

Structure of Quantum Wires on Au/Si(557)

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NSLS Lunch Seminar

Brookhaven, USA

Outline

- Surface Diffraction
- Crystal Truncation Rods
- Crystallography of Stepped Surfaces
- Quantum Wires
- Si(557) as a Facetted Template
- Au/Si(557) Structure

Beamline X16A of the National Synchrotron Light Source

Surface X-ray Diffraction

- Surface sensitivity comes from **symmetry**
- Buried interfaces equally accessible
- Kinematical diffraction is quantitative
- Ordered superstructure or “ 1×1 ”
- Direct methods under development

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)

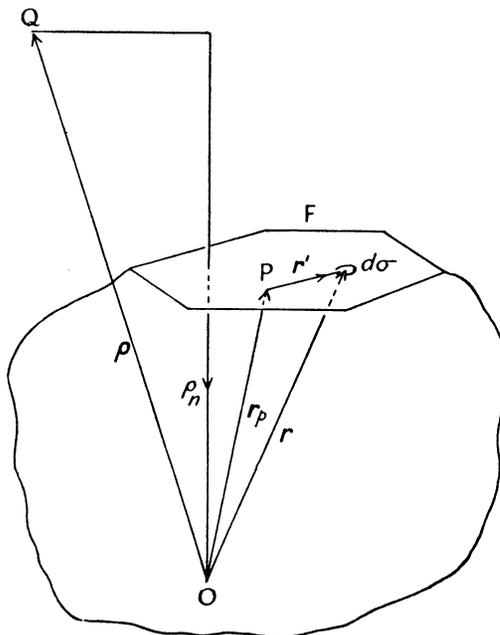
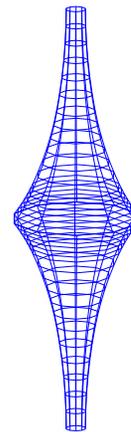
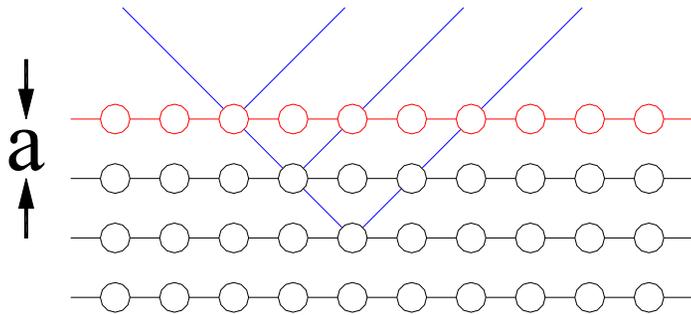


FIG. 200

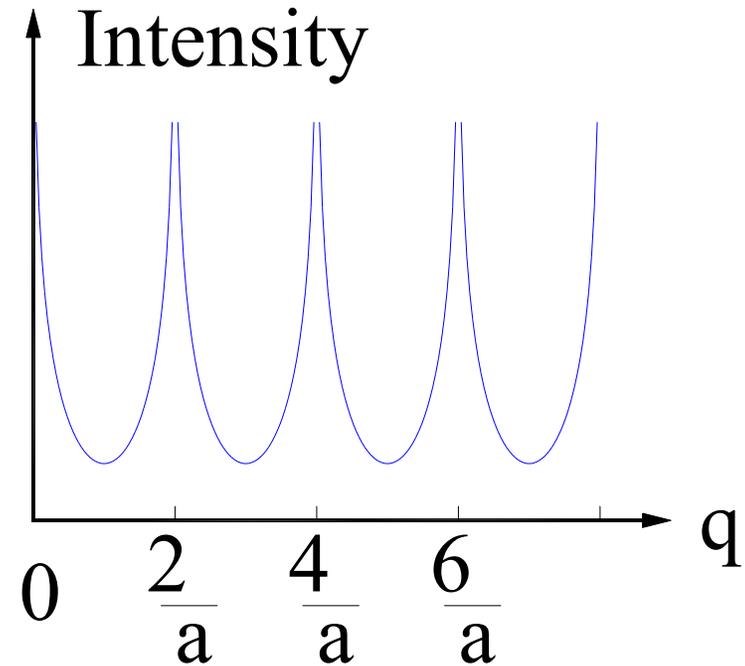


“Stacheln”

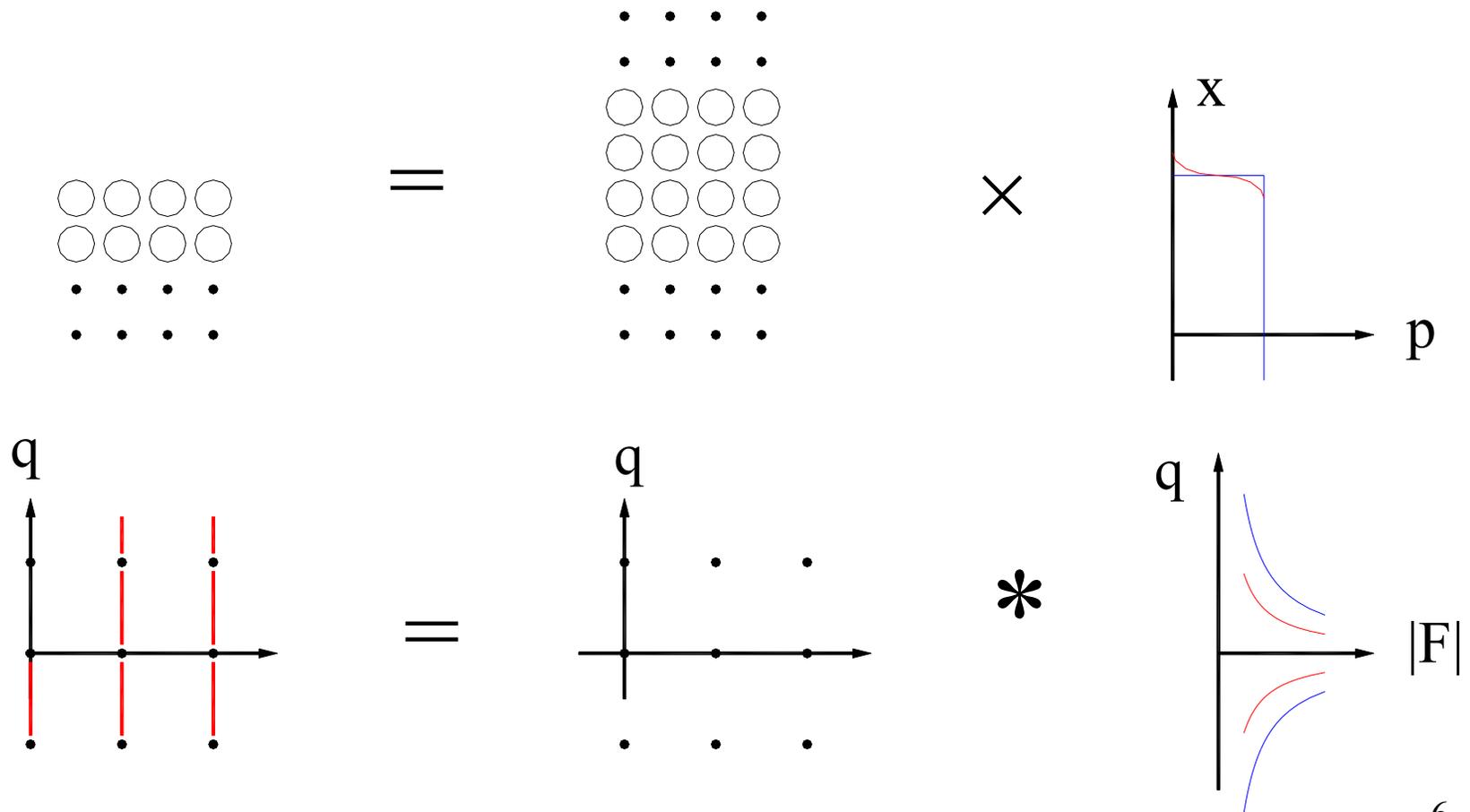
Origin of Truncation Rods



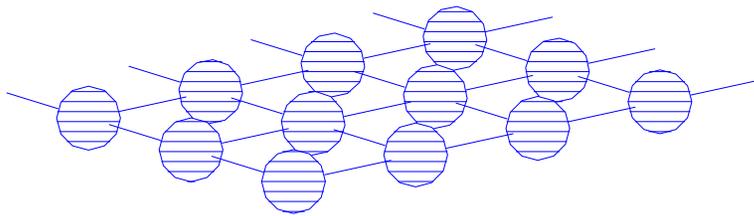
$$\begin{aligned} F_{CTR} &= \sum_{n=0}^{\infty} A_n \\ &= \sum_{n=0}^{\infty} f_L e^{inqa} \\ &= \frac{f_L}{1 - e^{iqa}} \end{aligned}$$



