Overview of Surface Diffraction

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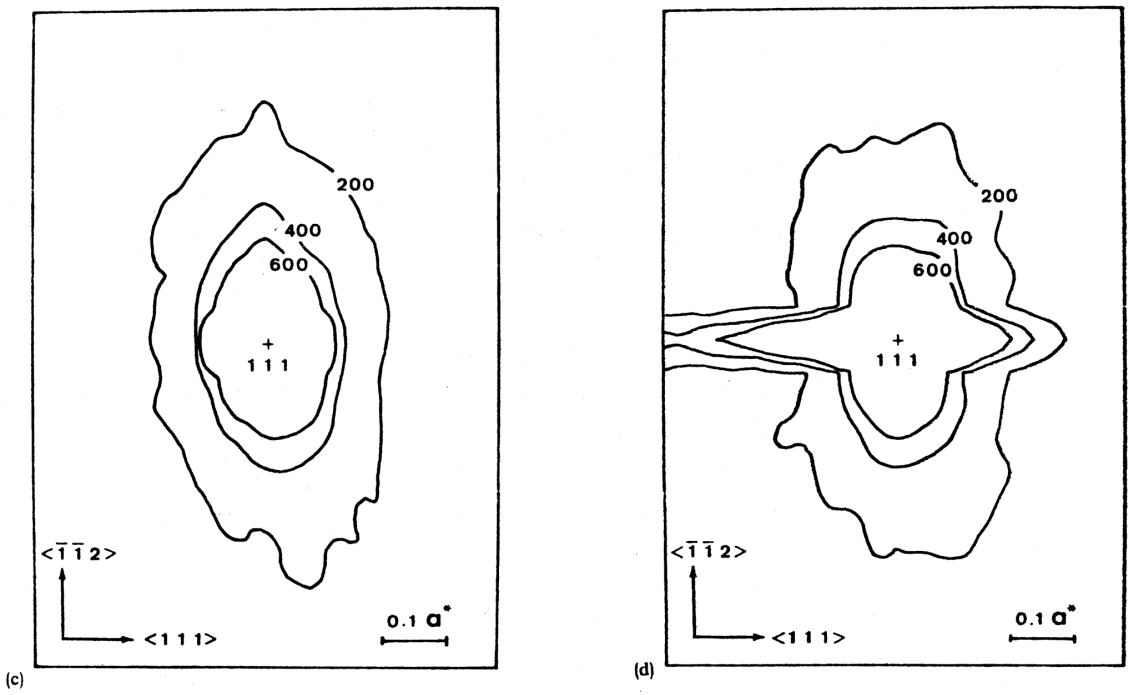
ESRF Workshop 4 March, 2004

Diffuse Scattering from Si Wafer



Unpolished wafer 40 microns removed

N. Kashiwagara, J. Harada and M. Ogino, J. Appl. Phys 54 2706 (1983)

Diffraction as a Surface Integral

Die äußere Form der Kristalle in ihrem Einfluß auf die Interferenzerscheinungen an Raumgittern

Von M. v. Laue

Annalen der Physik [5] 26 55 (1936)

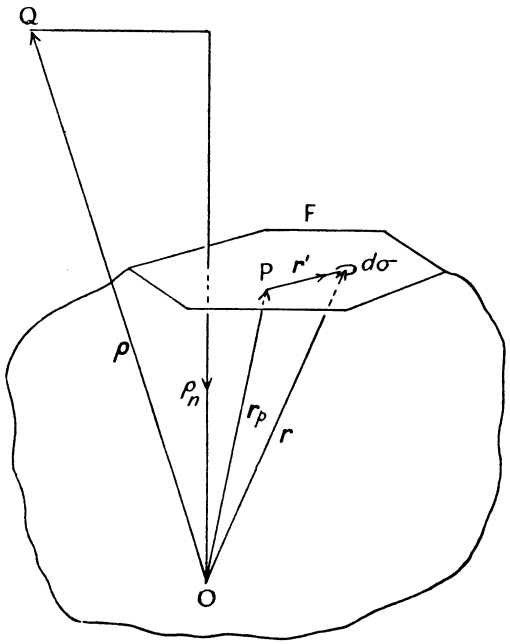
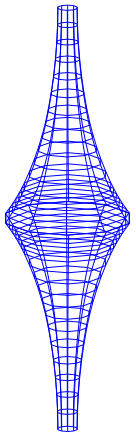
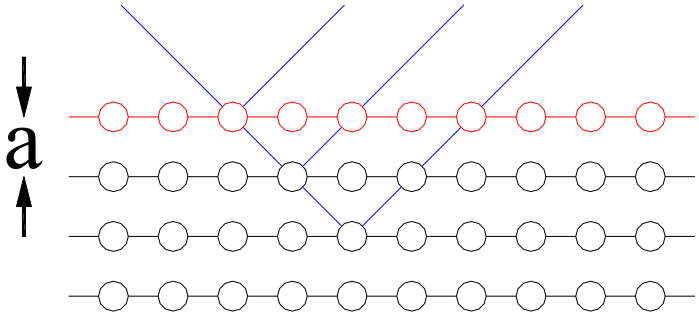


FIG. 200



"Stacheln"

