Surface Structure as a Foundation of Nanotechnology

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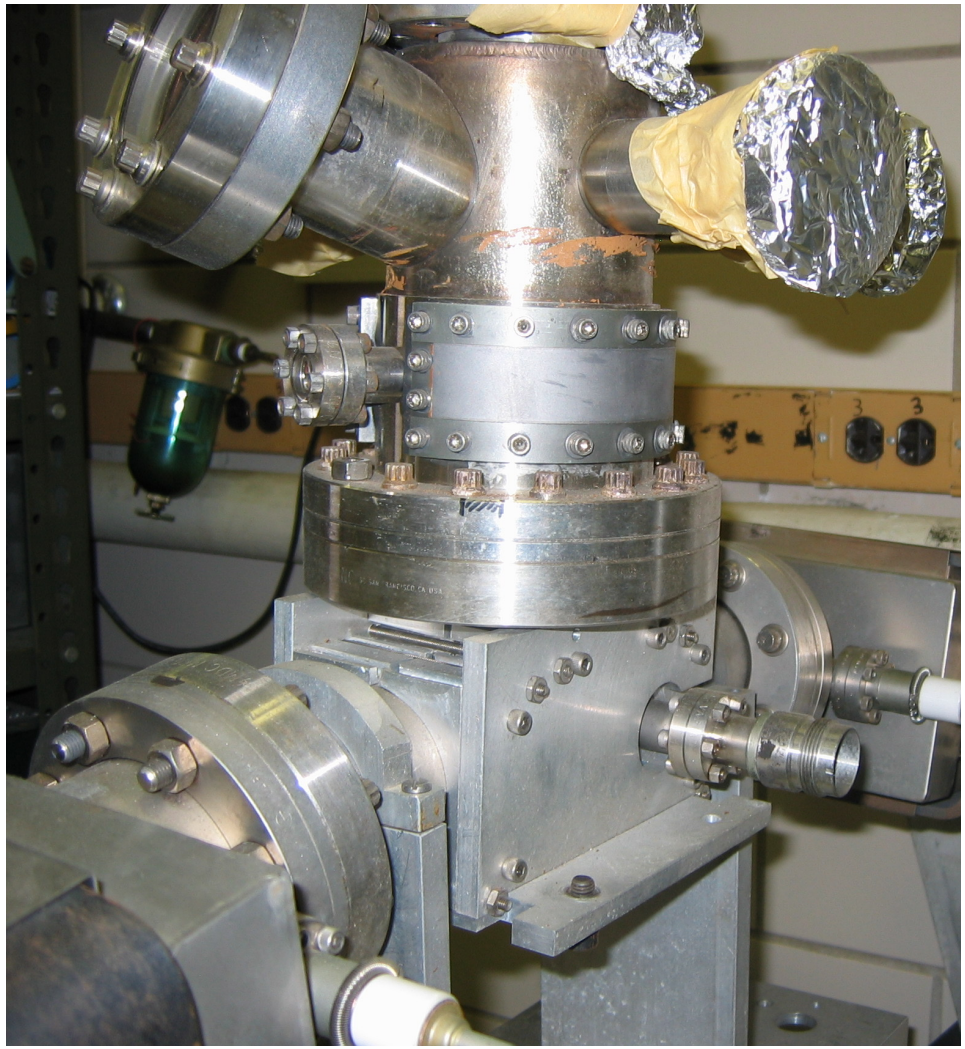
University College London

Diamond Light Source

Symposium on Condensed Matter Physics at Synchrotron Facilities: History as Prologue to the Future,

APS March Meeting, Denver, March 2007

First UHV Experiments



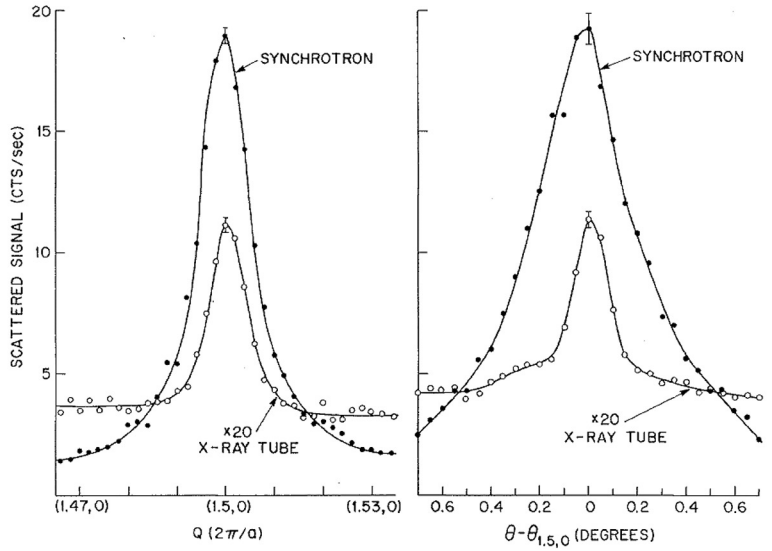
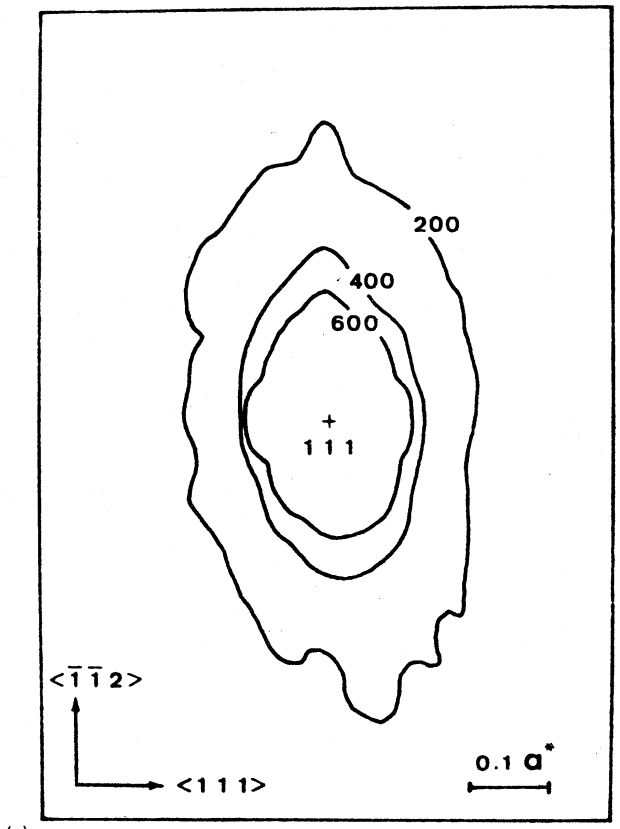


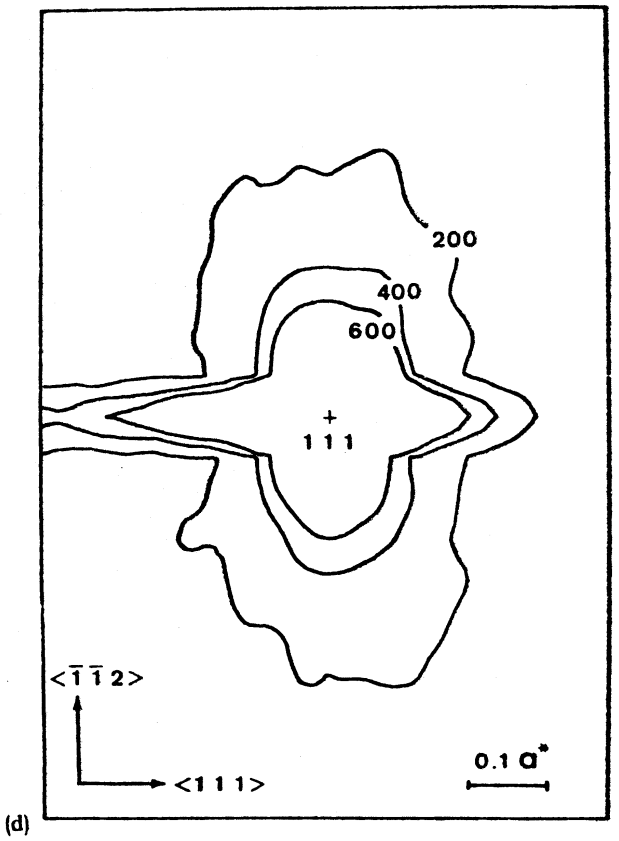
FIG. 1. A plot of the $(\frac{3}{2}, 0)$ Bragg reflection as a function of the momentum transfer $Q(2\pi/a)$ and the crystal's mosaic spread (deg).

P. Eisenberger and W. C. Marra,
PRL **46** 1081 (1981)
experiments done at SSRL

Diffuse Scattering from Si Wafer



Unpolished wafer



40 microns removed

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

Powders of 2D Crystallites

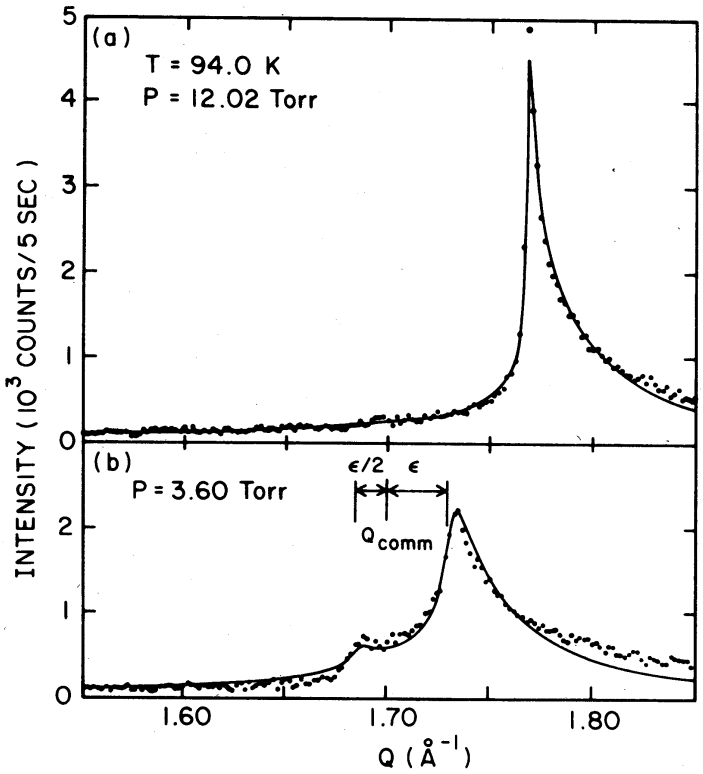
FIG. 4. Microphotometer record of the diffract pattern of a heat treated carbon black, showing t dimensional lattice reflections. Radiation Cu $K\alpha = 1.53$ monochromated by reflection from rocksalt.