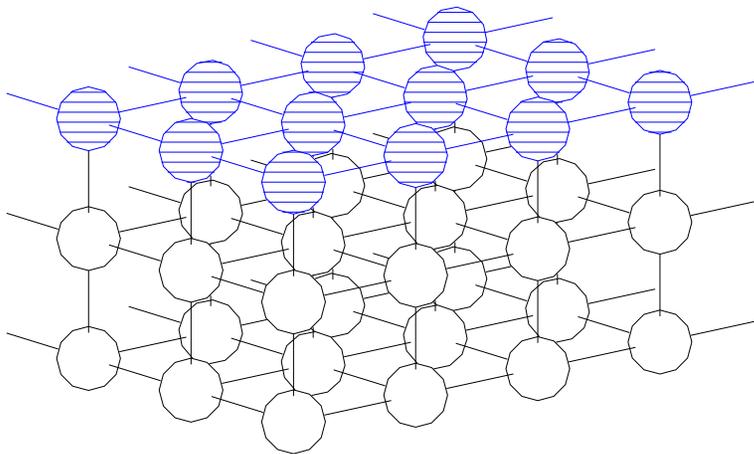
CTR as Convolution



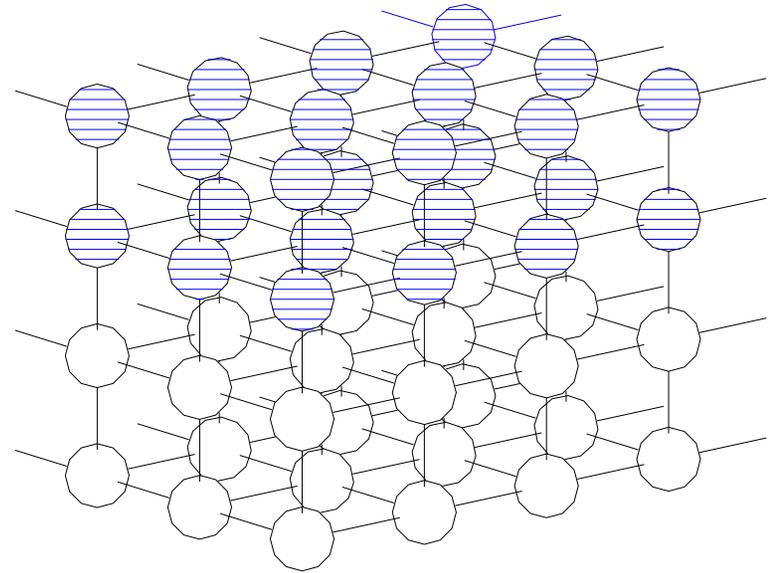
Surfaces and Interfaces



Isolated monolayer



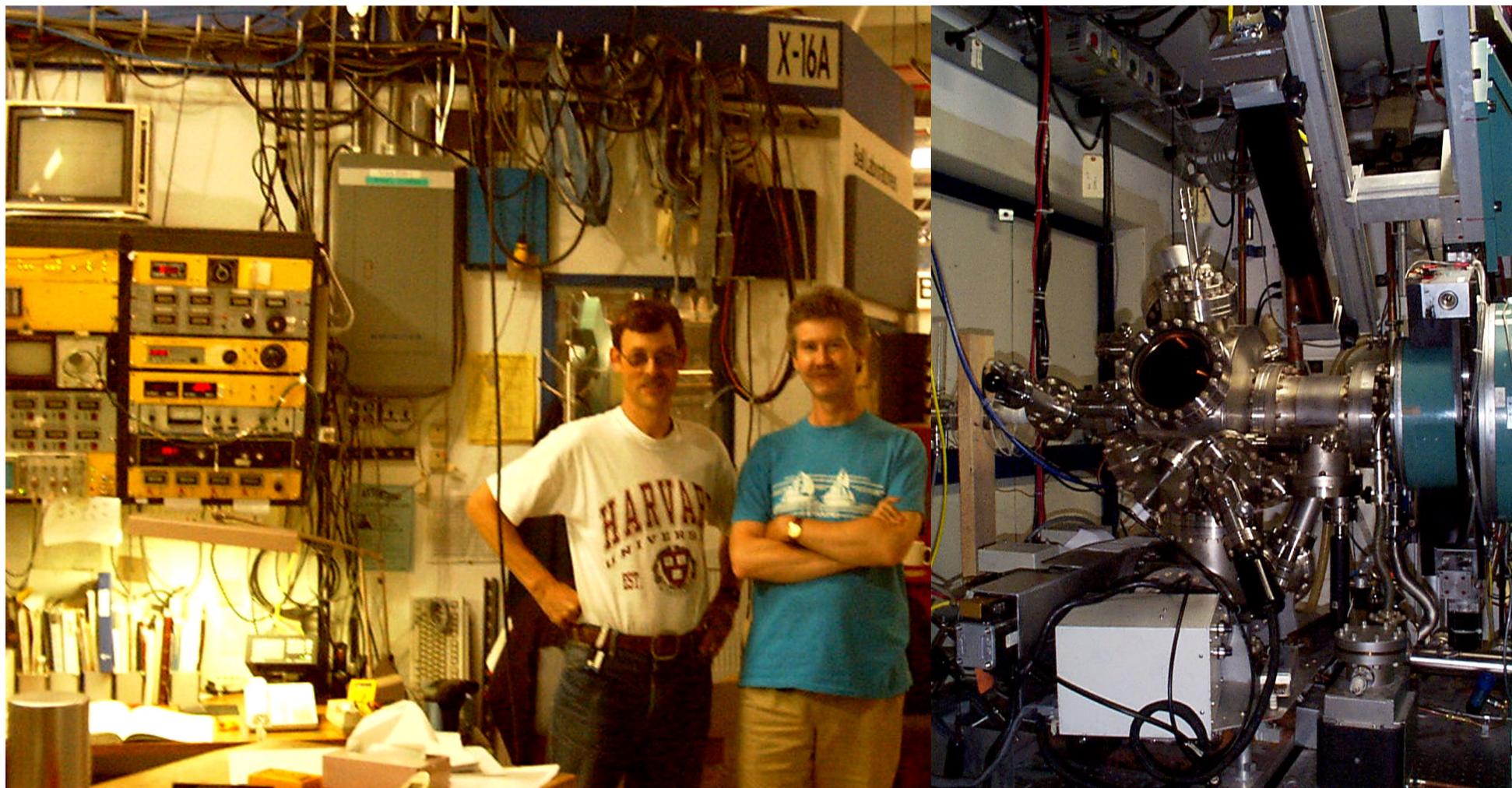
Surface of Crystal



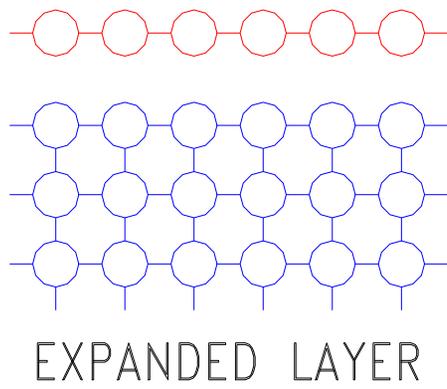
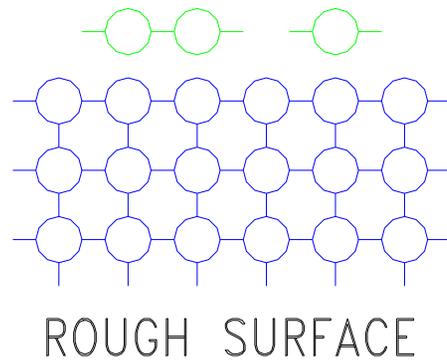
Crystal-Crystal Interface