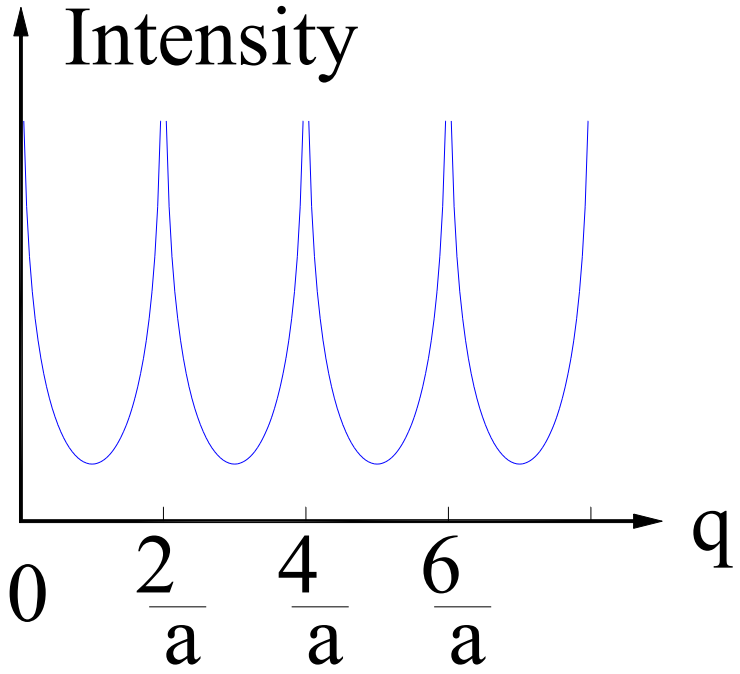
Origin of Truncation Rods



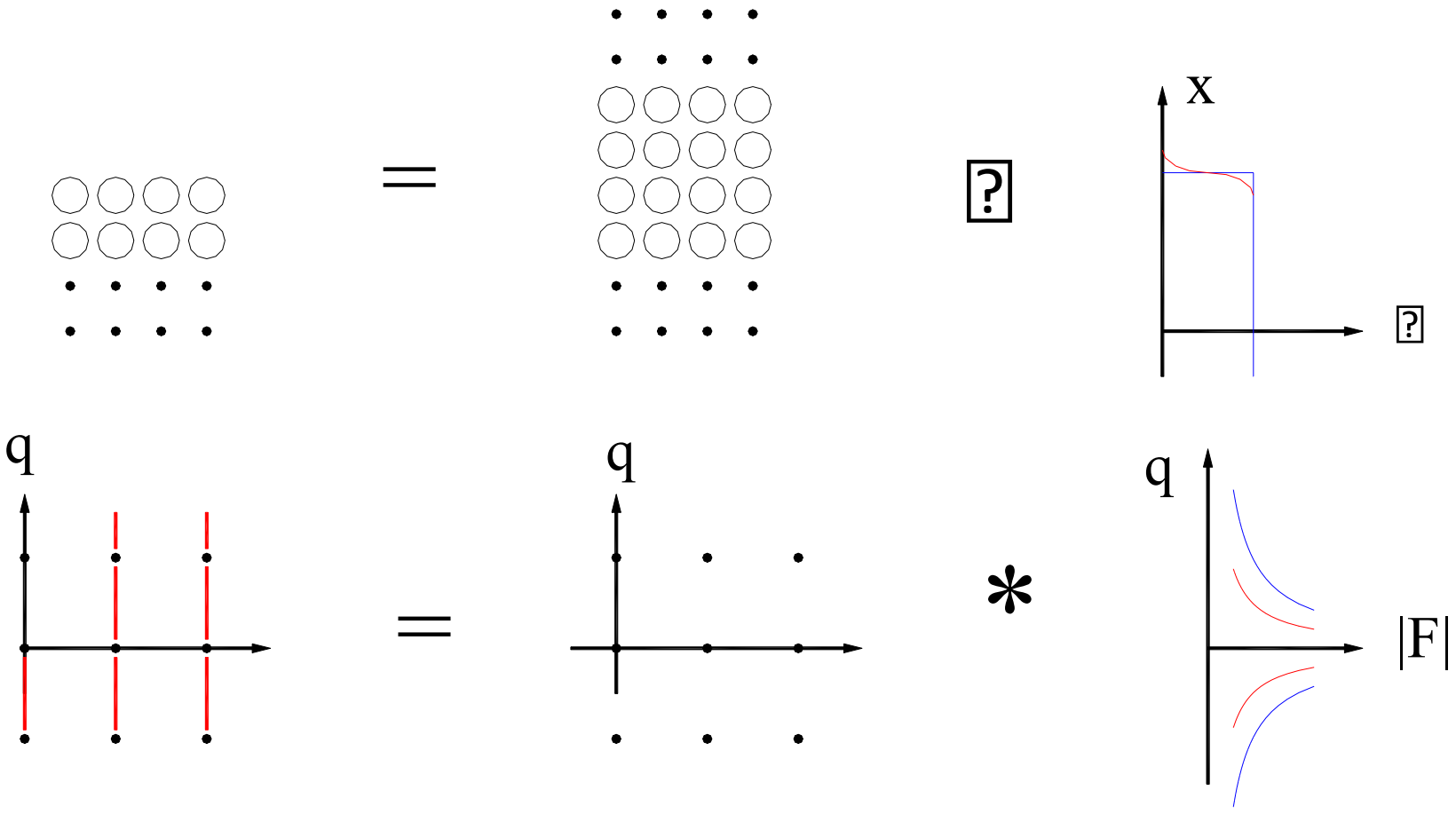
$$F_{CTR} = \sum_{n=0}^{\infty} A_n$$

$$= \sum_{n=0}^{\infty} f_L \; e^{inqa}$$

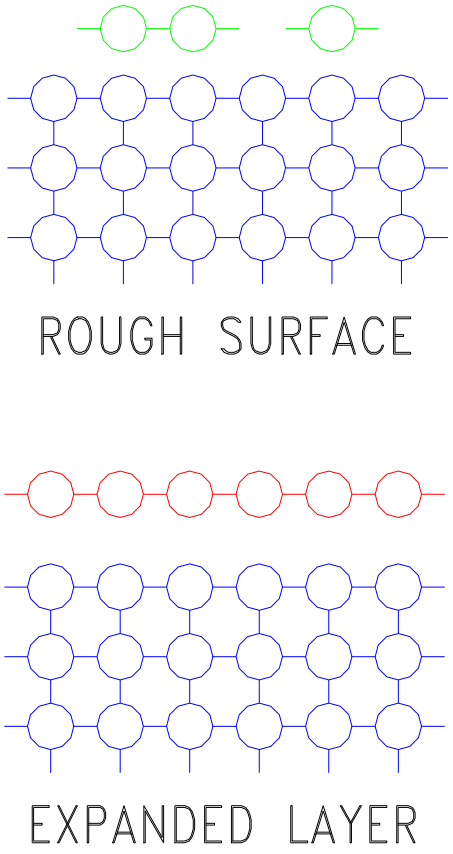
$$= \frac{f_L}{1 - e^{iqa}}$$

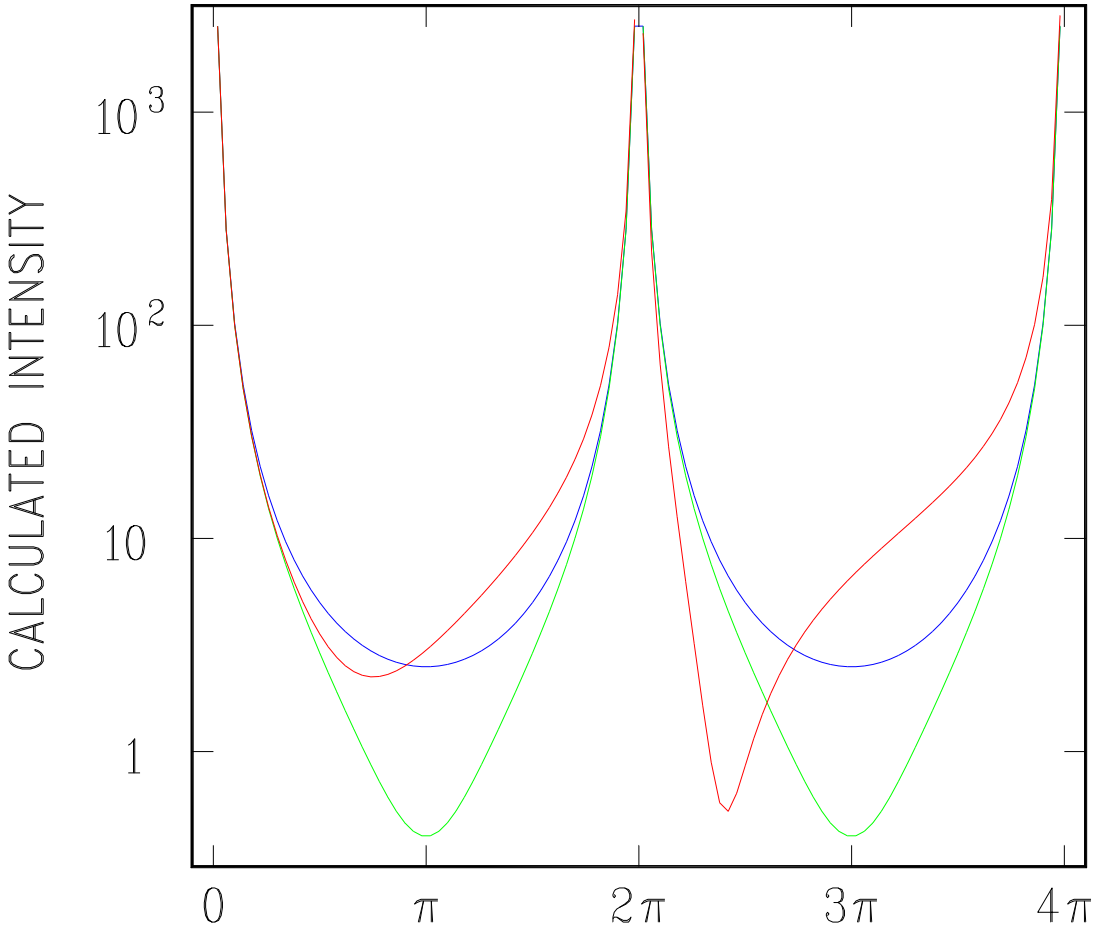


CTR as Convolution



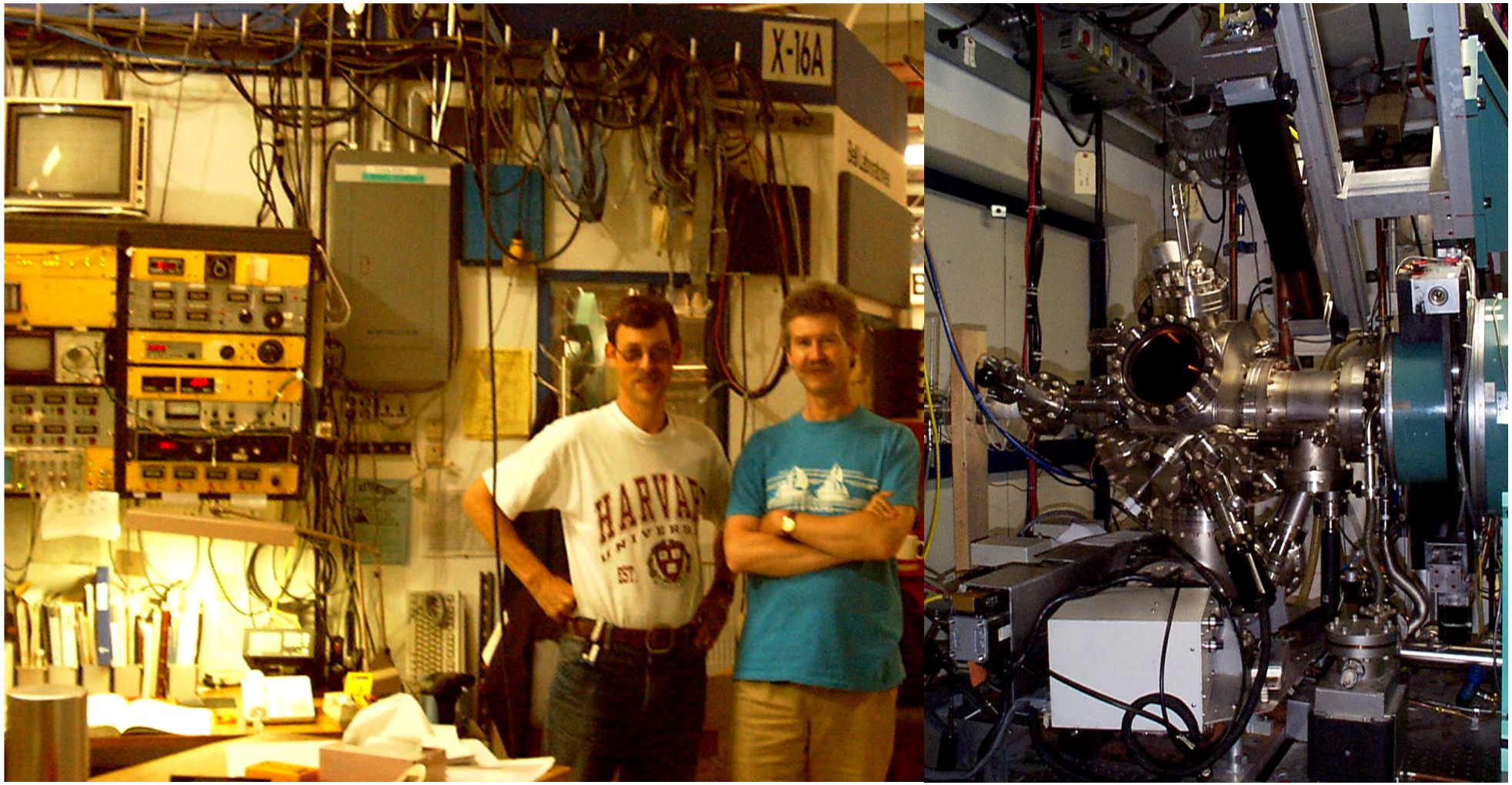
CTR is Sensitive to Surface Structure

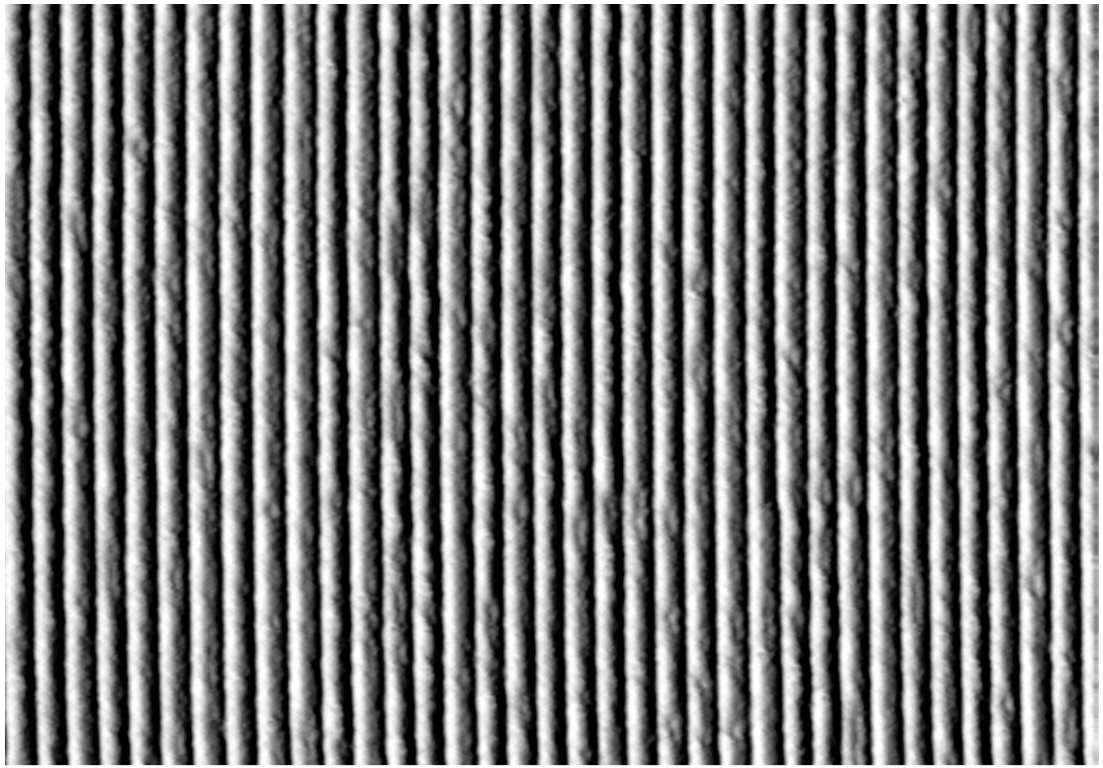


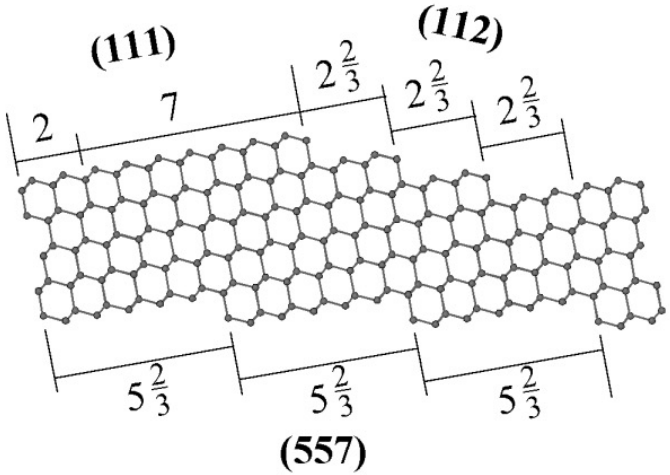


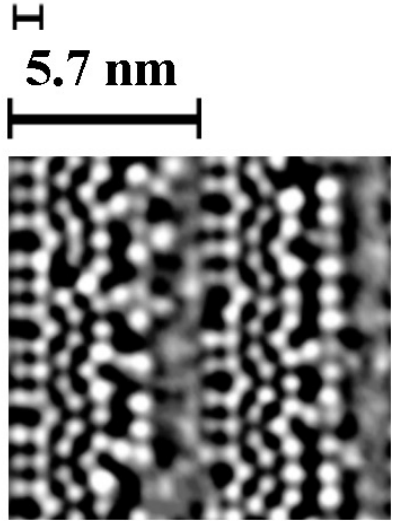
X16A Surface X-ray Diffraction

operating since 1987 ...

