Surface Structure using X-rays

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ICSOS Munich, July 2005

Important Contributions from

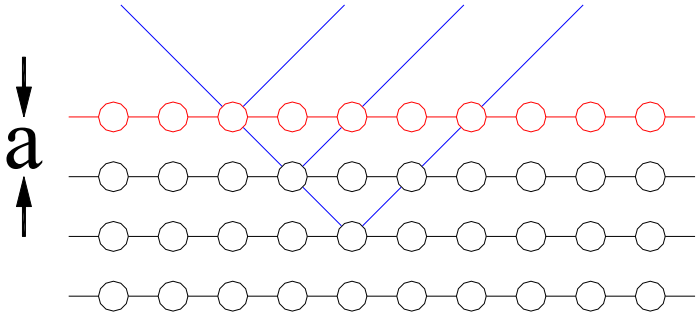
Sanjit Ghose	Urbana
Sebastien Boutet	Urbana
Peter Bennett	Arizona
Franz Himpsel	Wisconsin
Jia Wang	Brookhaven
Ratko Adzic	Brookhaven
Ben Ocko	Brookhaven
Marie-Claire St Lager	CNRS
Robert Baudouing-Savois	CNRS

Maurizio deSantis	CNRS
Pierre Dolle	CNRS
Bernard Croset	CNRS
M. Tabuchi	Nagoya
S. Hisadome	Nagoya
R. Oga	Nagoya
Y. Takeda	Nagoya
X16A, X22A	NSLS
BM32	ESRF

Surface Structure Menu

- Au quantum wires on Si(557)
- ‘Homometric’ structures of Pt(110)1x5
- Deep subsurface strain in Pt(111)/CO
- Direct methods for Heterostructures

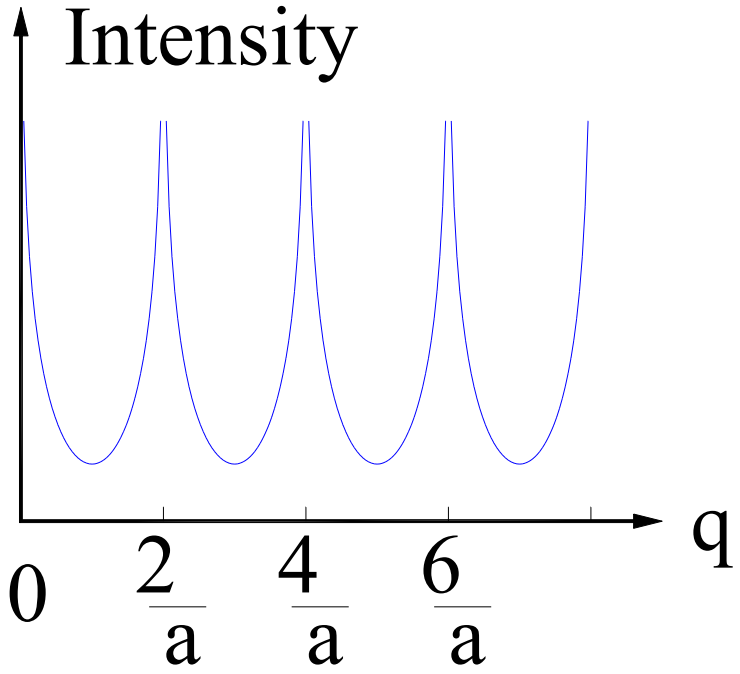
Origin of Truncation Rods



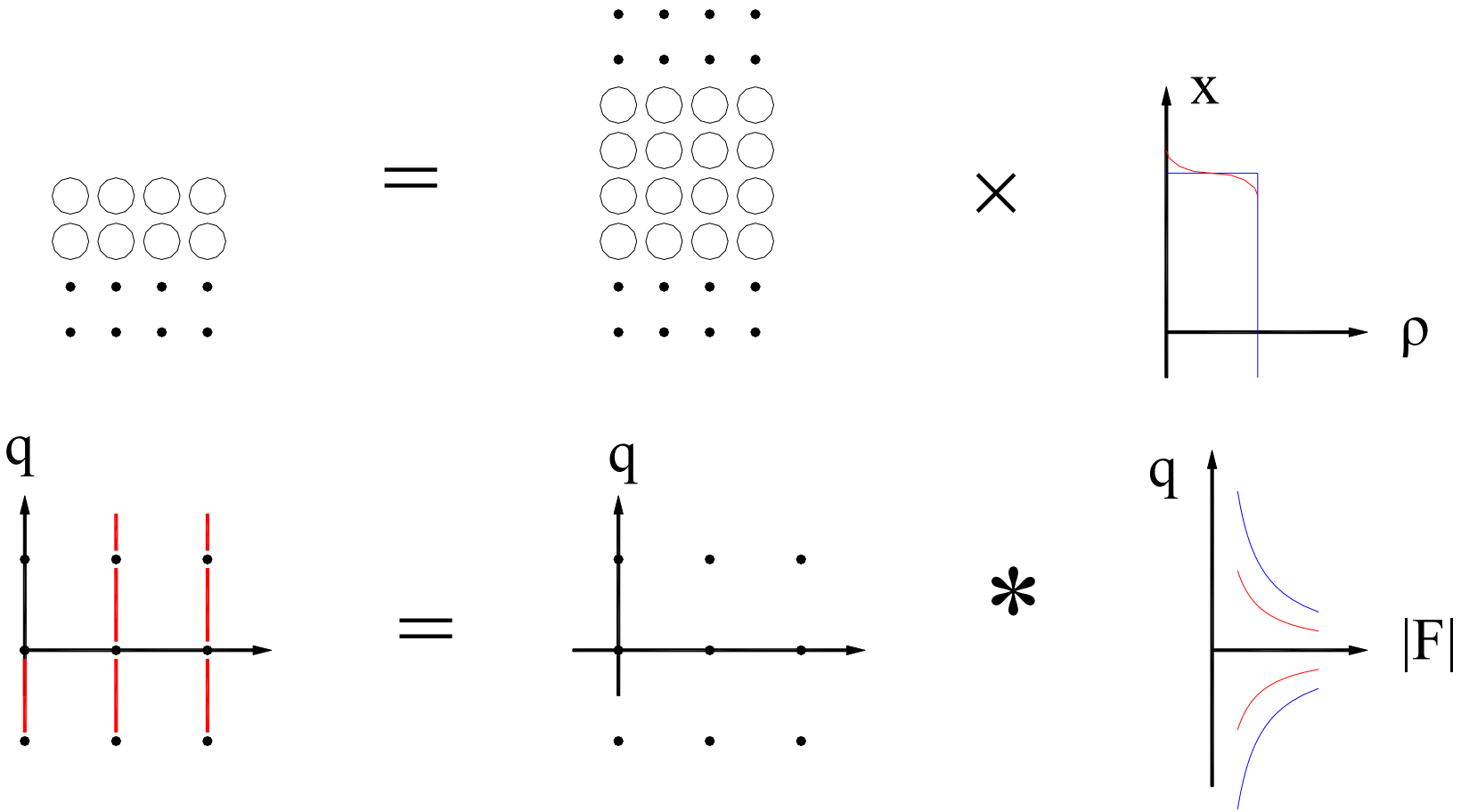
$$F_{CTR} = \sum_{n=0}^{\infty} A_n$$

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

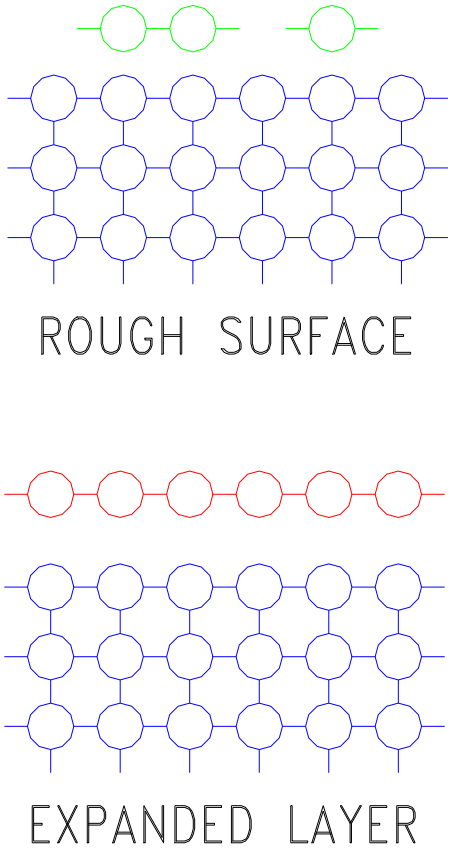
$$= \frac{f_L}{1 - e^{iqa}}$$

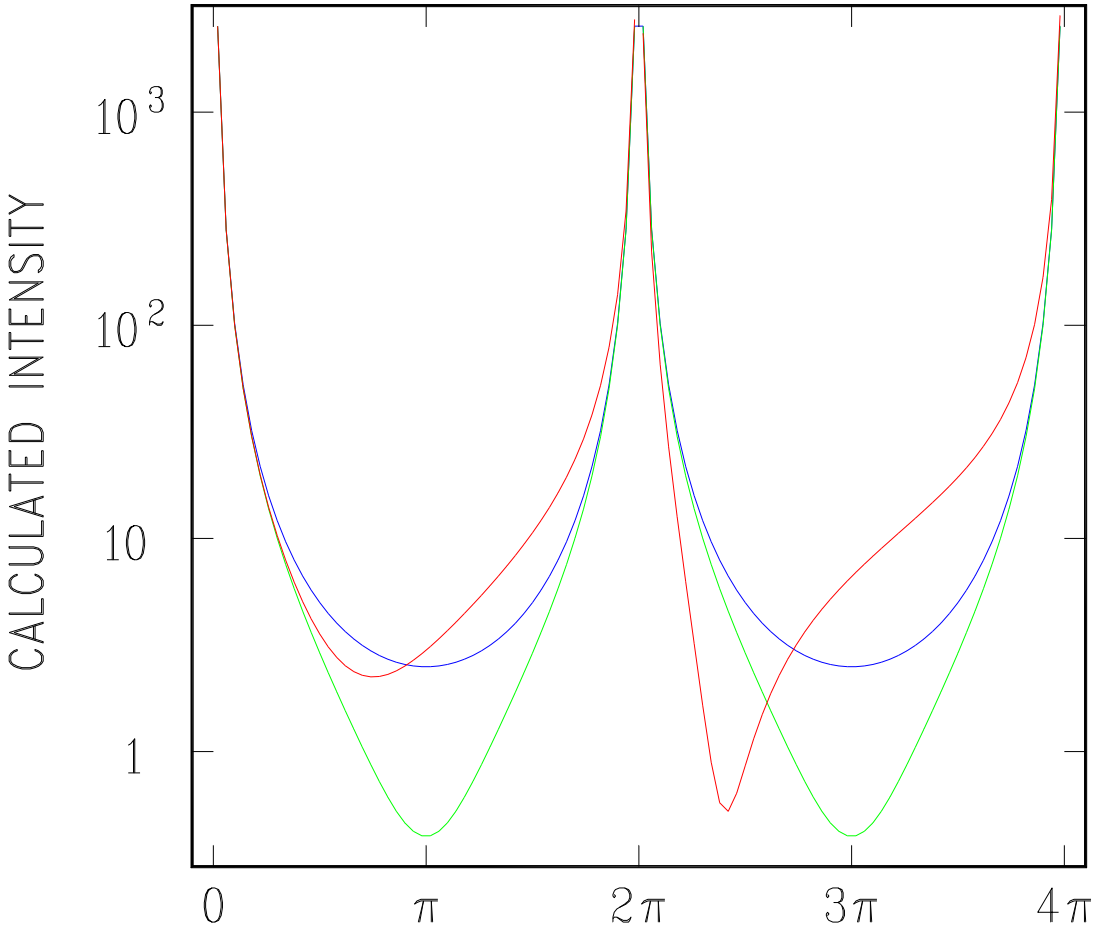


CTR as Convolution

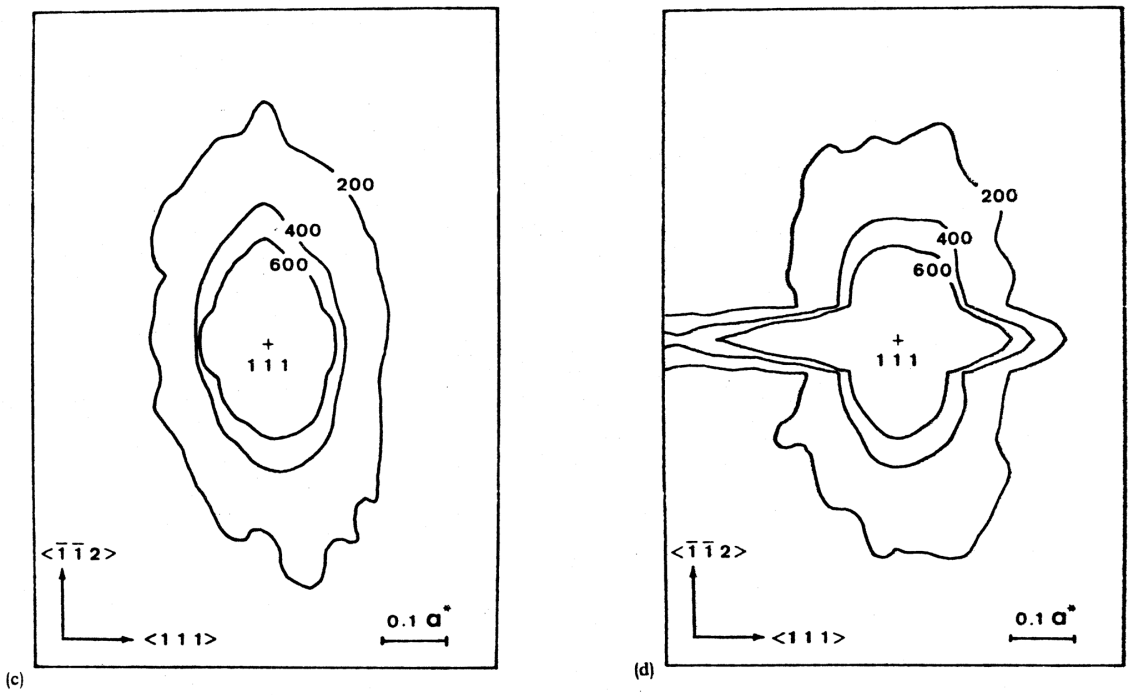


CTR is Sensitive to Surface Structure





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)

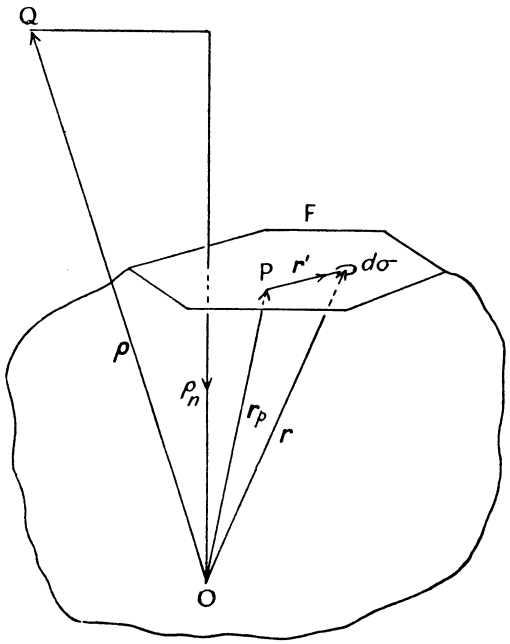
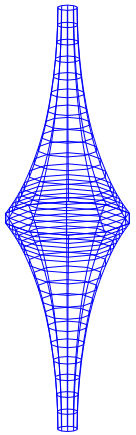


