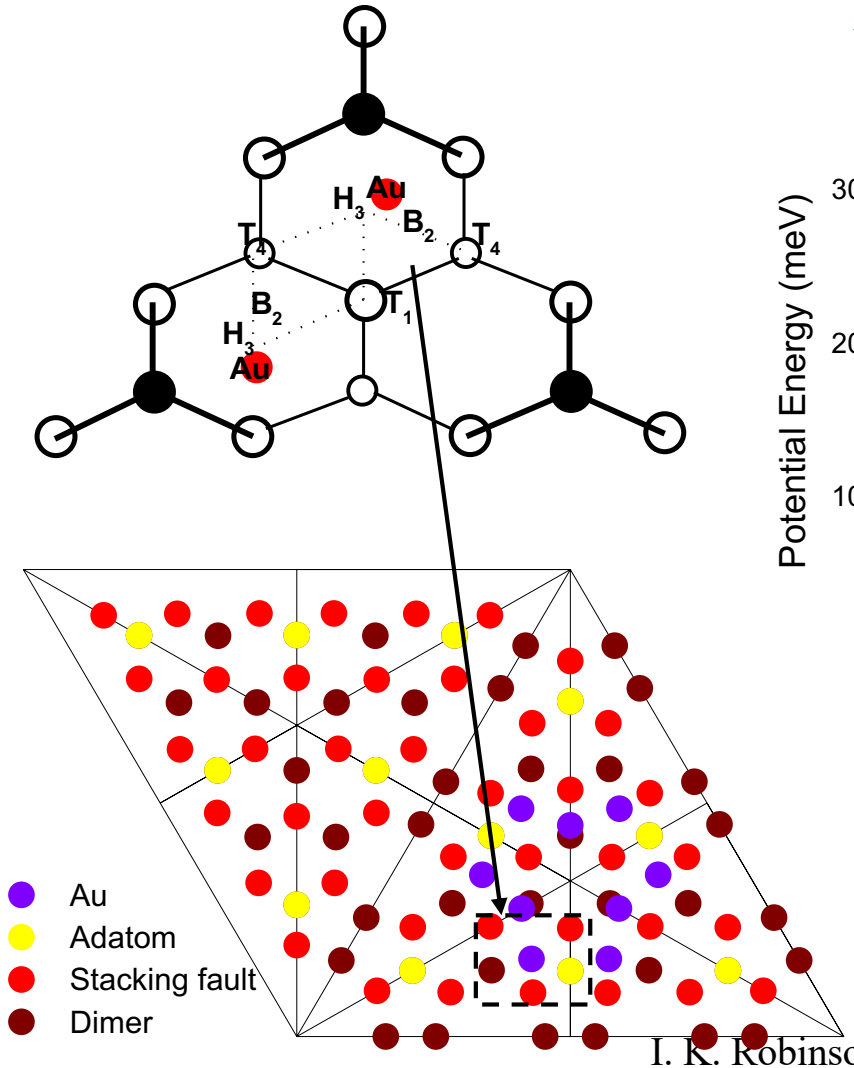
Potential Energy within Basin of Attraction



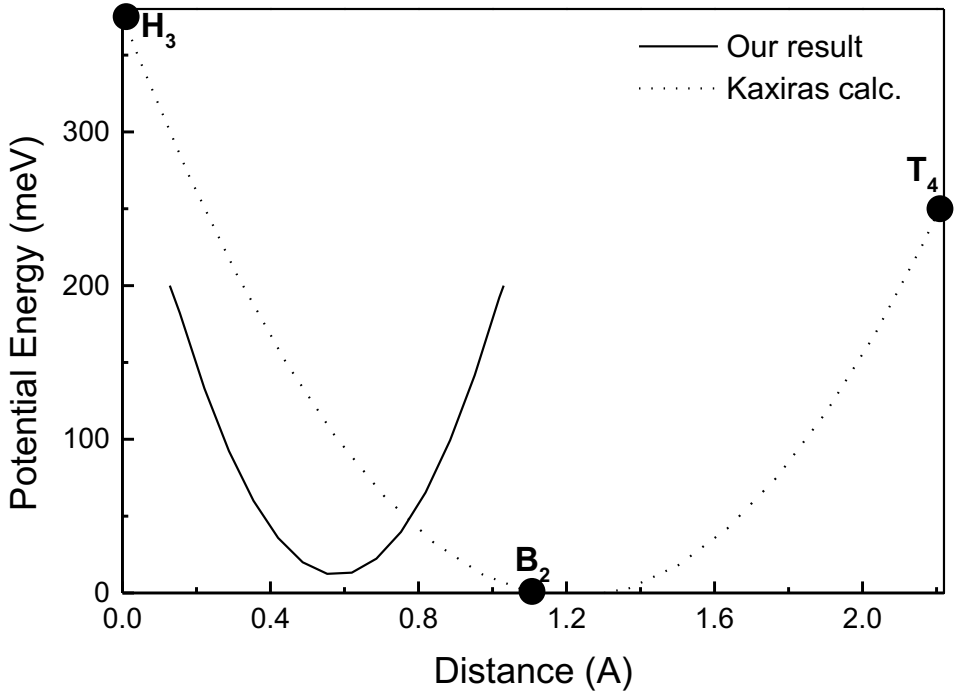
H. L. Meyerheim, I. K. Robinson and R. Schuster, Surf. Sci., 370,268(1997)

Comparison with Theory

Basin of Attraction



Potential Energy within Basin of Attraction



Kyeongjae Cho and Efthimios Kaxirax, Surf. Sci, 396, L261(1998)

Passivation of Si by Au?