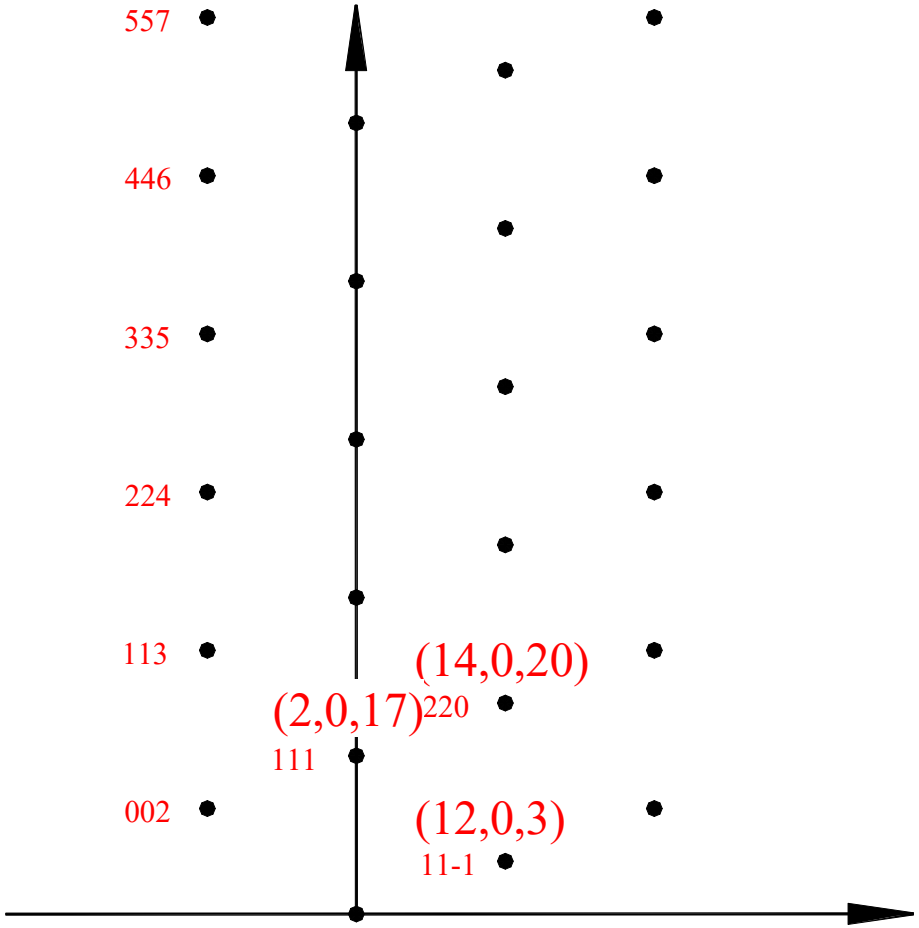




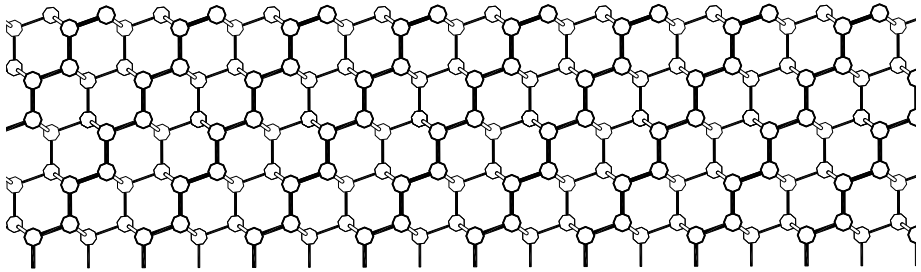

(111)
(112)
2
7
$2\frac{2}{3}$
$2\frac{2}{3}$
$2\frac{2}{3}$
$5\frac{2}{3}$
$5\frac{2}{3}$
$5\frac{2}{3}$
(557)

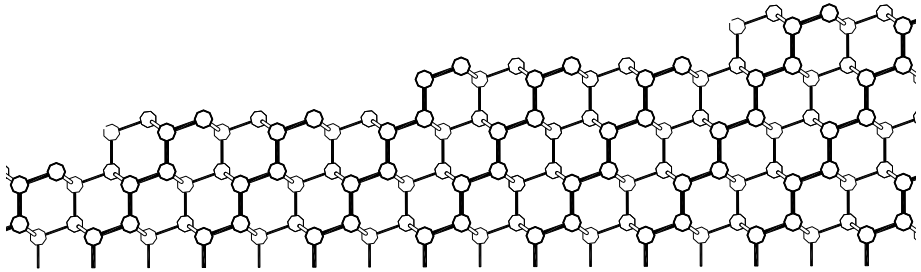

5.7 nm

Crystallography of Stepped Surfaces



Silicon (111)



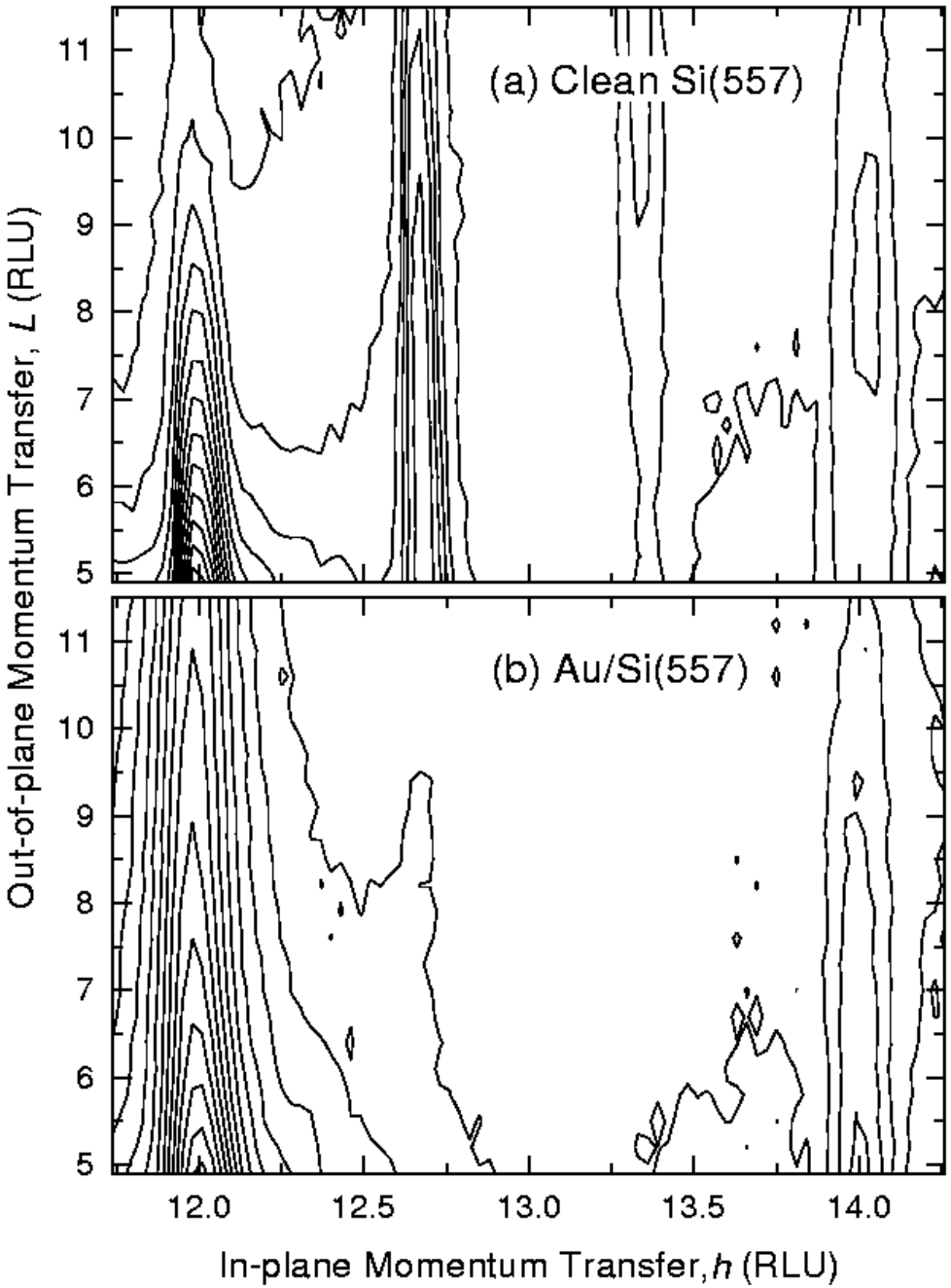


Si(557) surface

Alignment is Straightforward

```
CALCULATED PARAMETERS:
          A           B           C       ALFA    BETA    GAMMA
REC:  0.164431    1.63392    0.116412   90.06   90.03   89.93
DIR:   38.2118    3.84548     53.9736   89.94   89.97   90.07
          H    K     L     TTH      TH      PHI      CHI      ALP      CTS    ERROR
OR 1 = 12.0  0.0   3.0  21.938 112.920   50.308   -1.137    3.841    22456  0.0027
OR 2 = -5.0  1.0   7.0  20.284  97.018  307.482   -2.259    9.179    20719  0.0018
OR 3 = 14.0  0.0  20.0  26.411 113.142   40.844   -1.290   26.483    13639  0.0009
OR 4 = 12.0  2.0   3.0  43.135 110.470    4.520   -2.092    4.313    12772  0.0009
Lambda = 1.20913 A, wv = 5.19647, Energy = 10.2542 keV (FIXED)
Five-Circle Mode using alm = 2 and bem = 2:
```

Centered Orthorhombic unit cell contains two steps.