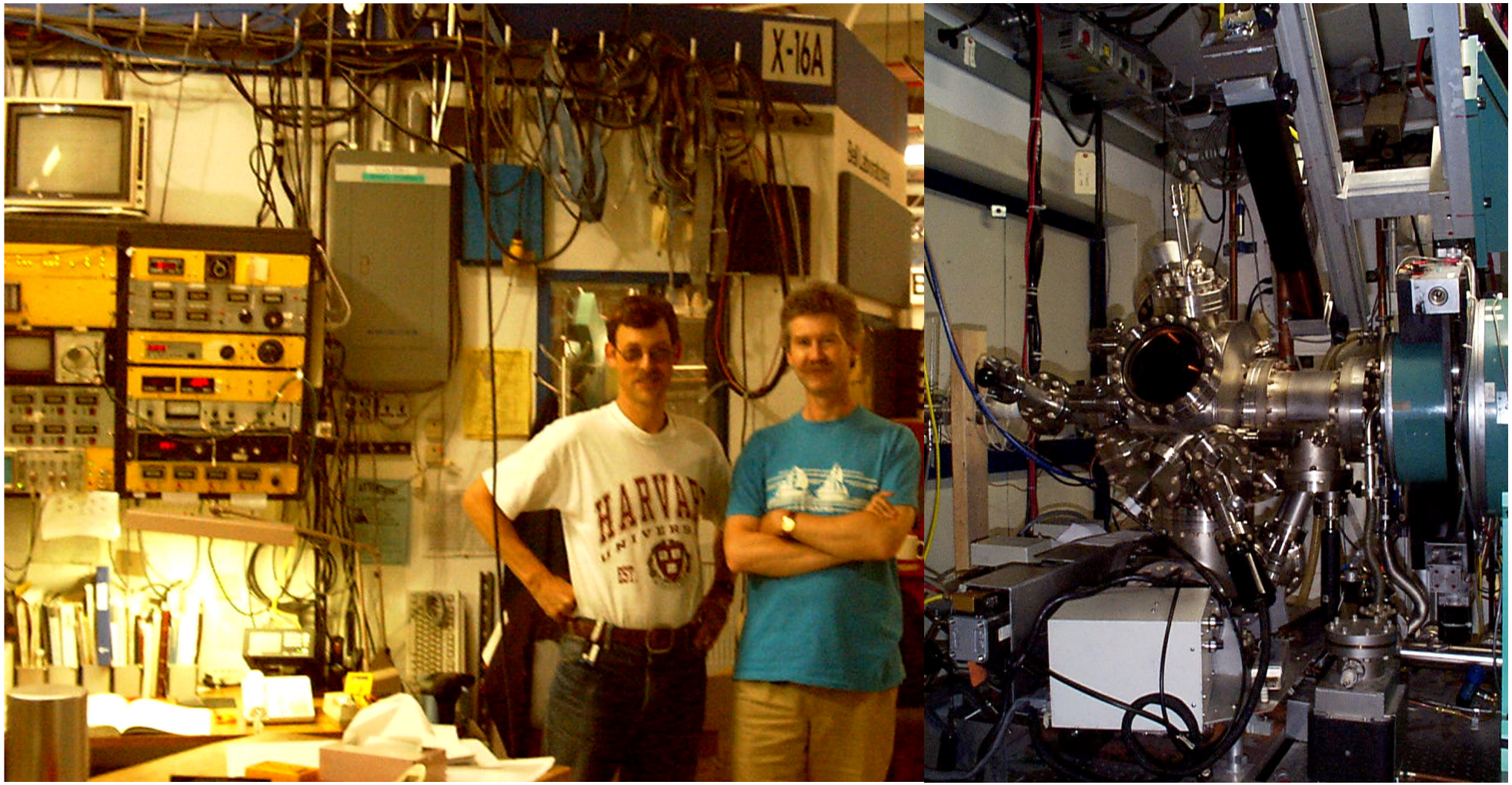
FIG. 200



"Stacheln"

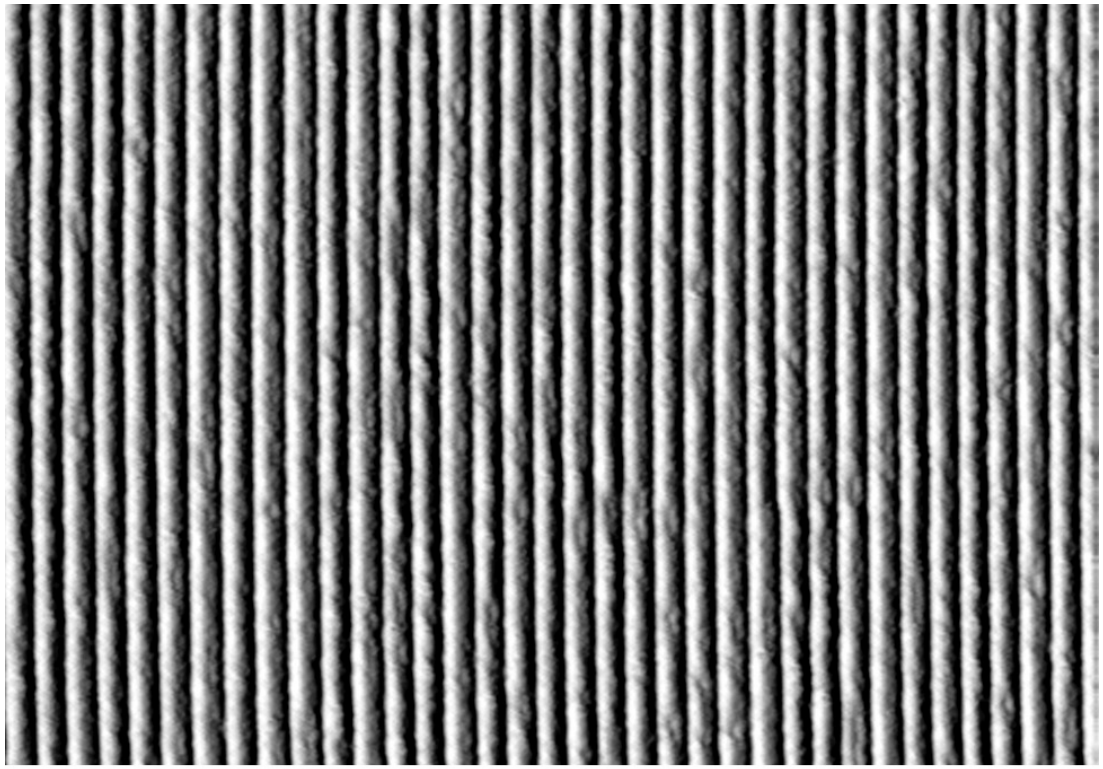
X16A Surface X-ray Diffraction

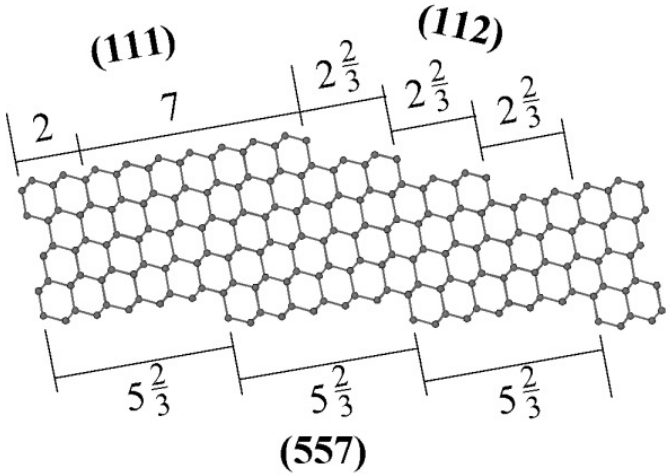
operating since 1987 ...

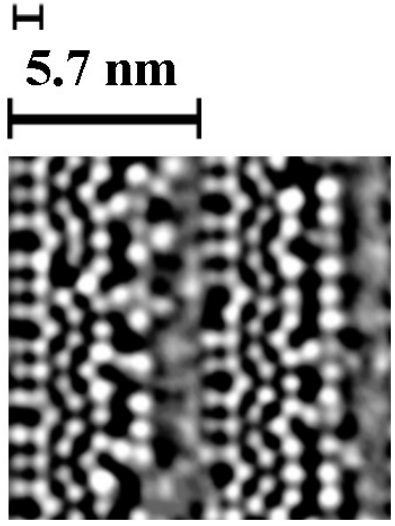


Surface Structure Menu

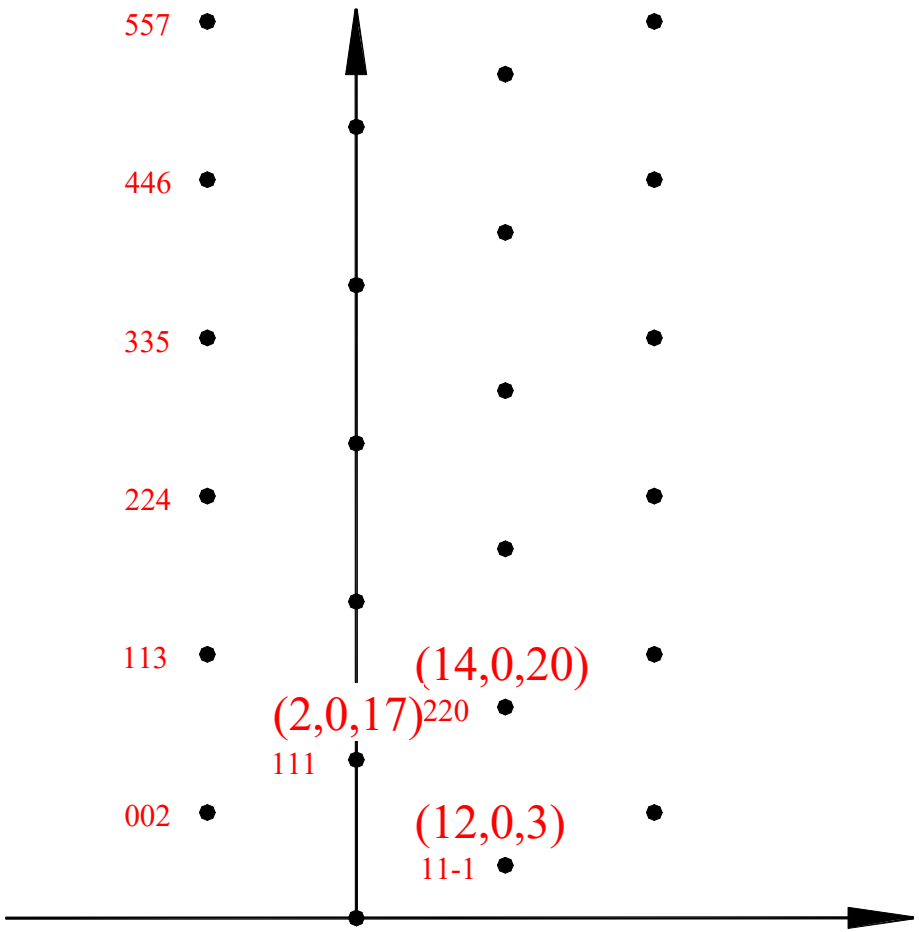
- Au quantum wires on Si(557)
- ‘Homometric’ structures of Pt(110)1x5
- Deep subsurface strain in Pt(111)/CO
- Direct methods for Heterostructures



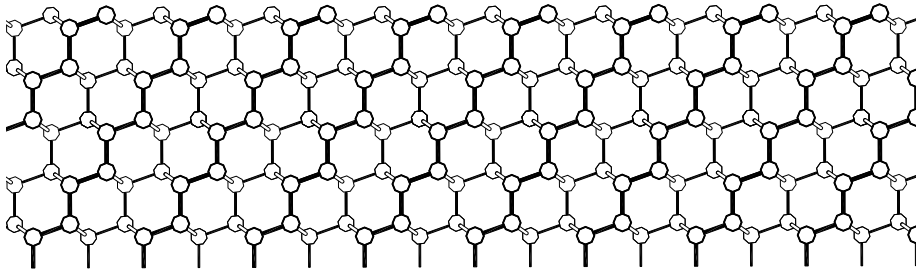

(111)
(112)
2
7
$2\frac{2}{3}$
$2\frac{2}{3}$
$2\frac{2}{3}$
$5\frac{2}{3}$
$5\frac{2}{3}$
$5\frac{2}{3}$
(557)

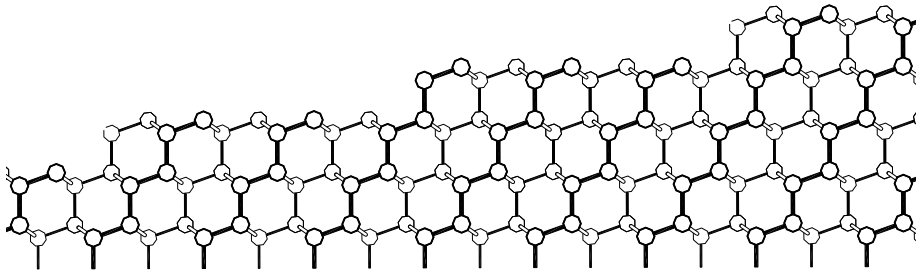

5.7 nm

Crystallography of Stepped Surfaces



Silicon (111)



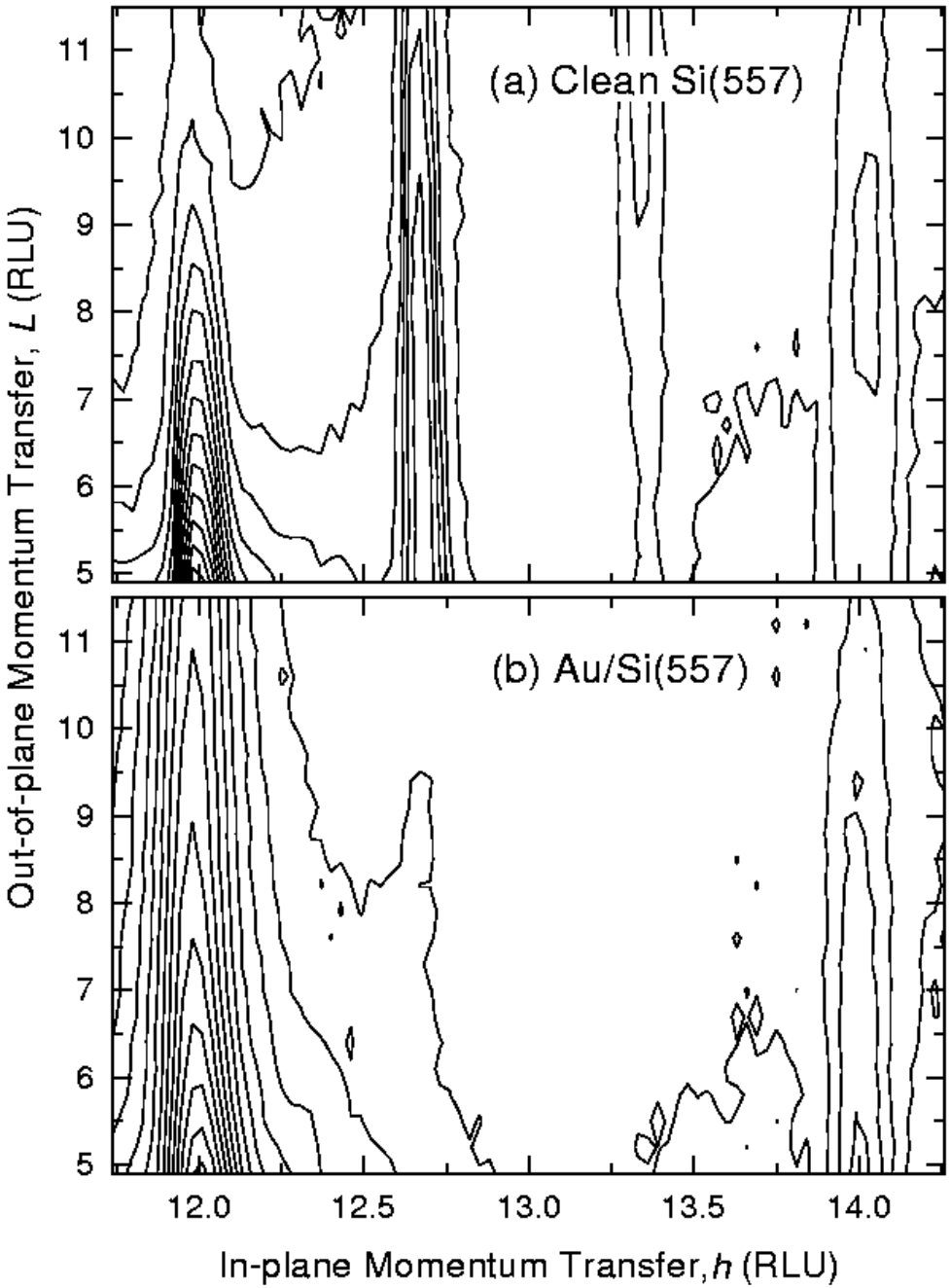


Si(557) surface

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.