- Passivation to oxygen in air or LEO?
- Start with well-defined Au/Si structure.
- Expose to increasing pressures of O_2
- Measure X-ray superstructure signal
- Structure stable in air: expose to AO source
- Result: no structure survived (so far)

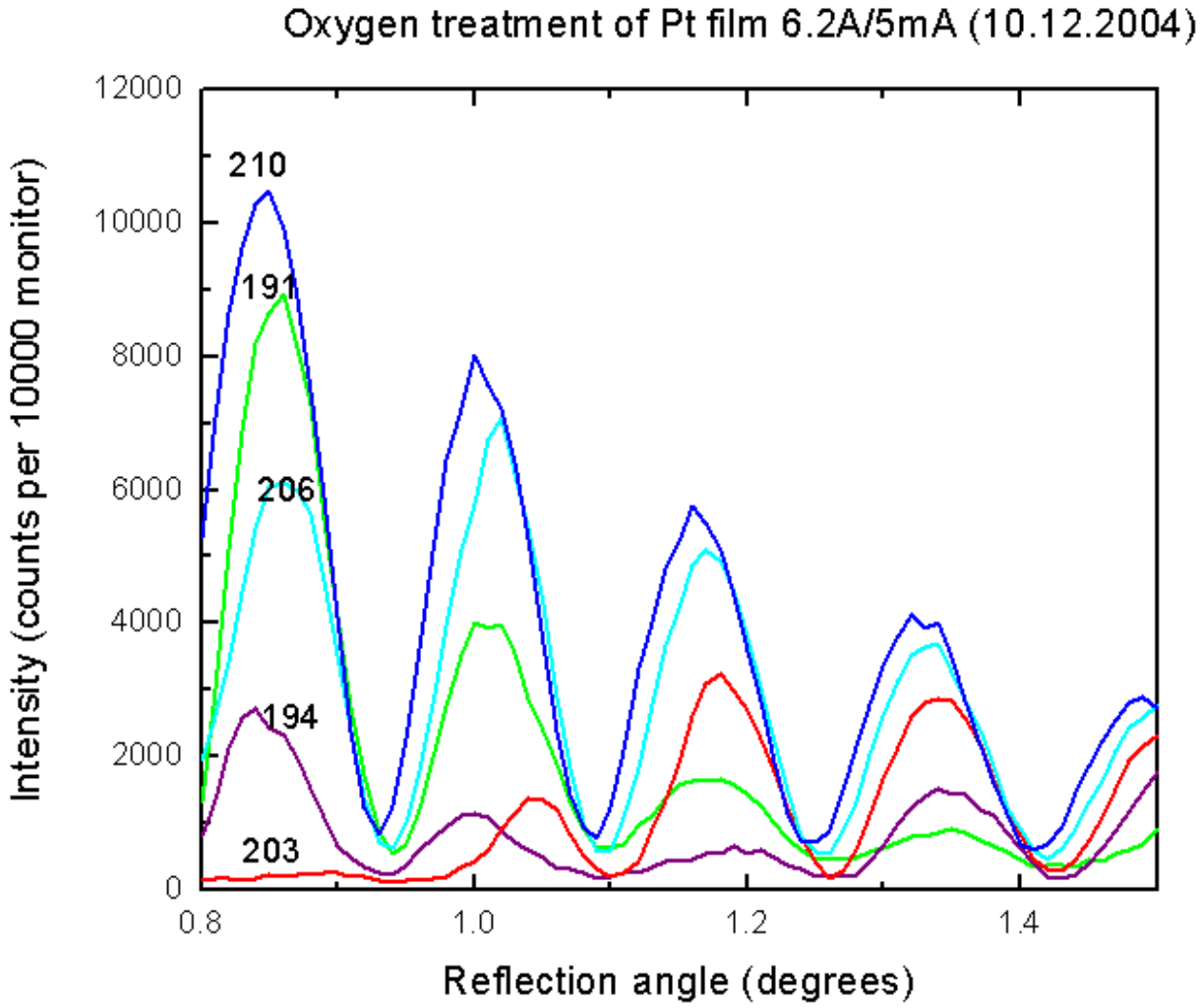
Future plans I

- Surface structures: insufficient material
- Grow thin films of Au on H-terminated Si(111)
- Establish minimum thickness stable in air
- Expose to AO source (Pittsburgh)
- Analyse integrity of film by X-ray reflectivity
- Correlate thickness and exposure dependences

Future Plans II

- Plasma oxidation of Pt thin films
- Collaboration with Andreas Stierle (MPI) and Jochen Rager (Bosch)
- UHV exposure at P~10^{-8} mbar, hot filament
- Pt forms oxide when 200C<T<450C?
- AO oxidation at RT??

X-ray Reflectivity of 200A Pt film



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Conclusions

- Two interesting Au/Si structures in publication
- No useful passivation effect so far on ordered Au/Si structures
- Thin films have less detailed information about structure, but may passivate
- Pt may be interesting new topic