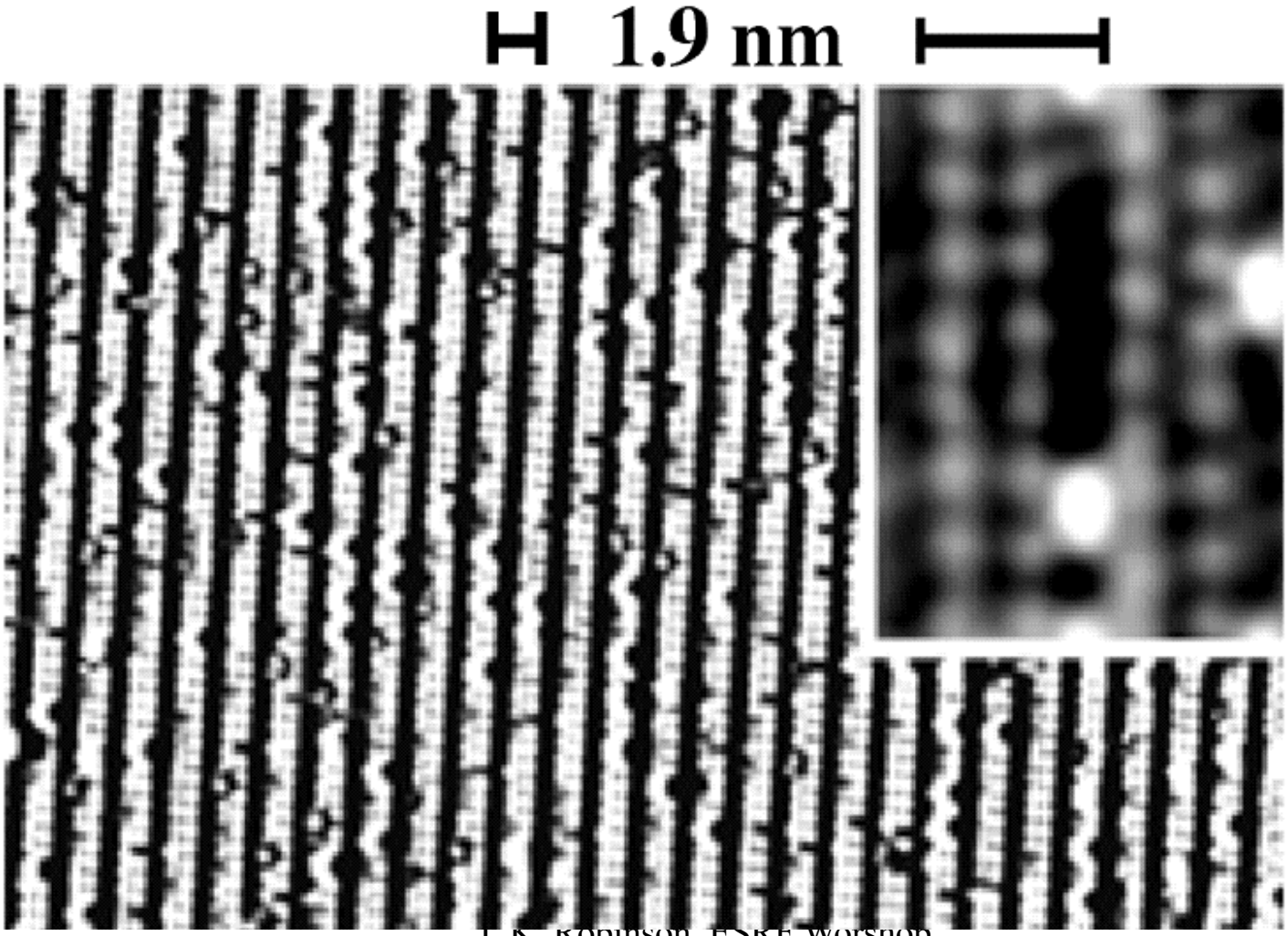


3×1 clean surface

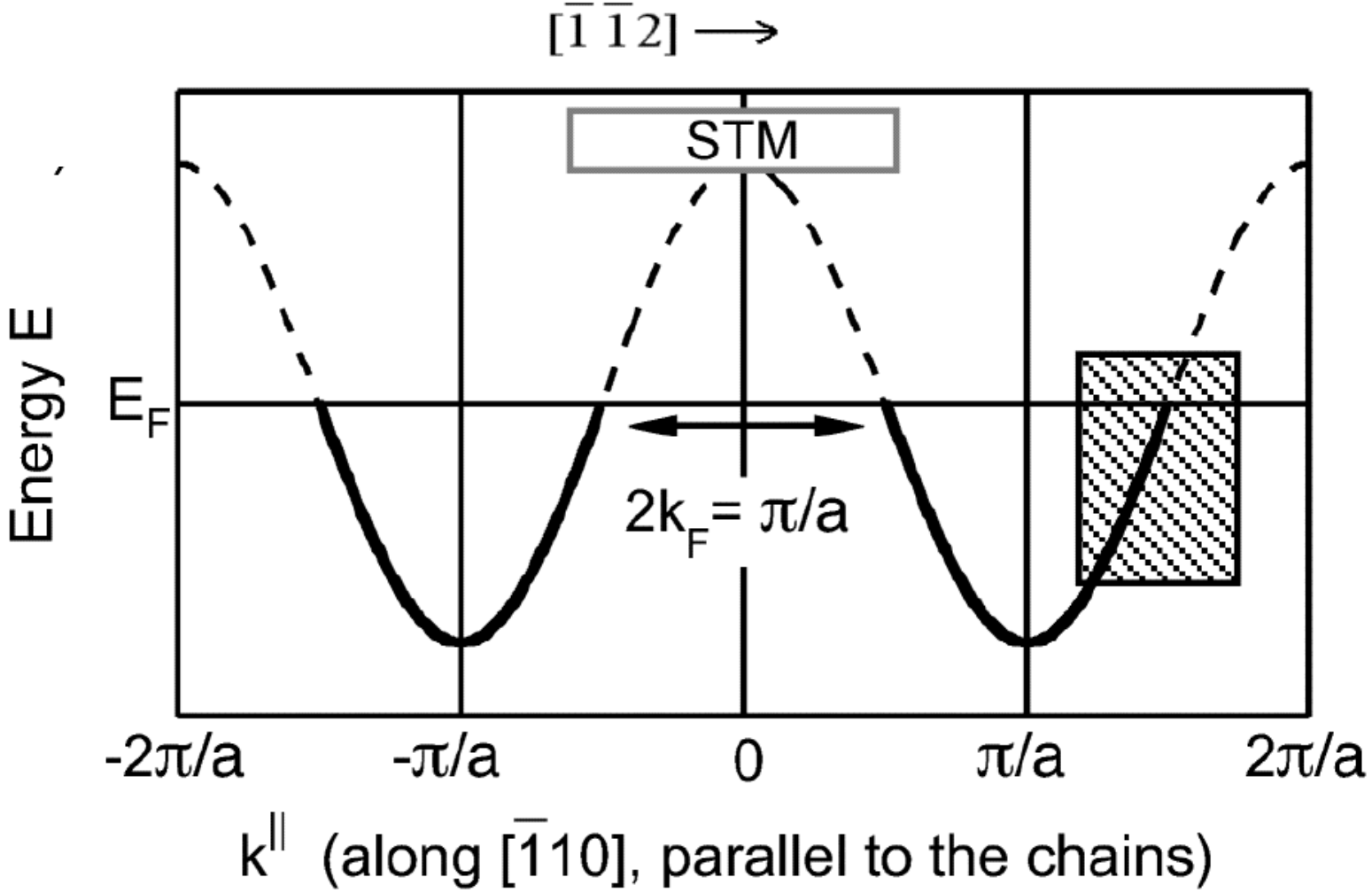
1×1 surface with 0.2ML Au at 600C

STM of Si(557)/Au

R. Losio, et. al., Phys. Rev. Lett. 86 4632 (2001)

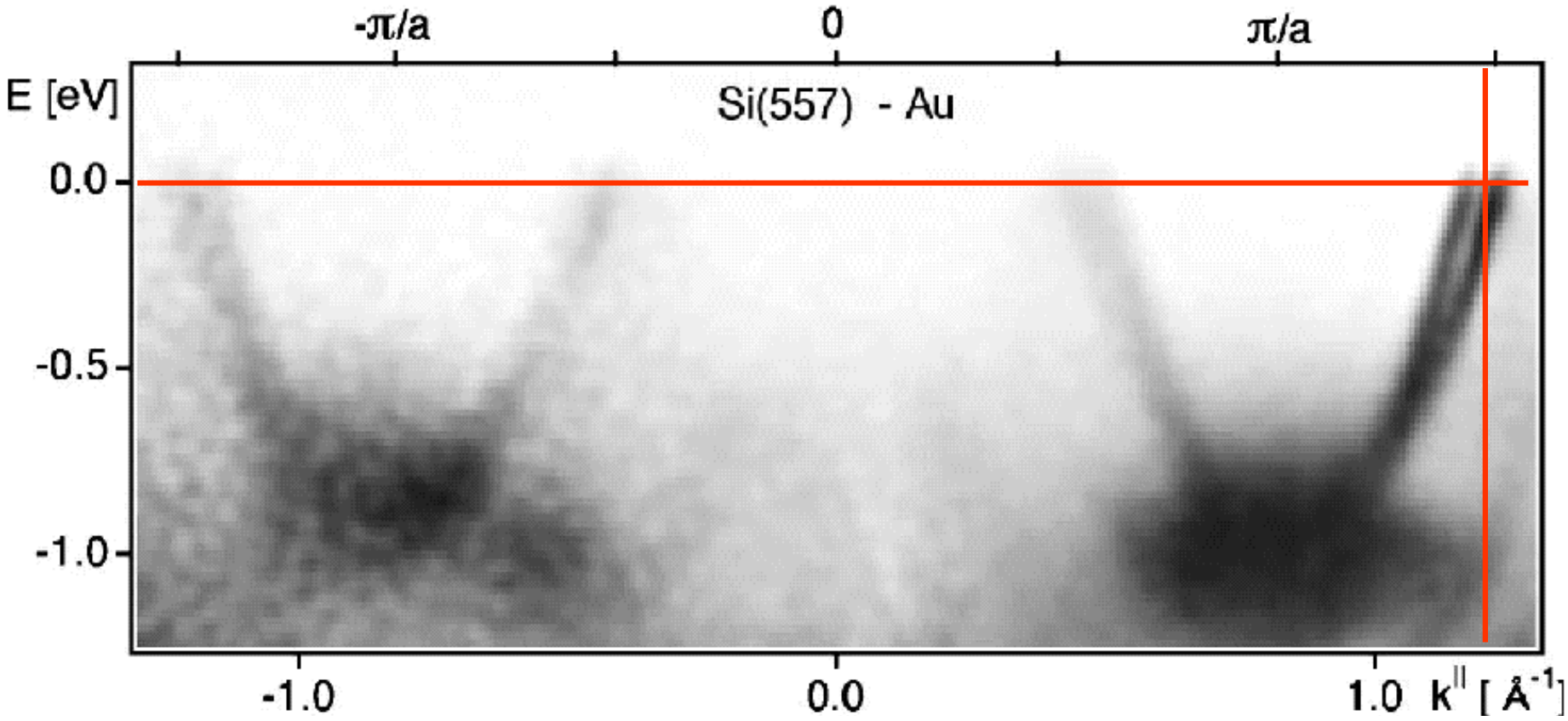


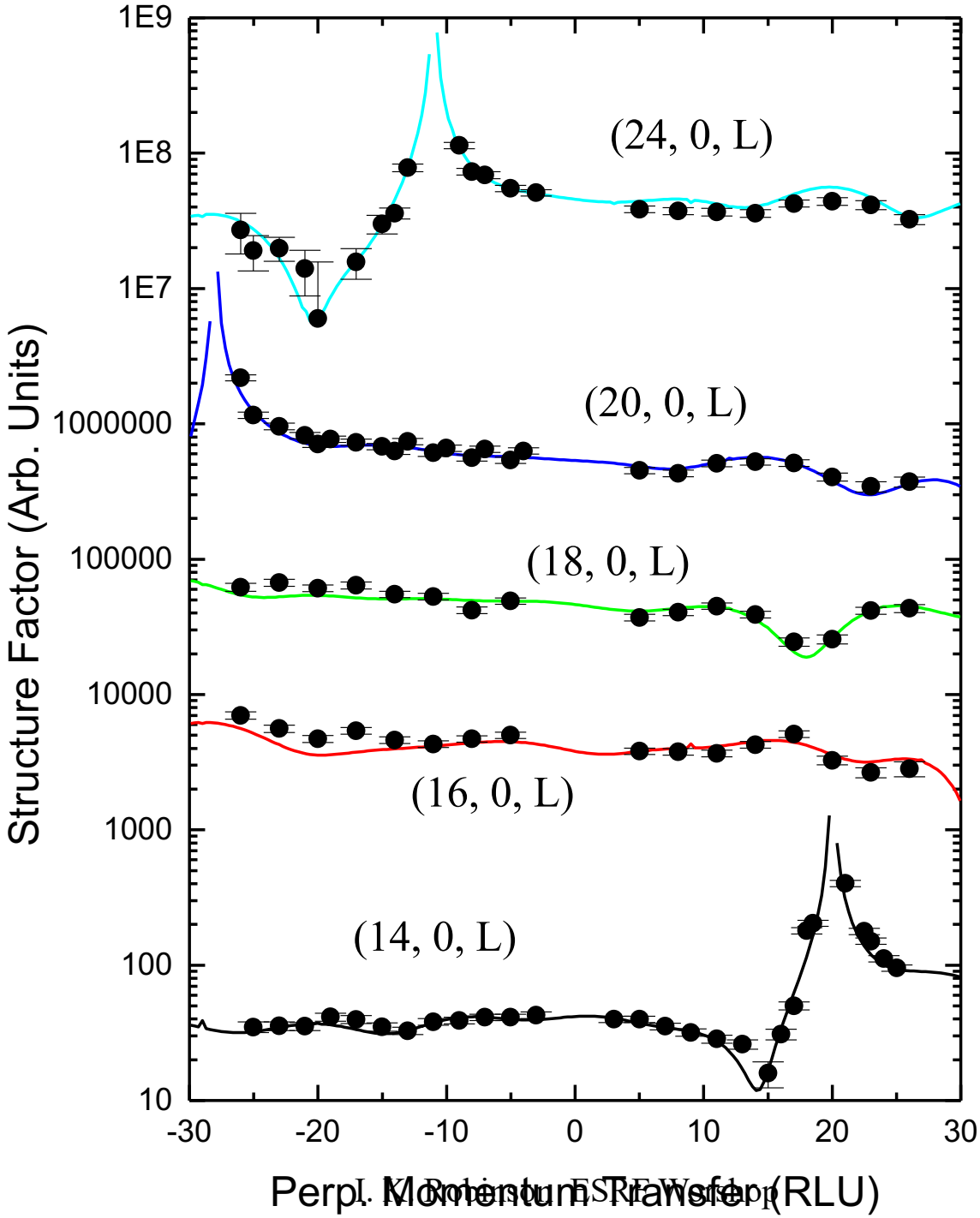
Schematic Band Topology for Au/Si(557)



Photoemission from Surface States Parallel to the Au Chains in Au/Si(557)

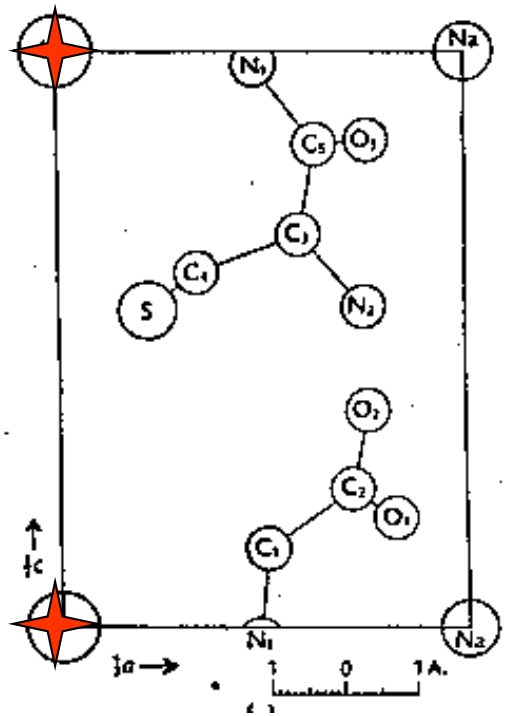
K. N. Altmann et. al. Phys Rev B 64 035406 (2001)



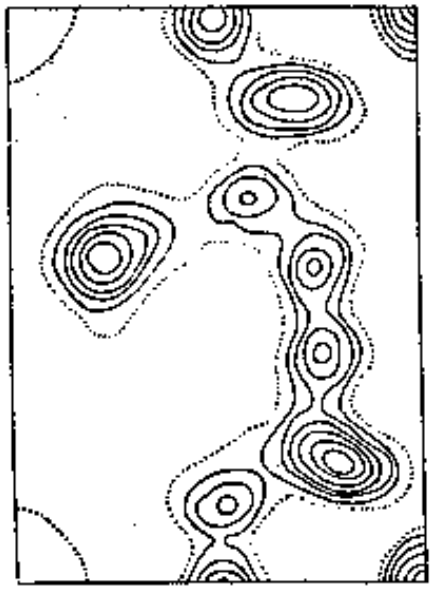

1E9
1E8
1E7
1000000
100000
10000
1000
100
10
(24, 0, L)
(20, 0, L)
(18, 0, L)
(16, 0, L)
(14, 0, L)
Structure Factor (Arb. Units)
-30
-20
-10
0
10
20
30
Perp. Momentum Transfer (RLU)

