Surface Crystallographic Structures at I-07

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University College London

I-07 User Working Group
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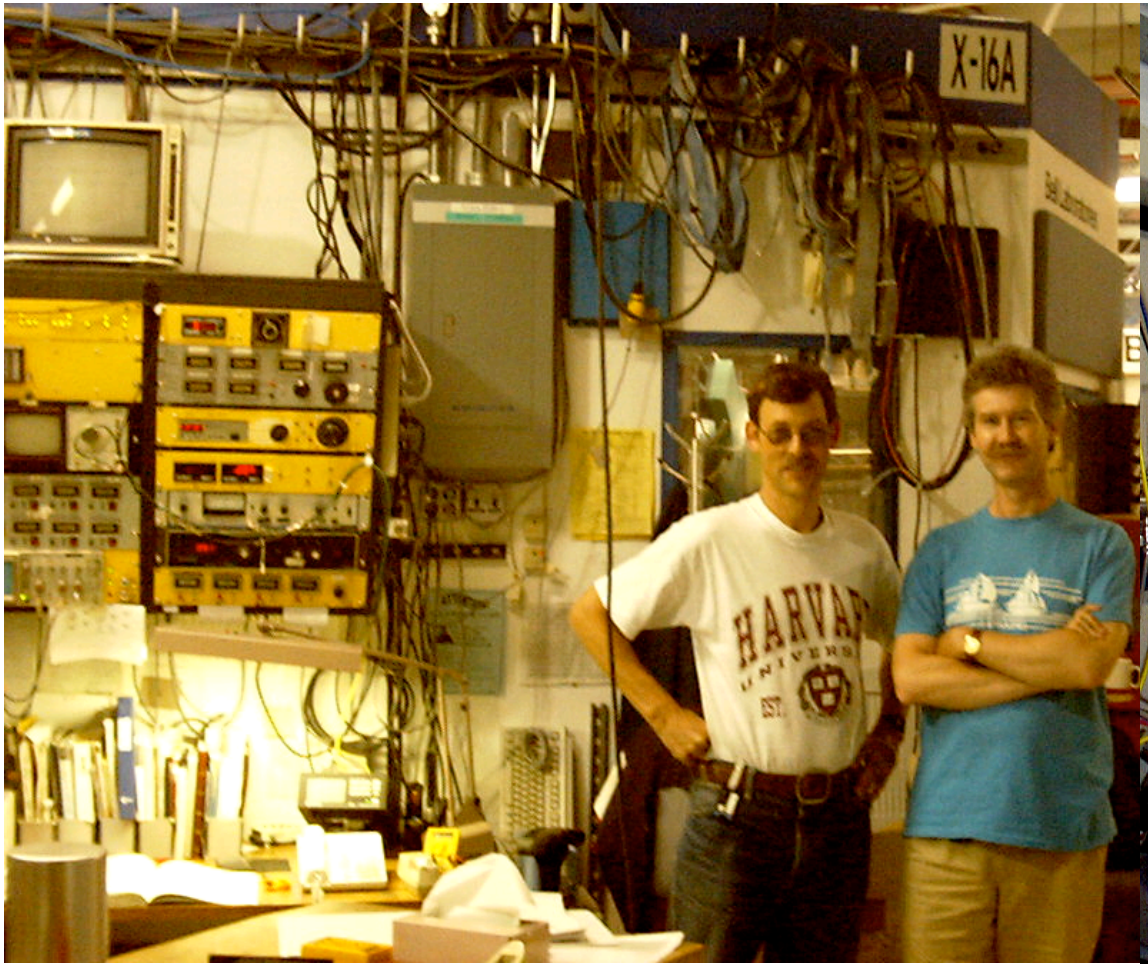
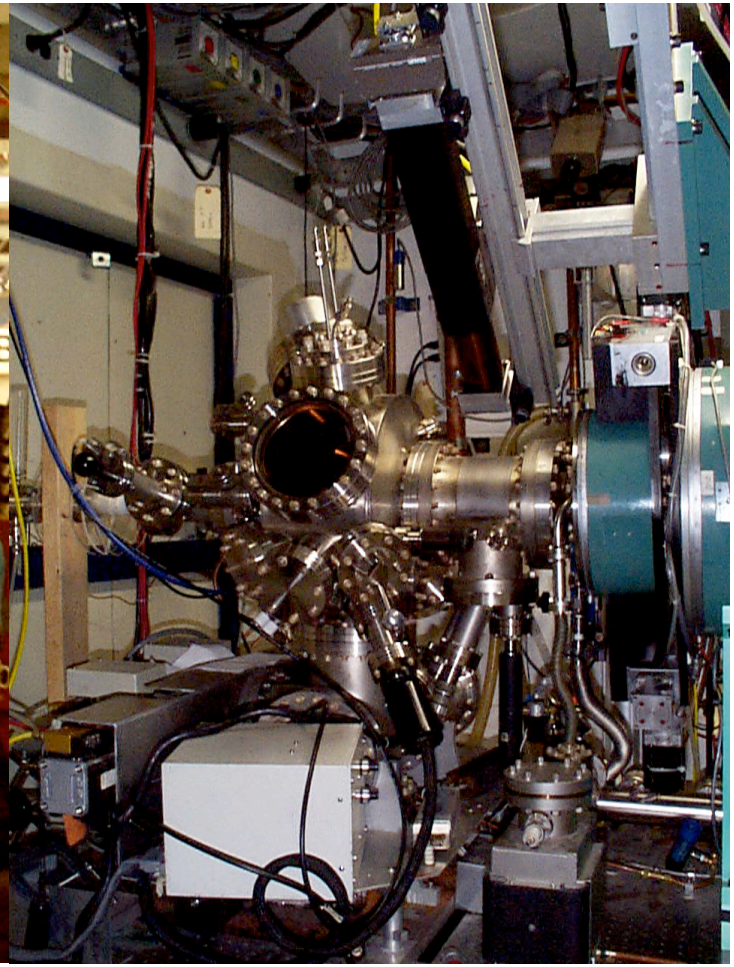
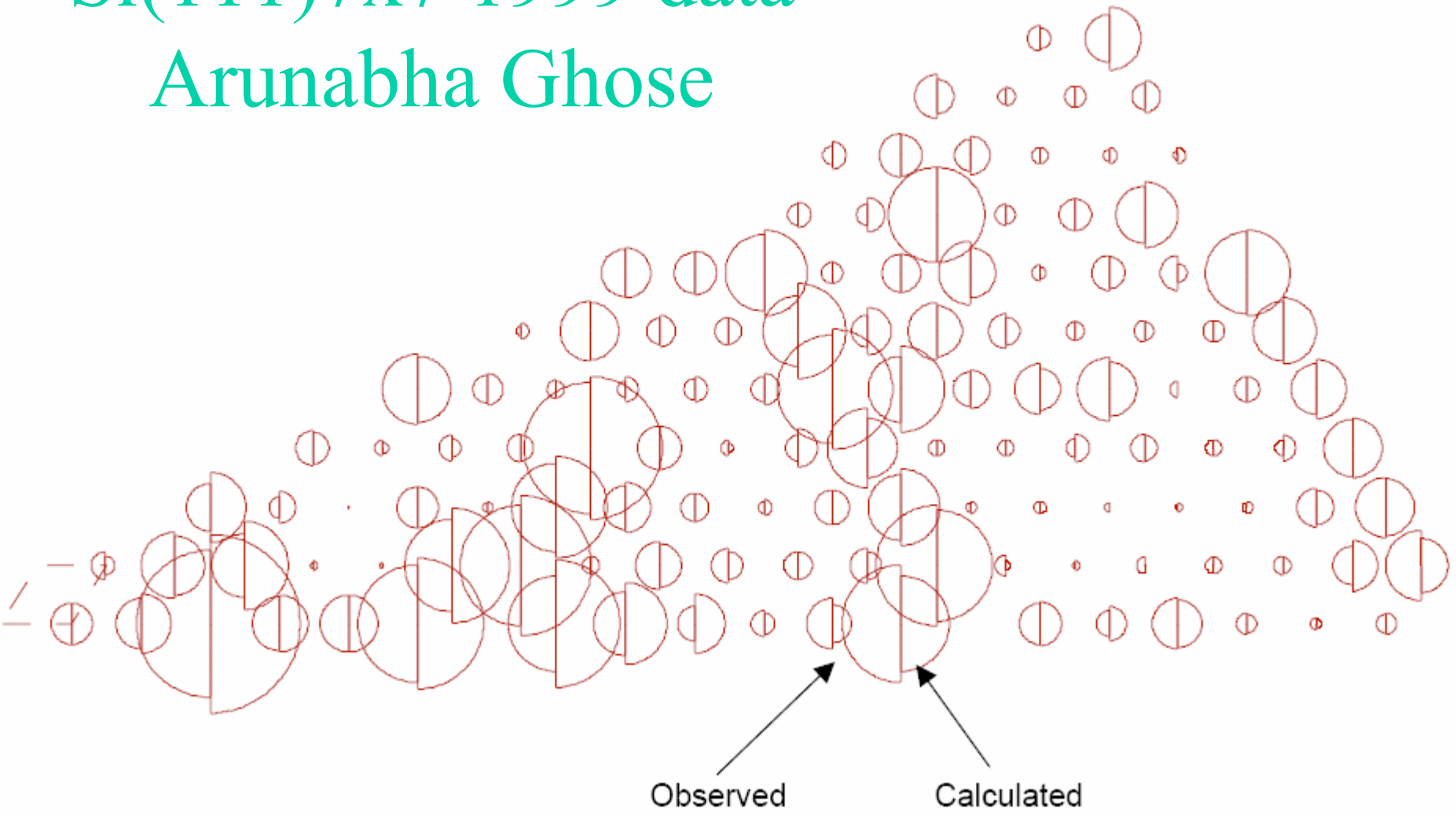
X16A Surface X-ray Diffraction