Carbon black

B. E. Warren, Phys. Rev. 59 693 (1941)

Kr on graphite

P. W. Stephens *et al*, Phys. Rev. B 29 3512 (1984)



Surfaces in Dynamical Diffraction

A. M. Afanas'ev *et. al.*, Acta Cryst **A40** 352 (1984)

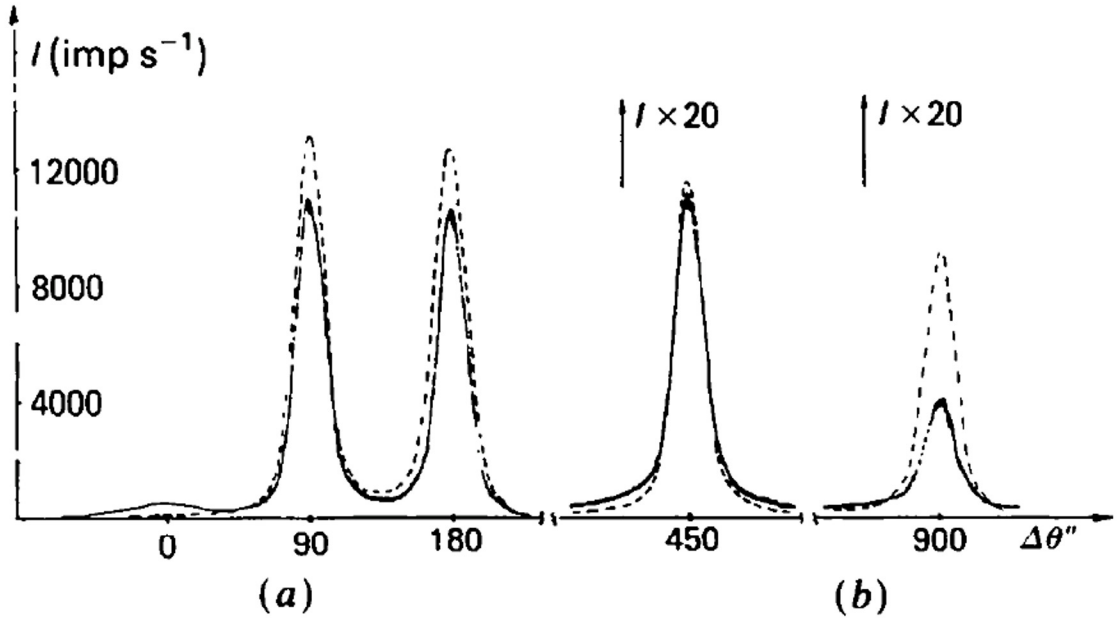
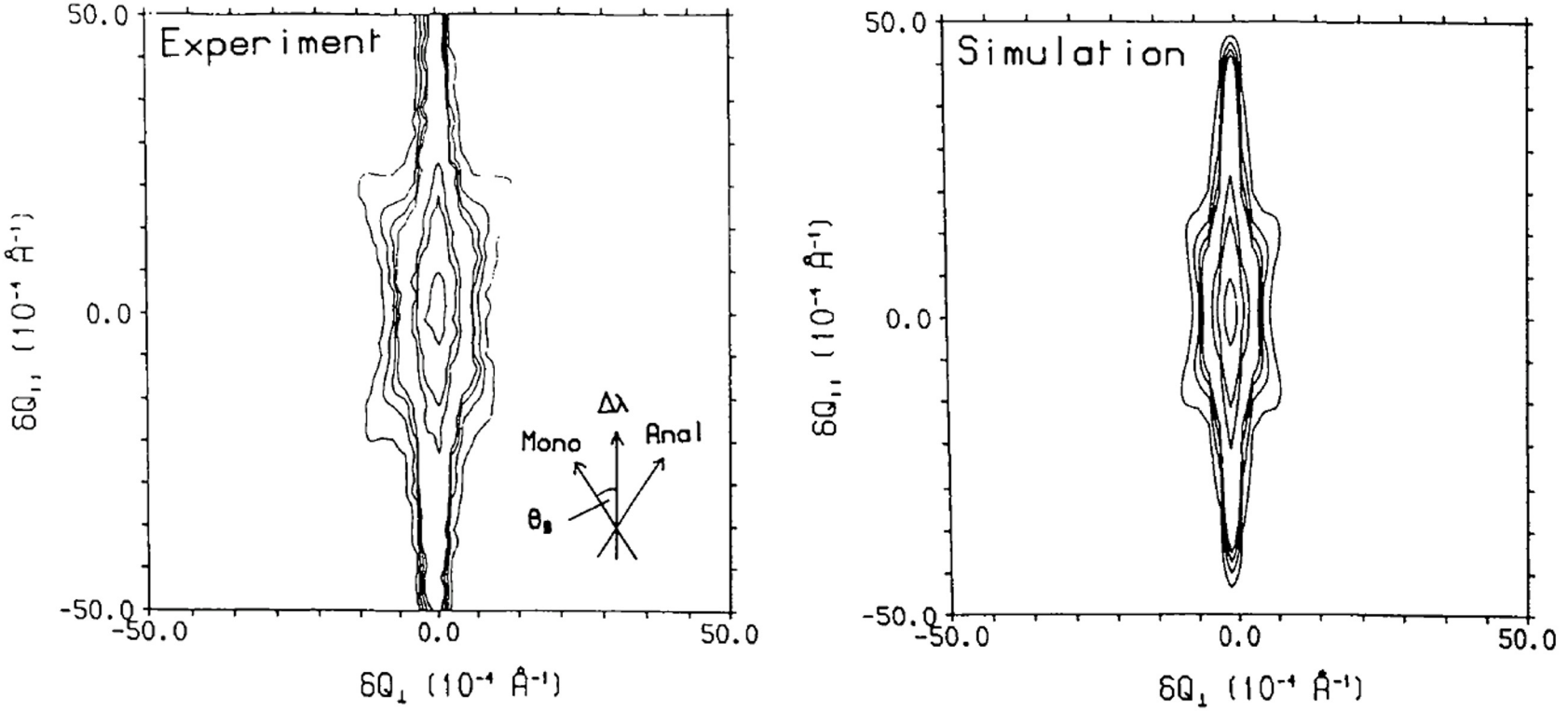


Fig. 2. TDC spectra from Ge(111) crystals, $(n, -n, n)$ arrangement, symmetric Bragg diffraction for (a) $\alpha = 90''$, (b) $\alpha = 450''$. Dashed line for ideal crystal, solid line for crystal first polished with diamond paste and then partially etched.

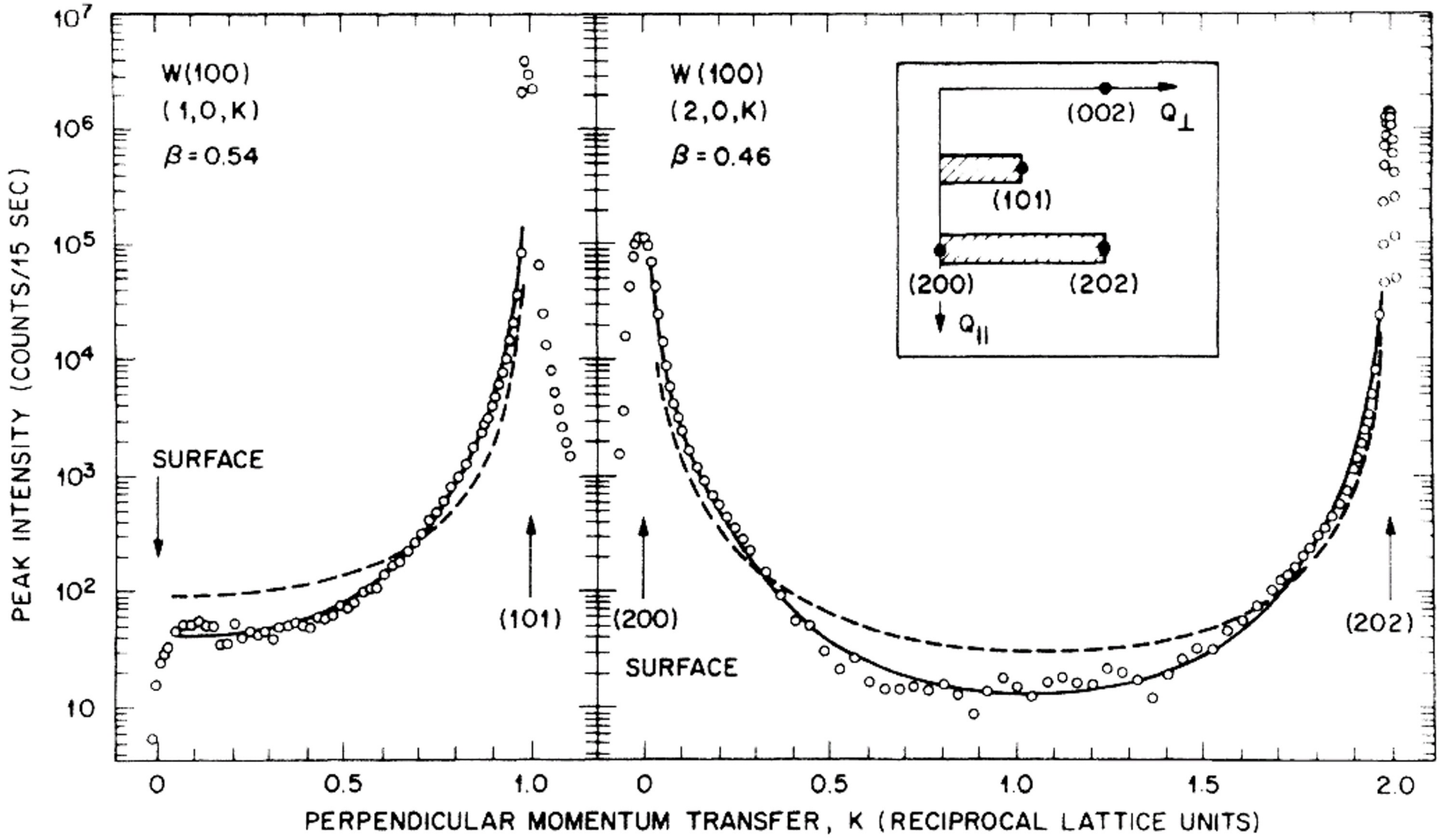
Effect of etching seen in triple-axis measurement of rocking curve

Resolution Function of the Triple-Axis Spectrometer

R. A. Cowley *et. al.*, Acta Cryst **A45** 415 (1989)



CRYSTAL TRUNCATION RODS AND SURFACE ROUGHNESS



I. K. Robinson APS March Meeting

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)

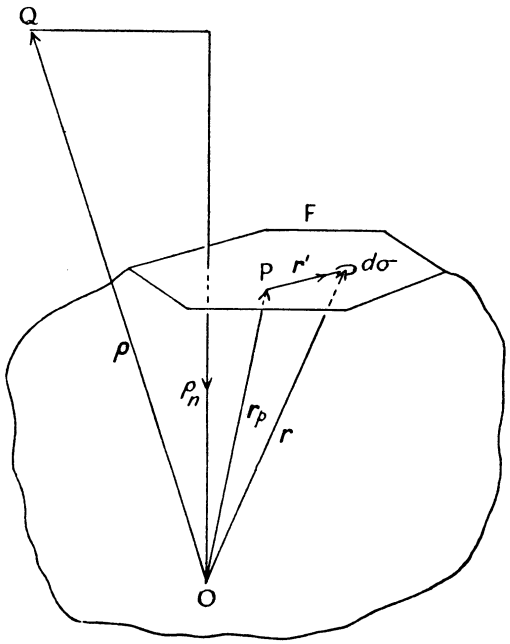
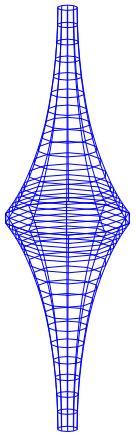
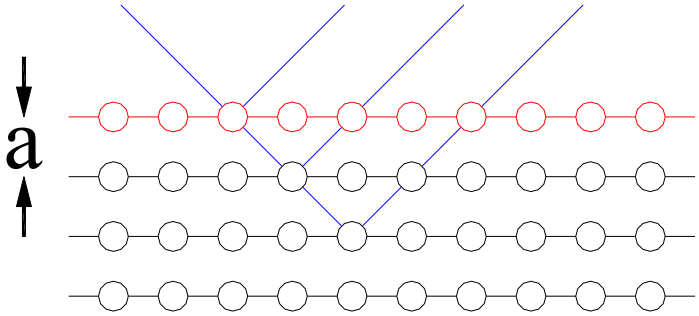


FIG. 200



"Stacheln"

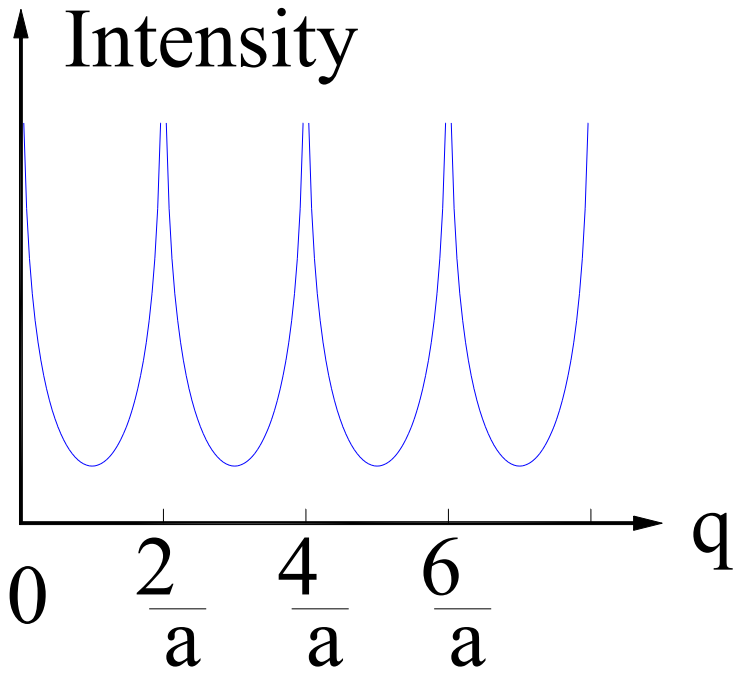
Origin of Truncation Rods



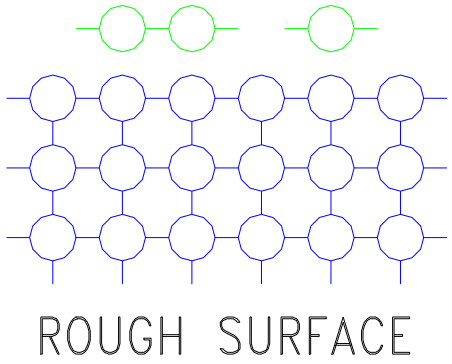
$$F_{CTR} = \sum_{n=0}^{\infty} A_n$$

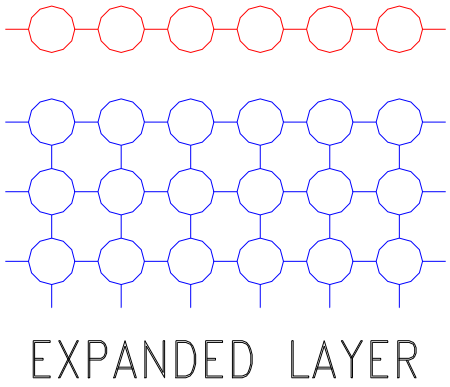
$$= \sum_{n=0}^{\infty} f_L \; e^{inqa}$$