Phasing by a Single Heavy Atom

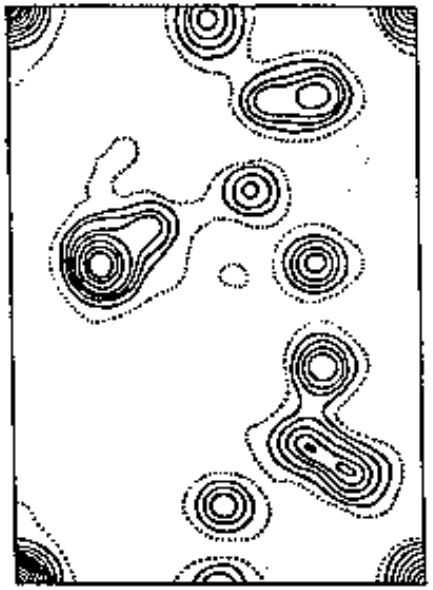
H. B. Dyer, Acta Cryst. 4 42 (1951)



Cysteinylglycine
sodium iodide

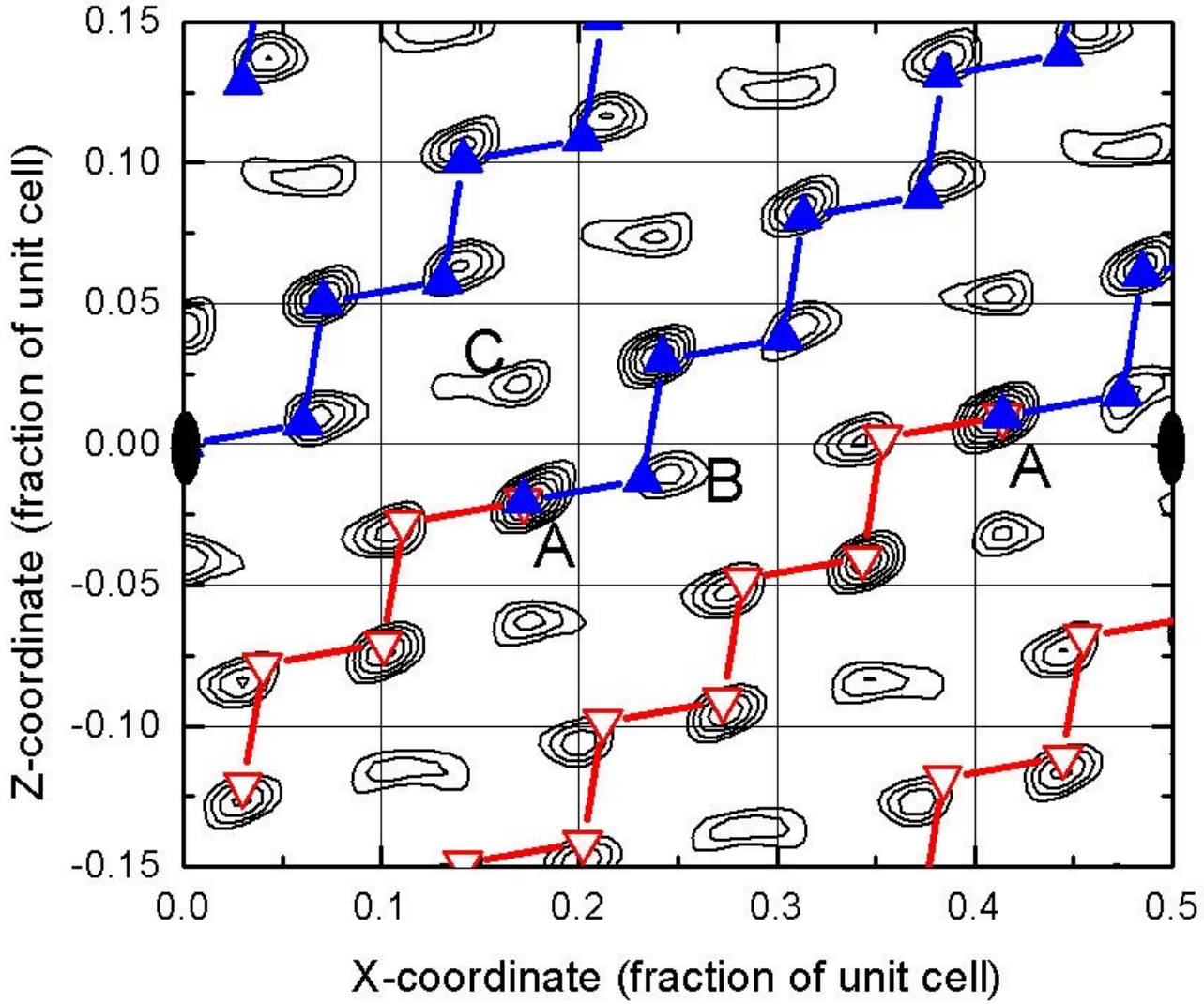


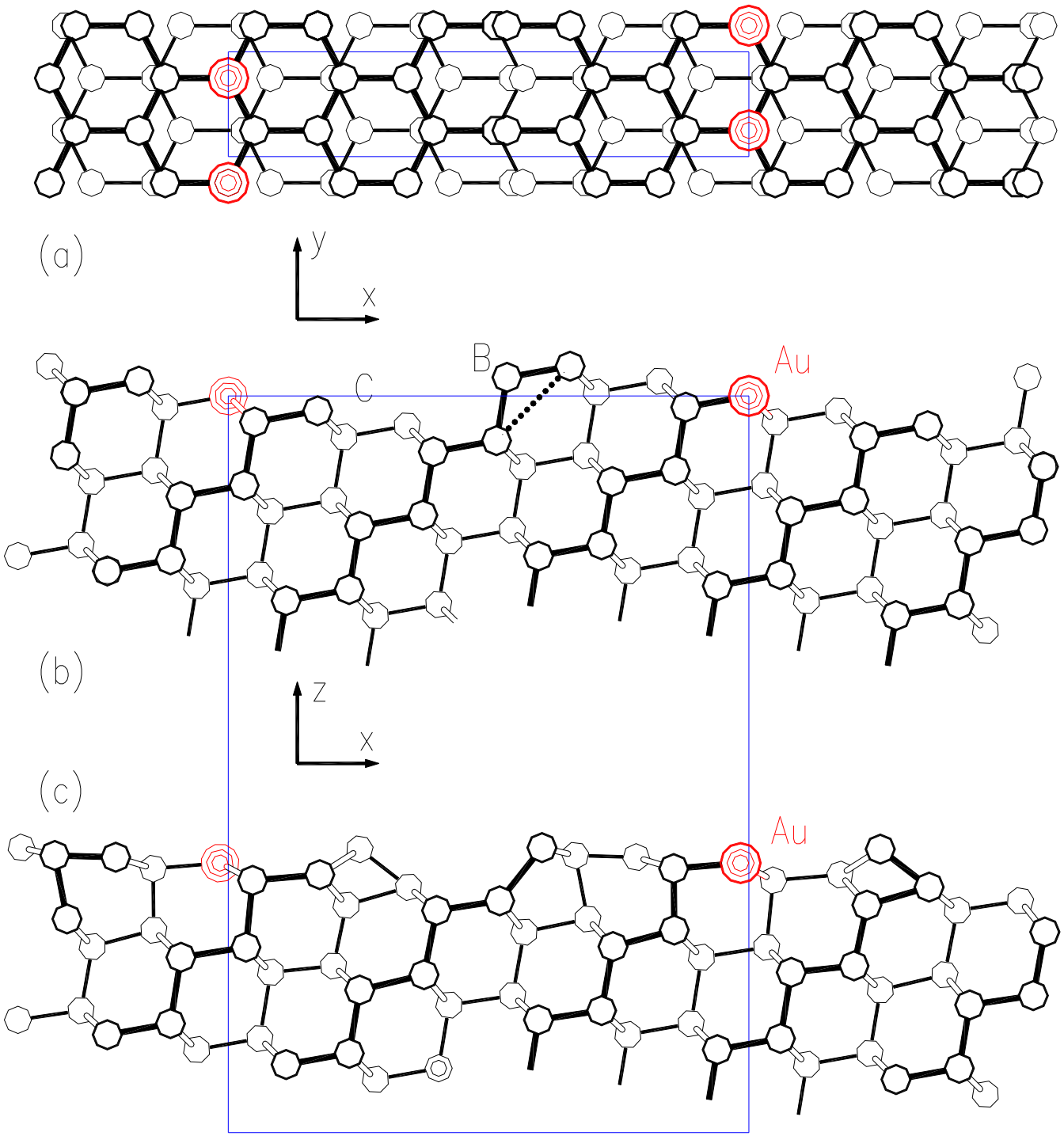
Patterson



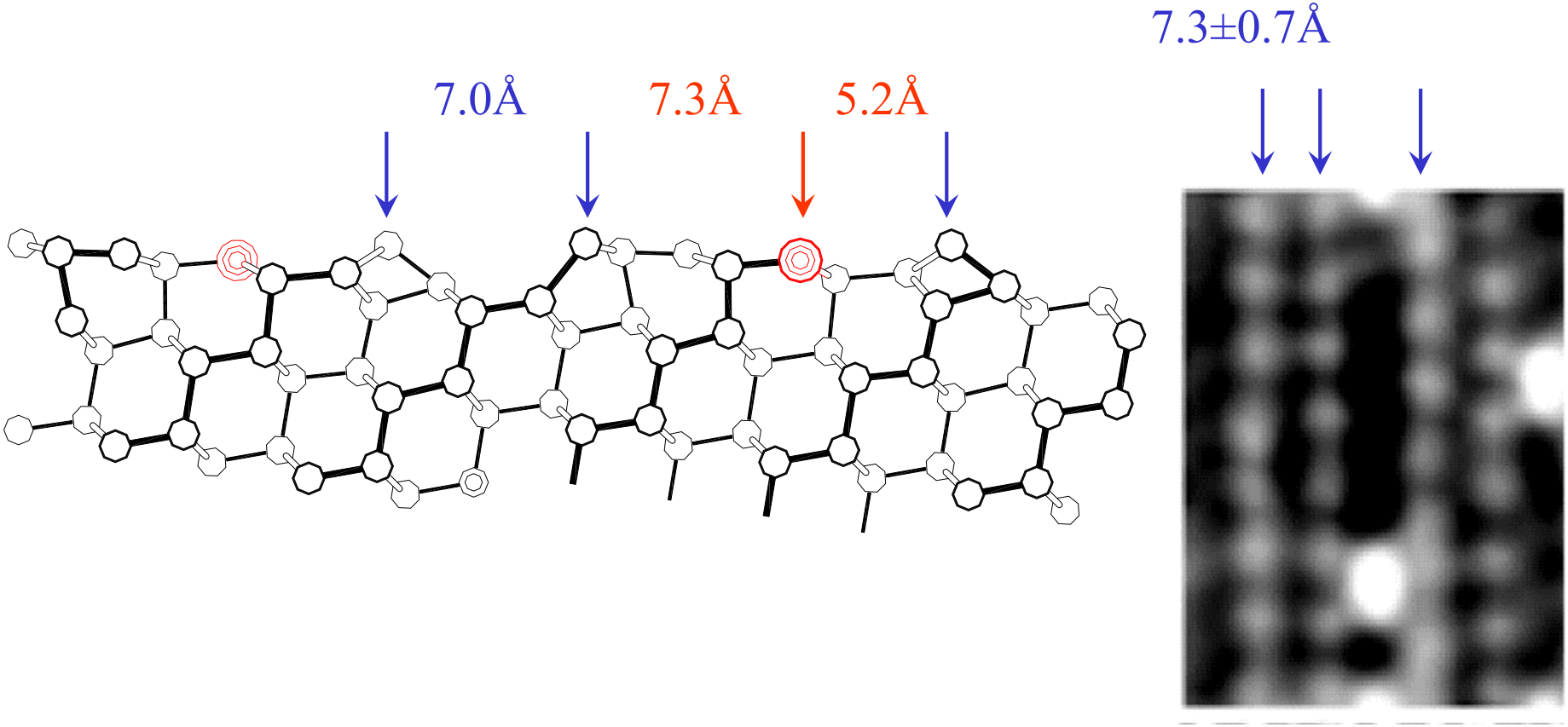
Electron density

X-Z Patterson of Au/Si(557)