X16A Surface X-ray Diffraction

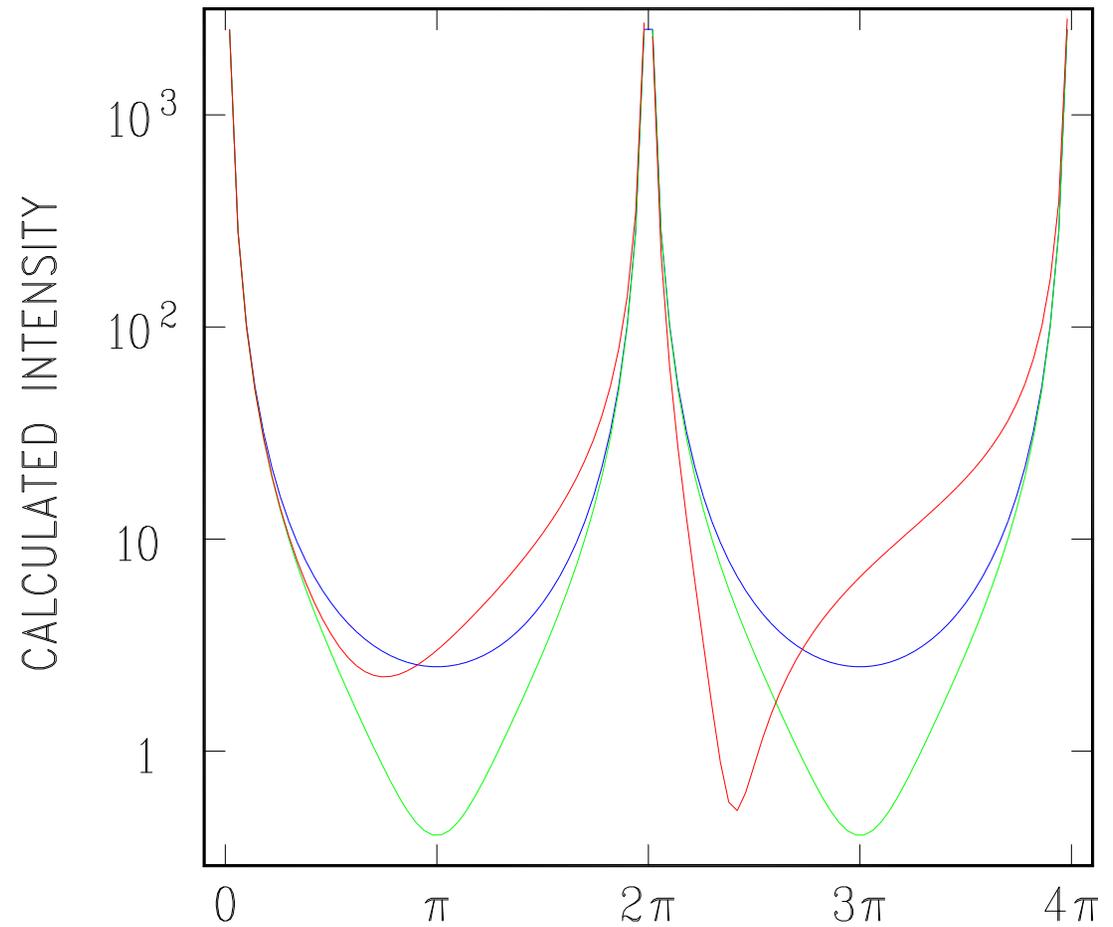
operating since 1987 ...

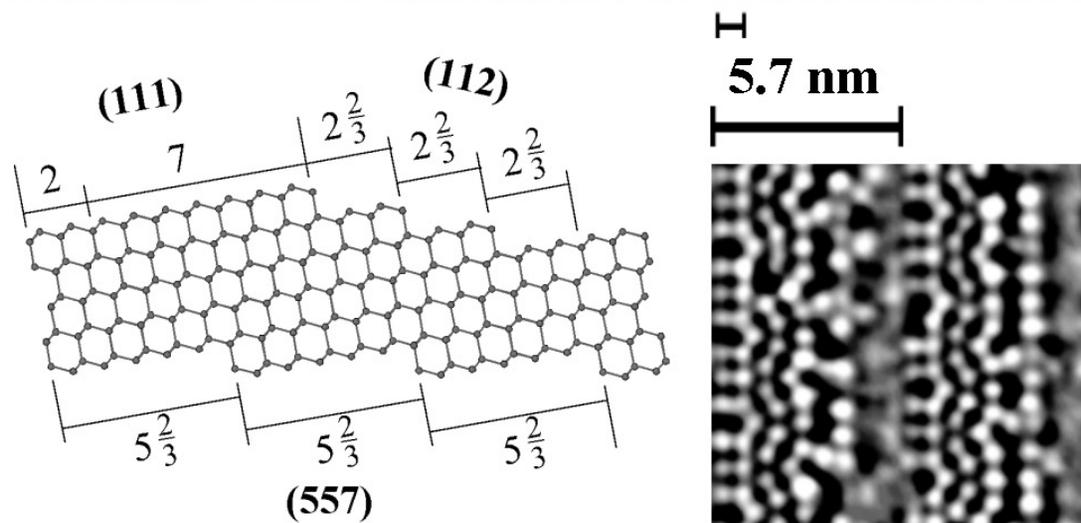
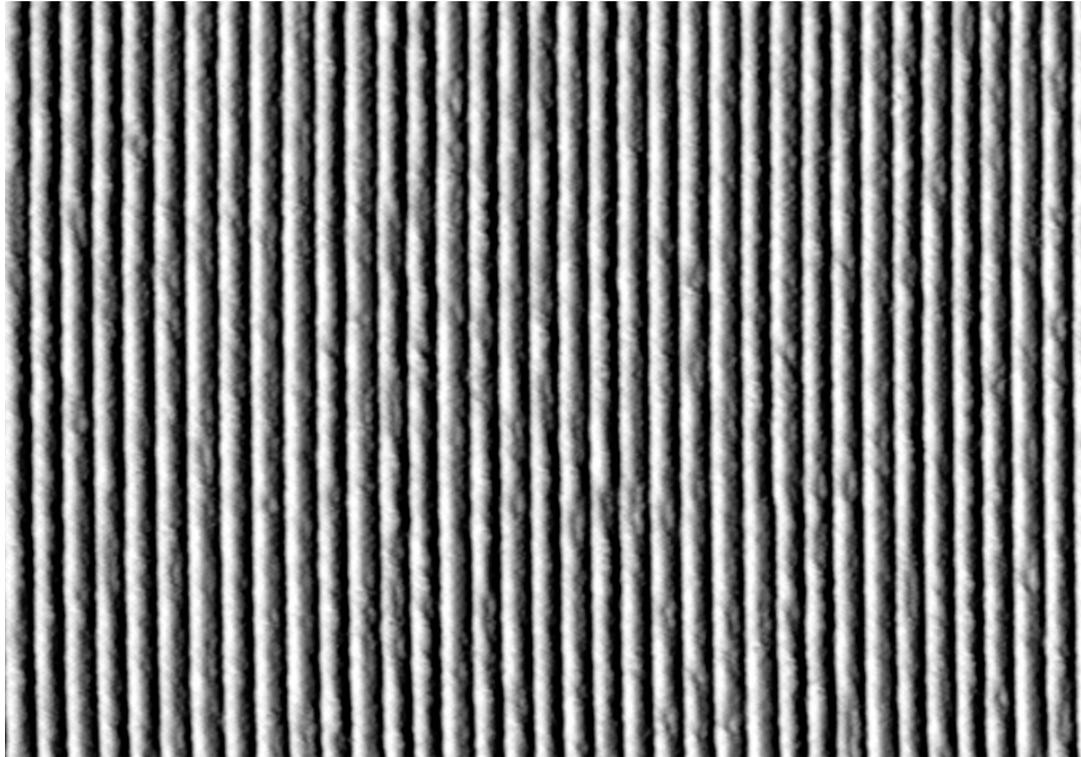


CTR is Sensitive to Surface Structure



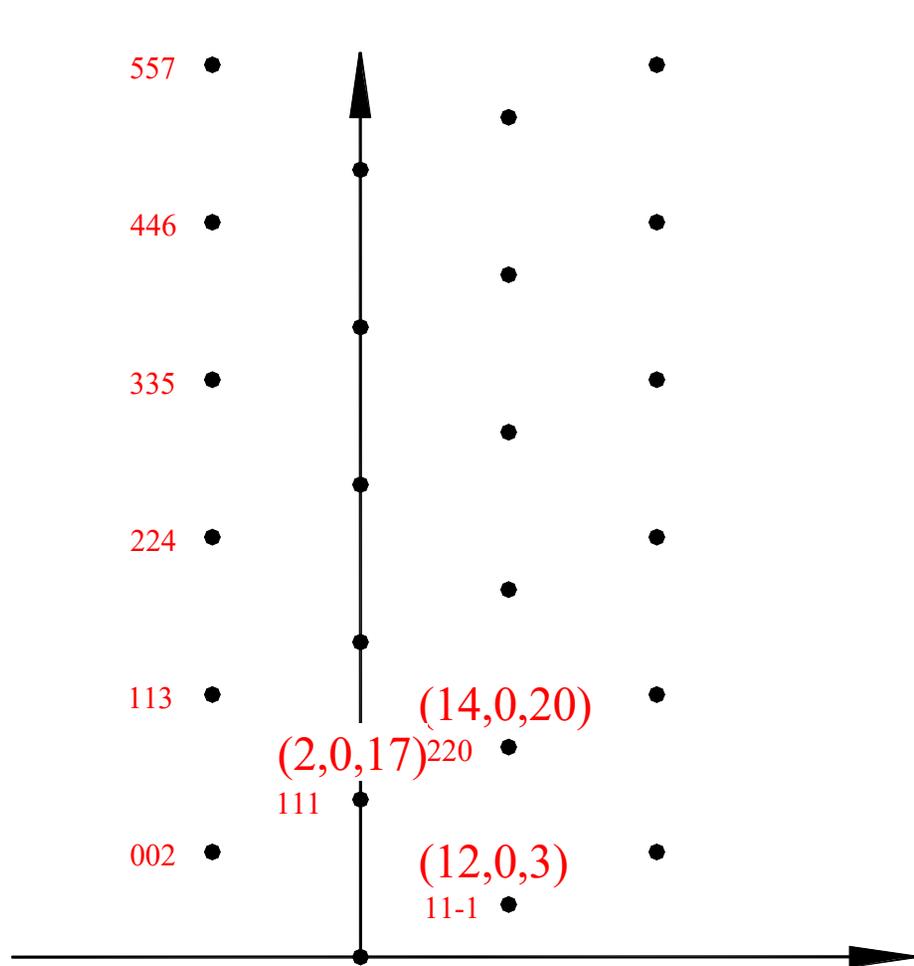
I.]