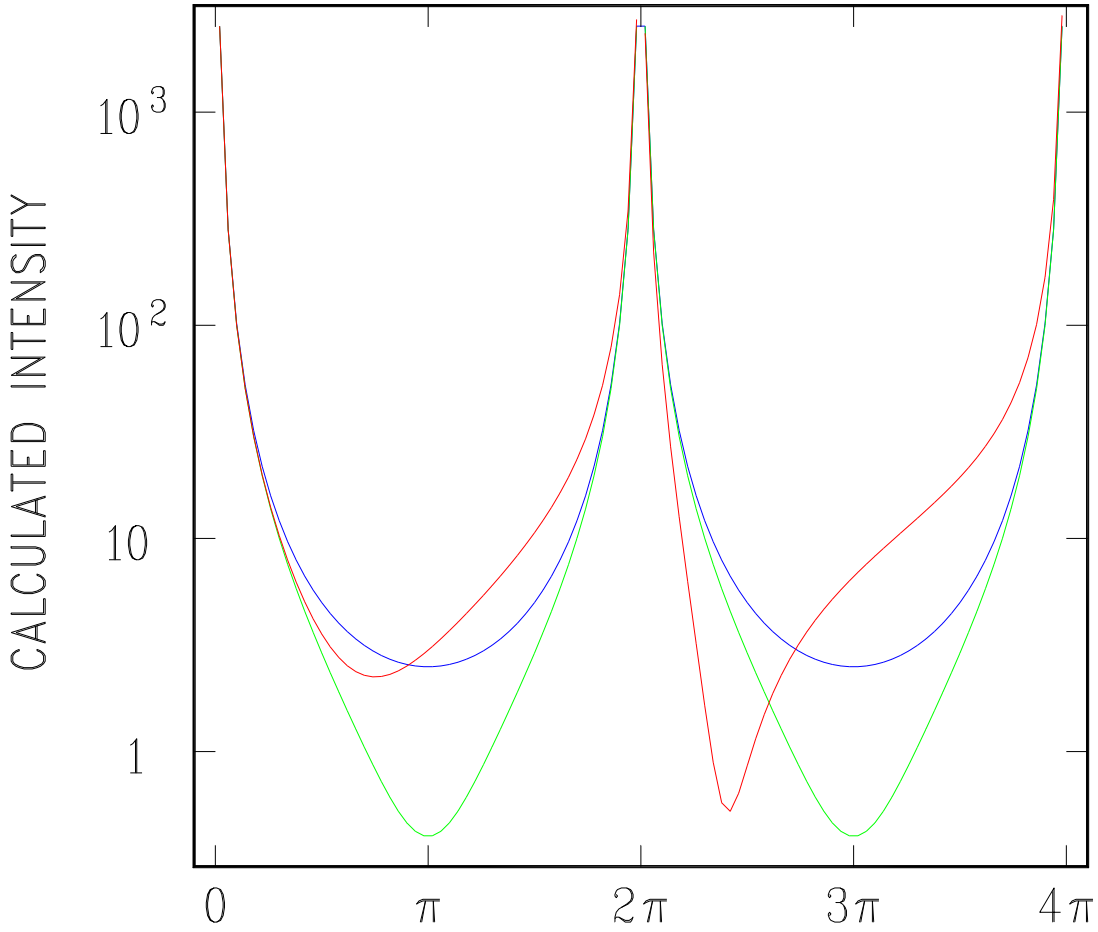
$$= \frac{f_L}{1 - e^{iqa}}$$



CTR is Sensitive to Surface Structure

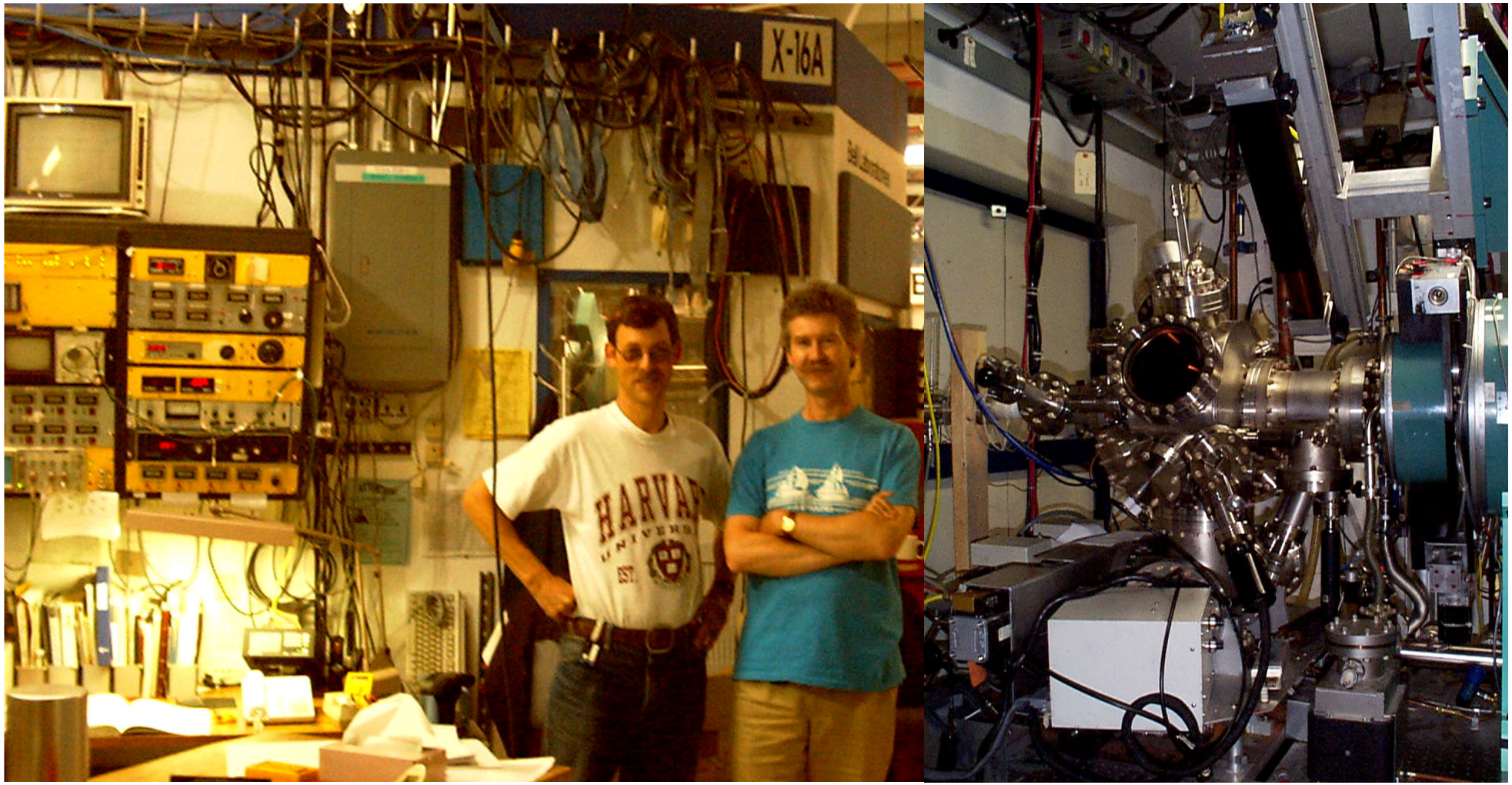


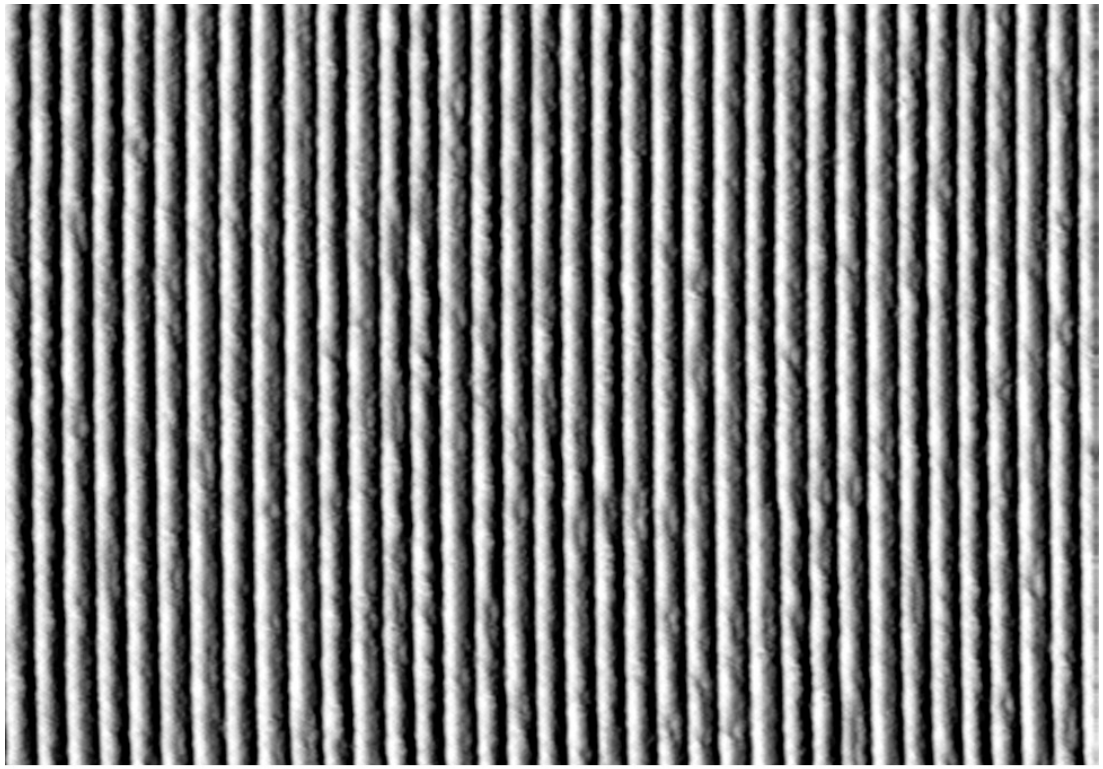


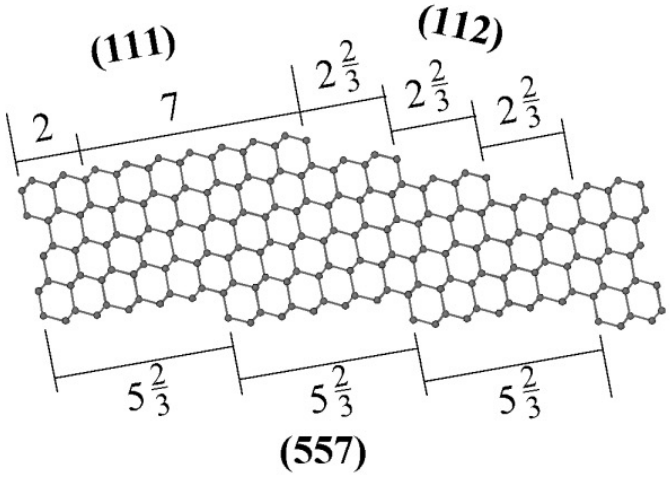


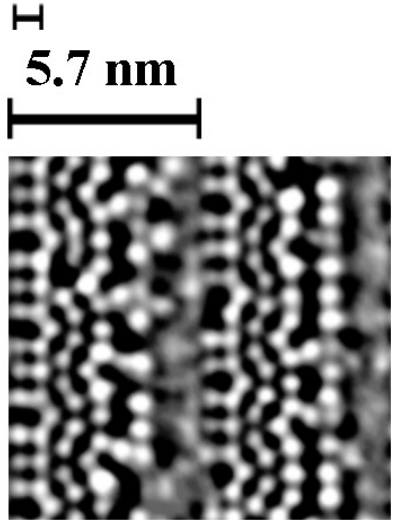
X16A Surface X-ray Diffraction

operating since 1987 ...