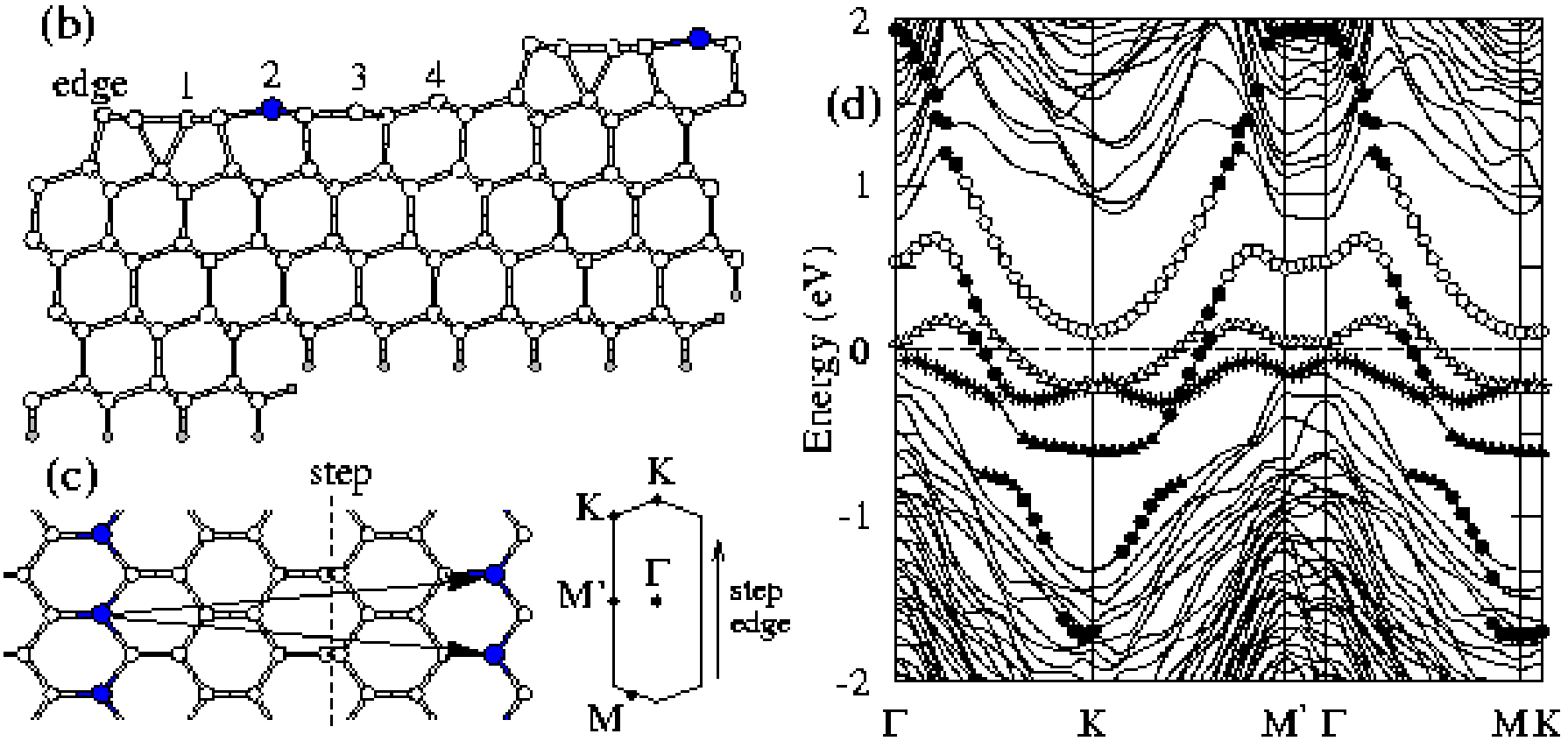

(a)
y
x
B
C
Au
(b)
z
x
(c)
Au

Comparison with STM

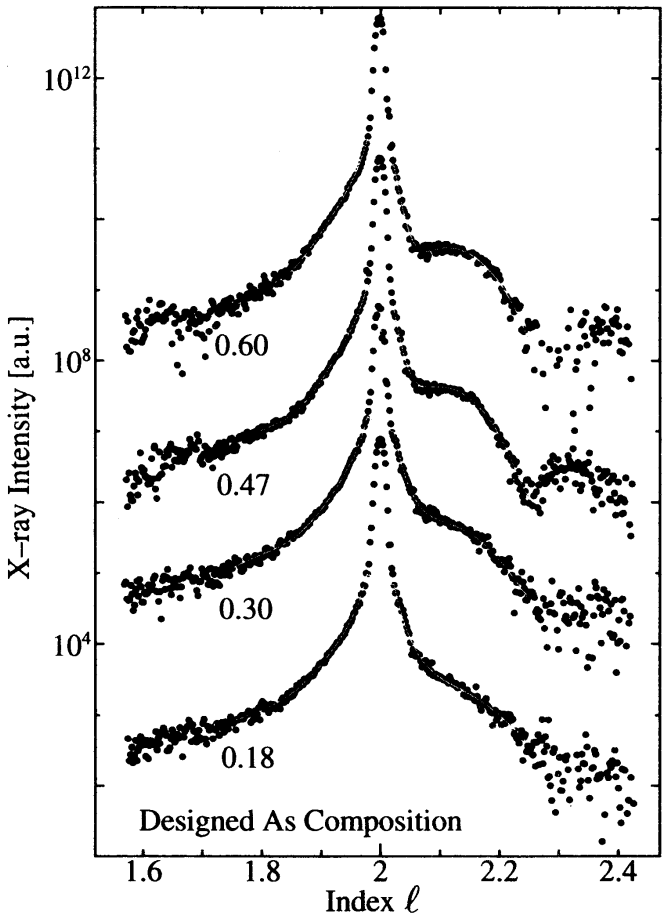


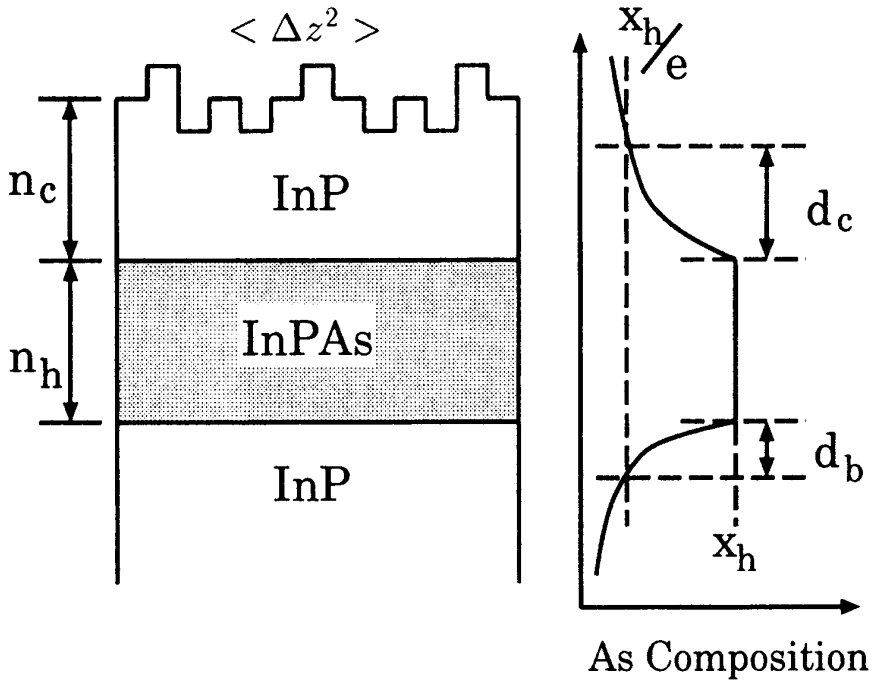
Calculated Electronic Band Structure of Au/Si(557) using SIESTA code