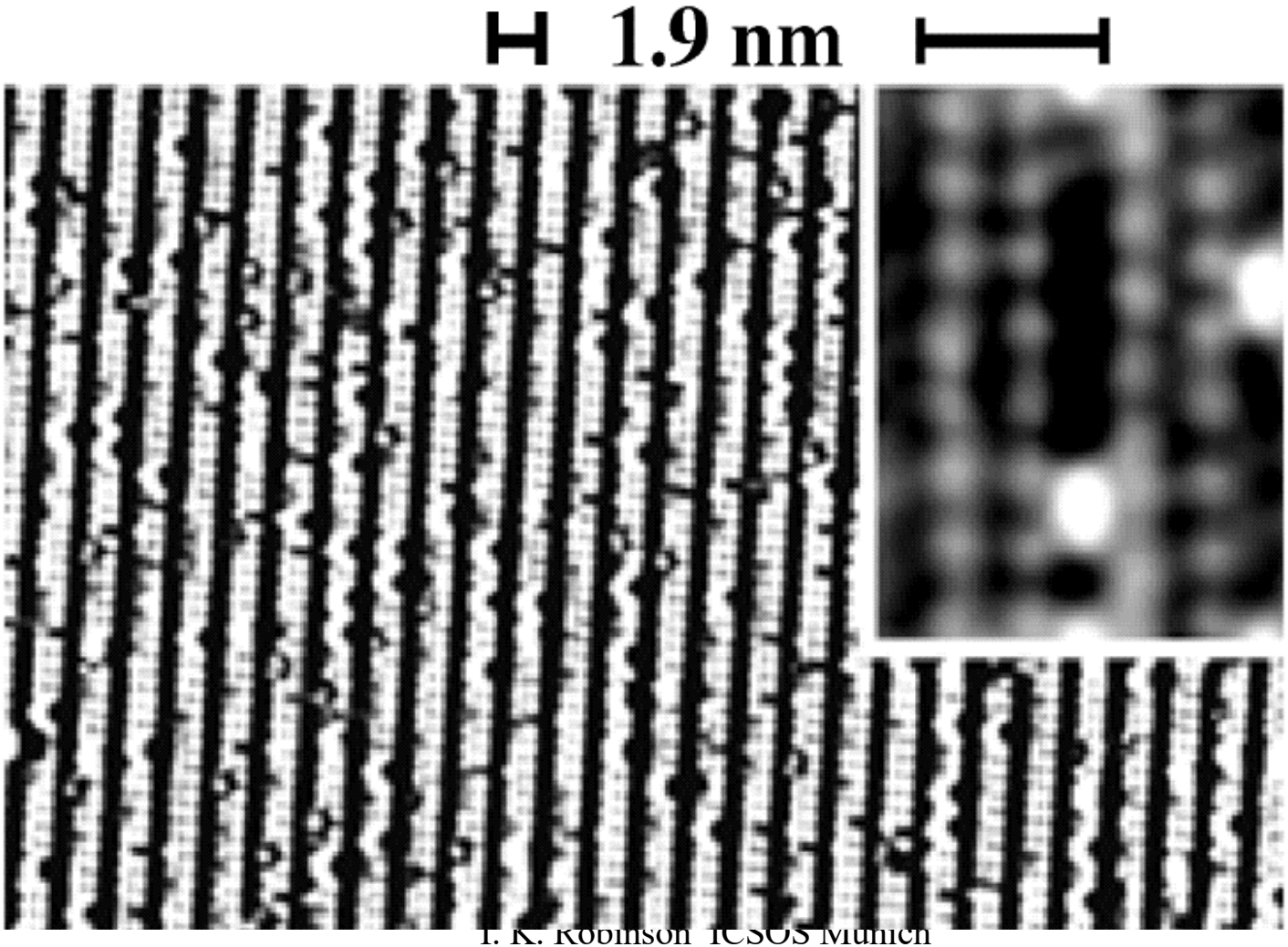


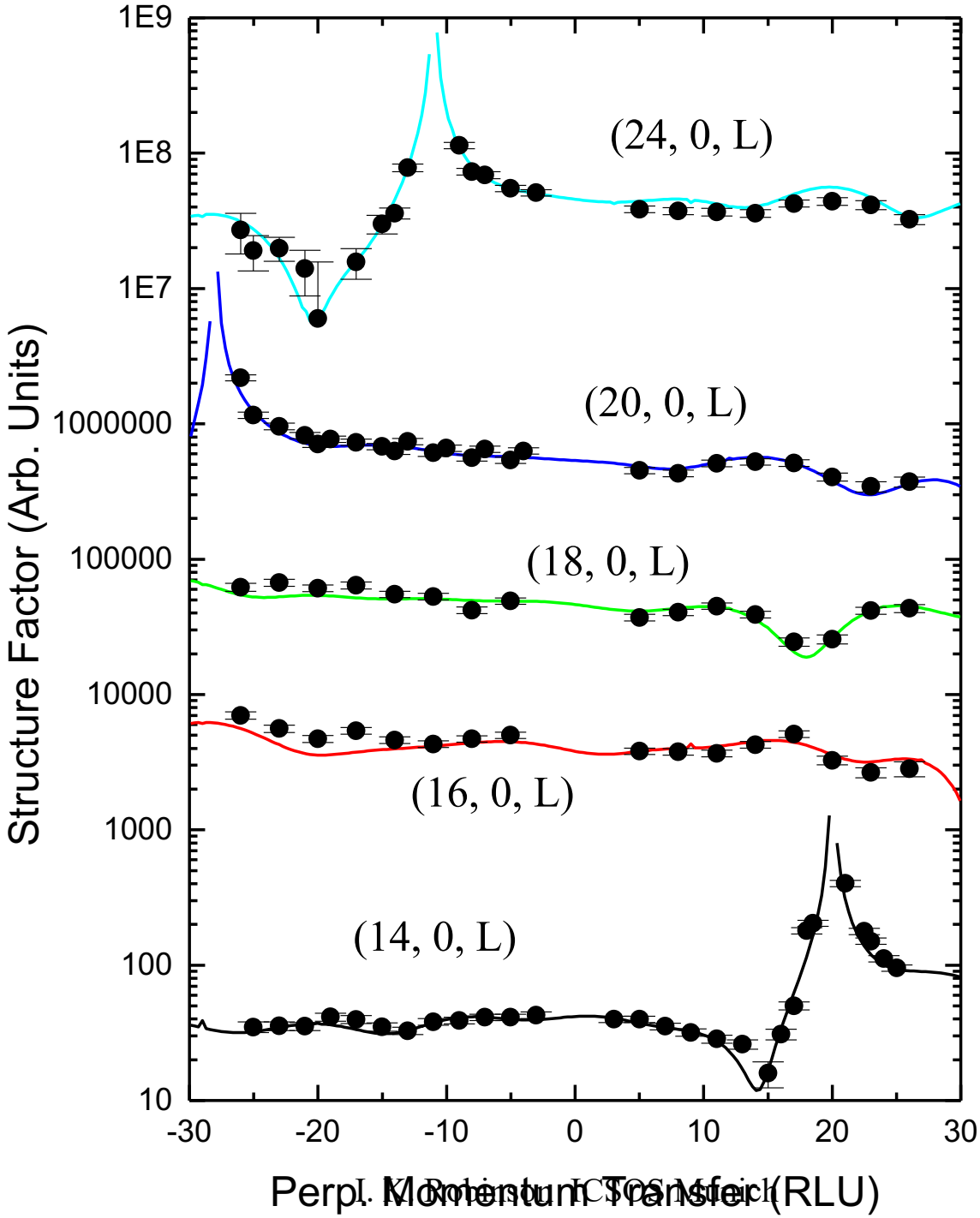
3×1 clean surface

1×1 surface with 0.2ML Au at 600C

STM of Si(557)/Au

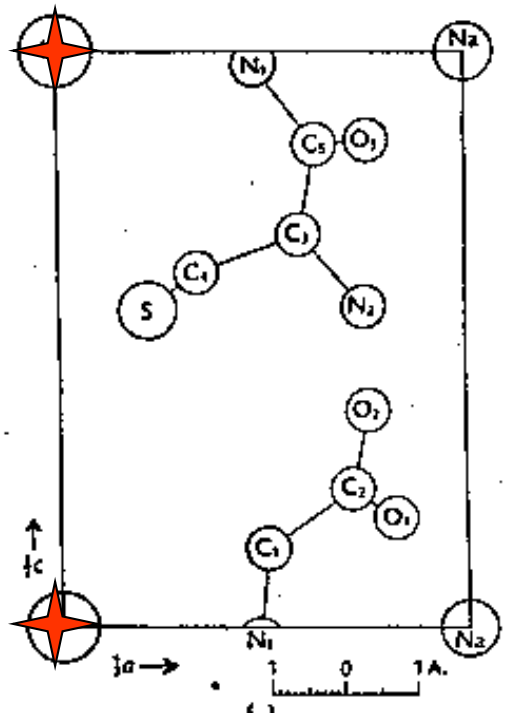
R. Losio, et. al., Phys. Rev. Lett. 86 4632 (2001)



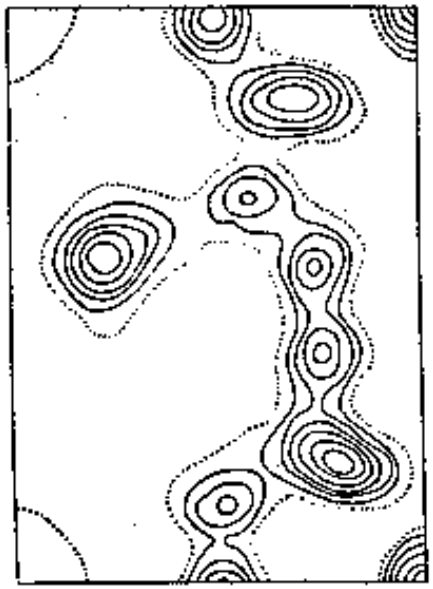

1E9
1E8
1E7
1000000
100000
10000
1000
100
10
(24, 0, L)
(20, 0, L)
(18, 0, L)
(16, 0, L)
(14, 0, L)
Structure Factor (Arb. Units)
-30
-20
-10
0
10
20
30
Perpendicular Momentum Transfer (RLU)

Phasing by a Single Heavy Atom

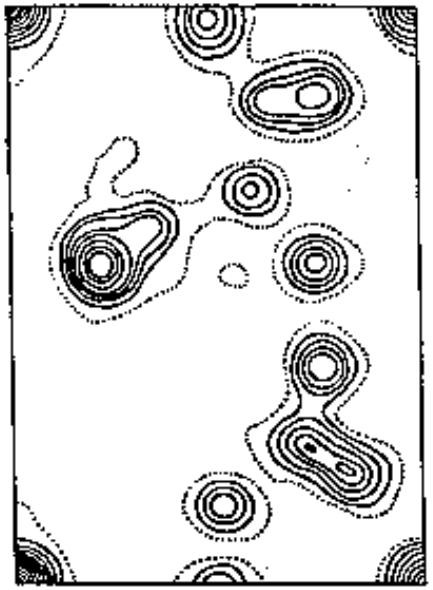
H. B. Dyer, Acta Cryst. 4 42 (1951)