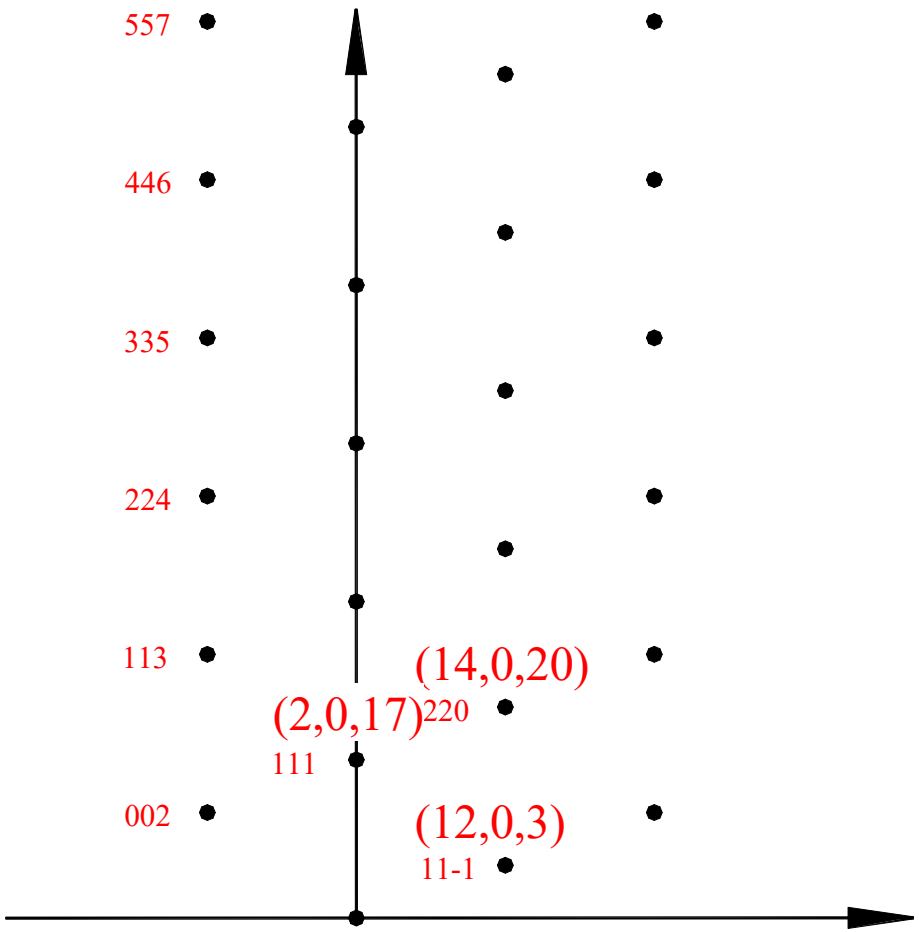




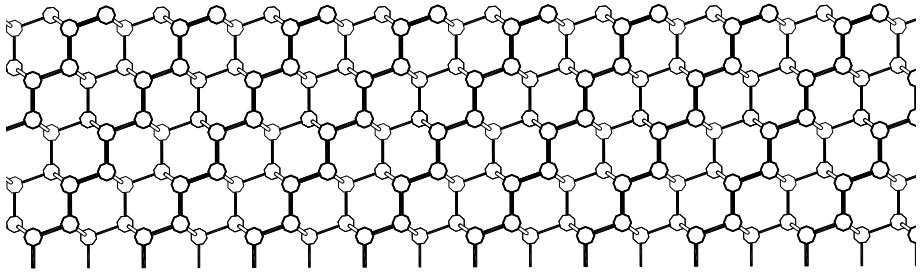

(111)
(112)
2
7
$2\frac{2}{3}$
$2\frac{2}{3}$
$2\frac{2}{3}$
$5\frac{2}{3}$
$5\frac{2}{3}$
$5\frac{2}{3}$
(557)

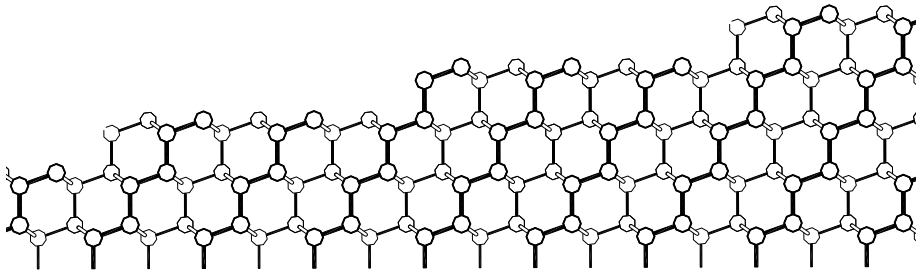

5.7 nm

Crystallography of Stepped Surfaces



Silicon (111)



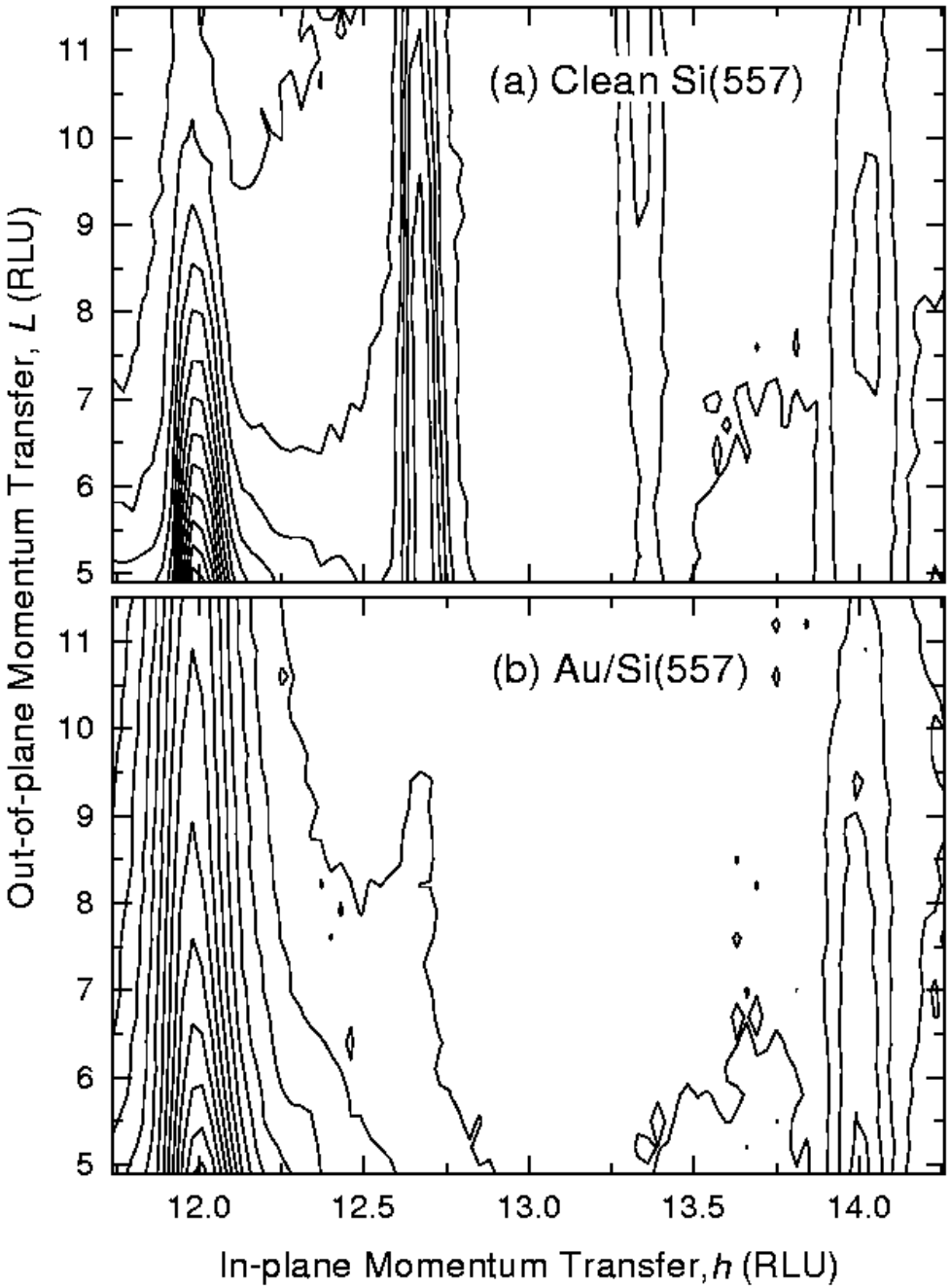


Si(557) surface

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.