D. Sanchez-Portal et. al. Phys. Rev. B **65**, 081401 (2002)



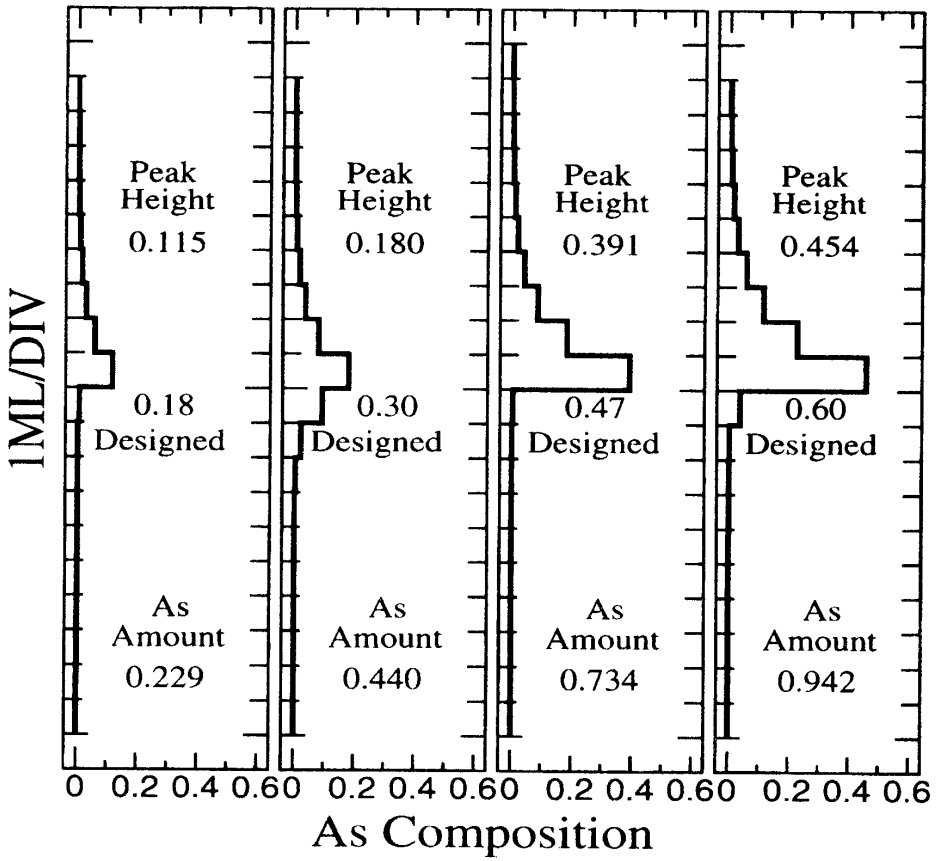
As in InP/InPAs heterostructure

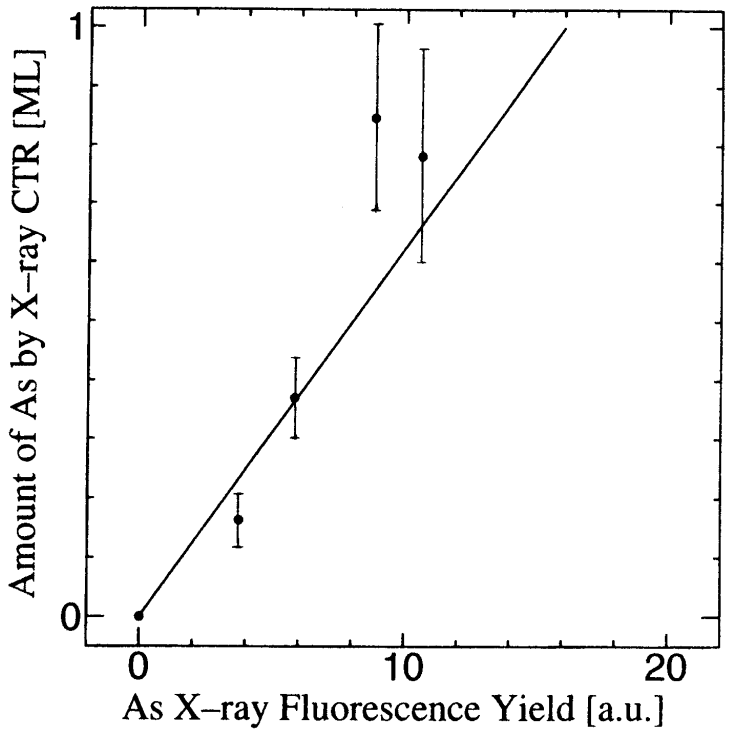




M. Tabuchi *et al* J. Appl. Phys 81 112 (1997)

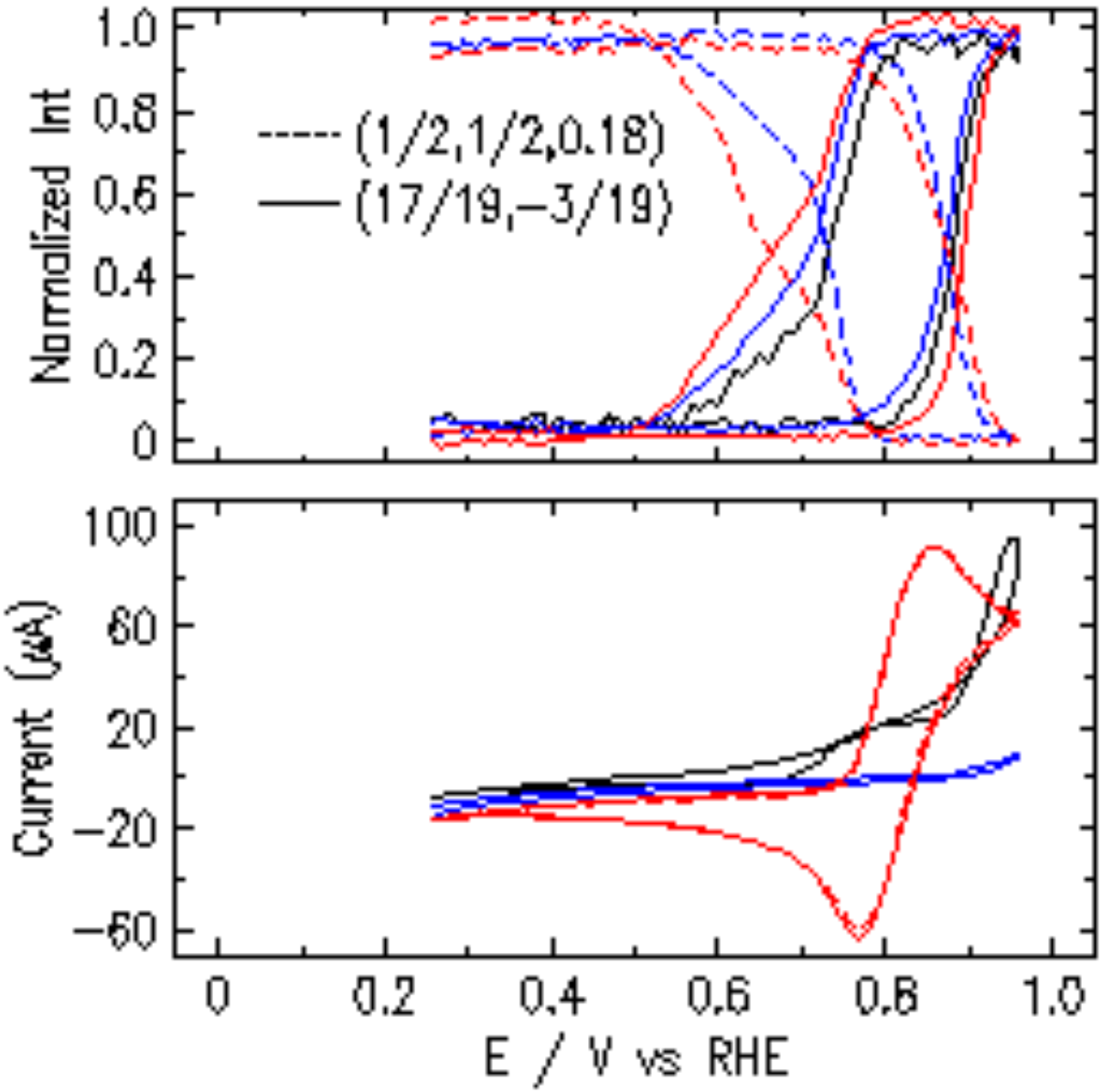
CTR agrees with Fluorescence



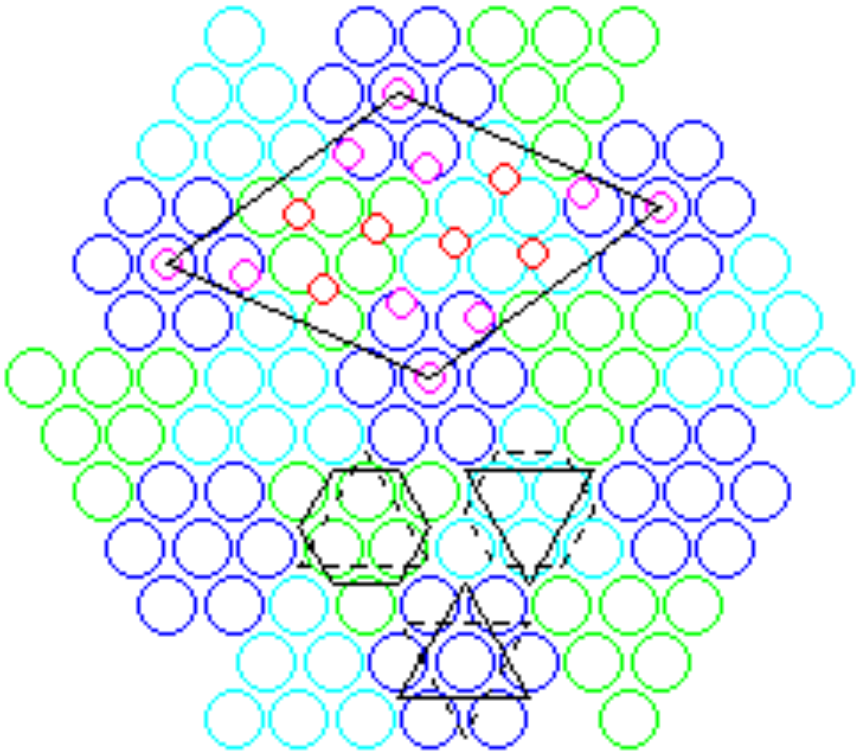


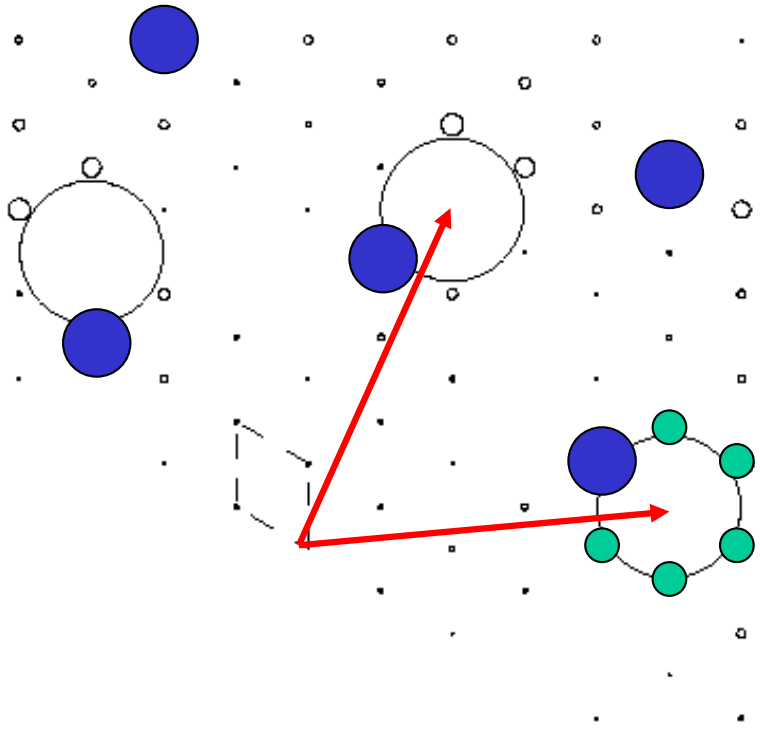
M. Tabuchi *et al* J. Appl. Phys 81 112 (1997)

CO dissolved in $HClO_4$ on Pt(111)

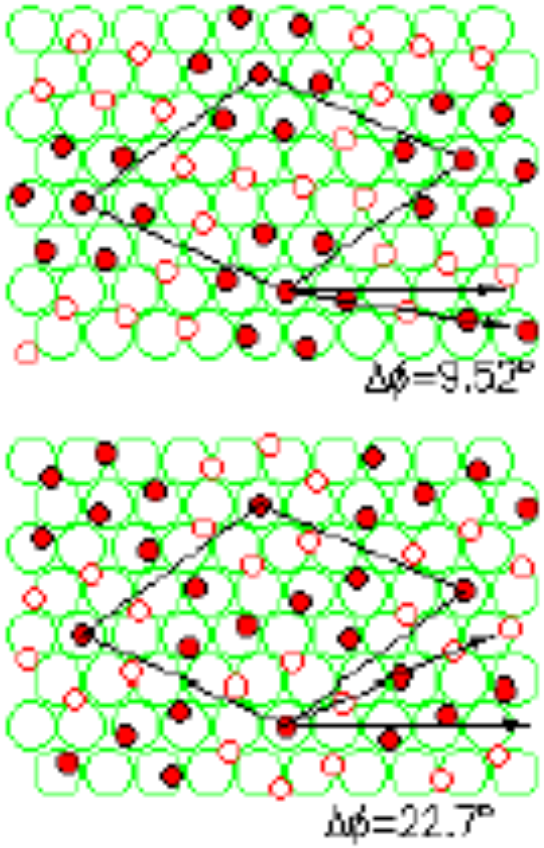


CO reciprocal lattice





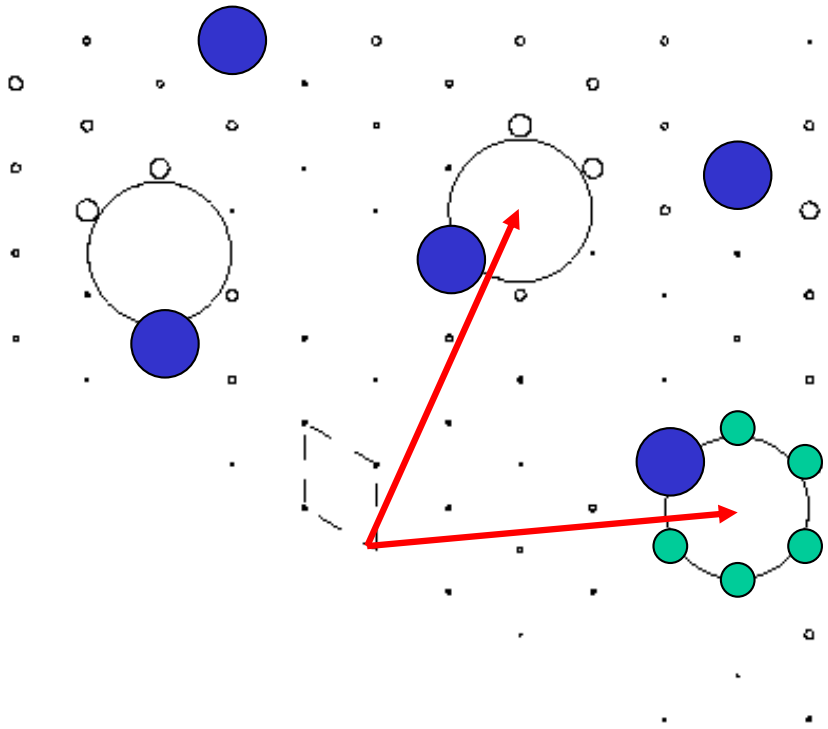
Two inequivalent packings of 13 CO's into rt(19) Pt(111) cell

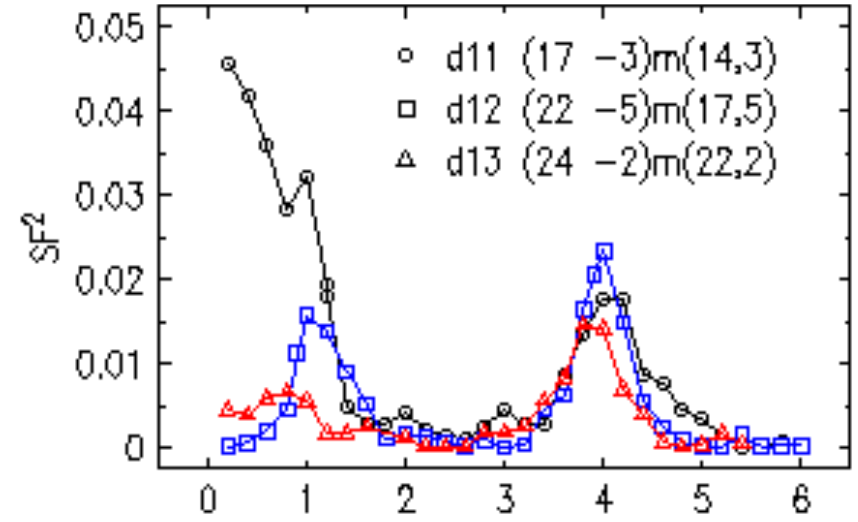


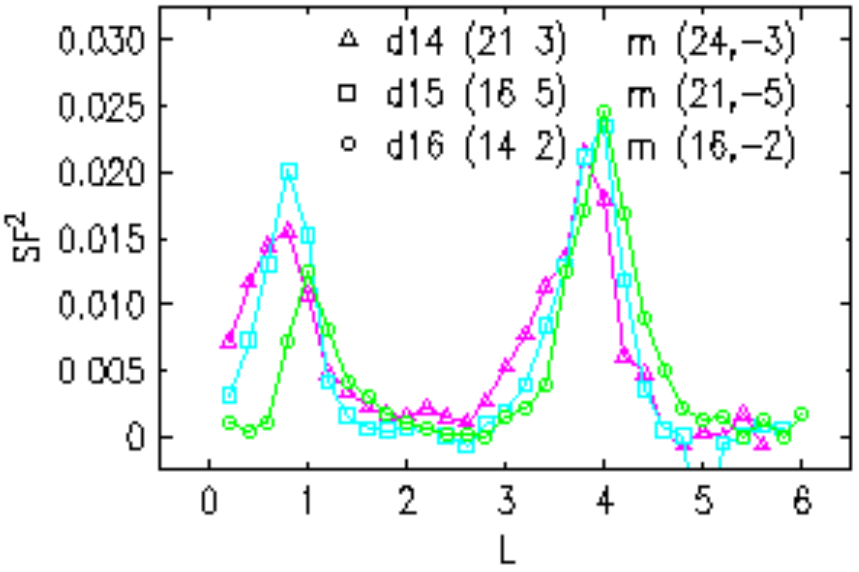
This 'patch' model is the only one observed, by the CO peak positions