Cysteinylglycine sodium iodide

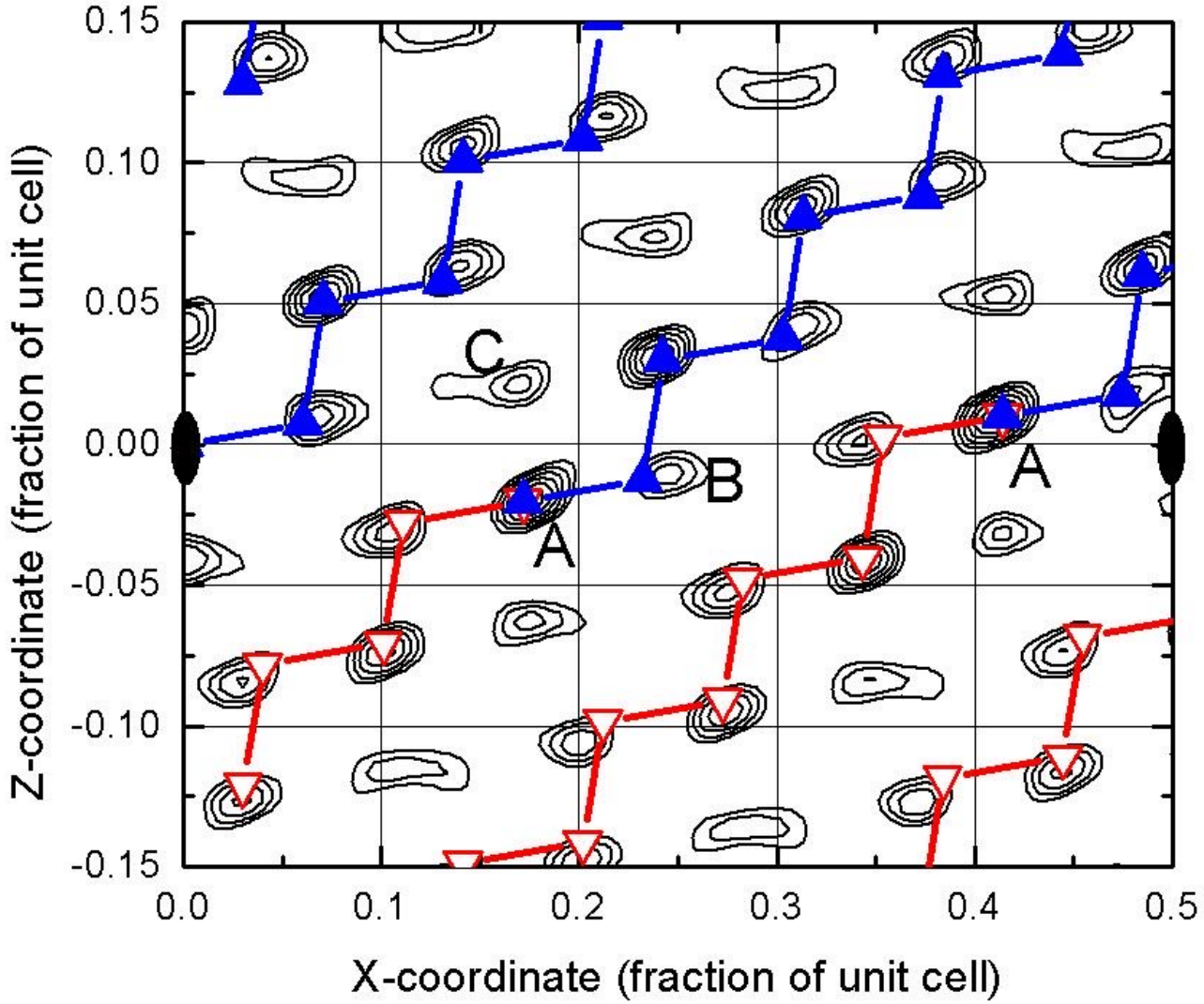


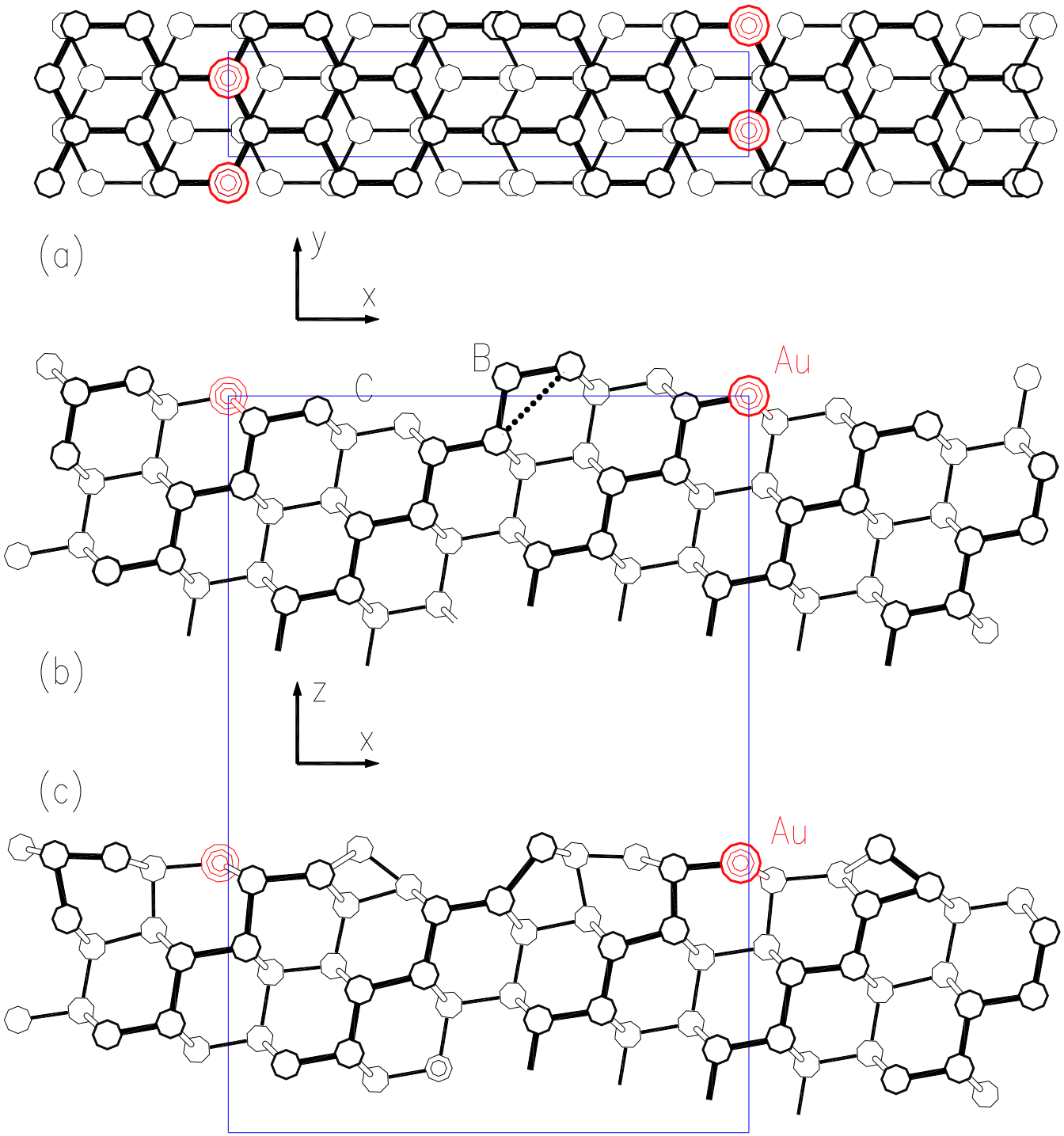
Patterson



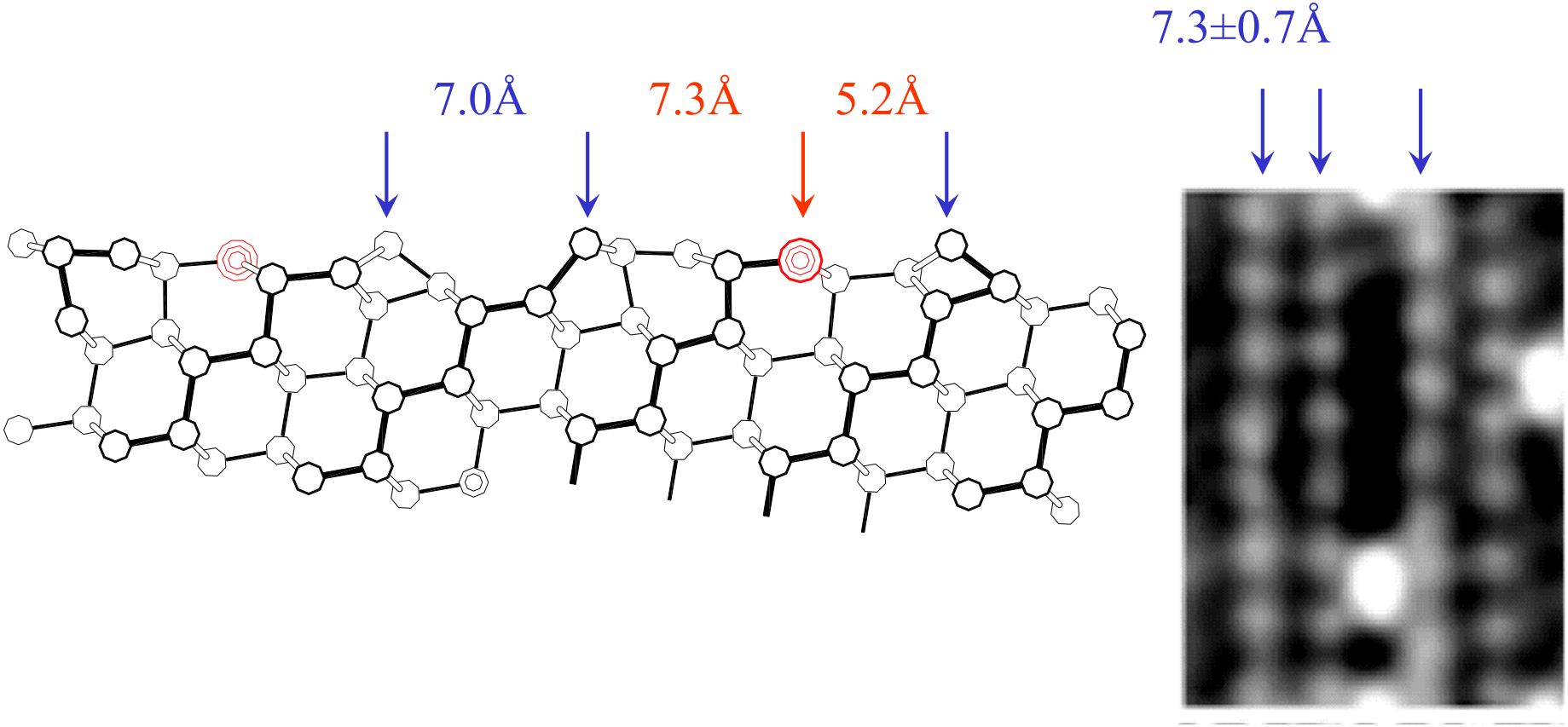
Electron density

X-Z Patterson of Au/Si(557)




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

Comparison with STM



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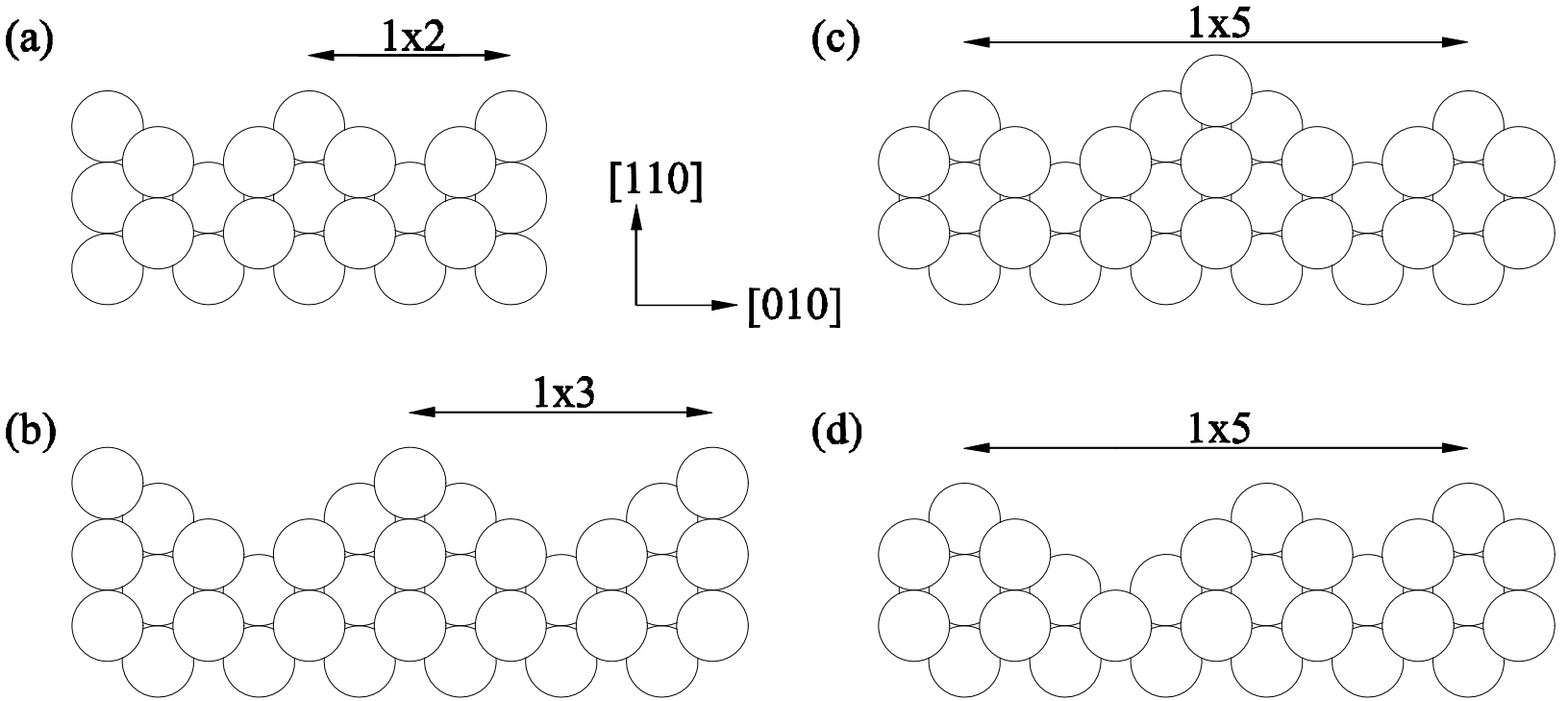
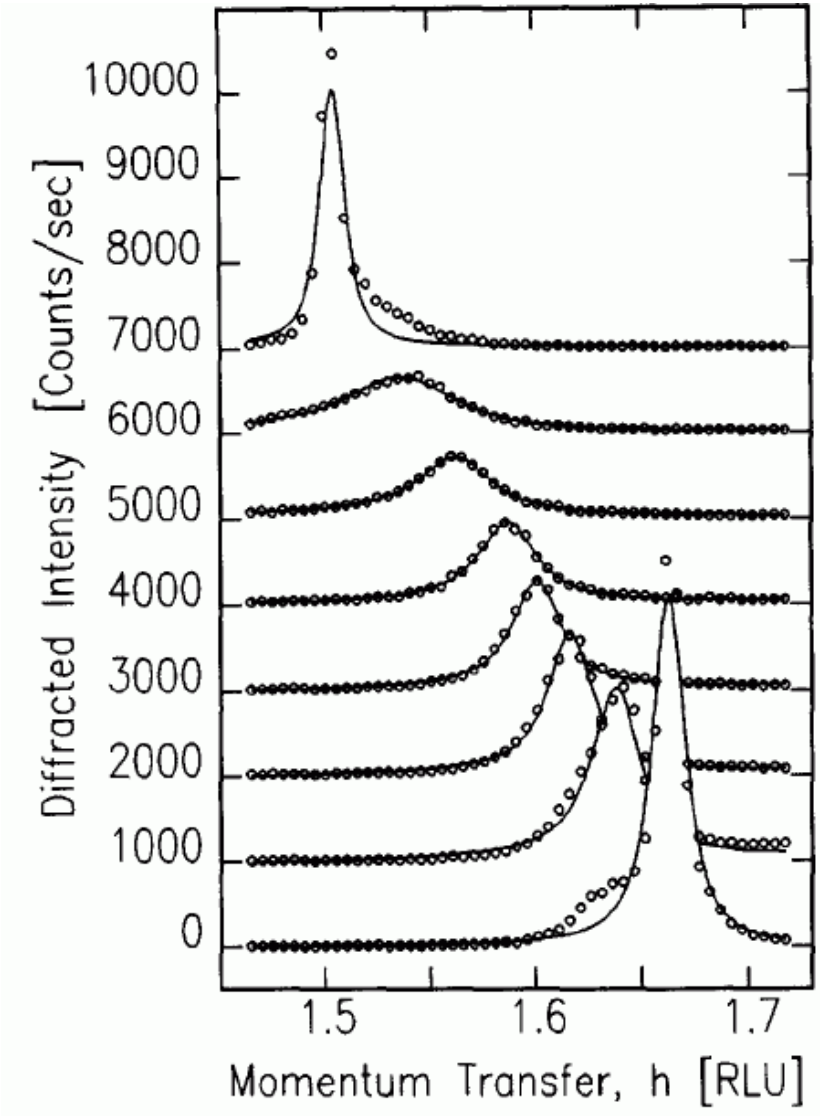
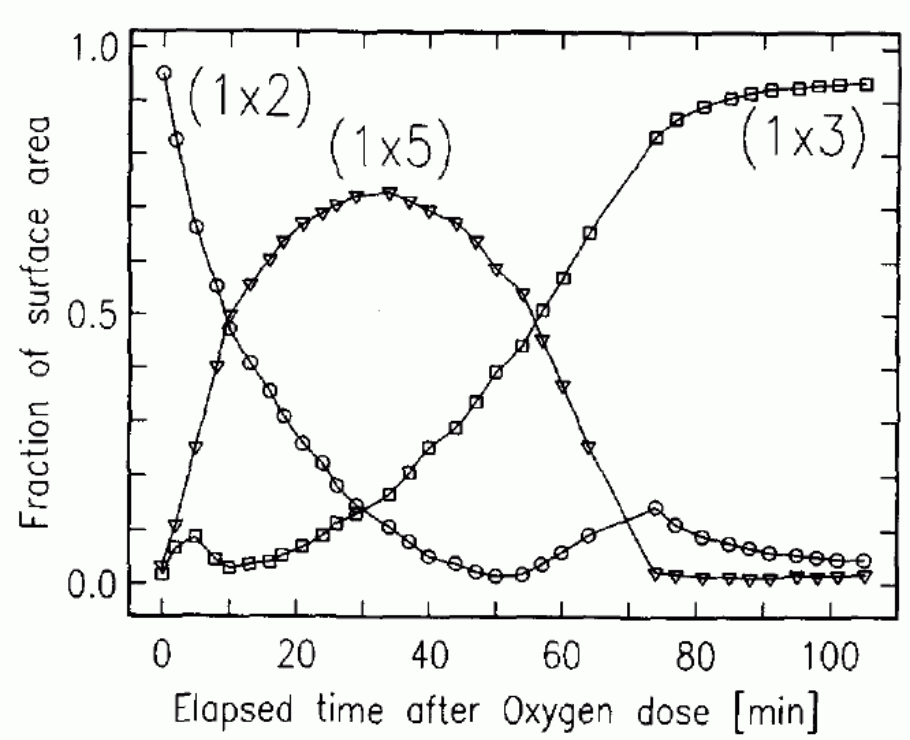
Missing Row structure of FCC(110)