operating since 1987 ...

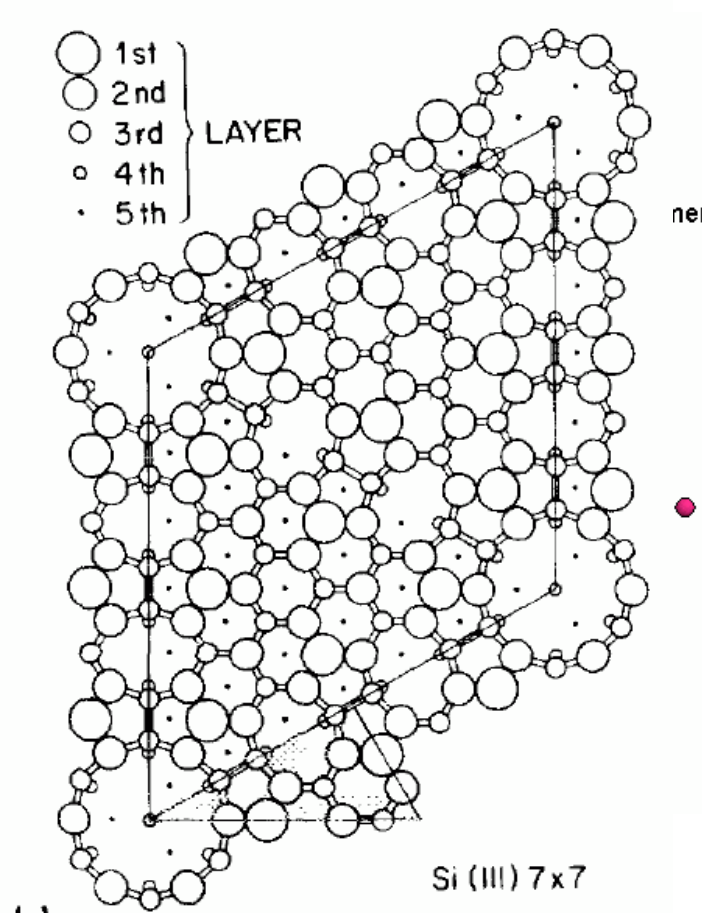


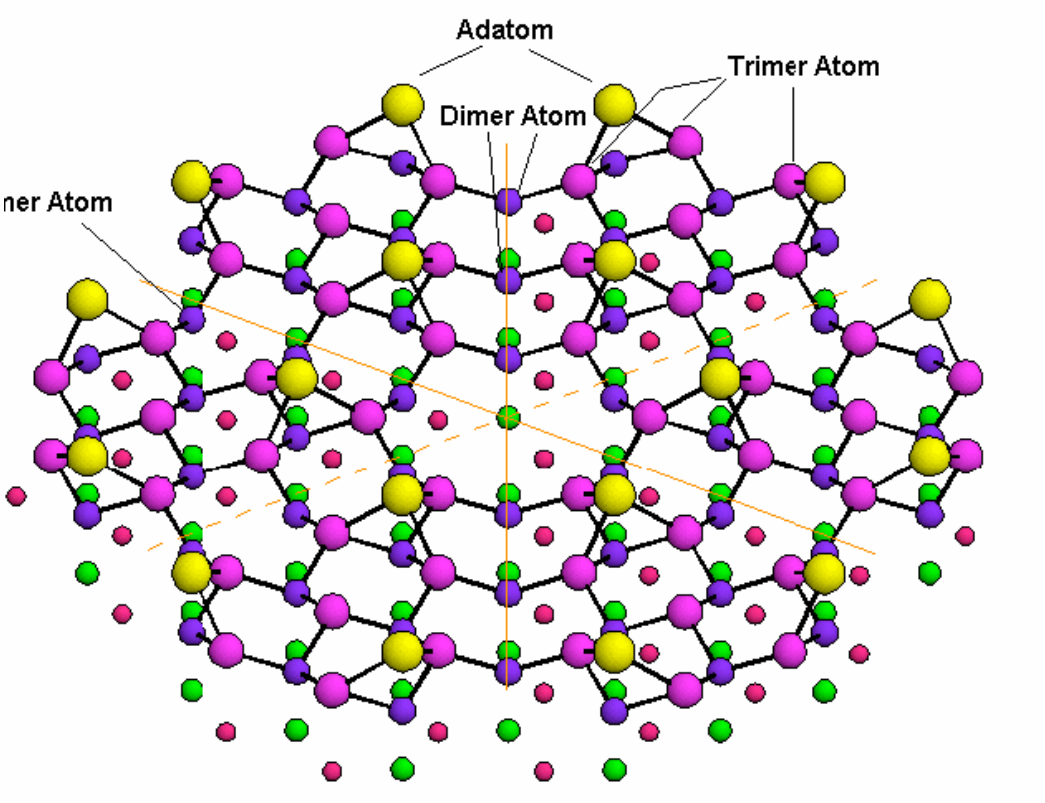


Si(111)7x7 1999 data
Arunabha Ghose

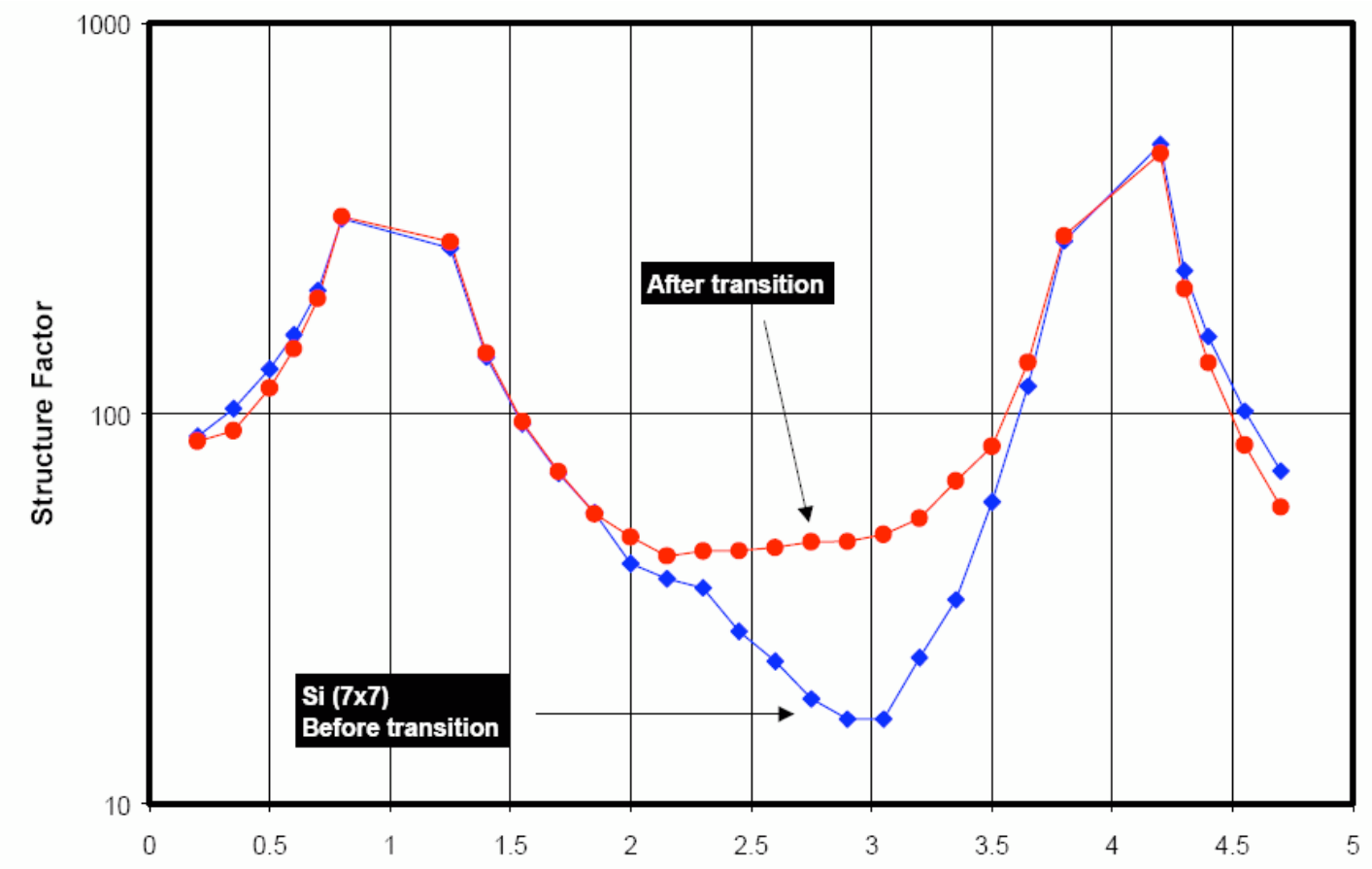


Dimer Adatom Stacking-fault model
K. Takayanagi (1985)