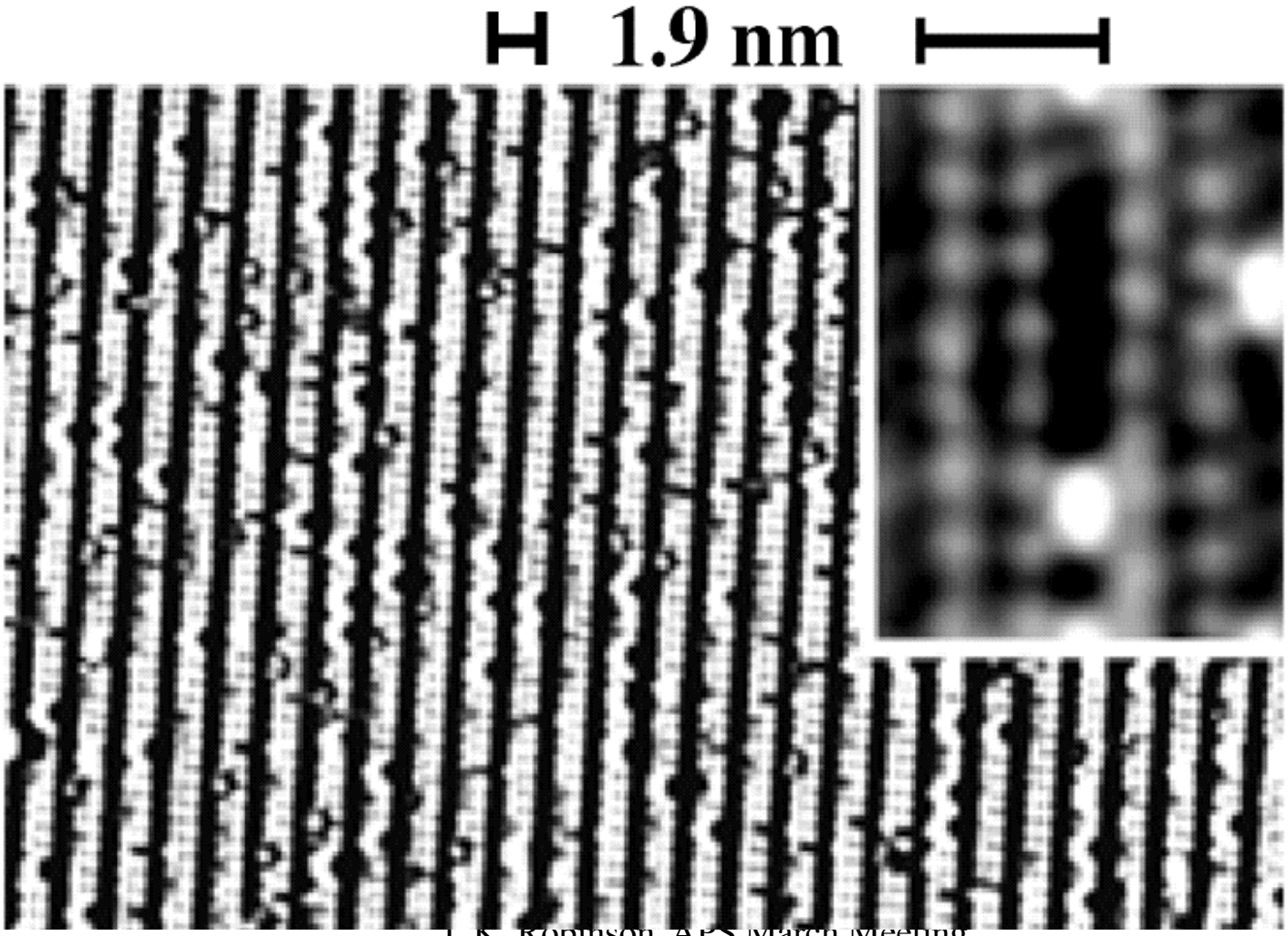


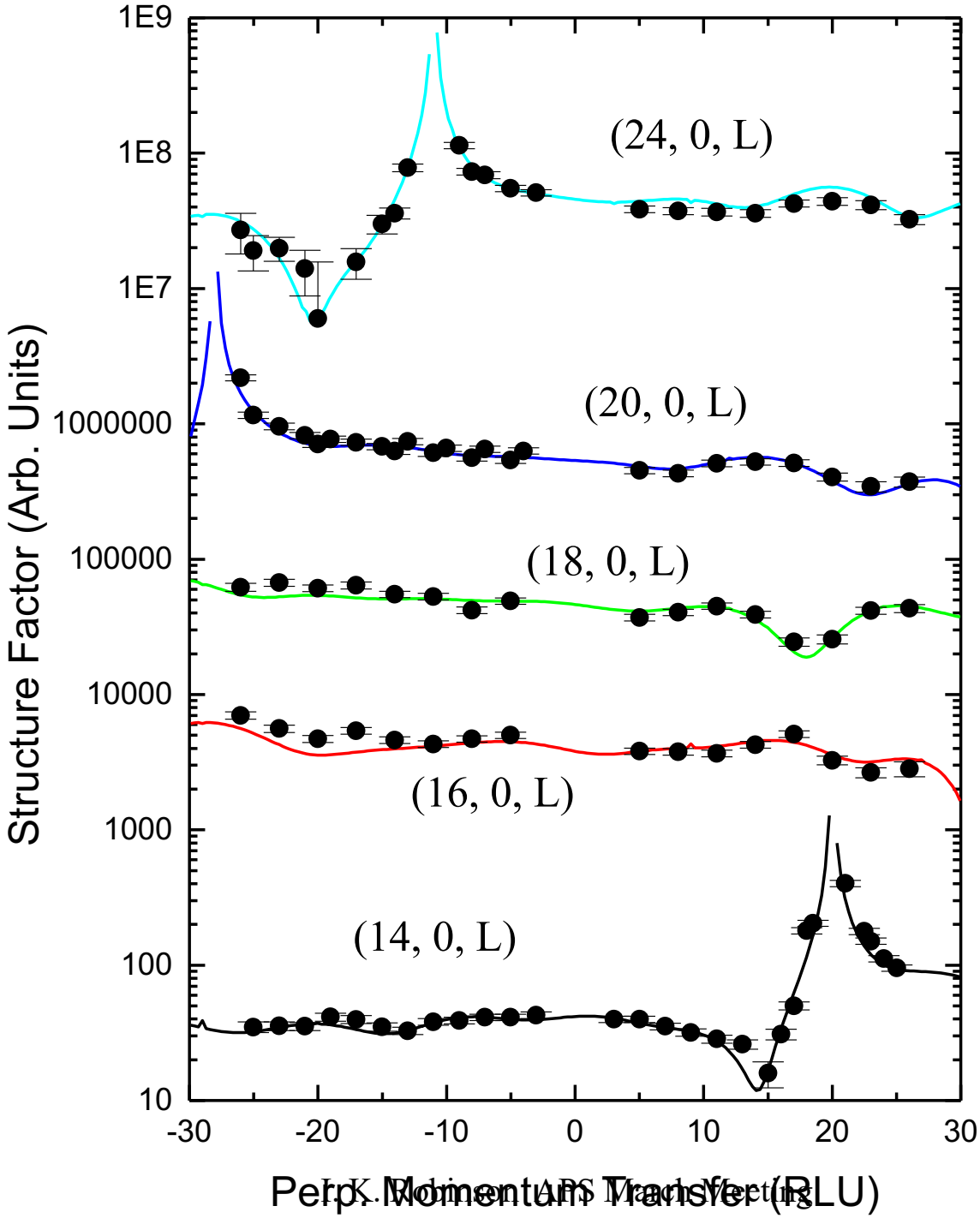
3×1 clean surface

1×1 surface with 0.2ML Au at 600C

STM of Si(557)/Au

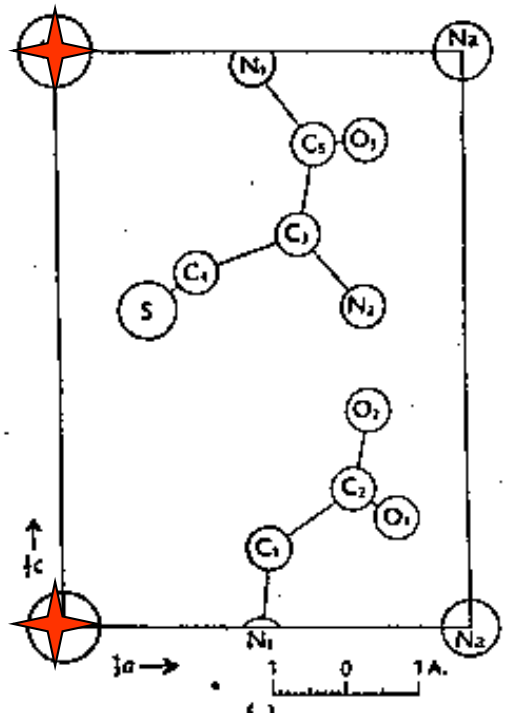
R. Losio, et. al., Phys. Rev. Lett. 86 4632 (2001)



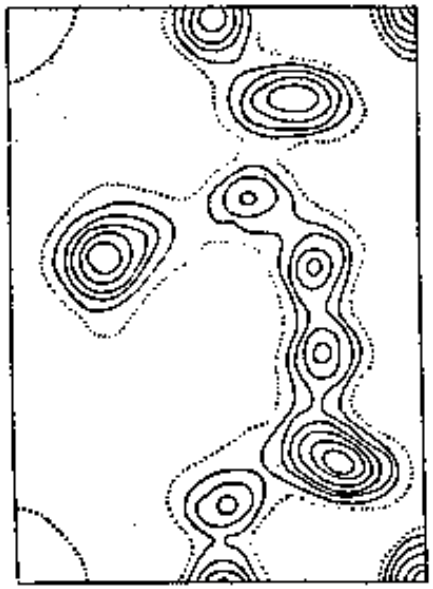

1E9
1E8
1E7
1000000
100000
10000
1000
100
10
Structure Factor (Arb. Units)
(24, 0, L)
(20, 0, L)
(18, 0, L)
(16, 0, L)
(14, 0, L)
-30
-20
-10
0
10
20
30
Perp. Momentum Transfer (RLU)

Phasing by a Single Heavy Atom

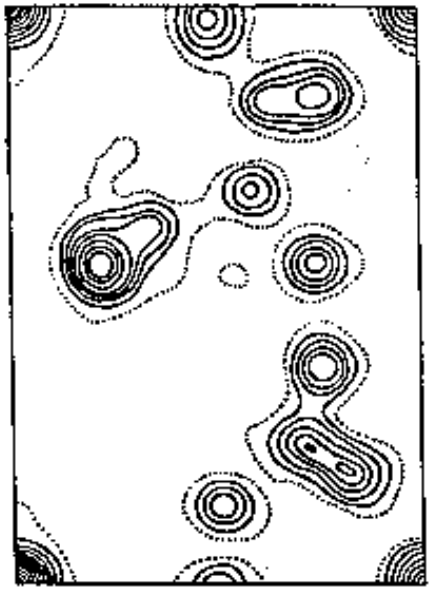
H. B. Dyer, Acta Cryst. 4 42 (1951)