Pt(110) during heating at 600C

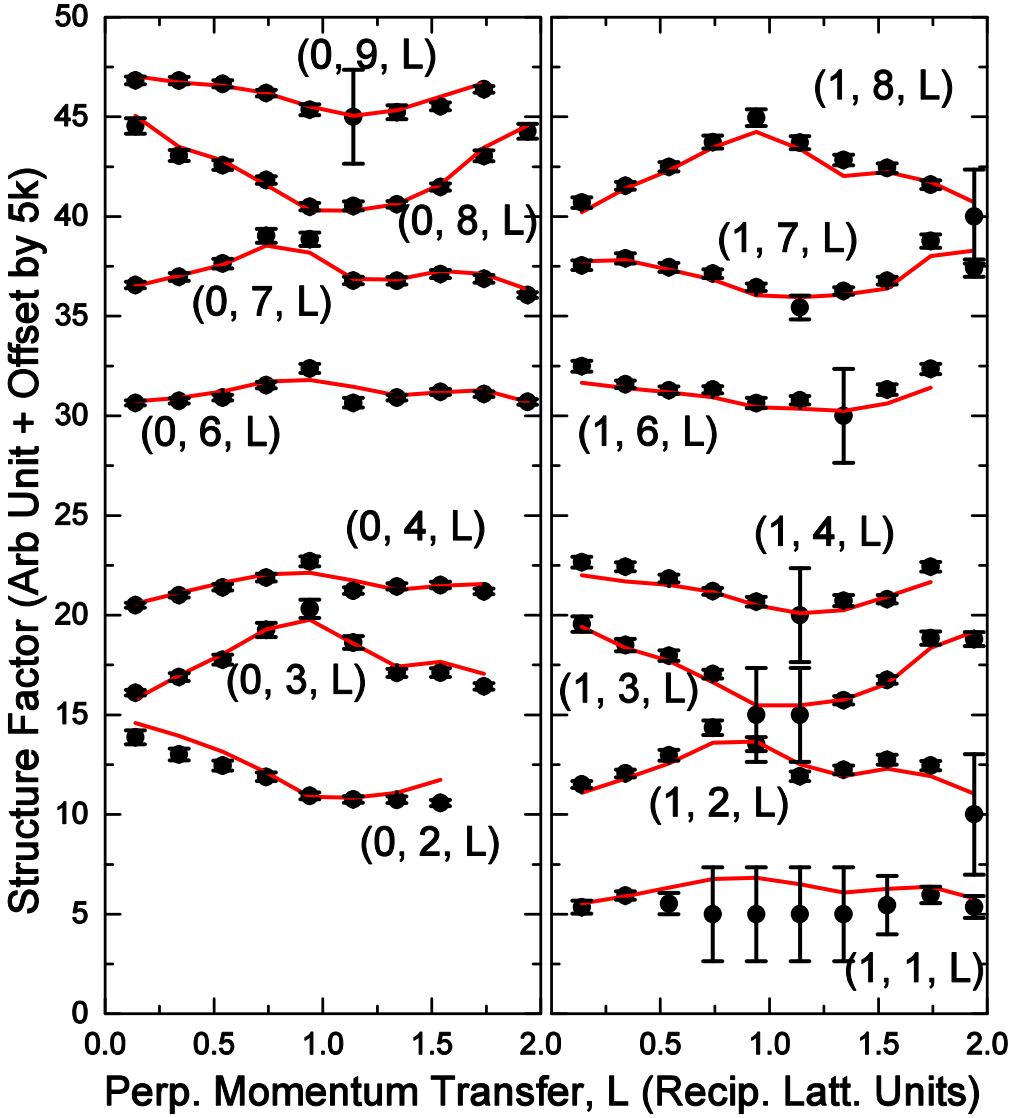
Accompanied by segregation of Carbon

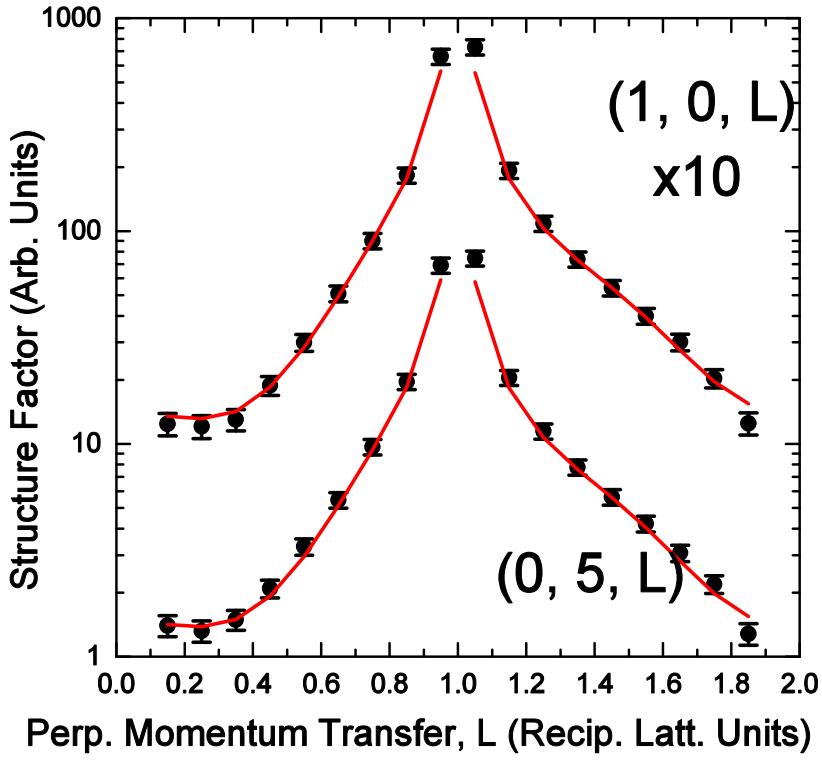




I. K. Robinson, P. J. Eng, C. Romainczyk and K. Kern, Surf. Sci. **367** 105-112 (1996)

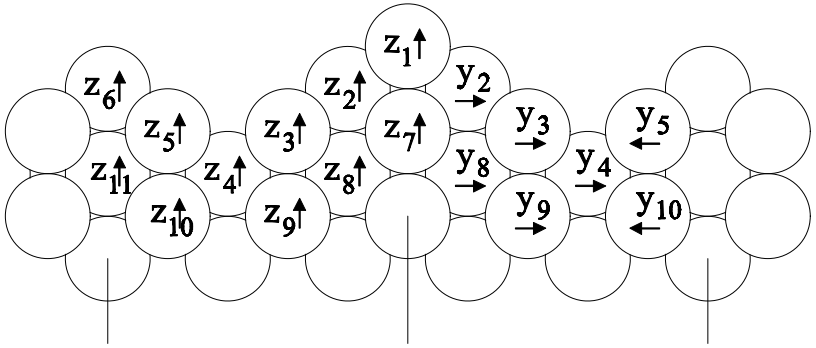
BM32 measurements of Pt(110)1x5



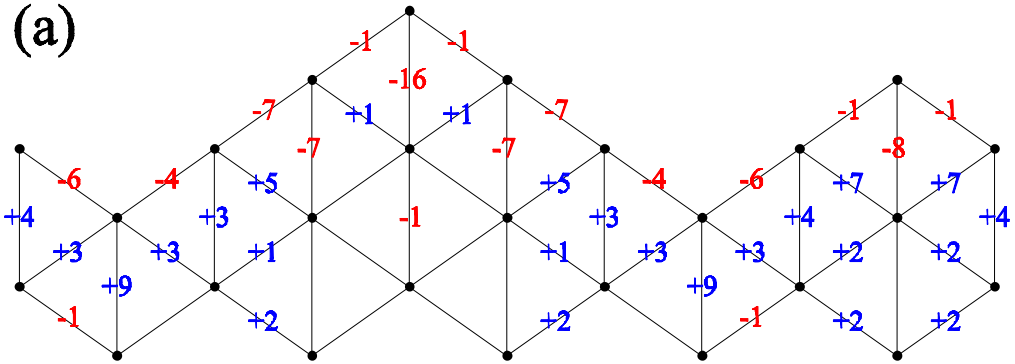


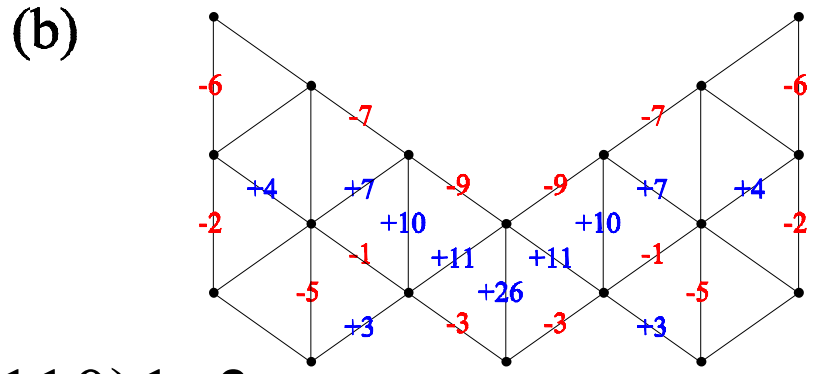
Displacements in final model

Pt(110)1x5 “hill” model



Chisq=2.7
90% hill, 10% valley
7% “1x1”





Pt(110)1x3

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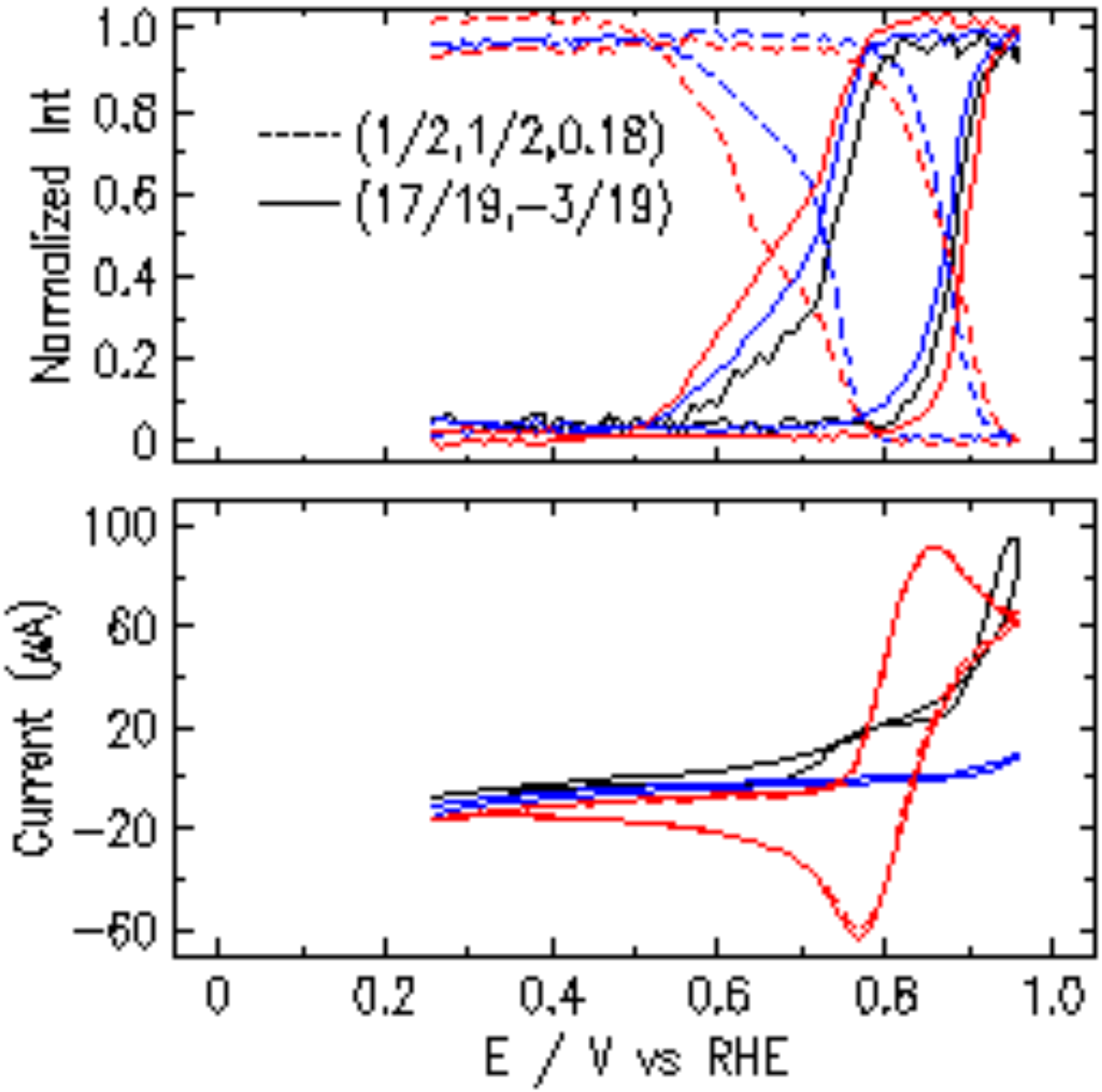
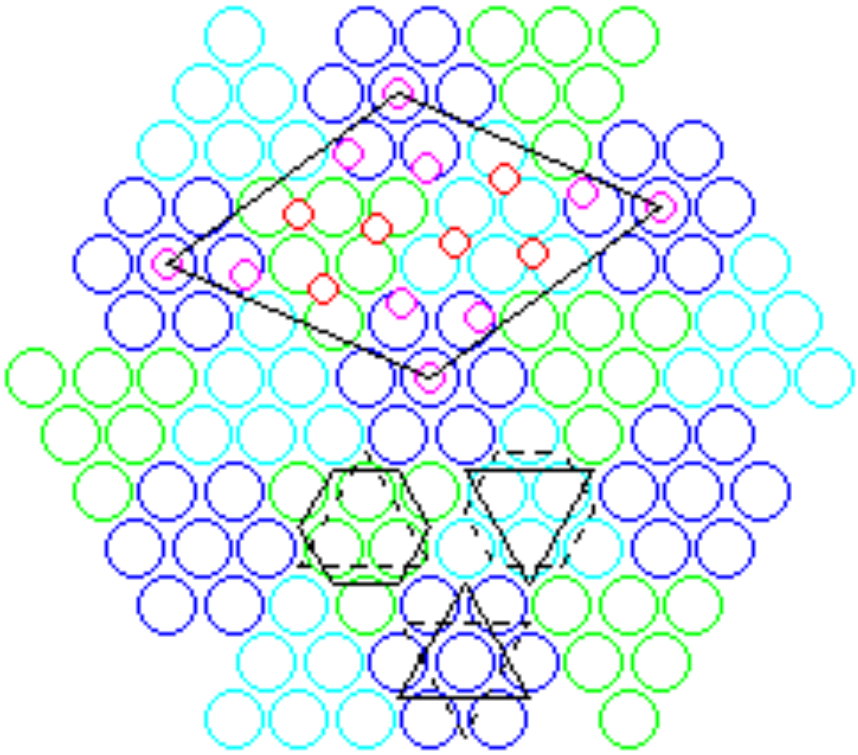
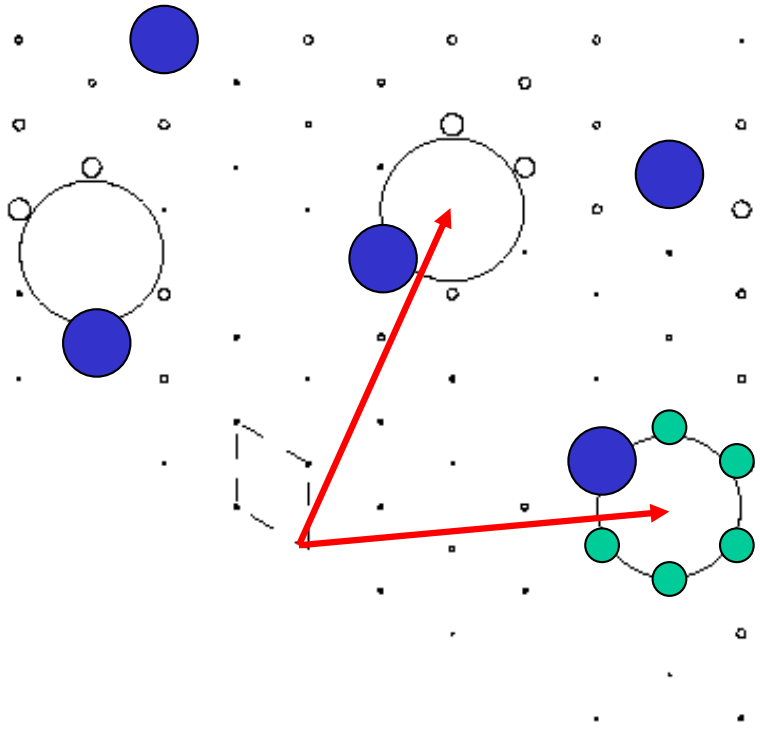
CO dissolved in $HClO_4$ on Pt(111)