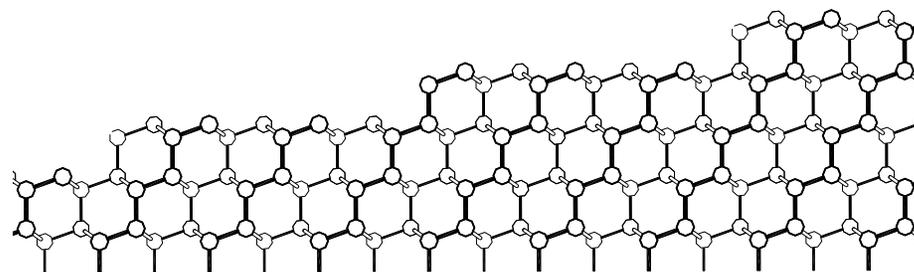
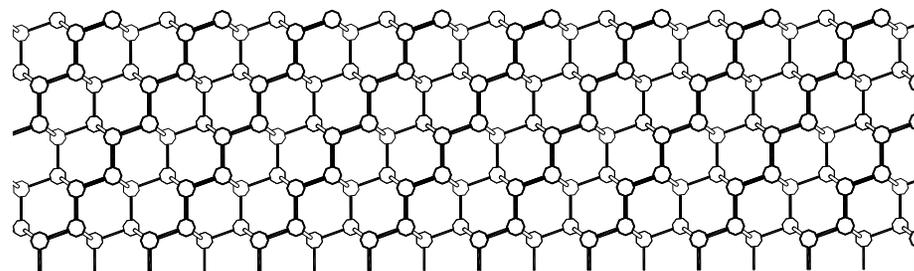


I. K. Robinson, NSLS Lunch Seminar

Crystallography of Stepped Surfaces



Silicon (111)



Si(557) surface

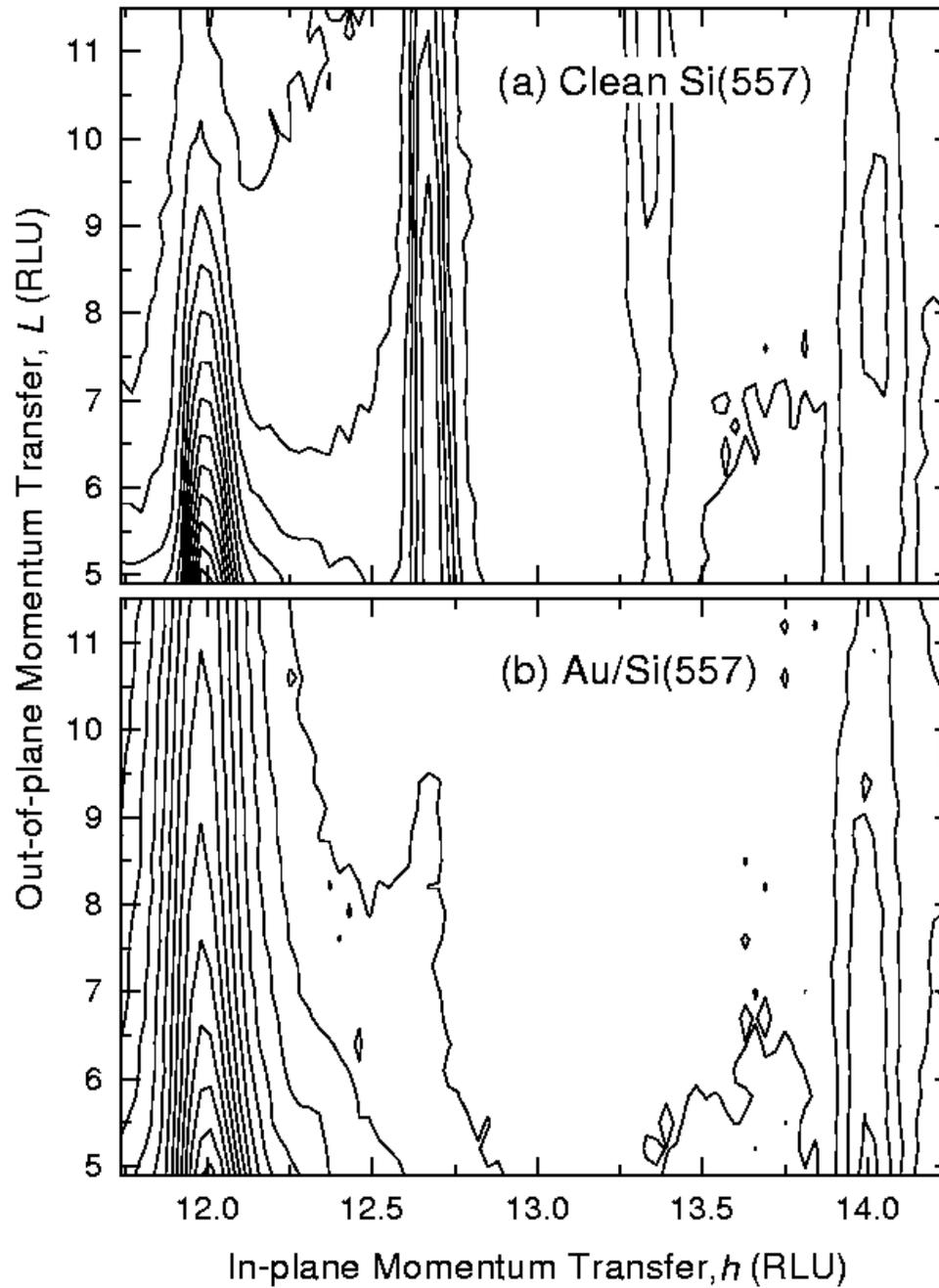
Alignment is Straightforward

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 Å, $wv = 5.19647$, Energy = 10.2542 keV (FIXED)
Five-Circle Mode using alm = 2 and bem = 2:

Centered Orthorhombic unit cell contains two steps.