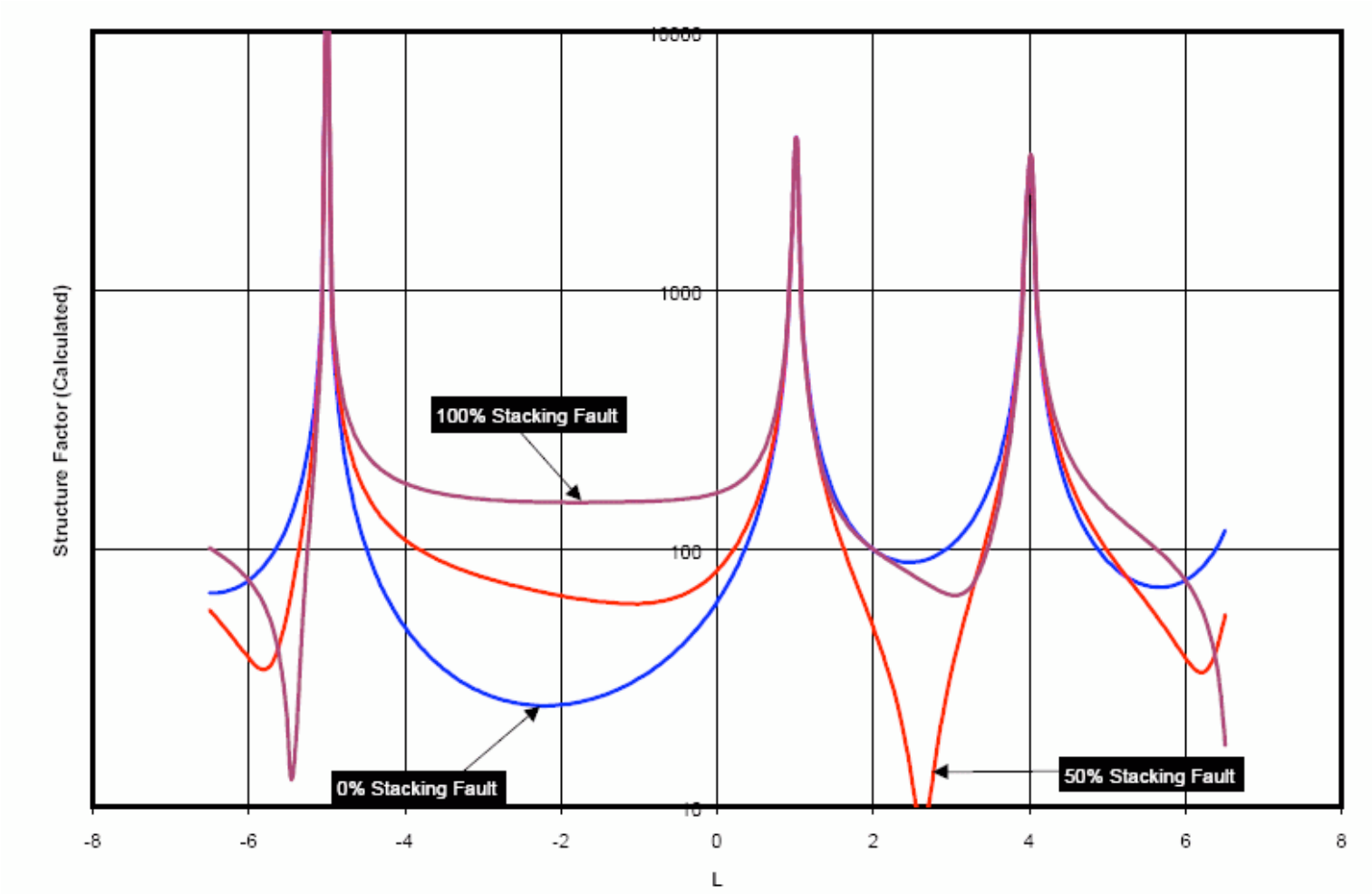




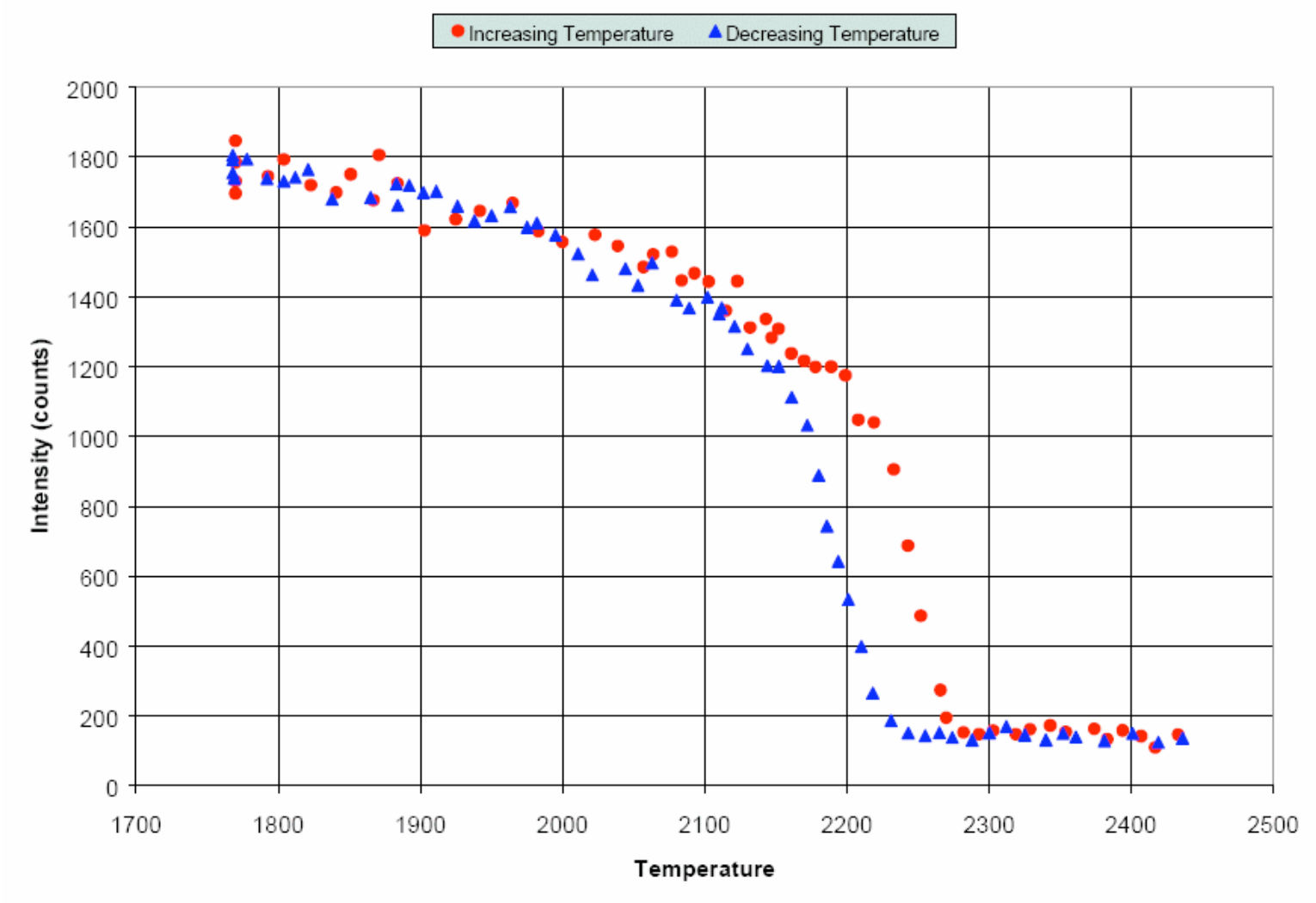
Si(111) phase transition



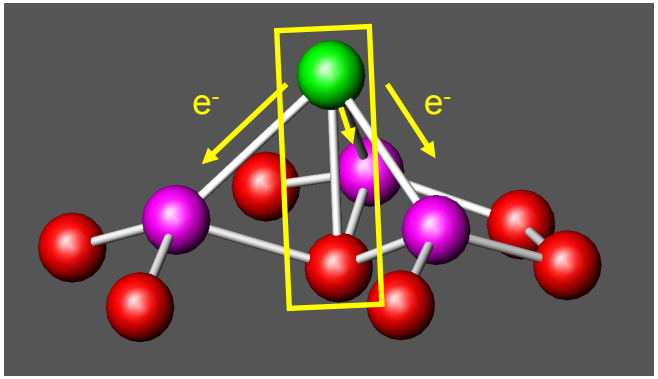
Si(111) CTR is sensitive to stacking faults