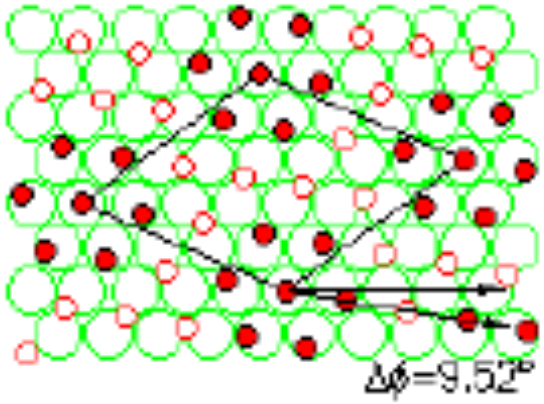


CO reciprocal lattice, rt19

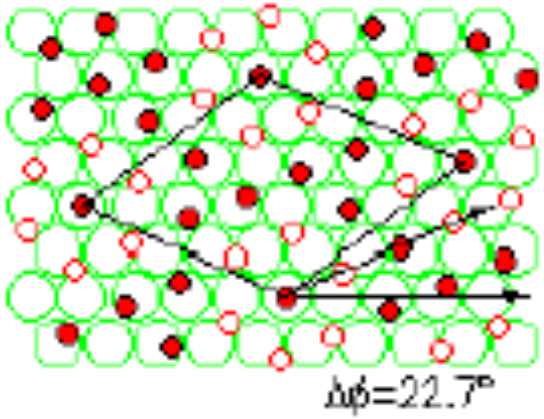




Two inequivalent packings of 13 CO's into rt(19) Pt(111) cell

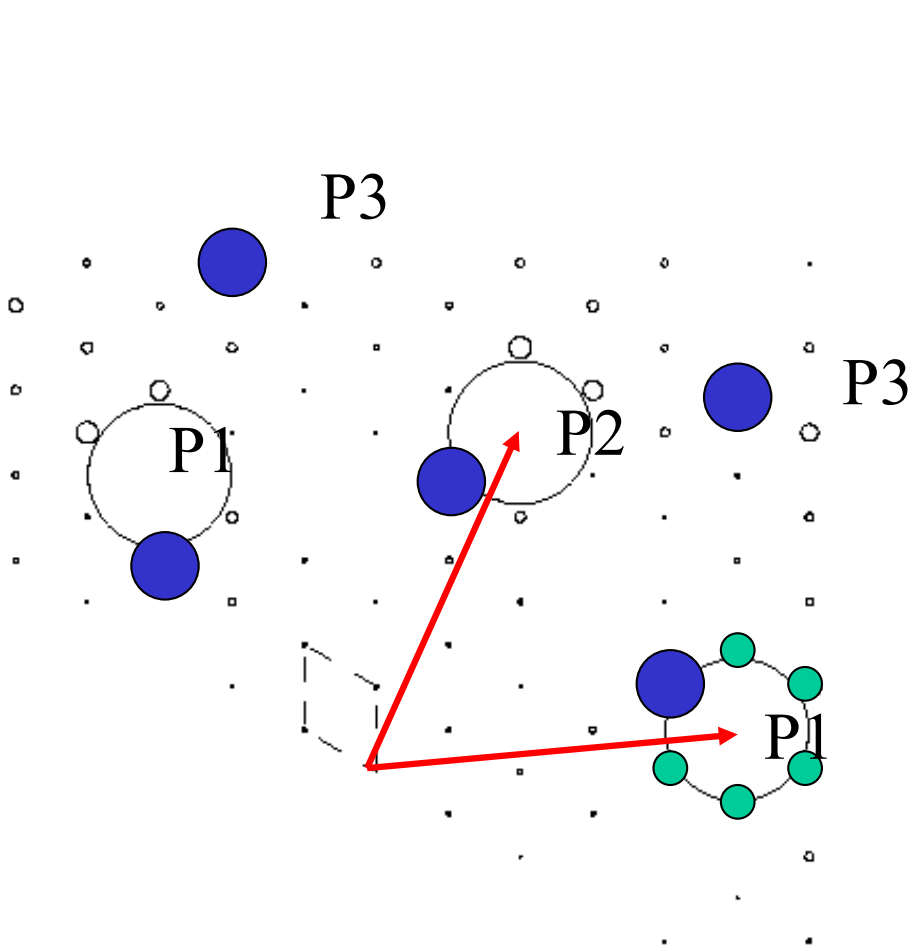


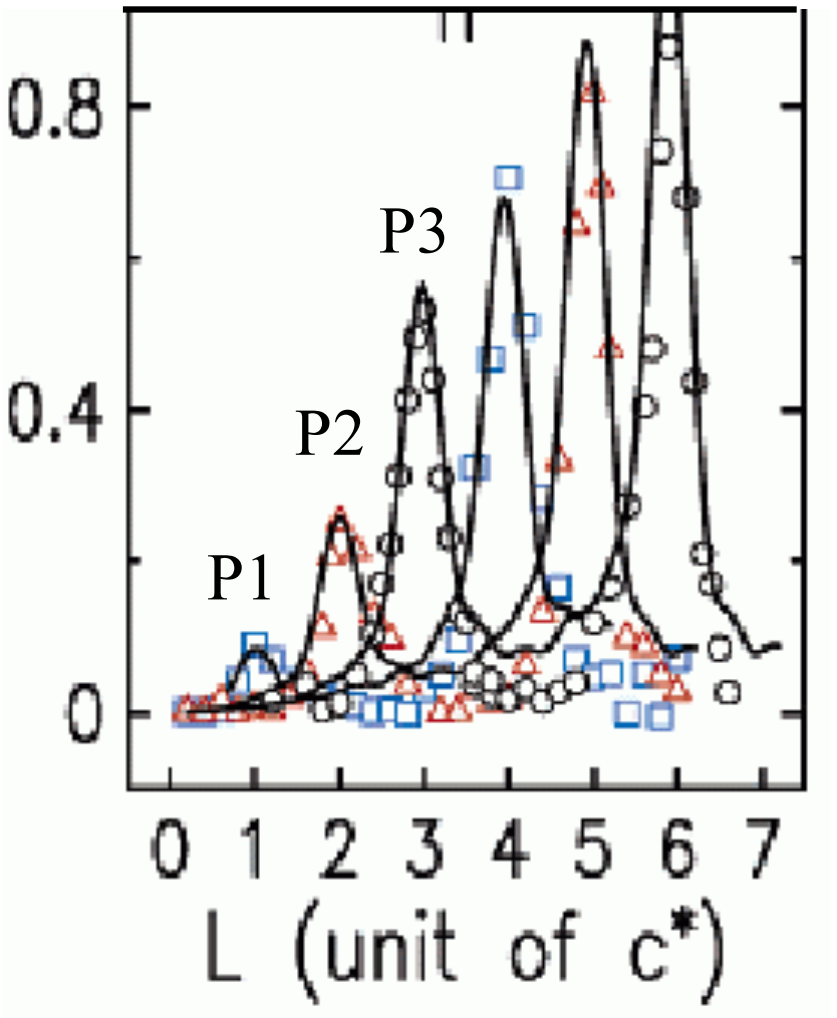
This 'patch' model is the only one observed, by the CO peak positions



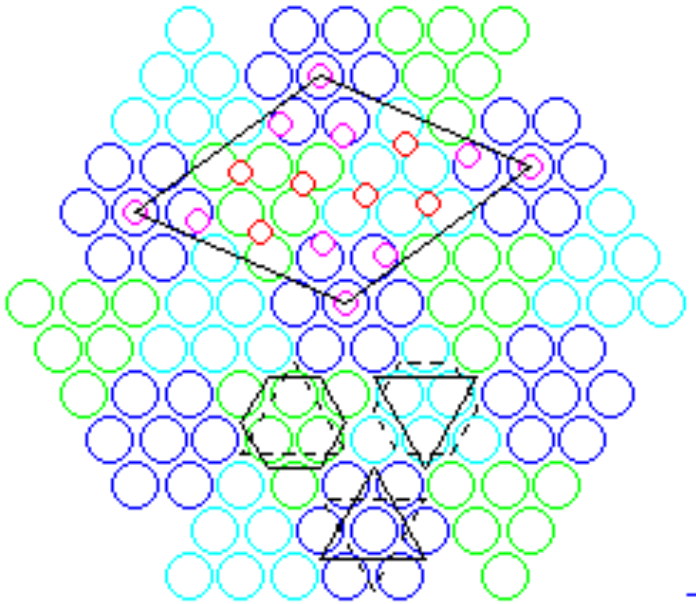
This 'ring' model is not seen.

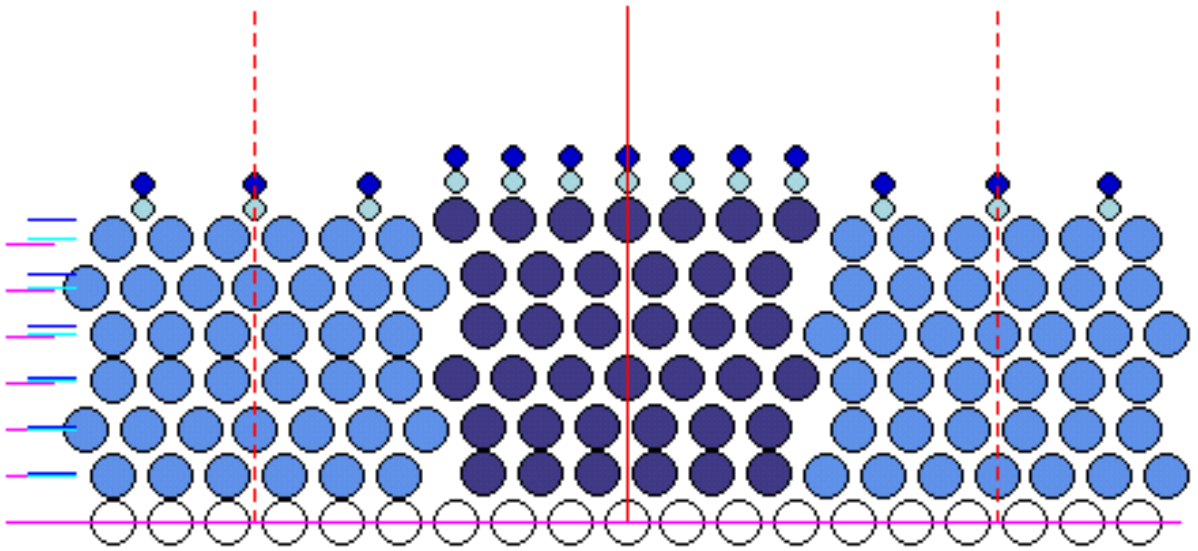
rt19×rt19 CO/Pt(111)