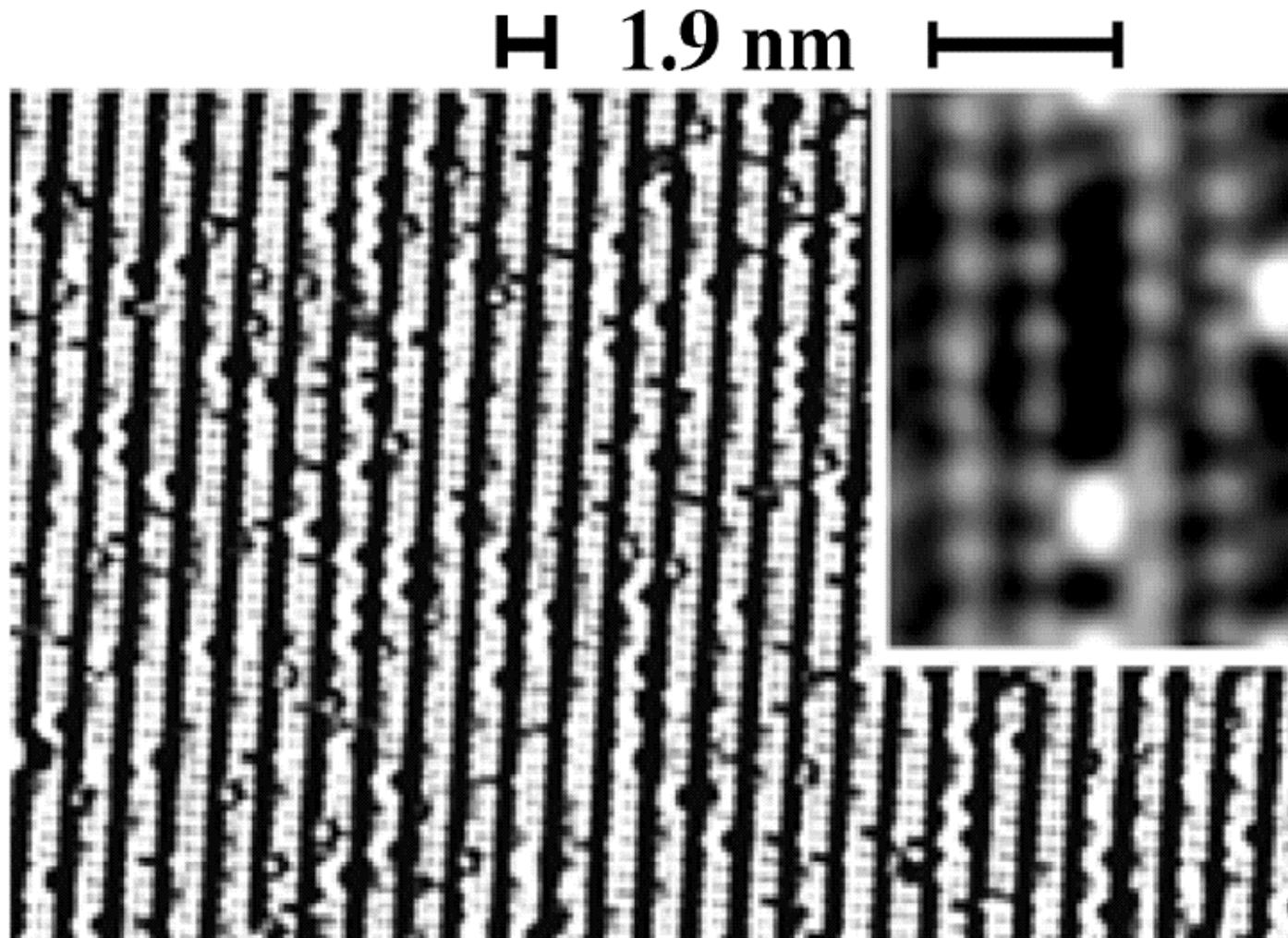


3×1 clean
surface

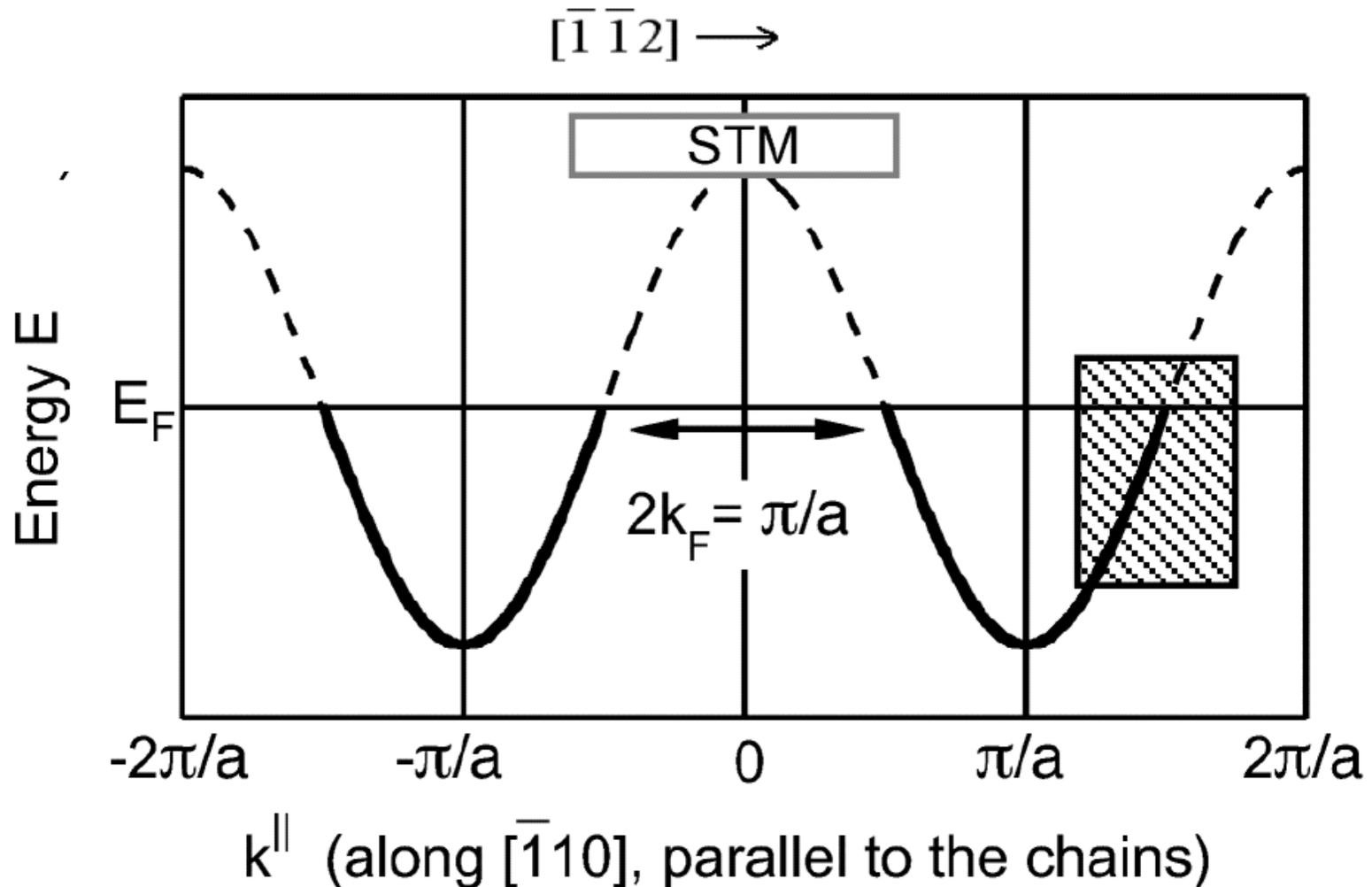
1×1 surface
with 0.2ML Au
at 600C

STM of Si(557)/Au

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

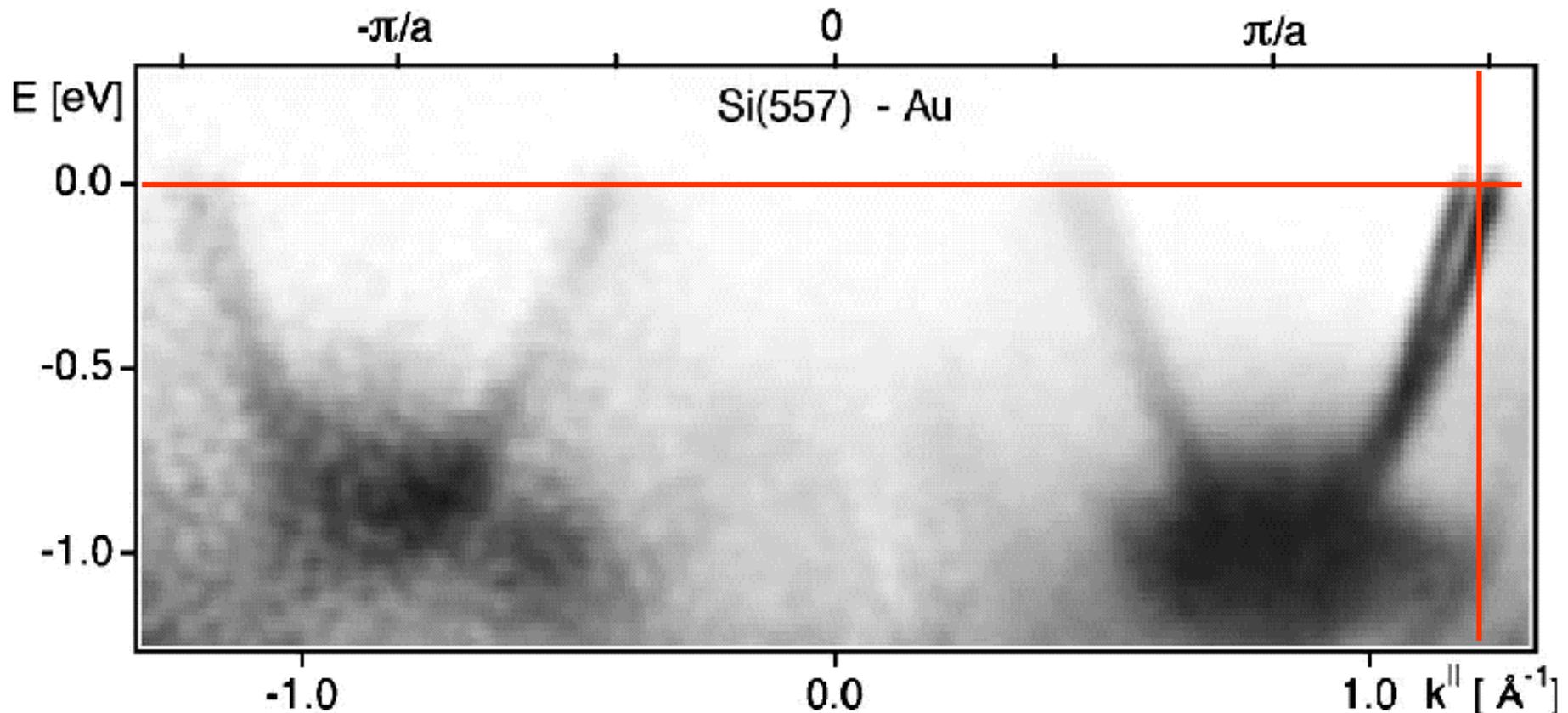


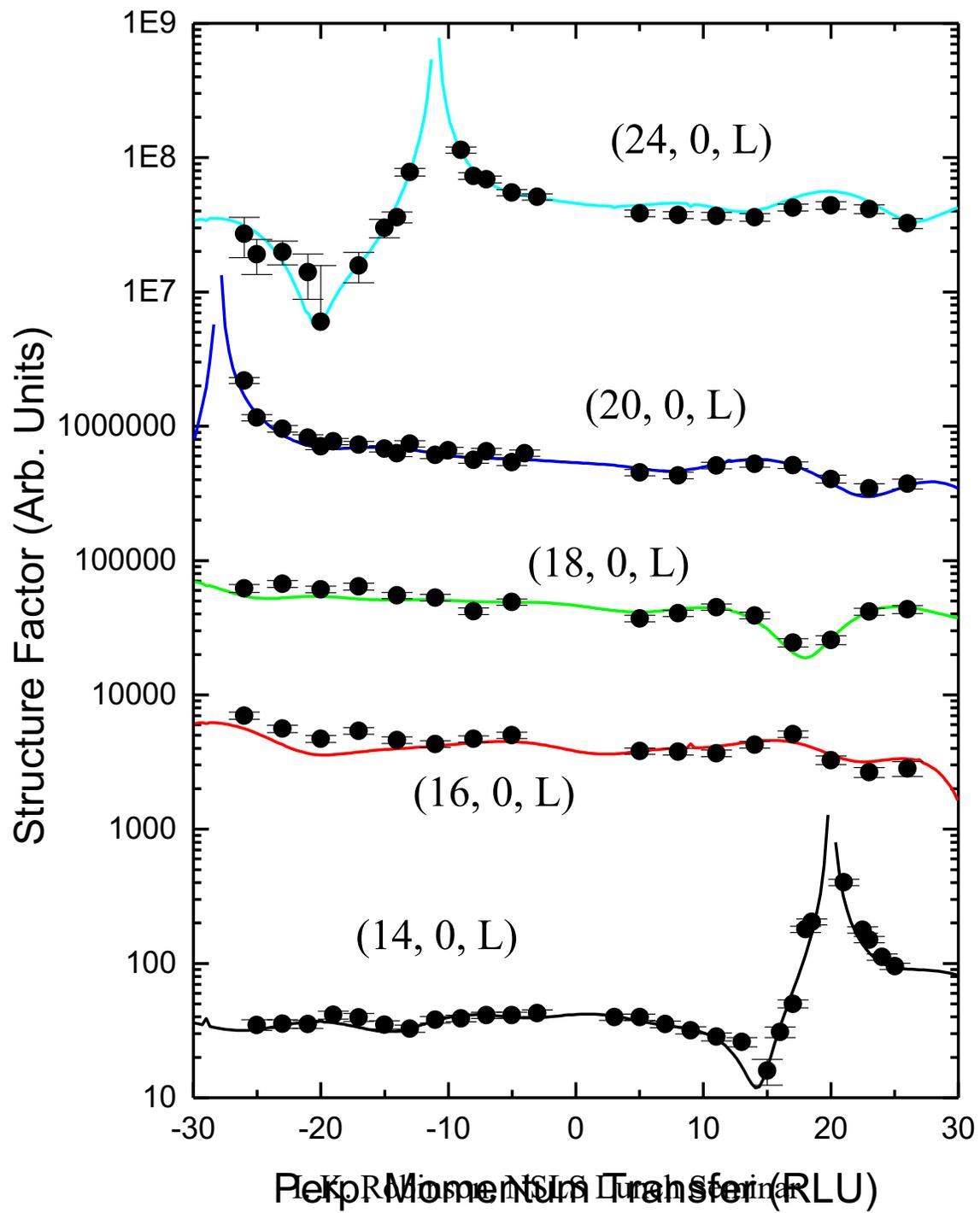