Cysteinylglycine sodium iodide

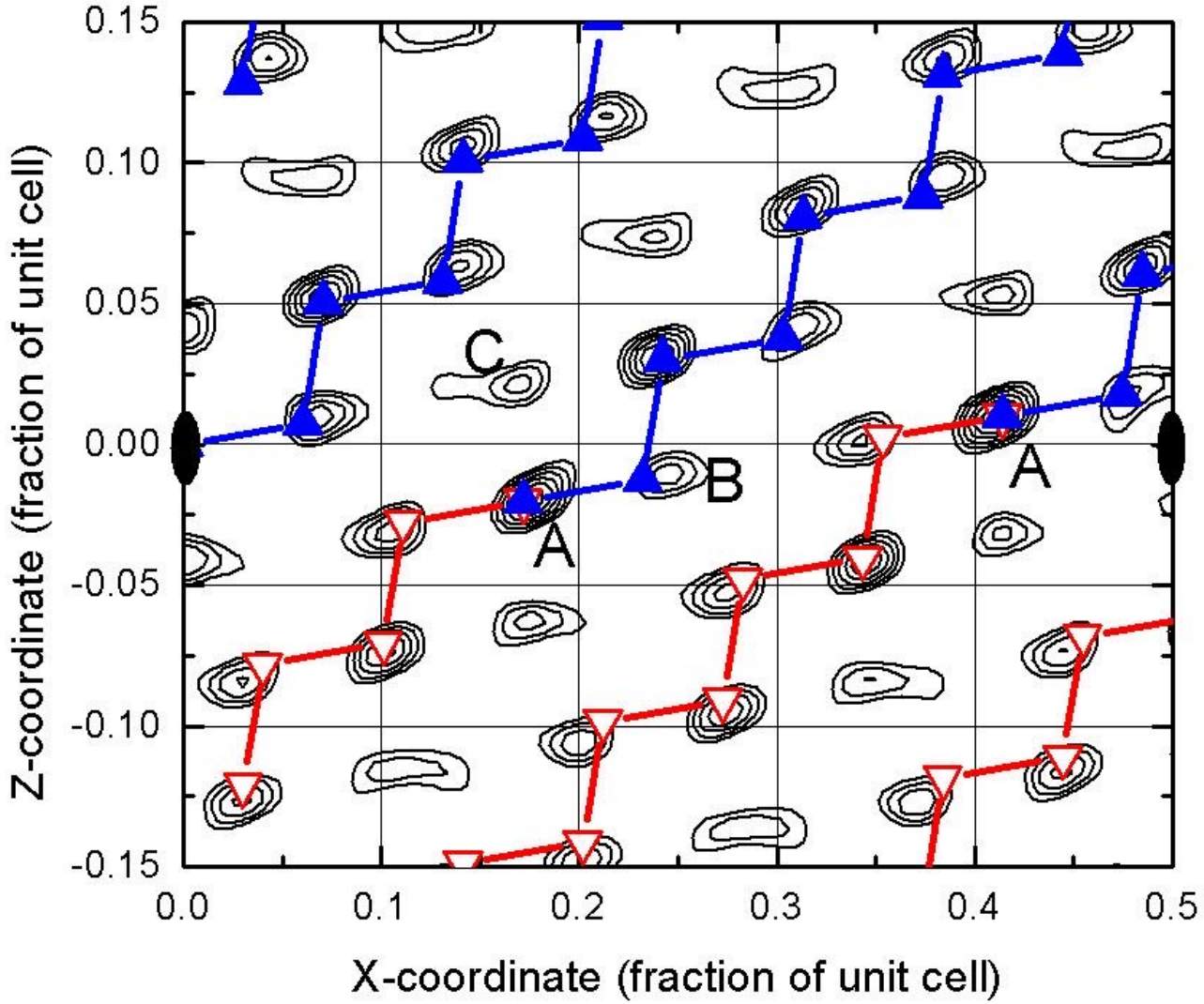


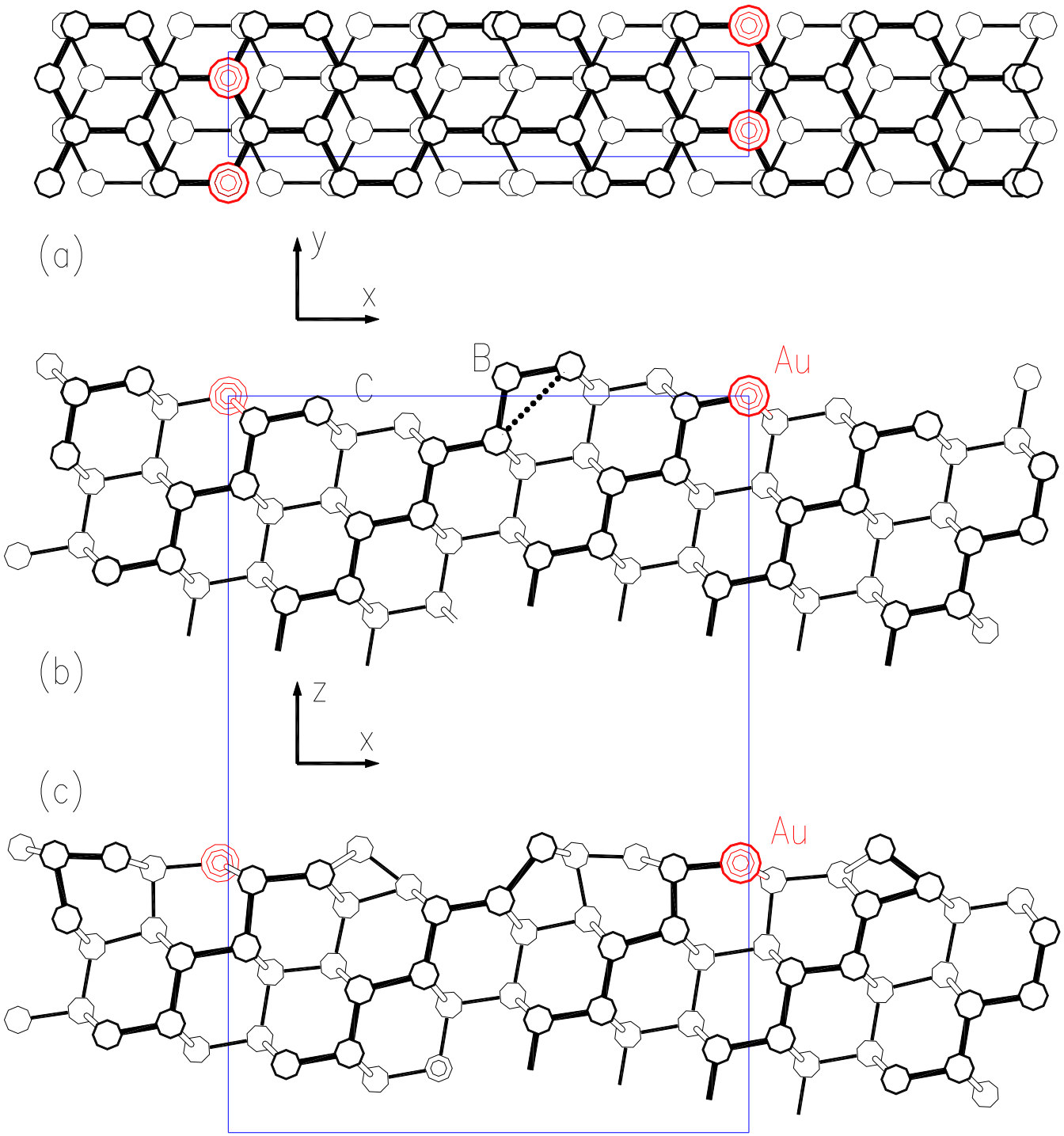
Patterson



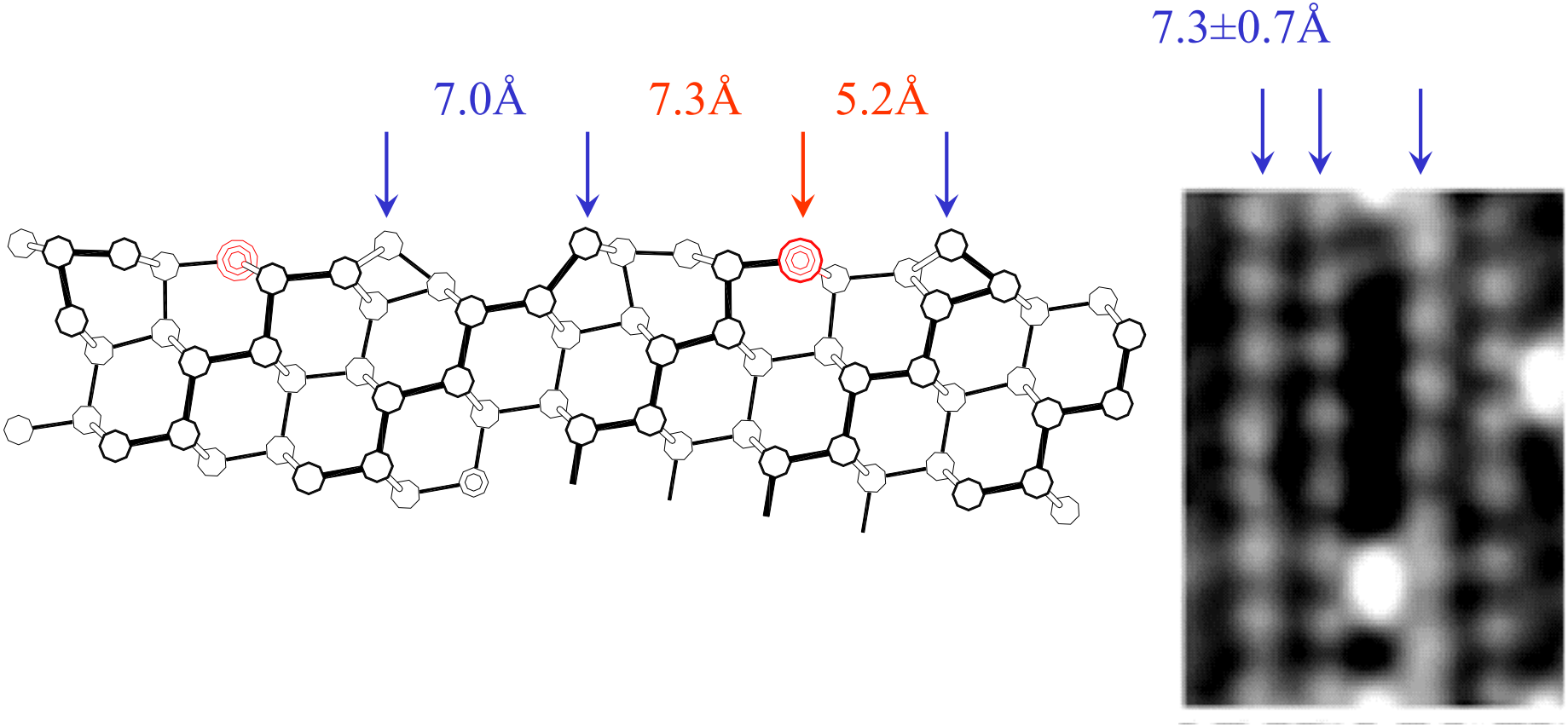
Electron density

X-Z Patterson of Au/Si(557)