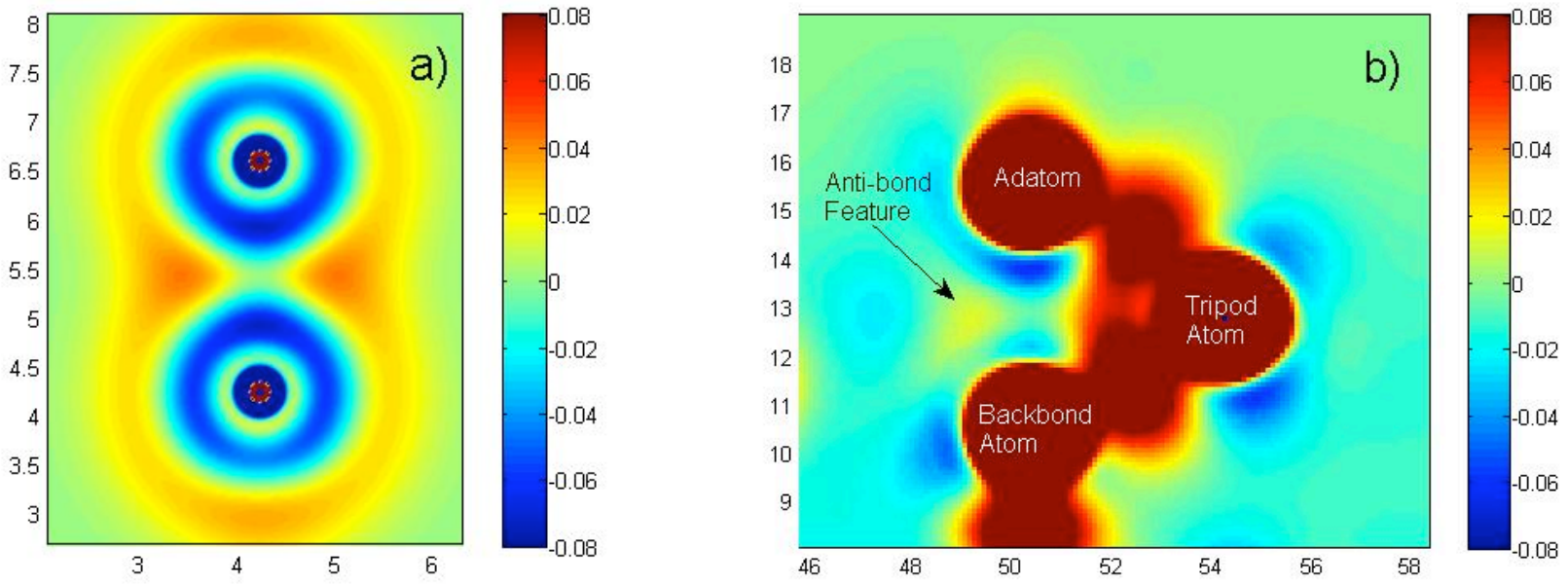
Si(111) phase transition



Adatom Geometry
Jim Ciston and Laurie Marks
Northwestern U



a) IAM-BCPA Anti-Bond feature difference map for an isolated Si-Si pair
b) (110) slice through an unfaulted central adatom (DFT difference map)