Schematic Band Topology for Au/Si(557)



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

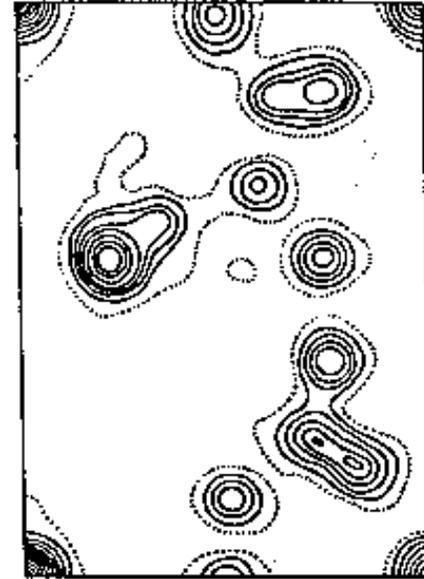
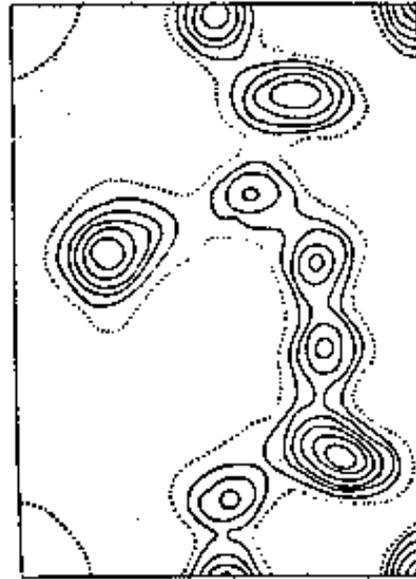
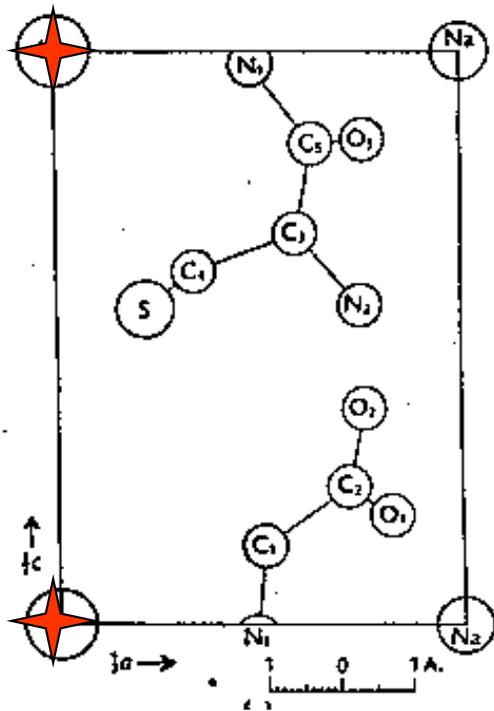
K. N. Altmann et. al. Phys Rev B 64 035406 (2001)