Top and Side Views of Model





Depth=1.8 layers

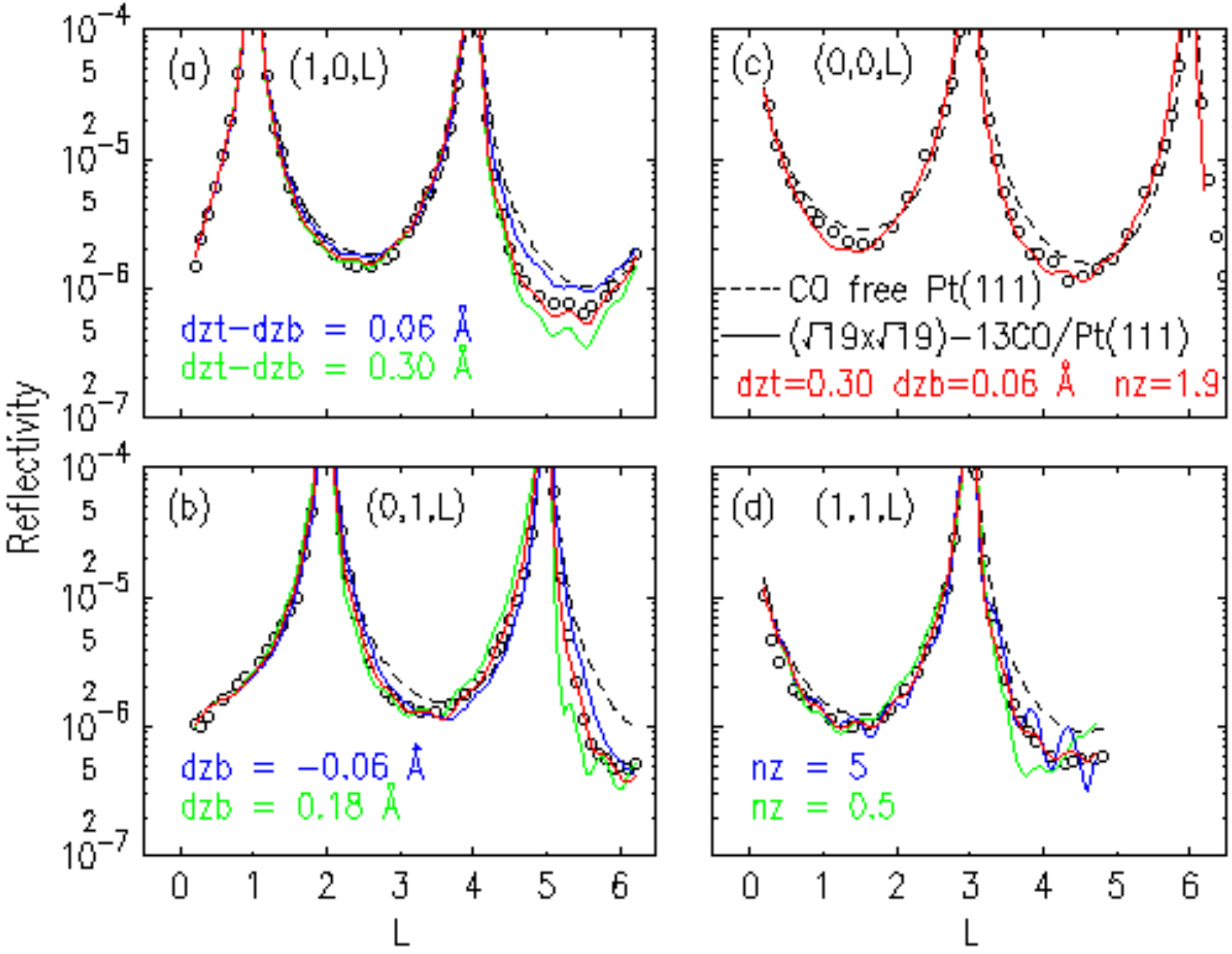
D_7=0.28 A

D_{6+6}=0.04 A

σ_{CO}=0.3 A

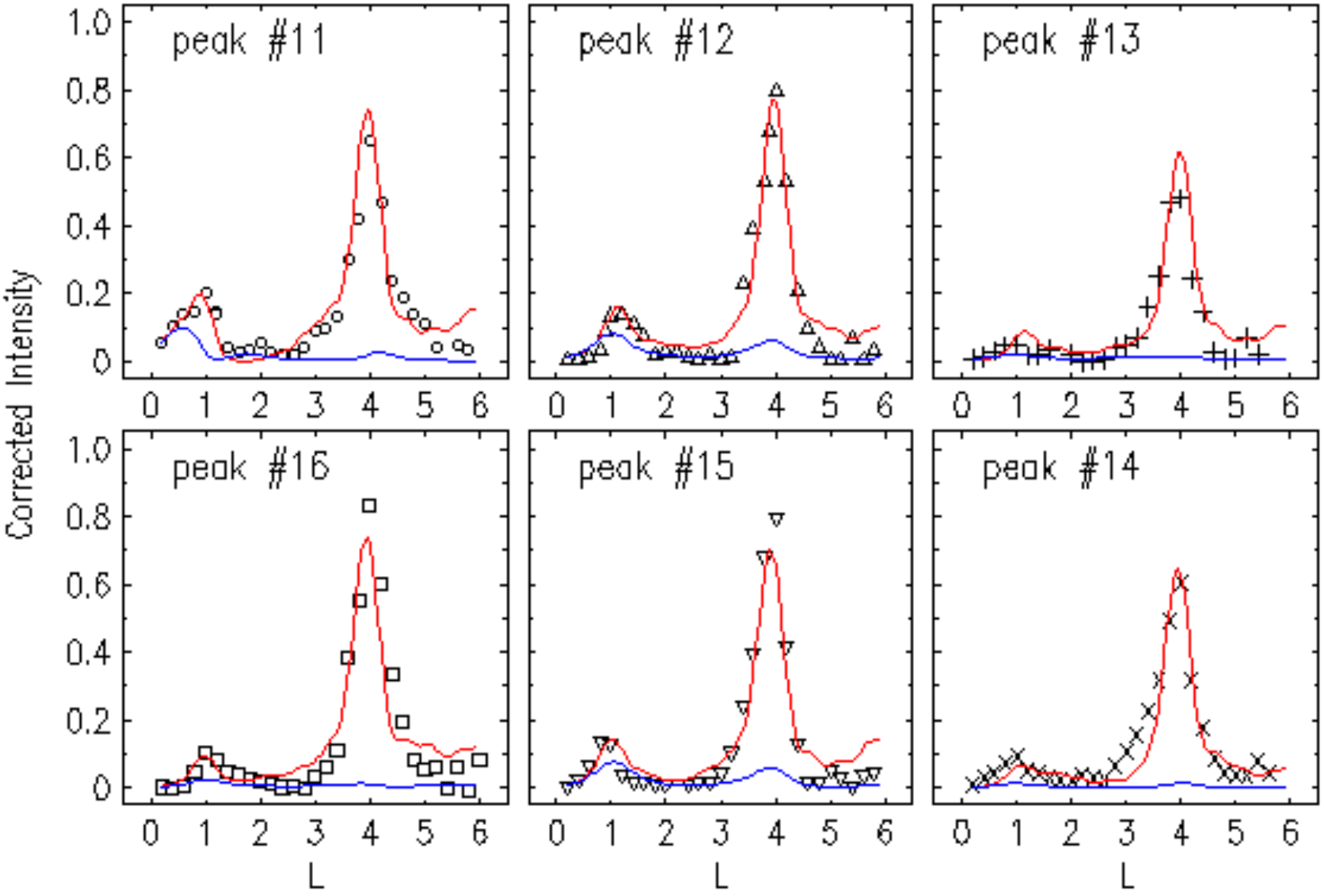
Fit of Model to CTR Data

Dashed curve is clean Pt(111)

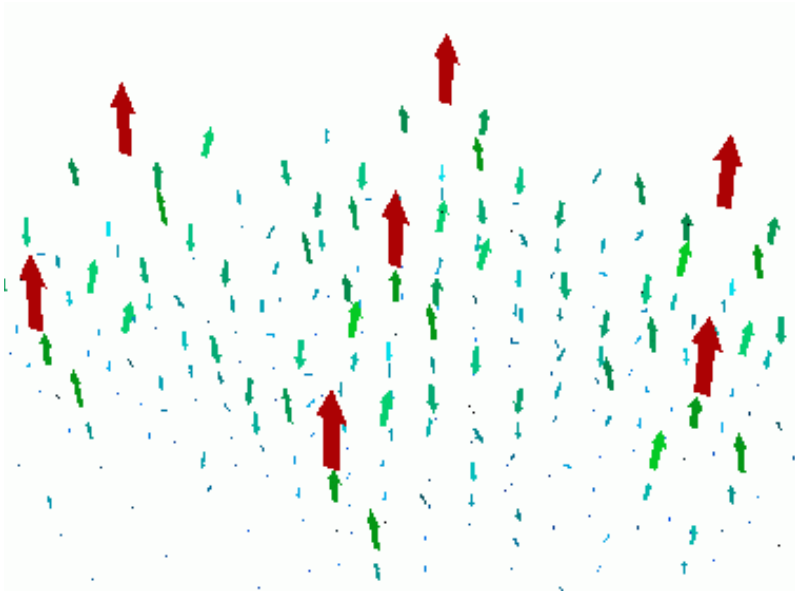


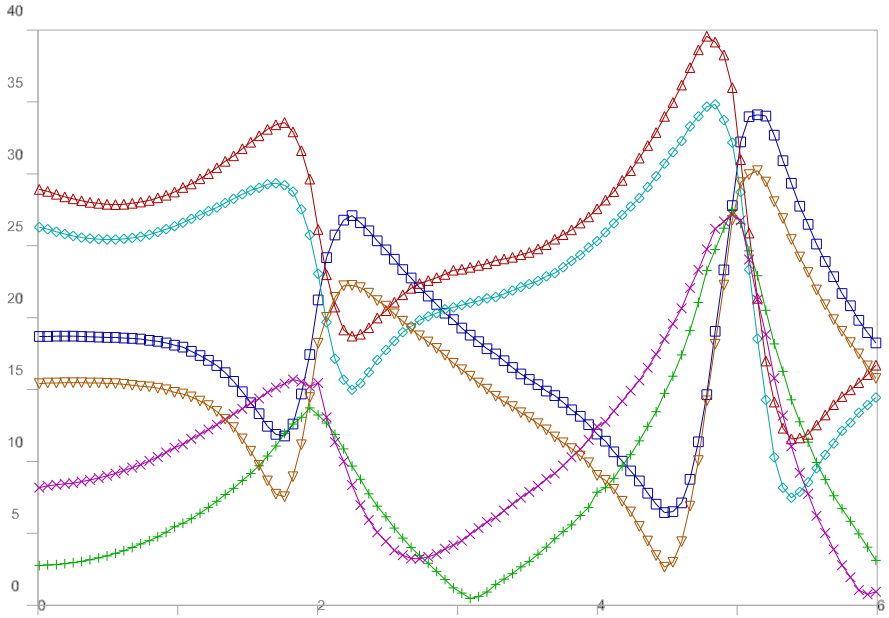
Fit of Model to Rt19 Data

Blue line has vertical relaxations turned off



Continuum Elasticity Calculation





L=2 L=5

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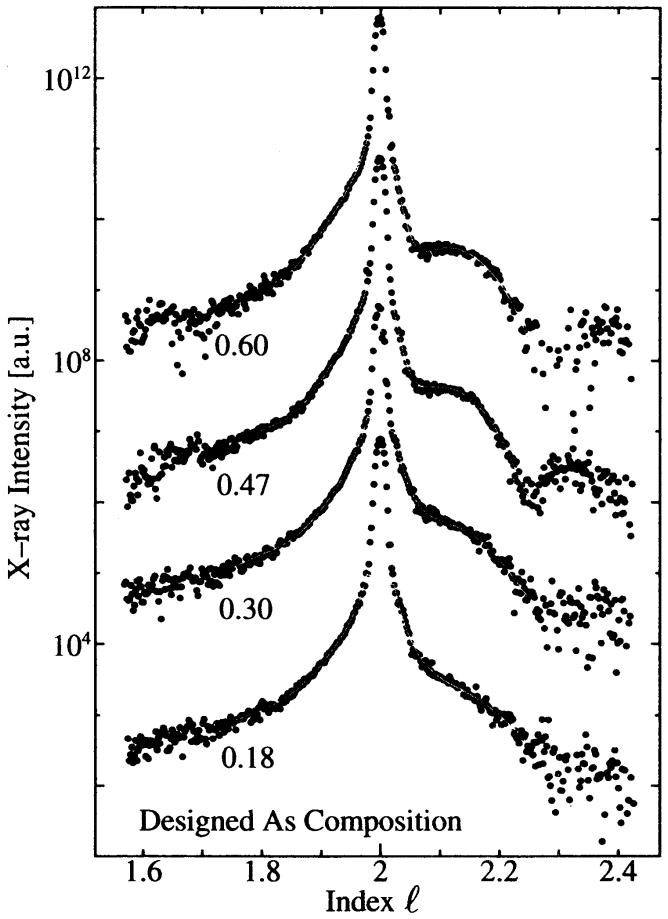
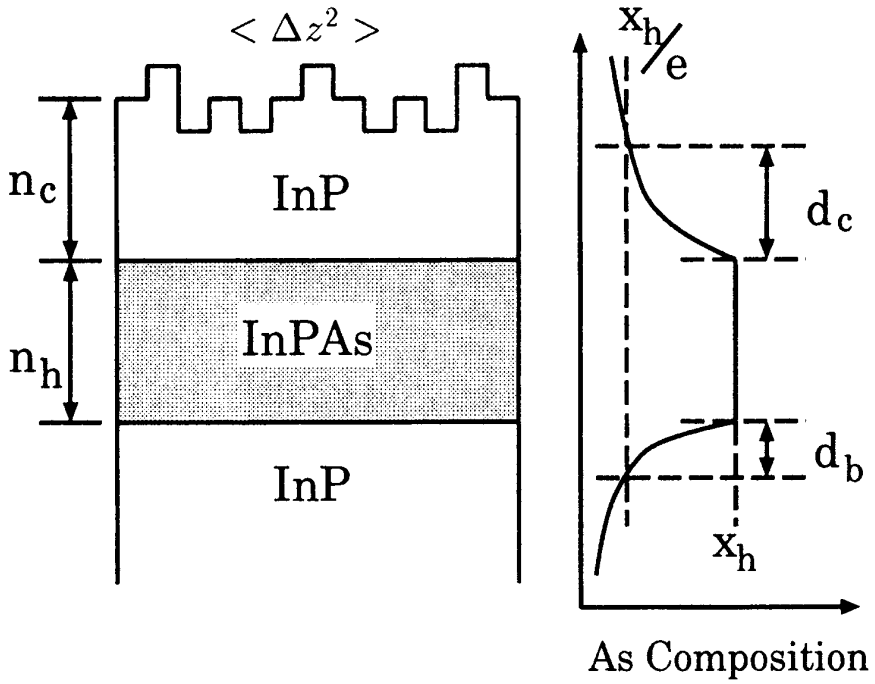
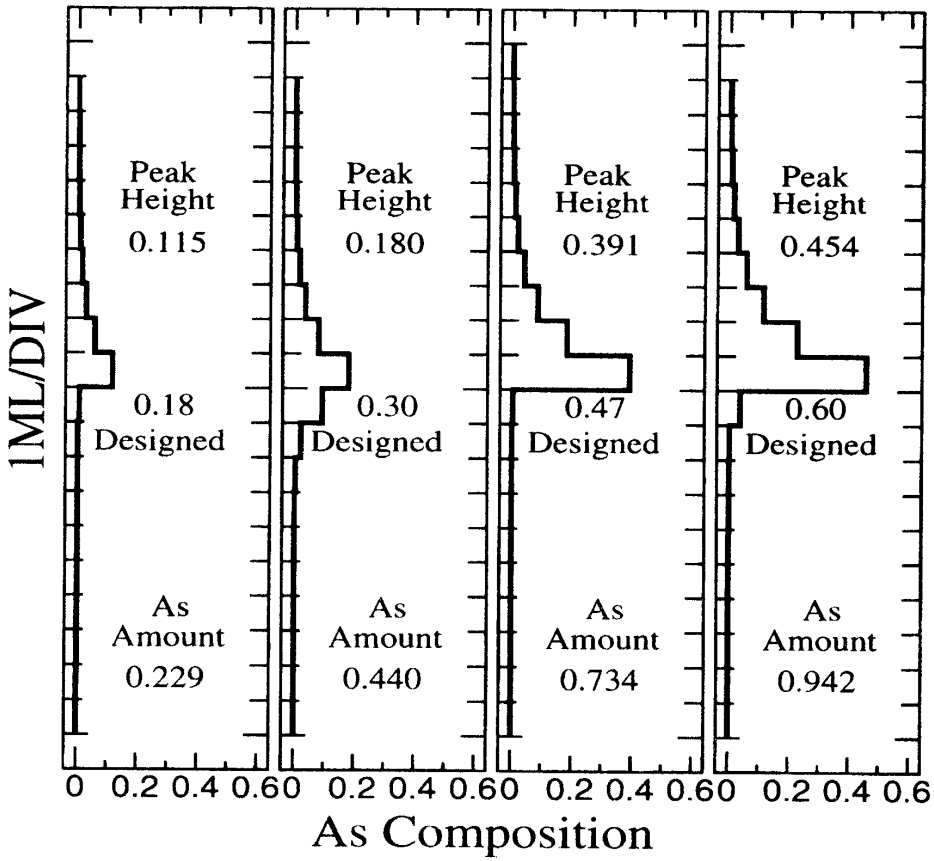
As in InP/InPAs heterostructure