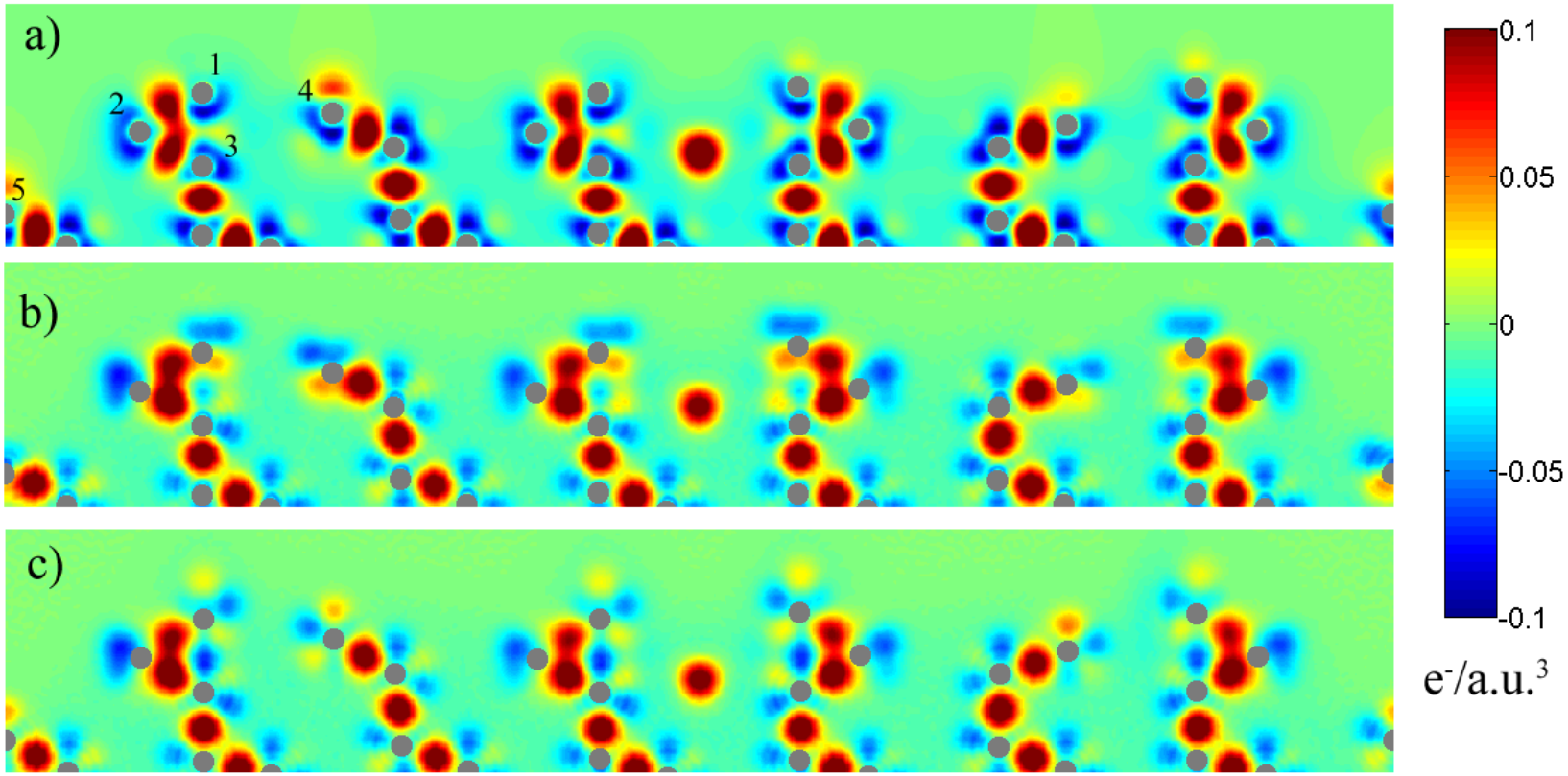


(110) slice of Si(111) 7x7 unit cell

a) the DFT difference density,

b) the difference density using just the conventional BCPA

c) a map of the charge density features fitted



$$F(Q) = F_1(Q)F_2(Q)$$

$$I(Q) = |F_1(Q)|^2|F_2(Q)|^2$$

$$F_j(Q) = \int \rho_j(x)e^{iqx}dx$$

$$F_j^*(Q) = \int \rho_j(-x)e^{iqx}dx$$

$$I(Q) = |\int \rho_1(x) \circ \rho_2(x)e^{iqx}dx|^2$$

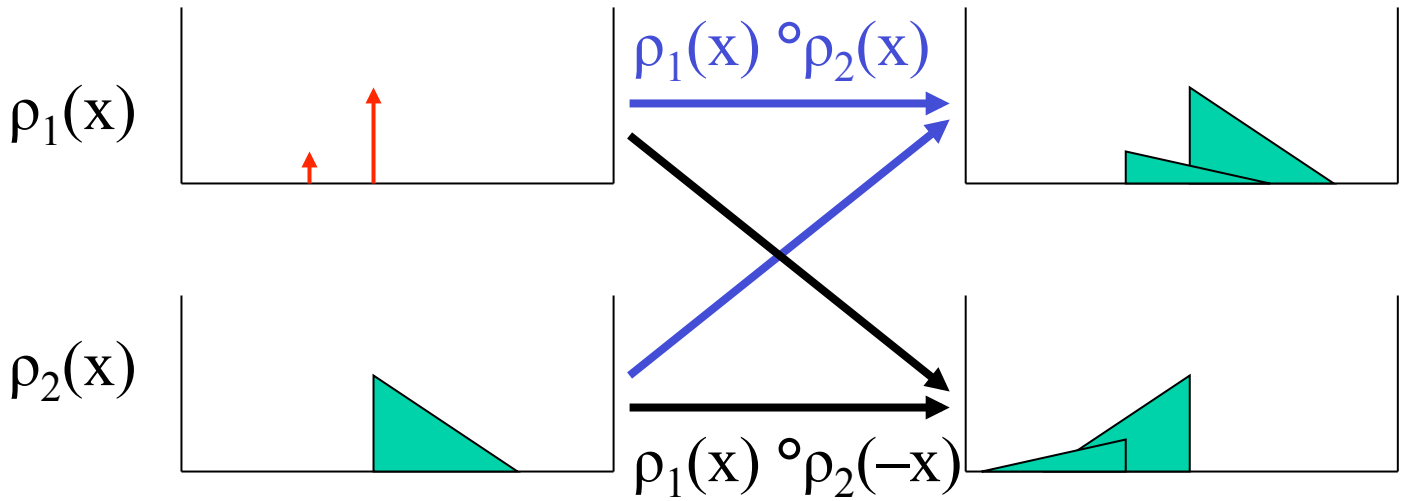
$$I(Q) = |\int \rho_1(-x) \circ \rho_2(x)e^{iqx}dx|^2$$

Homometric structures

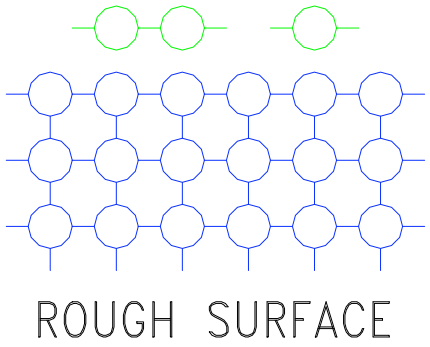
Identical diffraction from two structures whenever the structure factor is factorizable