Phasing by a Single Heavy Atom

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

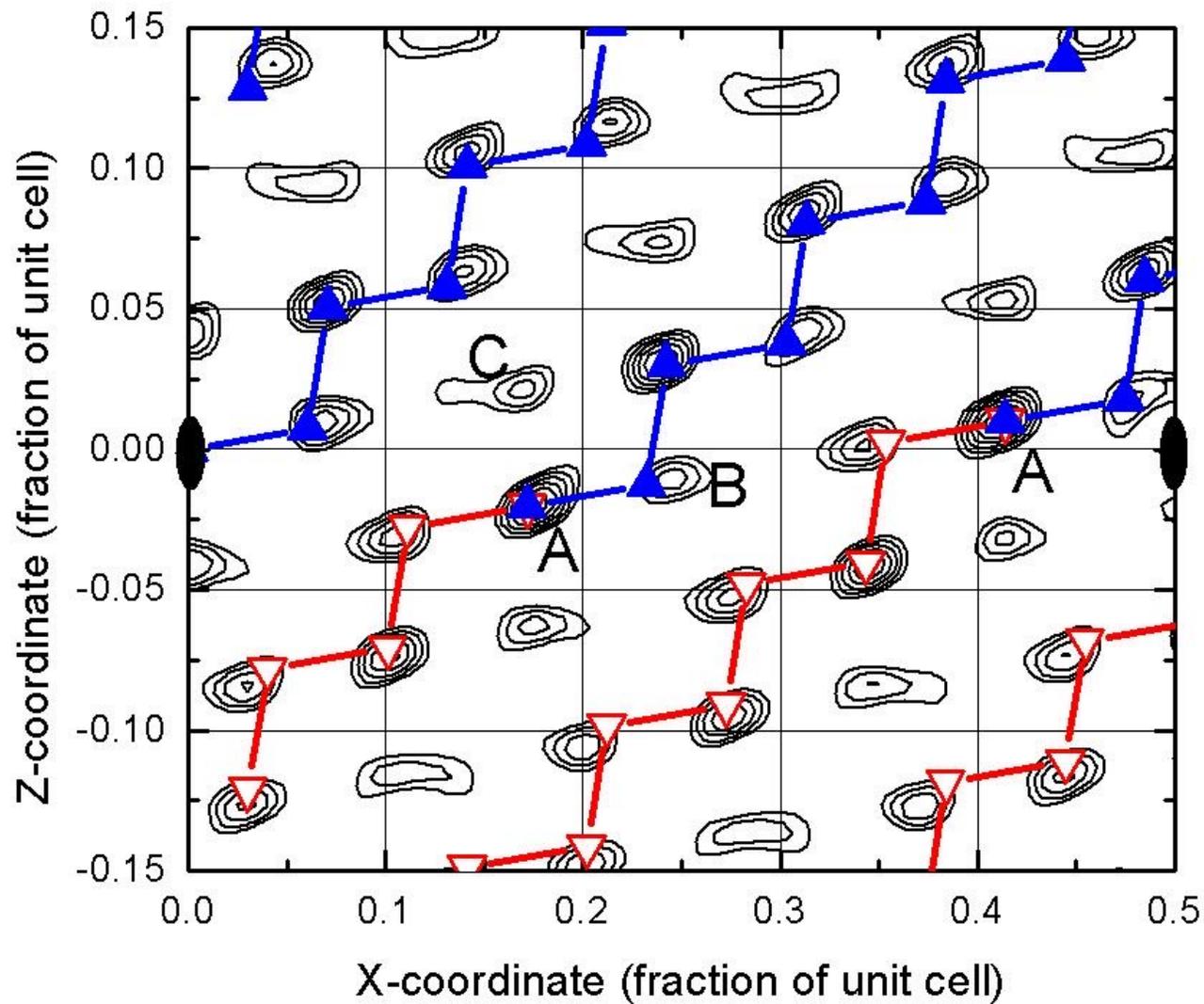


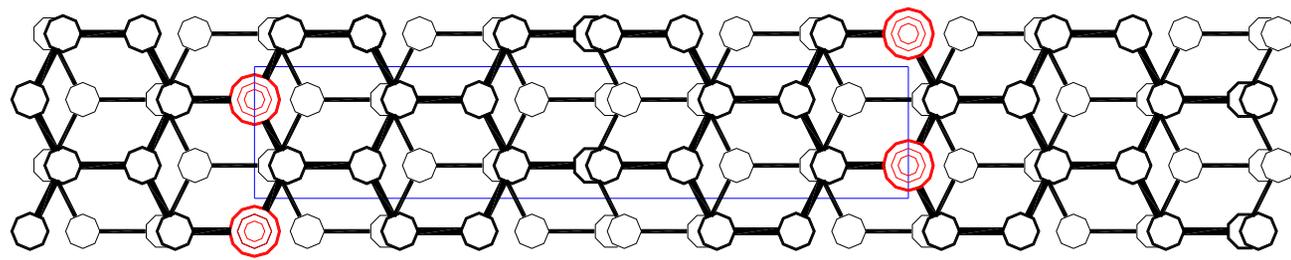
Cysteinylglycine
sodium iodide

Patterson

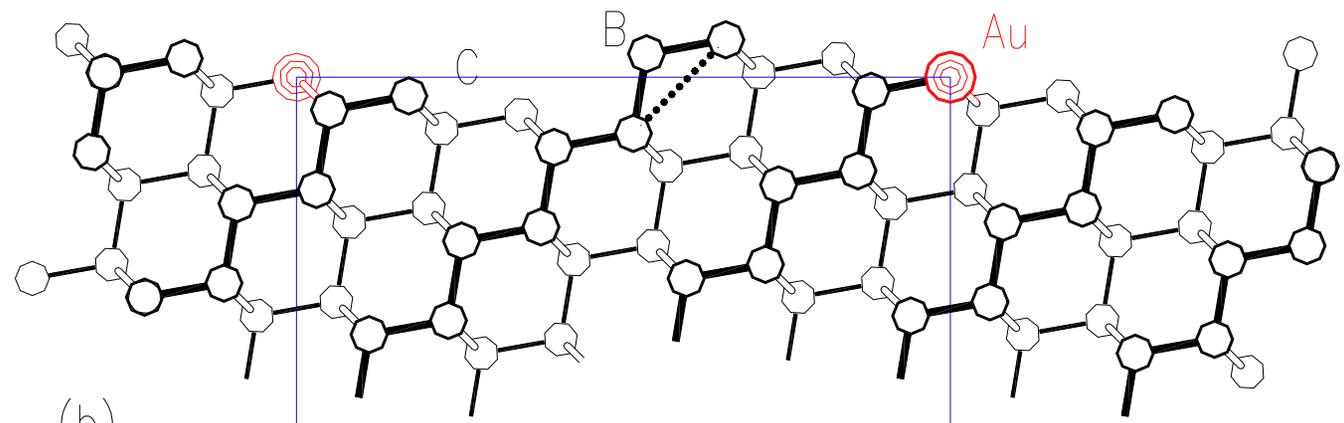
Electron density

X-Z Patterson of Au/Si(557)

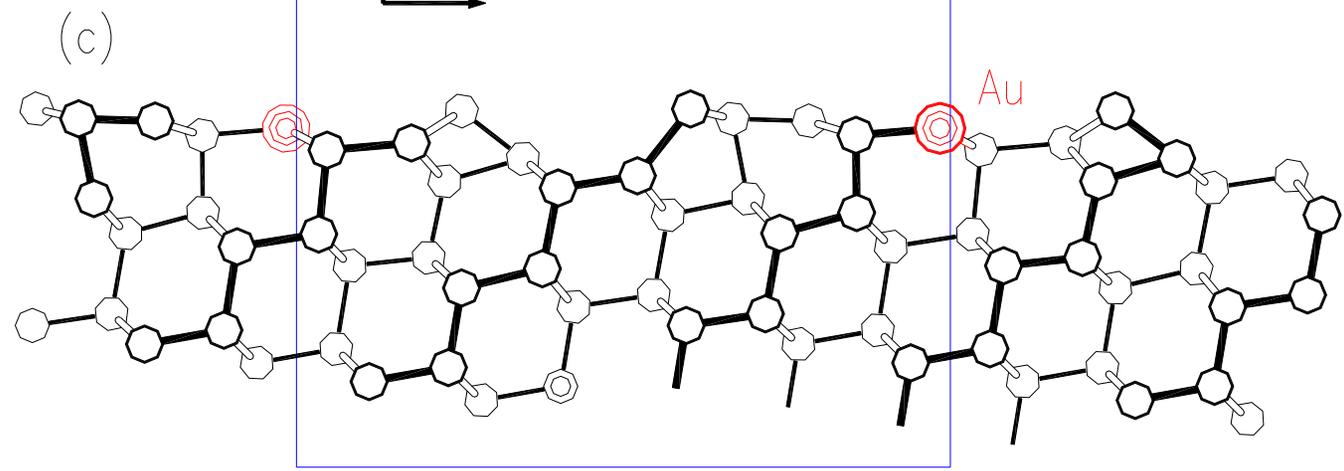




(a) A coordinate system with a vertical y-axis and a horizontal x-axis.

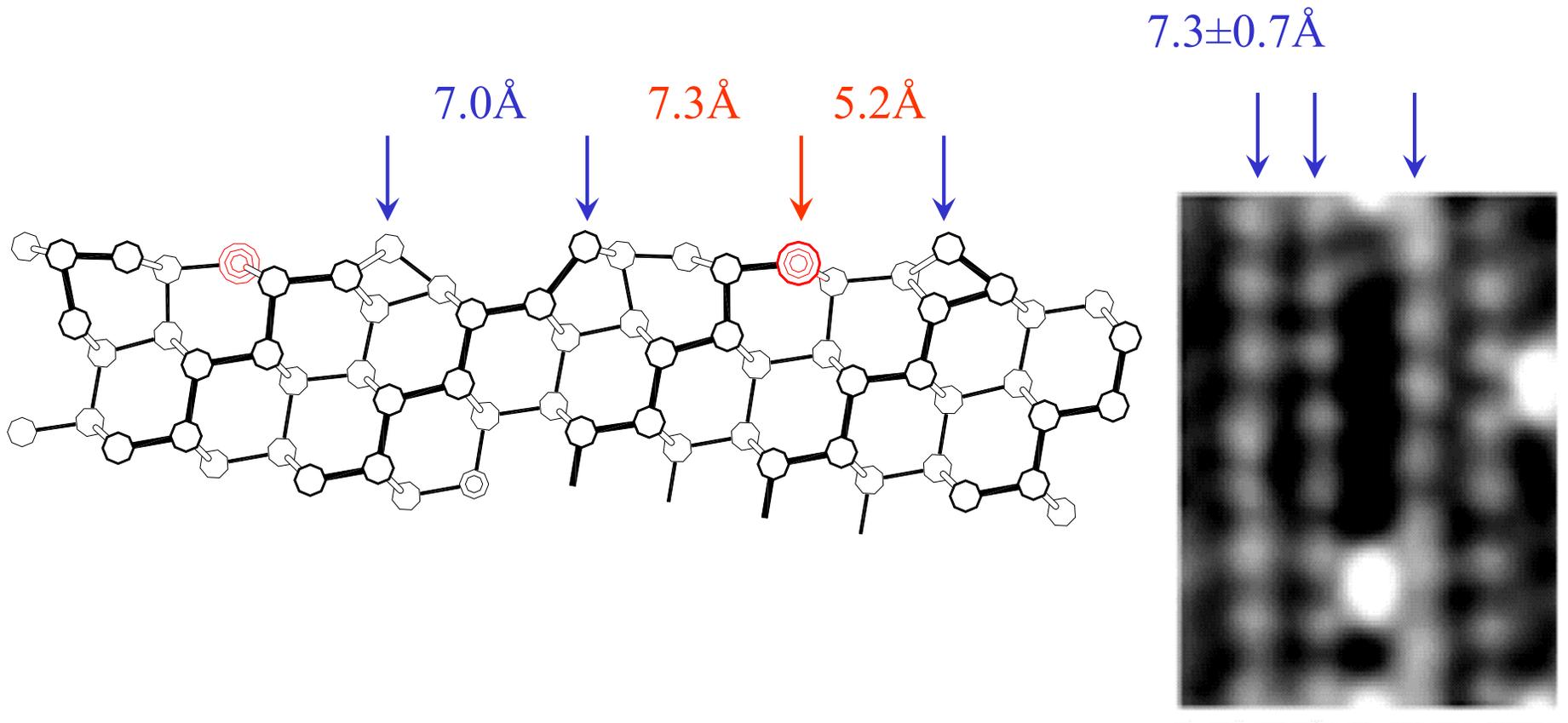


(b) A coordinate system with a vertical z-axis and a horizontal x-axis.