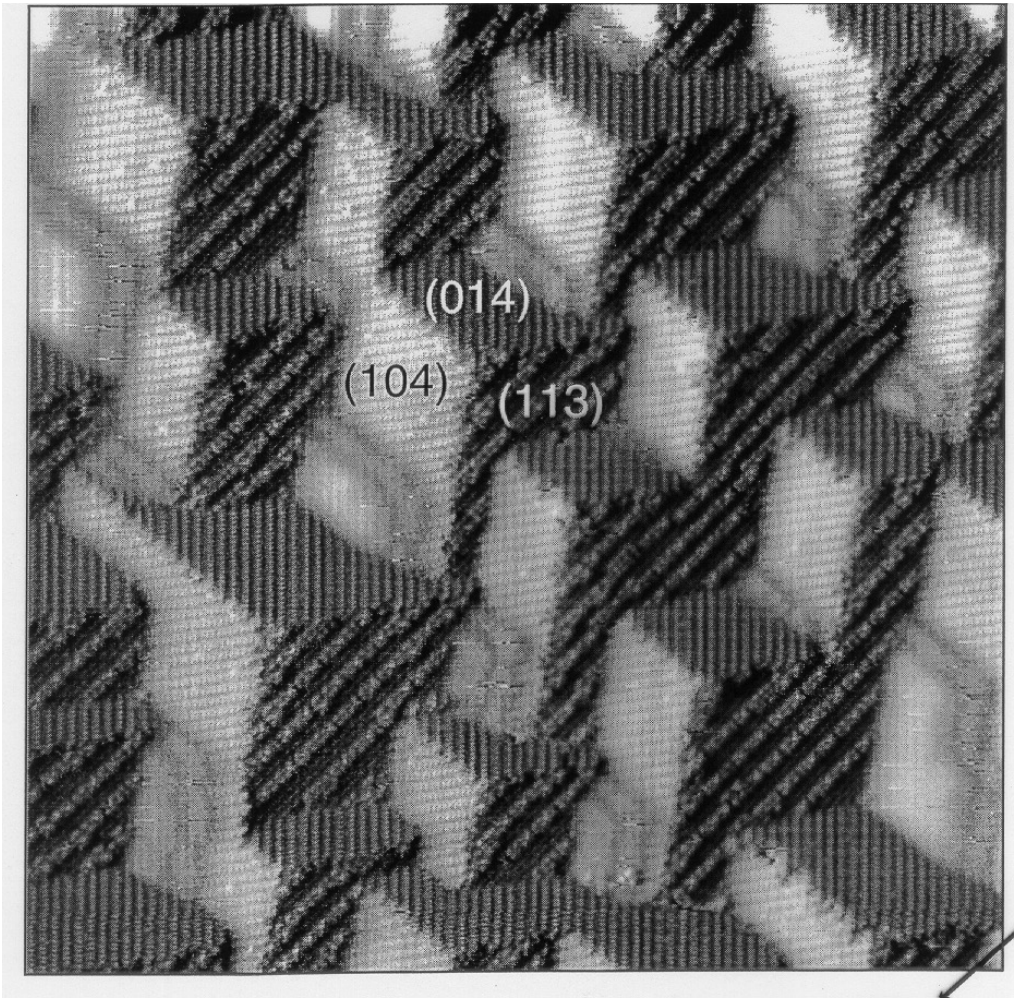

(a)
y
x
B
C
Au
(b)
z
x
(c)
Au

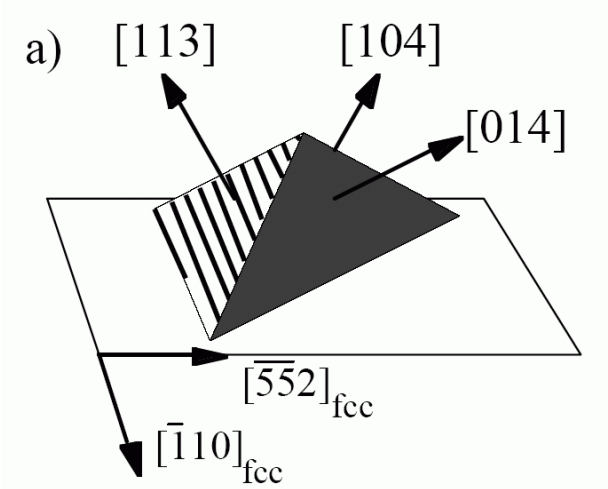
Comparison with STM

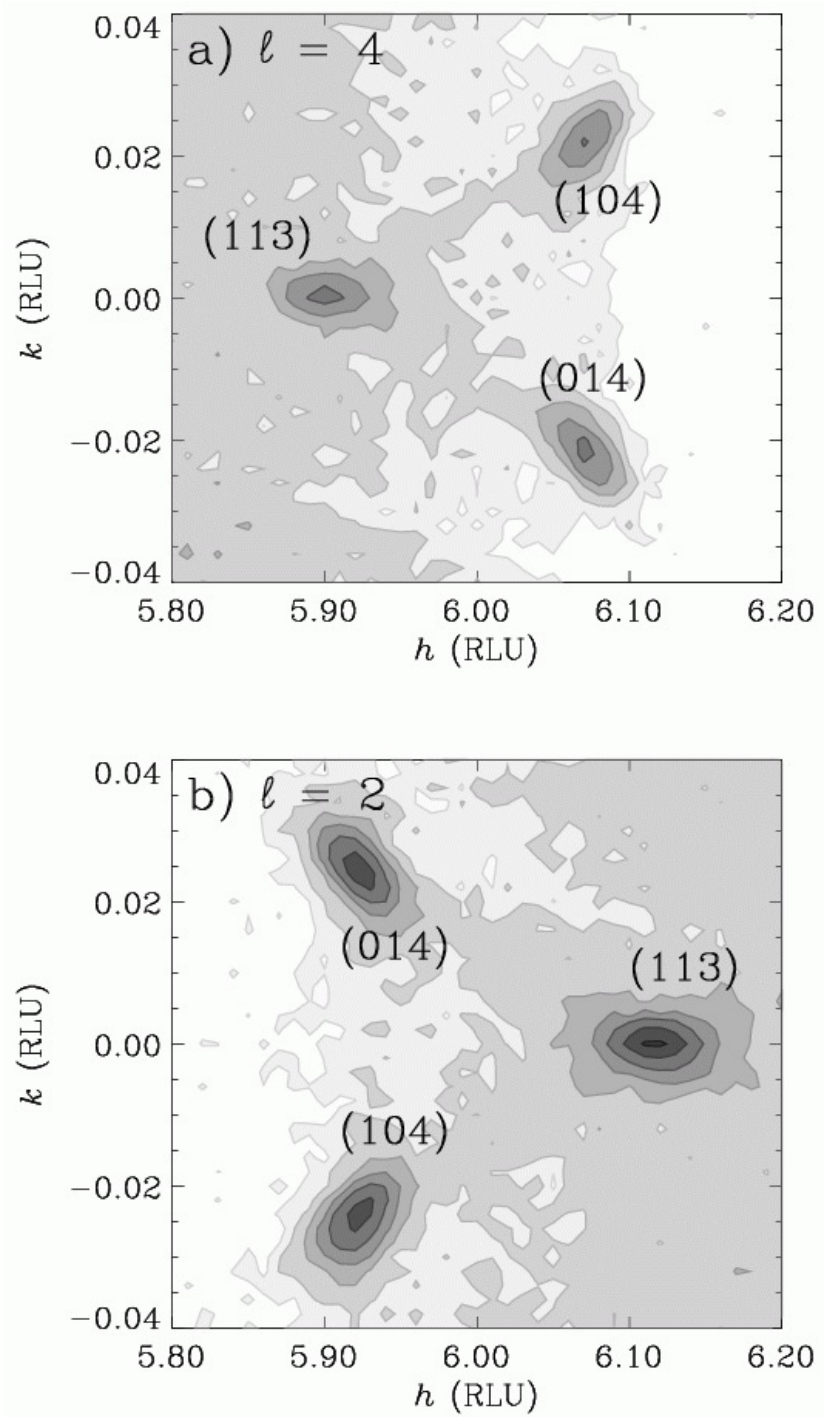


Cu(115) after Oxidation: STM

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



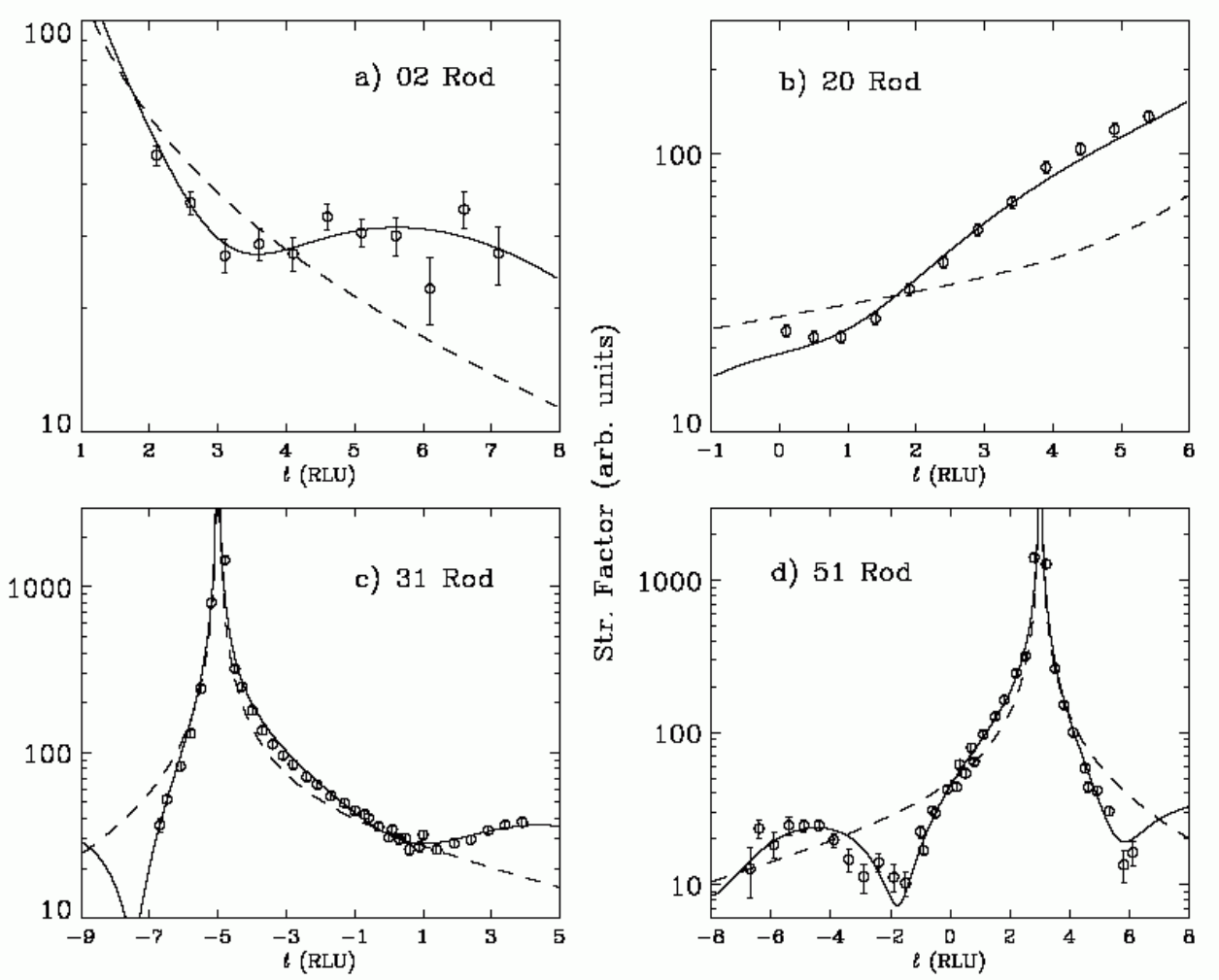




Cu(115) after Oxidation: X16A

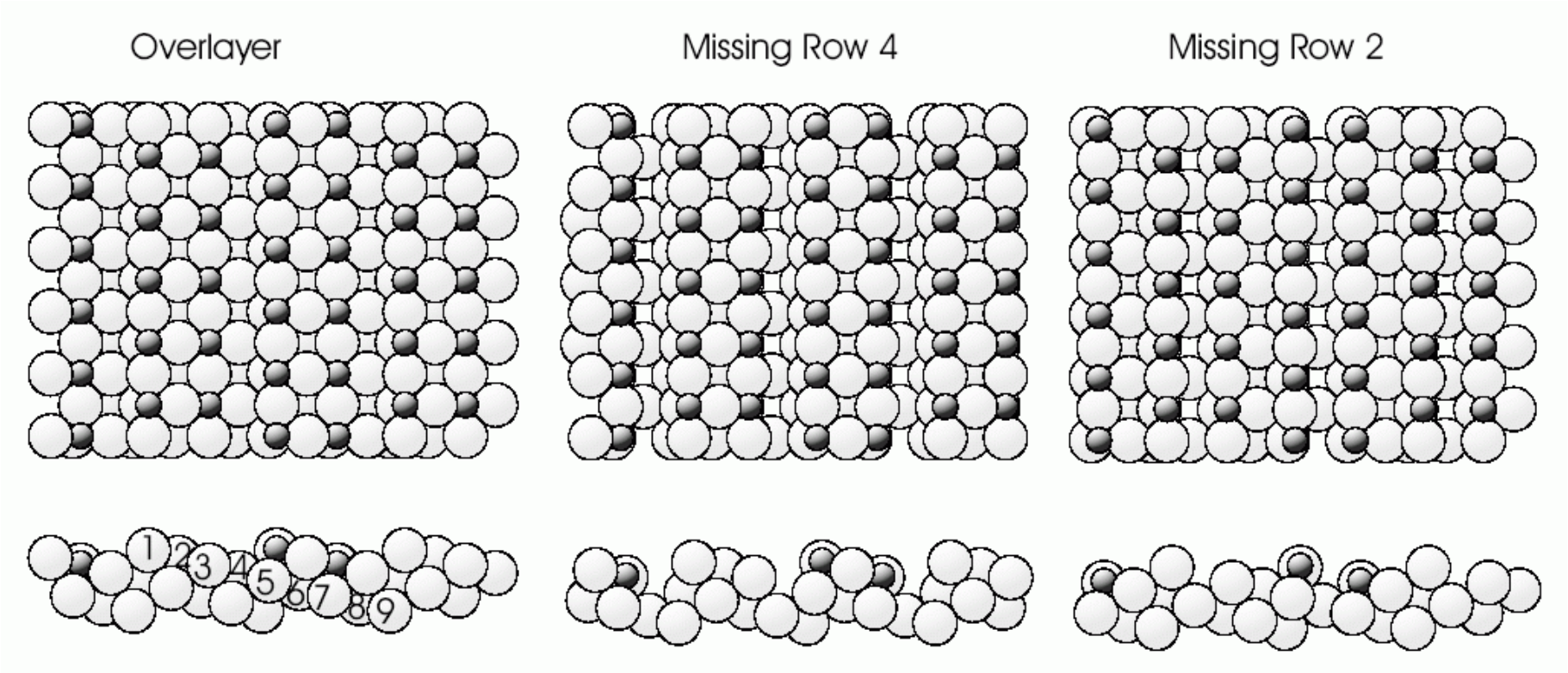
Don Walko, UIUC PhD Dissertation (2000)

Re-index CTRs for Cu(104) facets



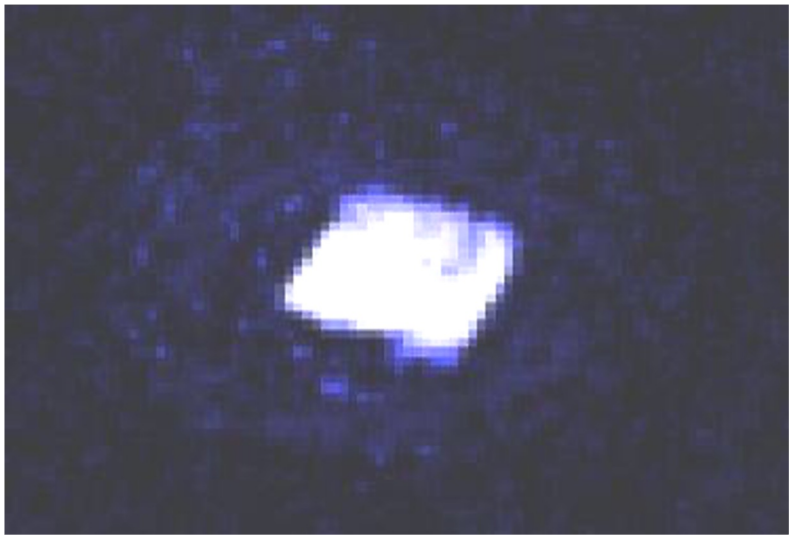
Surface Structures of Cu(104)-O

E. Vlieg, S. M. Driver, P. Goedtkindt, P. J. Knight, W. Liu, J. Luedecke, K. A. Mitchell, V. Murashov, I. K. Robinson, S. A. de Vries and D. P. Woodruff, Surface Science **516** 16-32 (2002)