This 'ring' model is not seen.

rt19×rt19 CO/Pt(111)

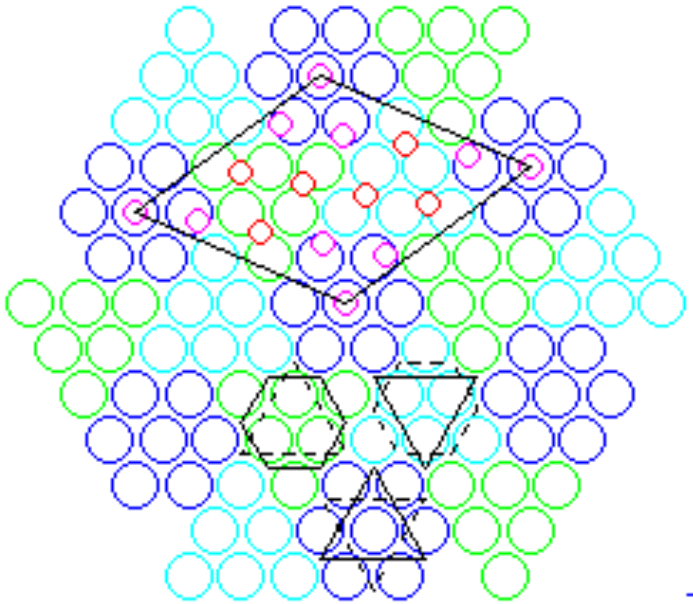


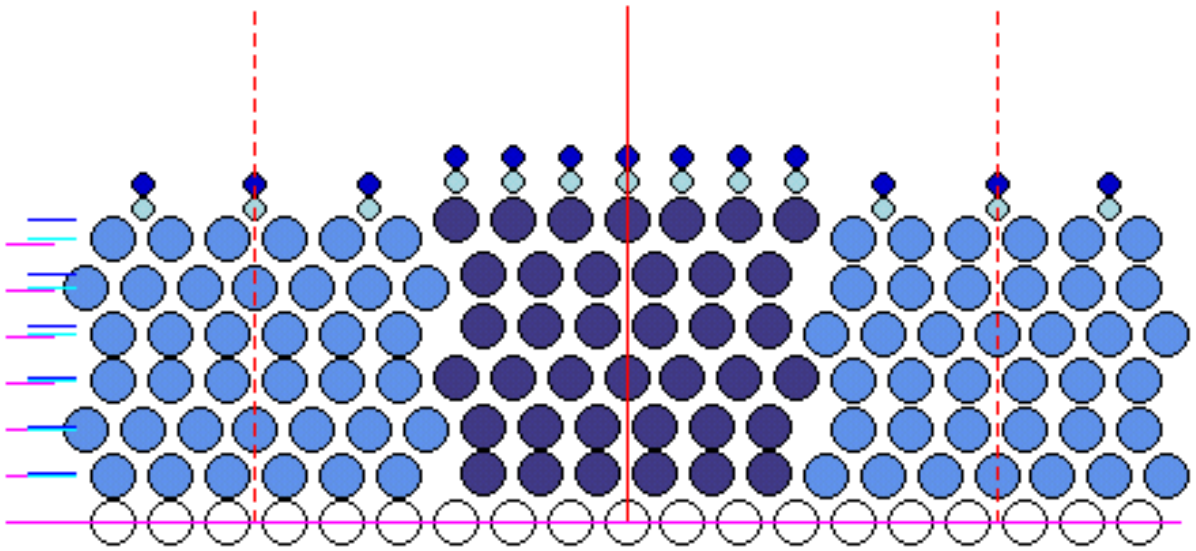




I. K. Robinso

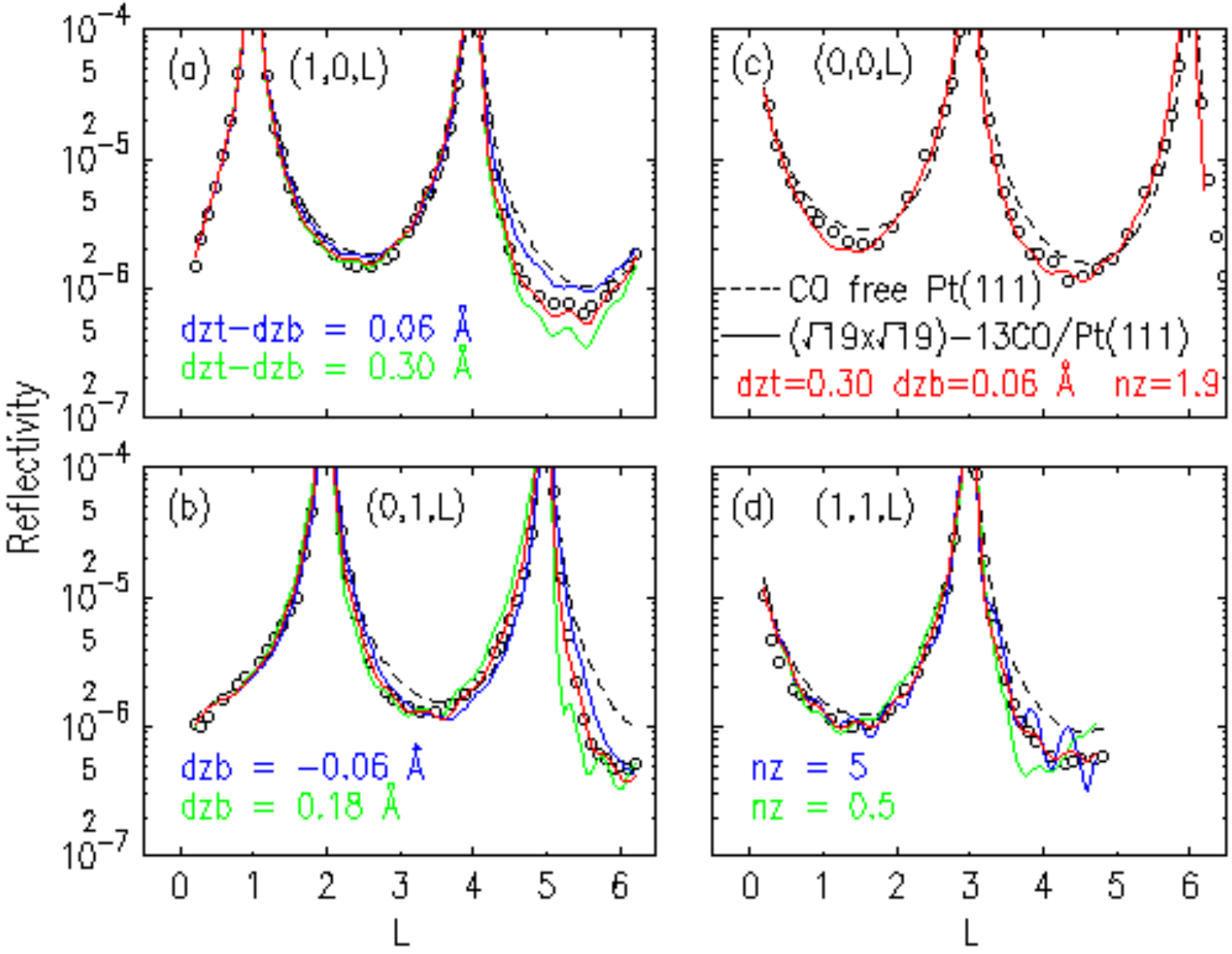
Top and Side Views of Model





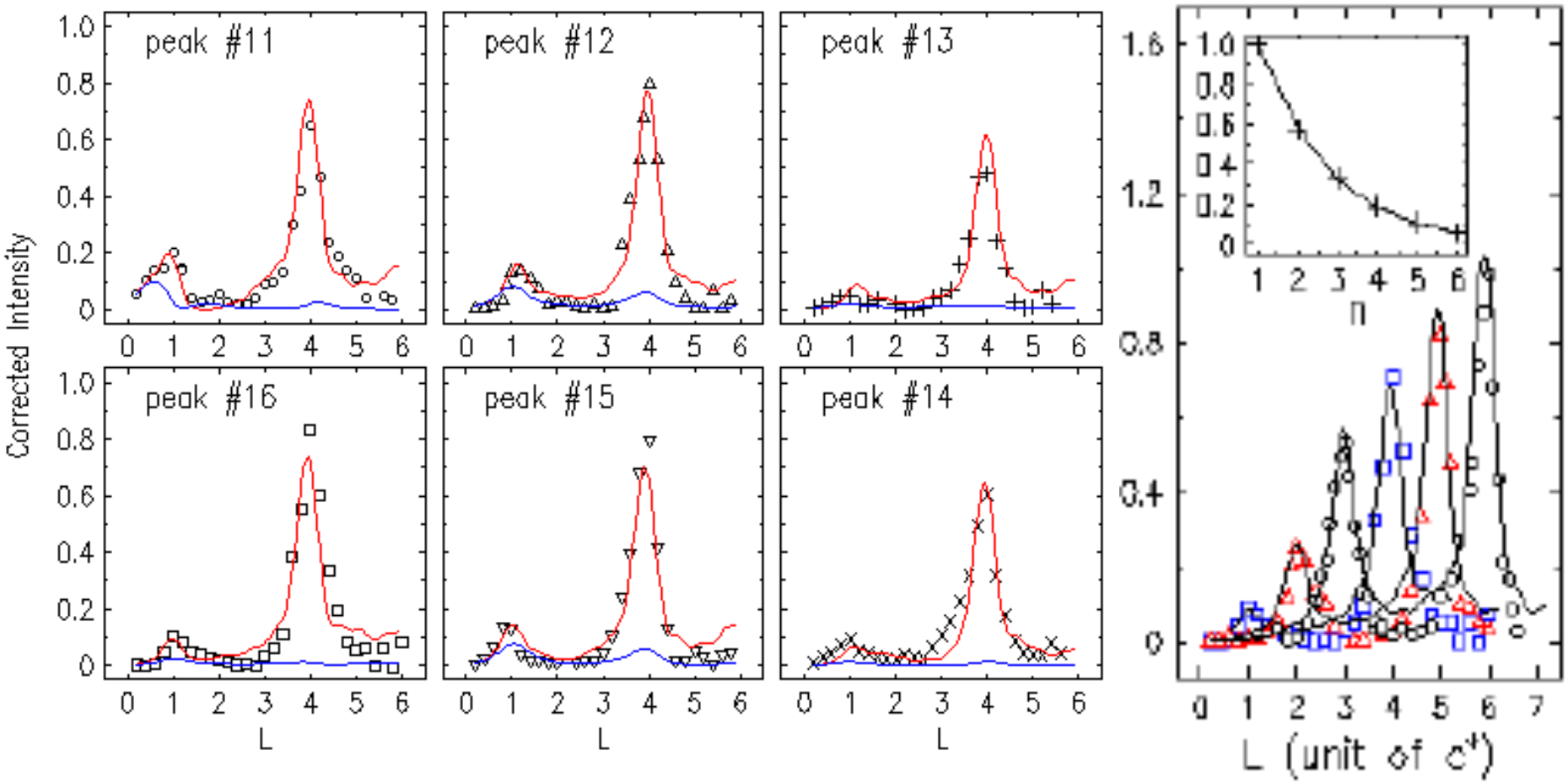
Fit of Model to CTR Data

Dashed curve is clean Pt(111)



Fit of Model to Rt19 Data

Blue line has vertical relaxations turned off



Important Contributions from

Peter Bennett	Arizona
Franz Himpsel	Wisconsin
Sanjit Ghose	Urbana
Jia Wang	Brookhaven
Ratko Adzic	Brookhaven