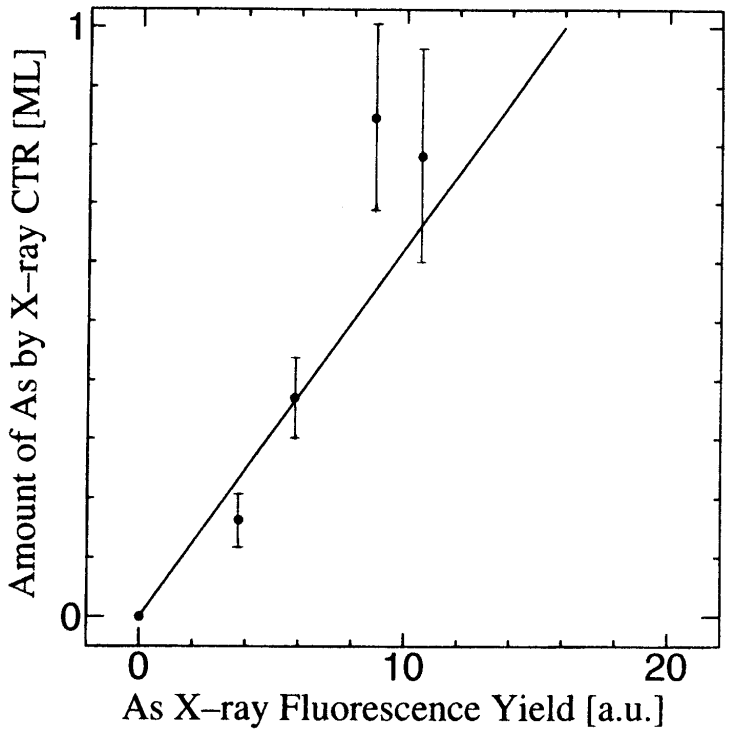




M. Tabuchi *et al* J. Appl. Phys 81 112 (1997)

CTR agrees with Fluorescence





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

CTR of double-step structure

$$A_1(Q) = \sum_{j=0}^{\infty} \rho_1 e^{iQaj} + \sum_{j=n}^{\infty} \rho_2 e^{iQaj}$$
$$= (\rho_1 + \rho_2 e^{iQan}) \frac{1}{1-e^{iQa}}$$
$$= M_1(Q) \frac{1}{1-e^{iQa}}.$$

Perturbation limit: $\rho_2 << \rho_1$

$$|M_1(Q)| = |\rho_1 + \rho_2 e^{iQan}|$$

$$\simeq \rho_1 + \rho_2 \cos(Qan)$$

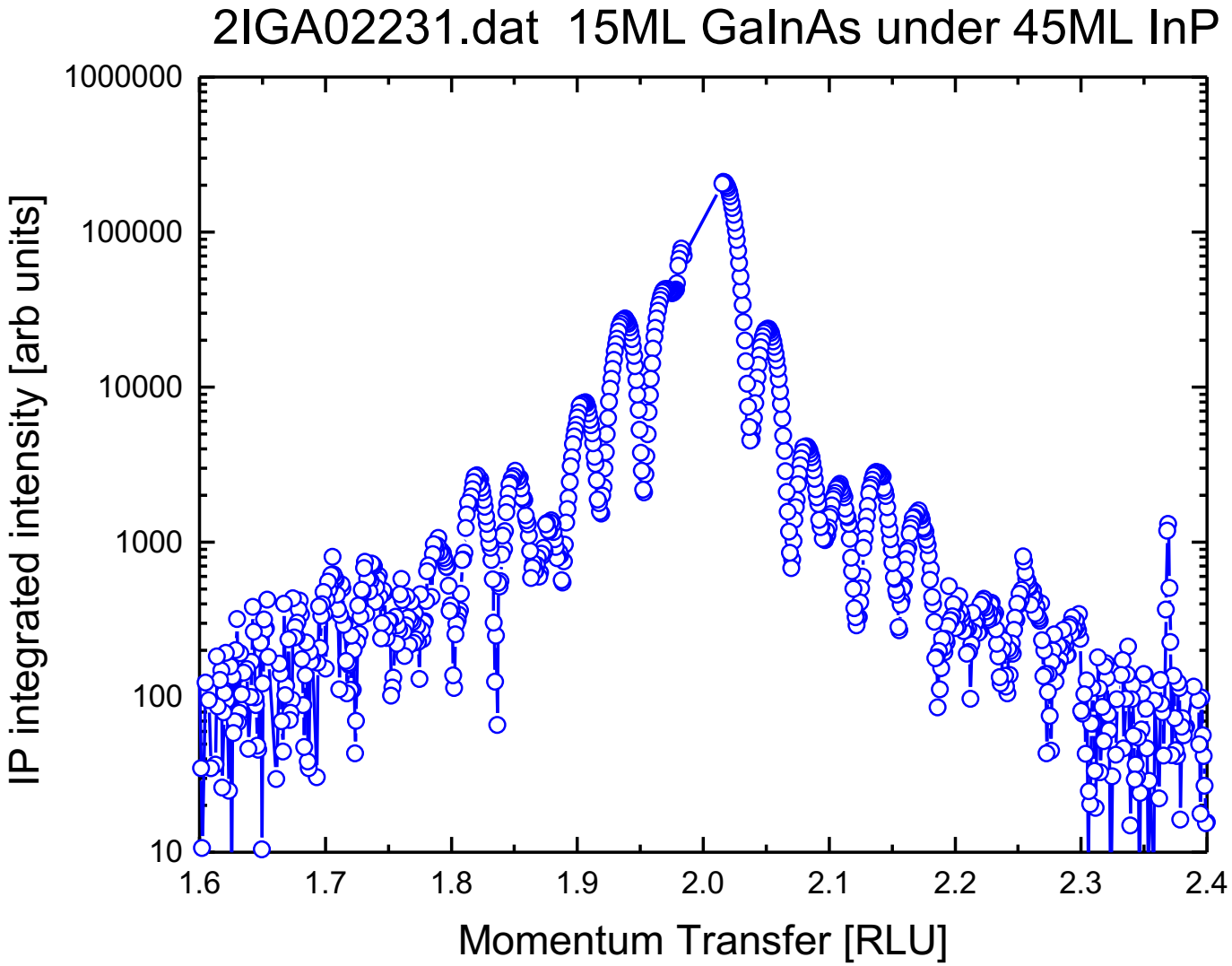
Data Analysis Procedure

$$M(Q) = \sqrt{I(Q)}/|A_0(Q)|$$

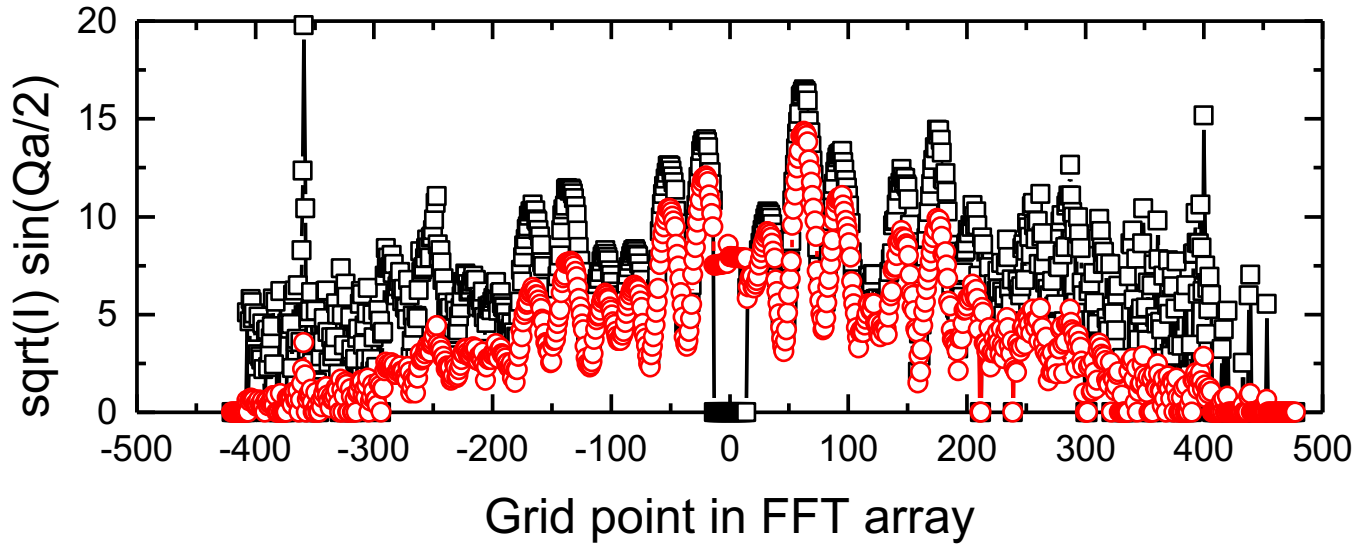
$$= \sqrt{I(Q)}\sin(Qa/2).$$

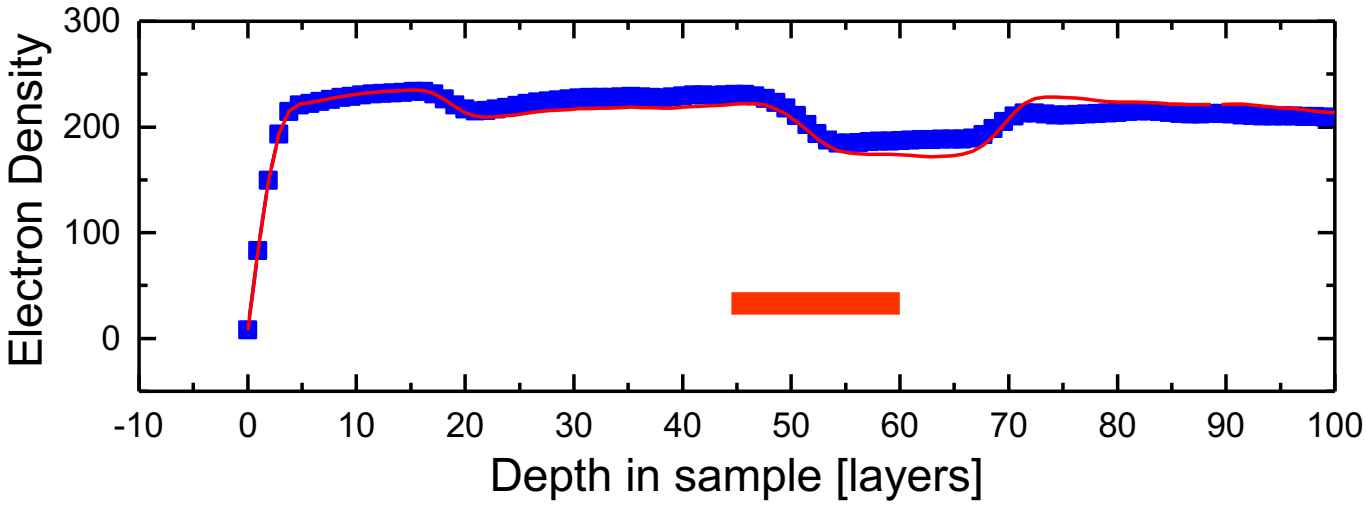
$$\rho(z) = \int_0^z \mathcal{F}\{\sqrt{I(Q)}\sin(Qa/2)\}dz'$$

Test InP/GaAs/InP heterostructure

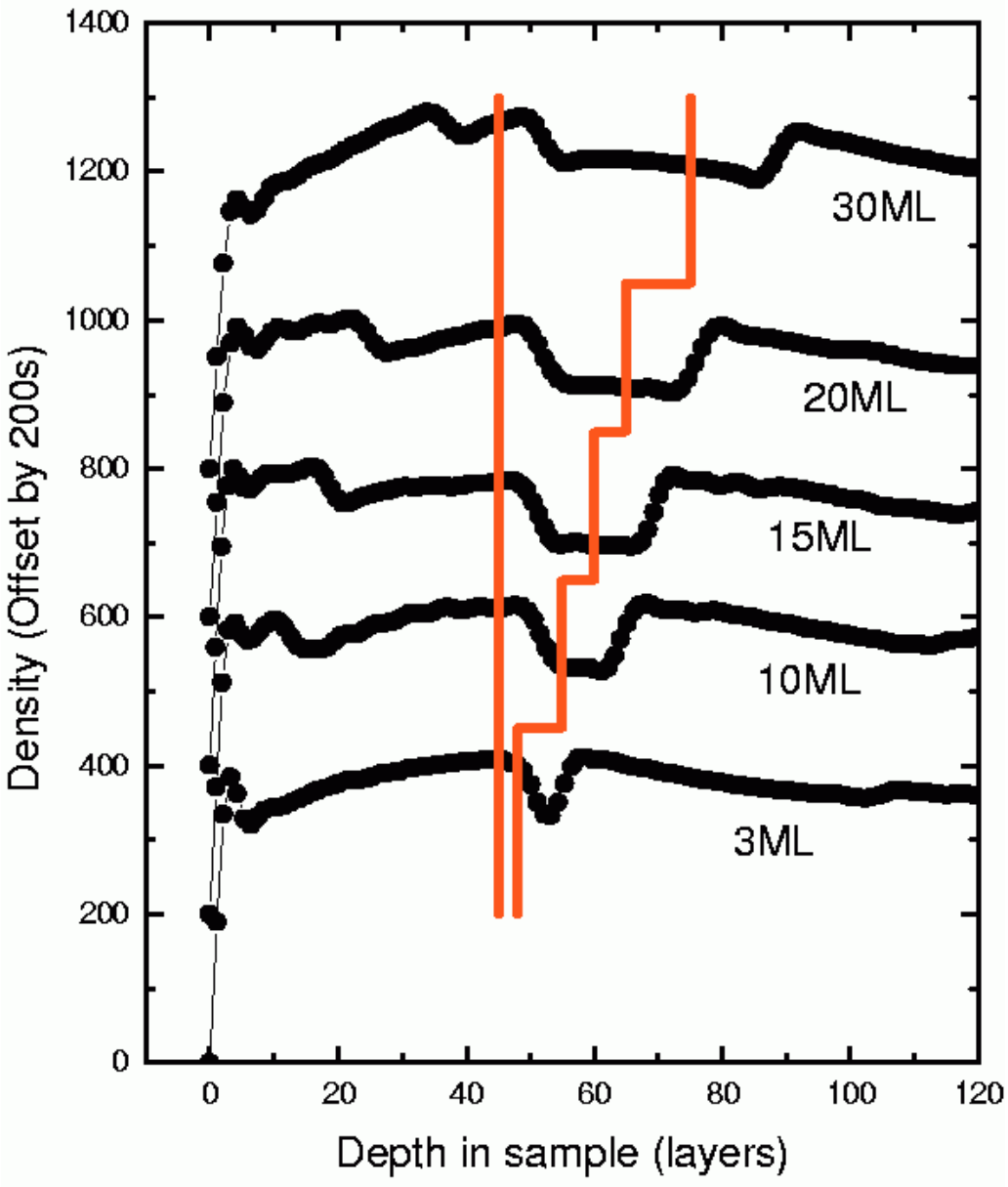


Input and Output of FFT





Thickness Variation



Conclusions and Outlook

- Au quantum wires on Si(557)
- ‘Homometric’ structures of Pt(110)1x5
- Deep subsurface strain in Pt(111)/CO
- Direct methods for Heterostructures
- Needs better way to Parameterize Strain