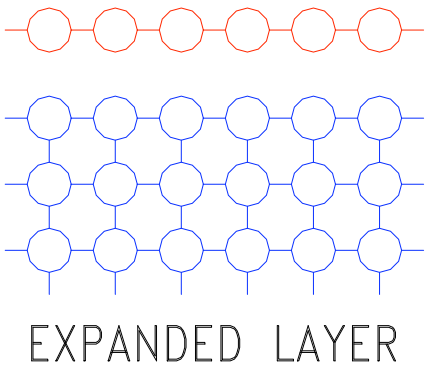
Homometric structures II

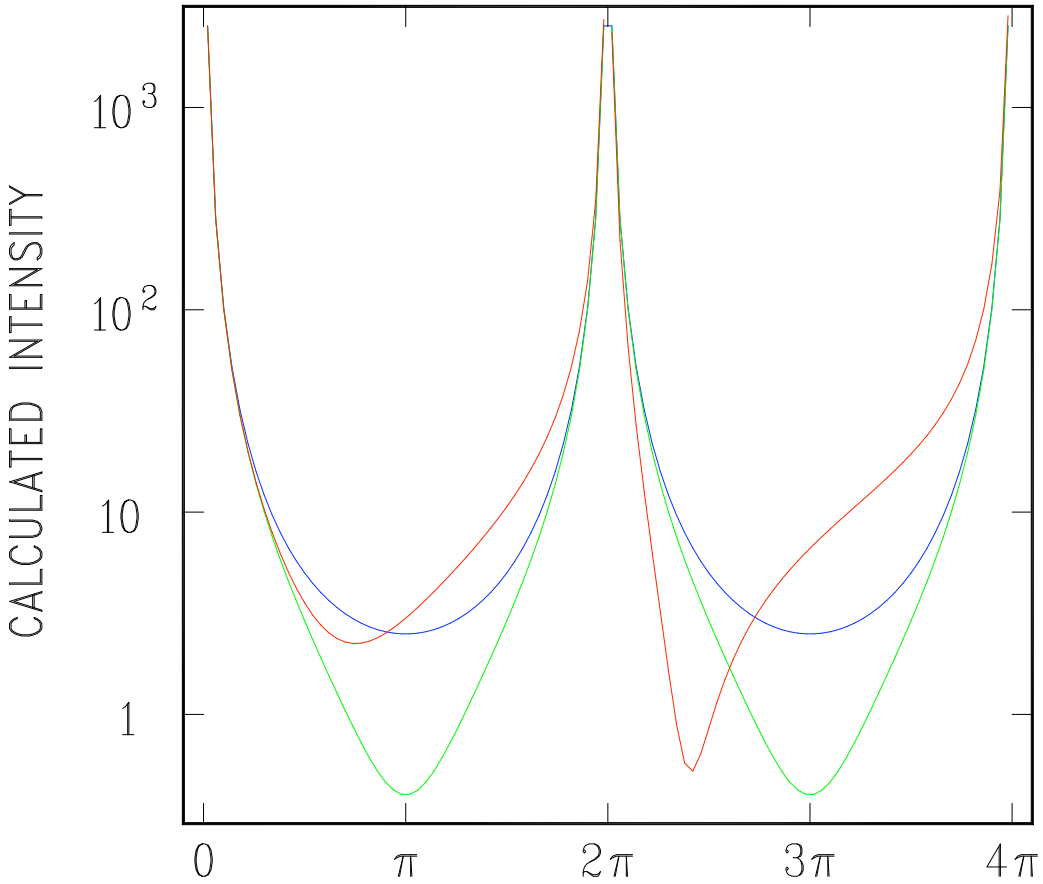
Convolution of two structures without mirror symmetry