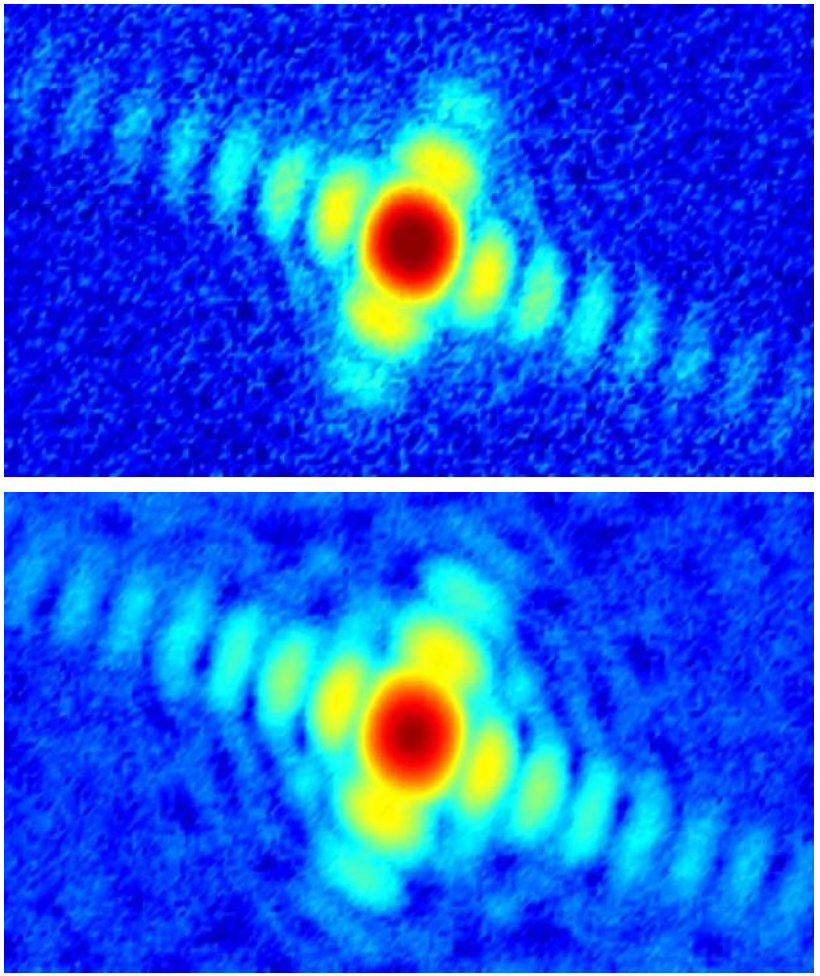


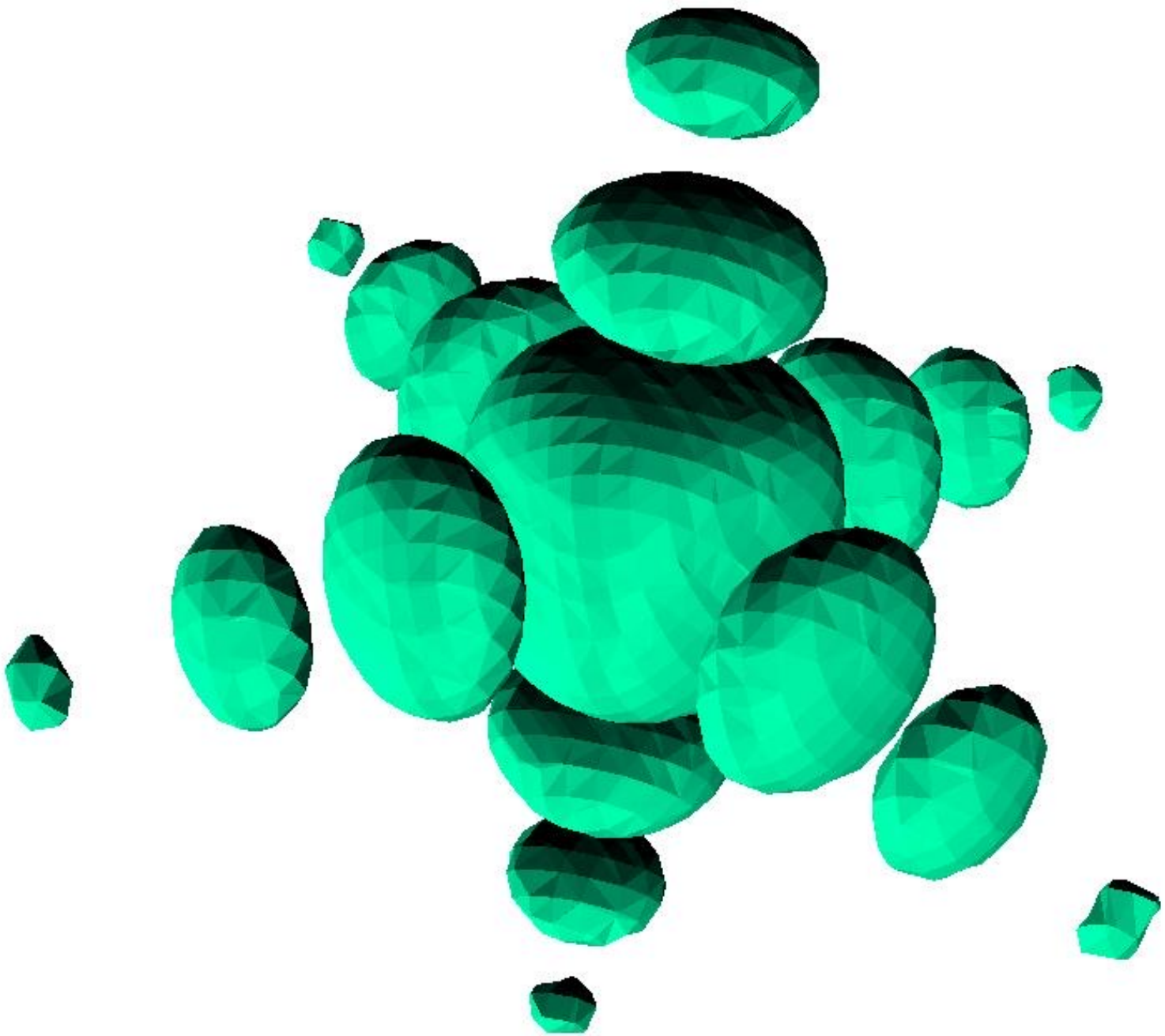
Perderau and Rhead | Robinson et al | Woodruff et al

Reconstruction of Ag Nanocrystal



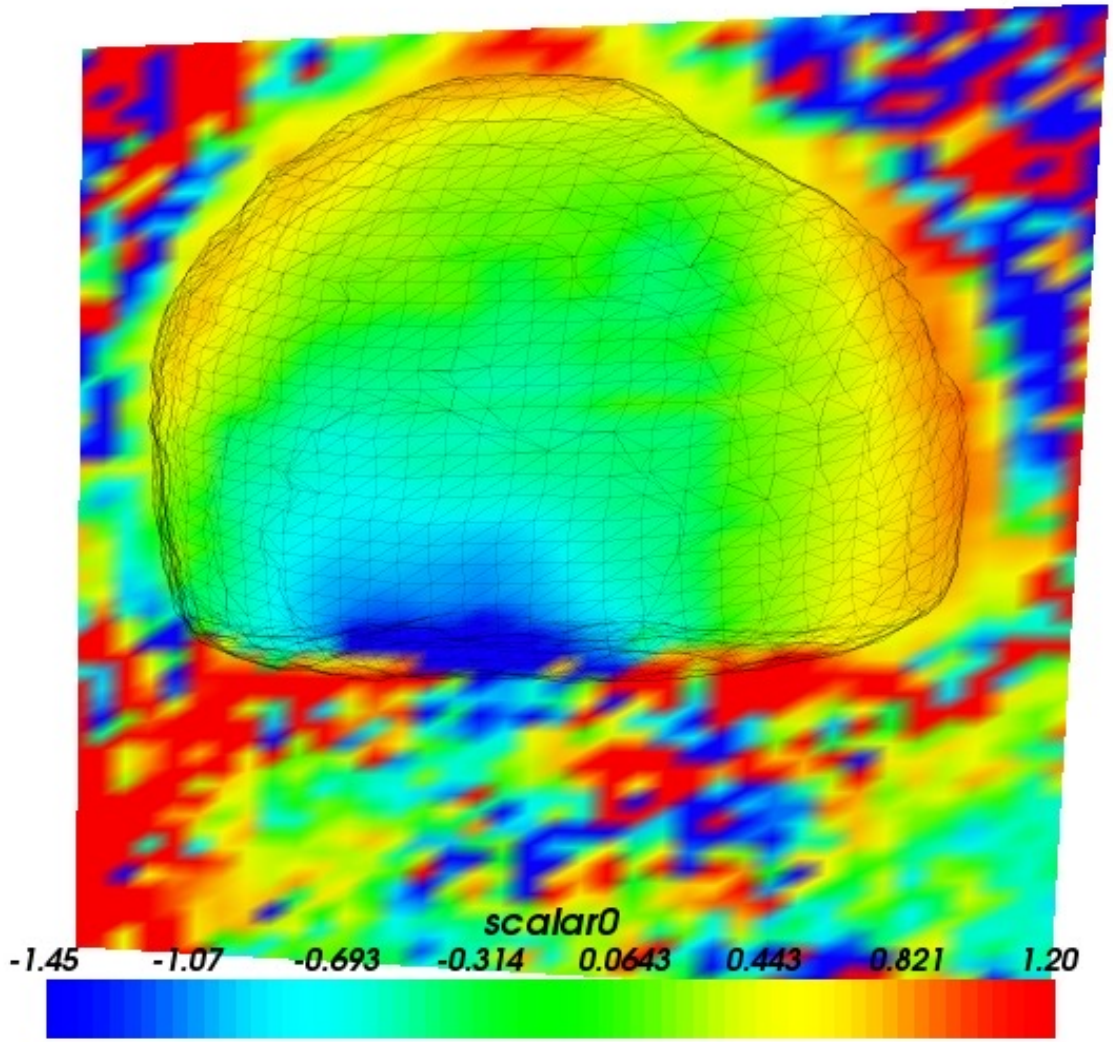
200nm





Contours showing Positive Phase

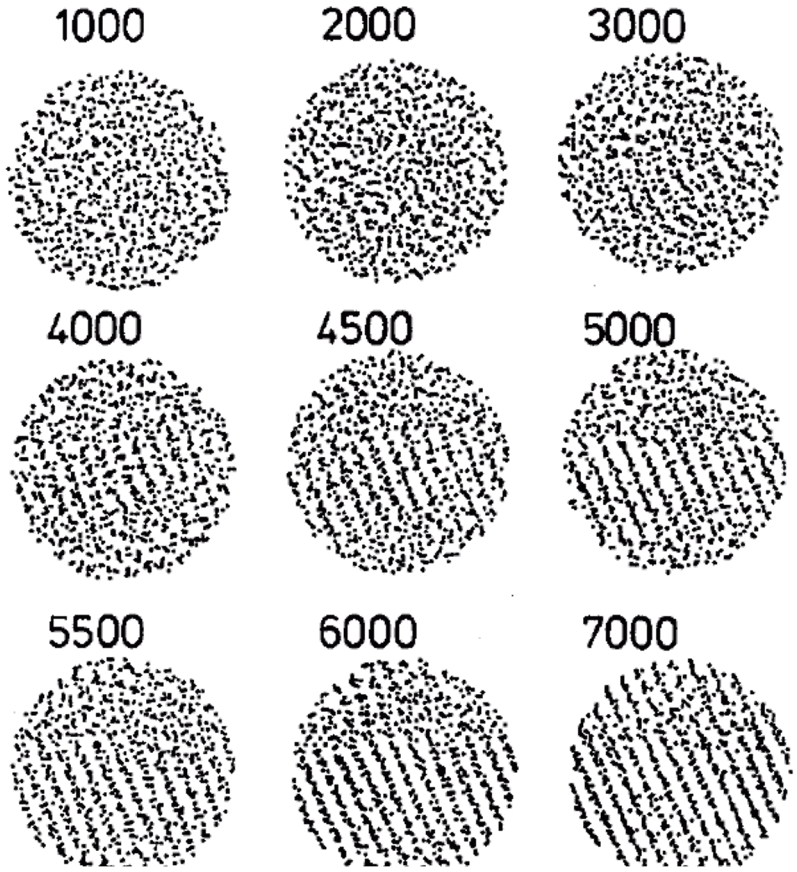
including correction for refraction by crystal

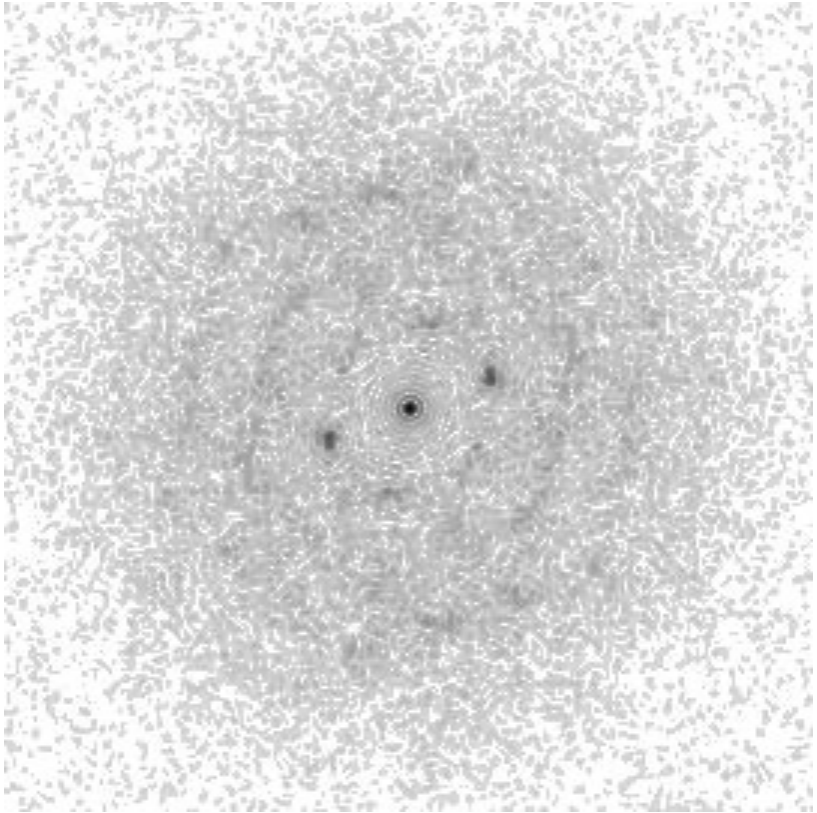


MD simulation of freezing

LJ liquid of 864 atoms. Time steps after T-Jump

S. Nose and F. Yonezawa, JCP 84 1893 (1986)





Important Contributions from

Paul Fuoss	Argonne
Peter Bennett	Arizona
Doon Gibbs	Brookhaven
Ben Ocko	Brookhaven
Peter Eng	Chicago
Robert Feidenhans'l	Copenhagen
Jens Als-Nielsen	Copenhagen
Mike Altman	HKUST
Elias Vlieg	Nijmegen
Sunny Sinha	San Diego
Don Walko	Urbana
Franz Himpsel	Wisconsin

Conclusions

- Au quantum wires on Stepped Si
- Facetting of Cu(115) seen in CTRs
- Nanocrystal: paradigm of Surface/Bulk
- Future: snapshots of condensed matter

Future of Surface Diffraction

- Nanocrystal Structure CXD
- Buried interfaces, such as solid-liquid CTR
- Quantum dots and wires CXD
- Fluctuating surfaces, capillary waves XPCS
- Nanostructured rough surfaces GISAXS, XPCS
- Continuum models of strain and defects CXD
- Automated techniques CCD