CTR is Sensitive to Surface Structure

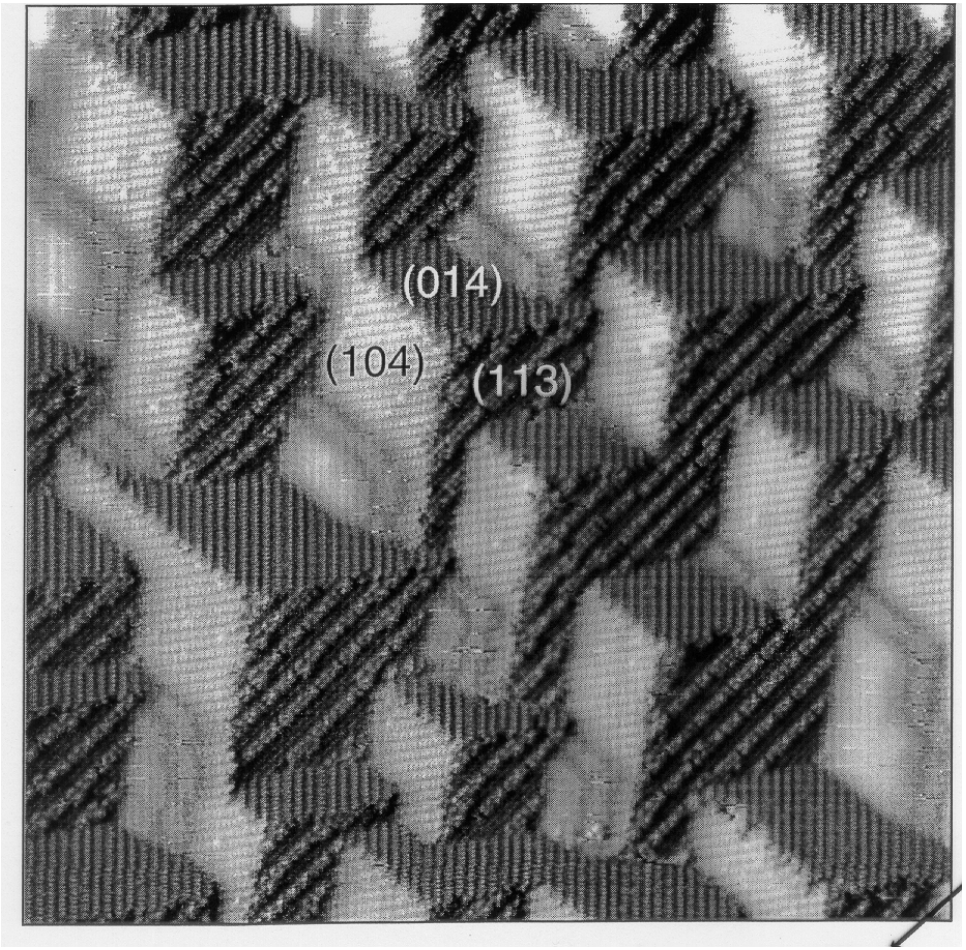


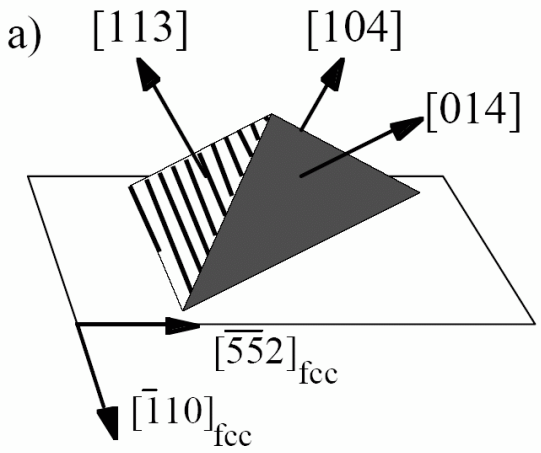


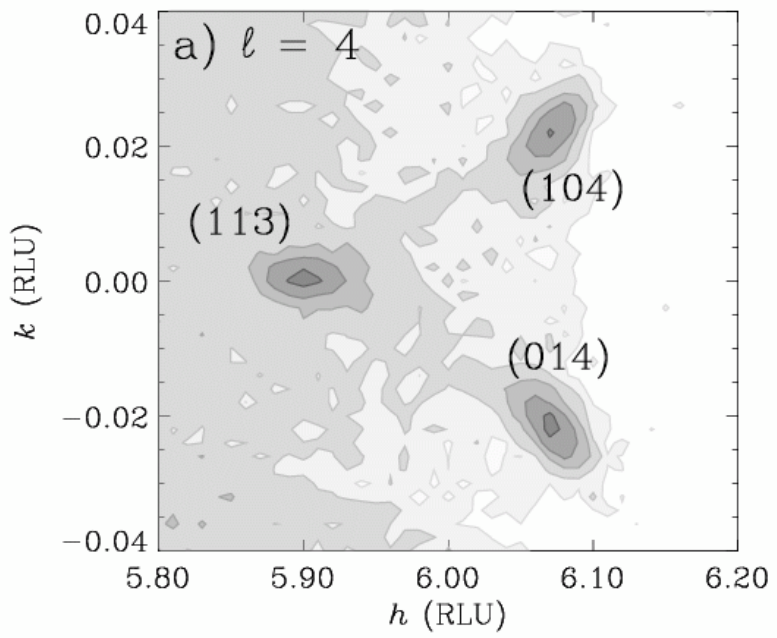


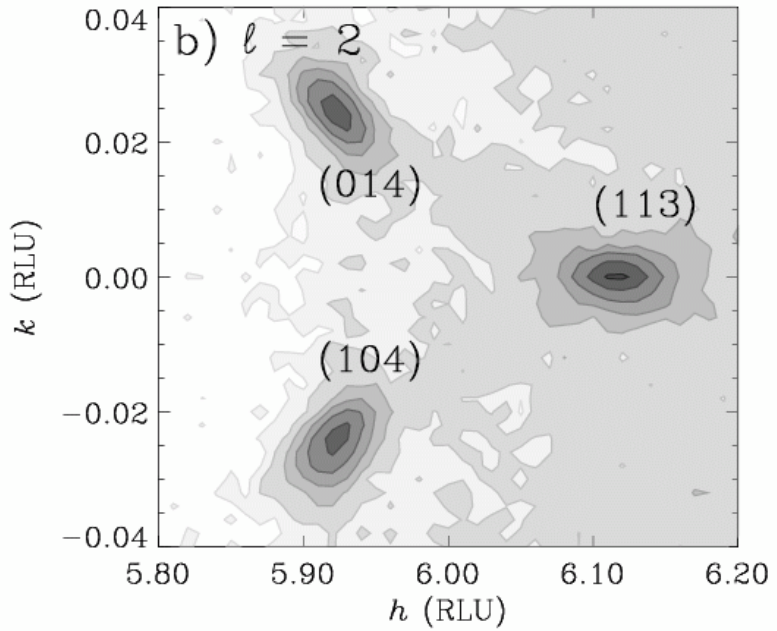
Cu(115) after Oxidation: STM

S. Reiter and E. Taglauer, Surf. Sci. **367** 33 (1996)





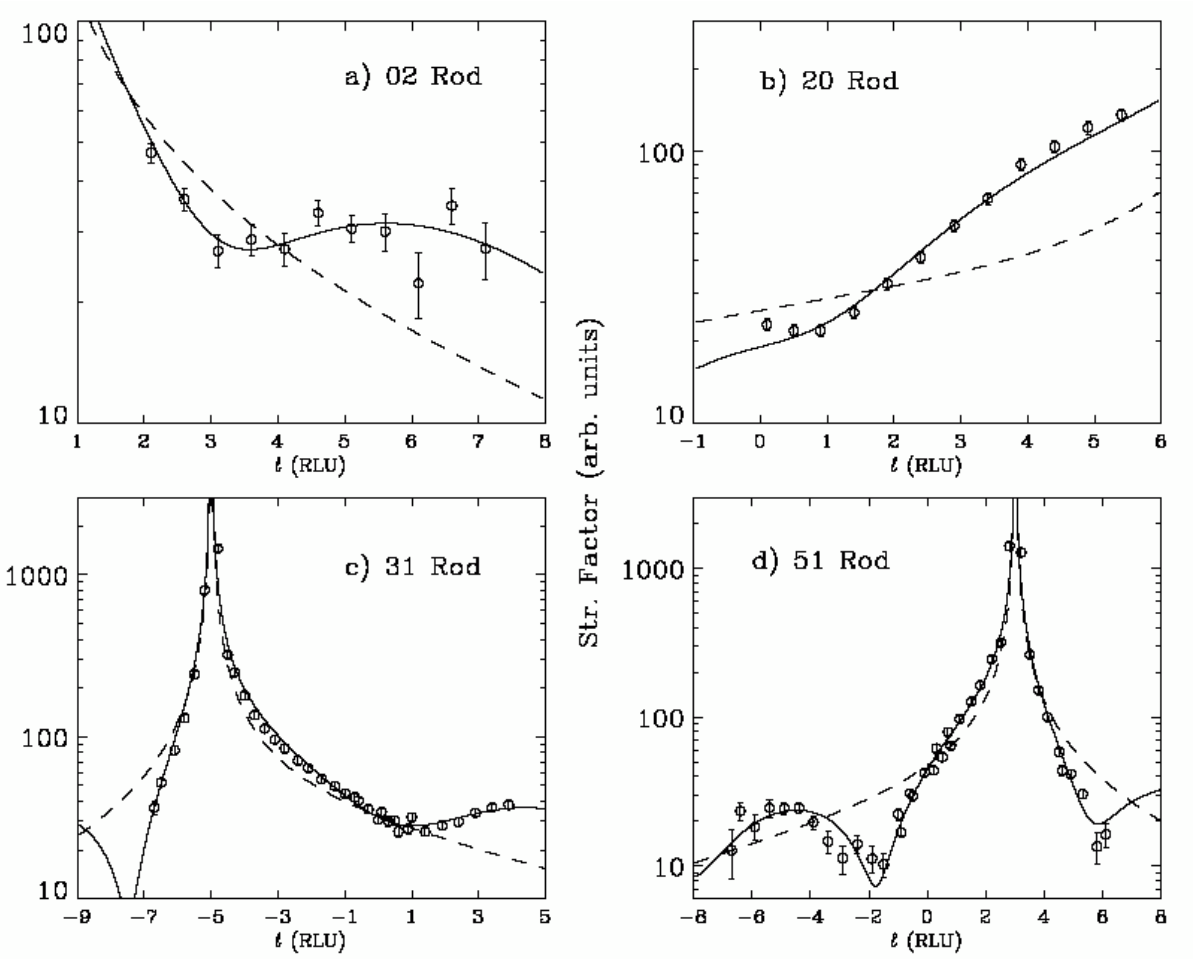




Cu(115) after Oxidation: X16A

Don Walko, UIUC PhD Dissertation (2000)

Re-index CTRs for Cu(104) facets



Future Directions
(verbatim from review in 9/2005)

- Surfaces of light elements
- Buried interfaces, such as solid-liquid
- Quantum dots and wires CXD
- Fluctuating surfaces, capillary waves XPCS
- Nanostructured rough surfaces GISAXS, XPCS
- Continuum models of strain
- Improved parallel techniques for large datasets CCD