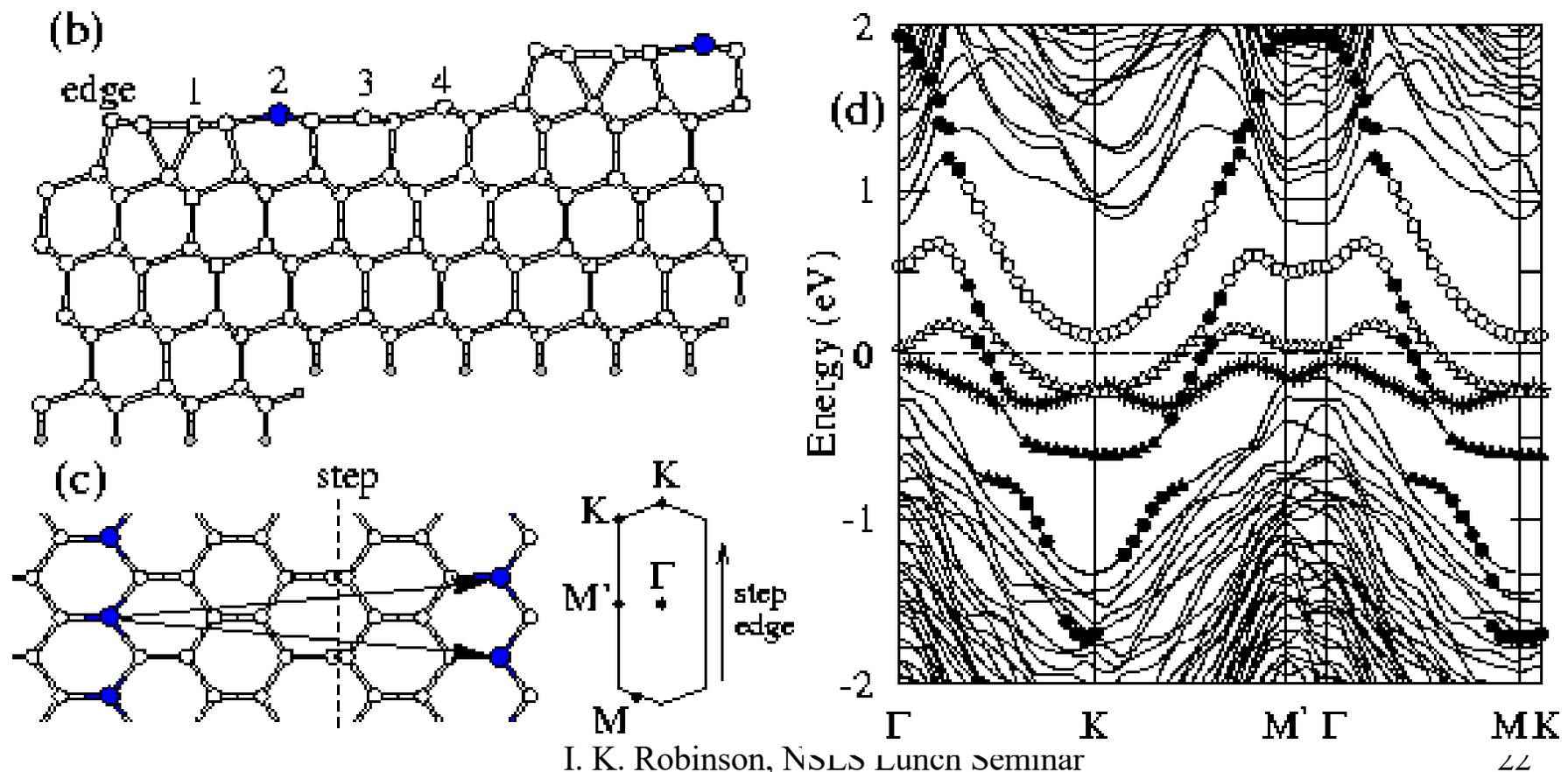
(c)

Comparison with STM



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

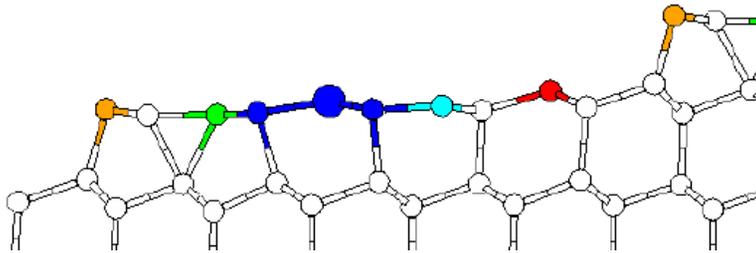
D. Sanchez-Portal et. al. Phys. Rev. B **65**, 081401 (2002)



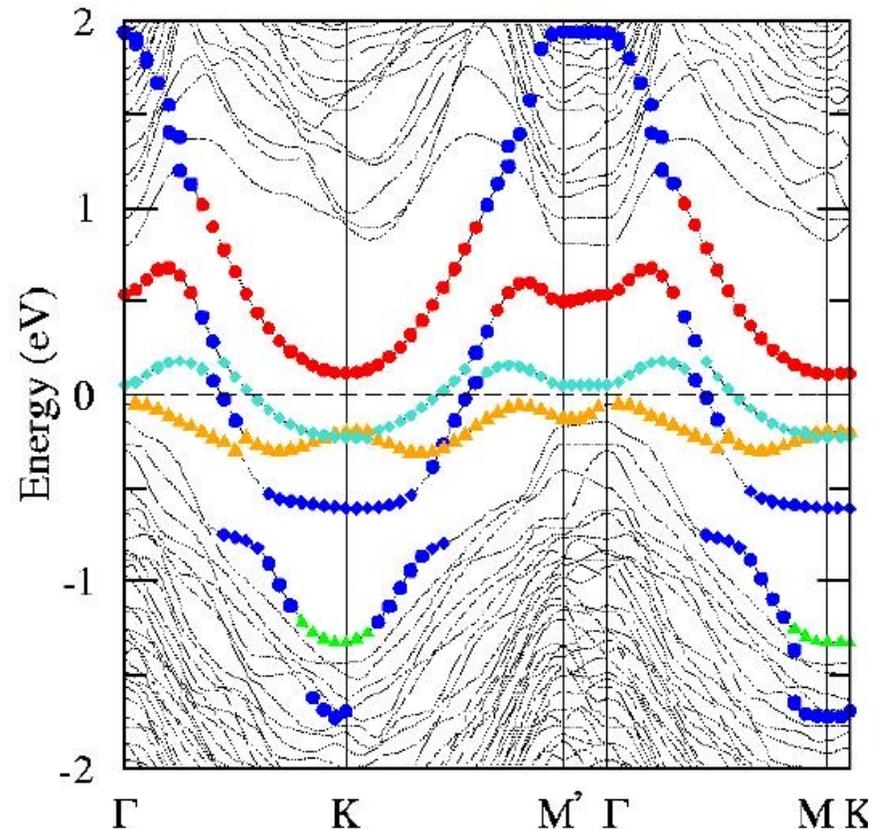
Si(557)-Au: calculated band structure

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

Mulliken populations allow to identify the origin of each band



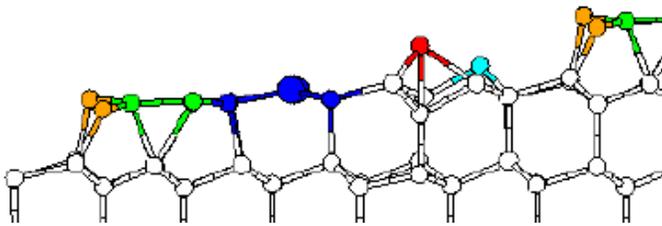
- Directions Γ - K - M' and Γ - M are parallel to the gold chains
- “Gold bands” (blue) are strongly hybridized with the Si neighboring atoms
- Orange band corresponds to the step edge
- Red and cyan bands are due to dangling bonds in the terraces
- The inclusion of adatoms saturating some of the Si dangling-bonds do not modify the main features of this band structure.



Si(557)-Au: role of adatoms

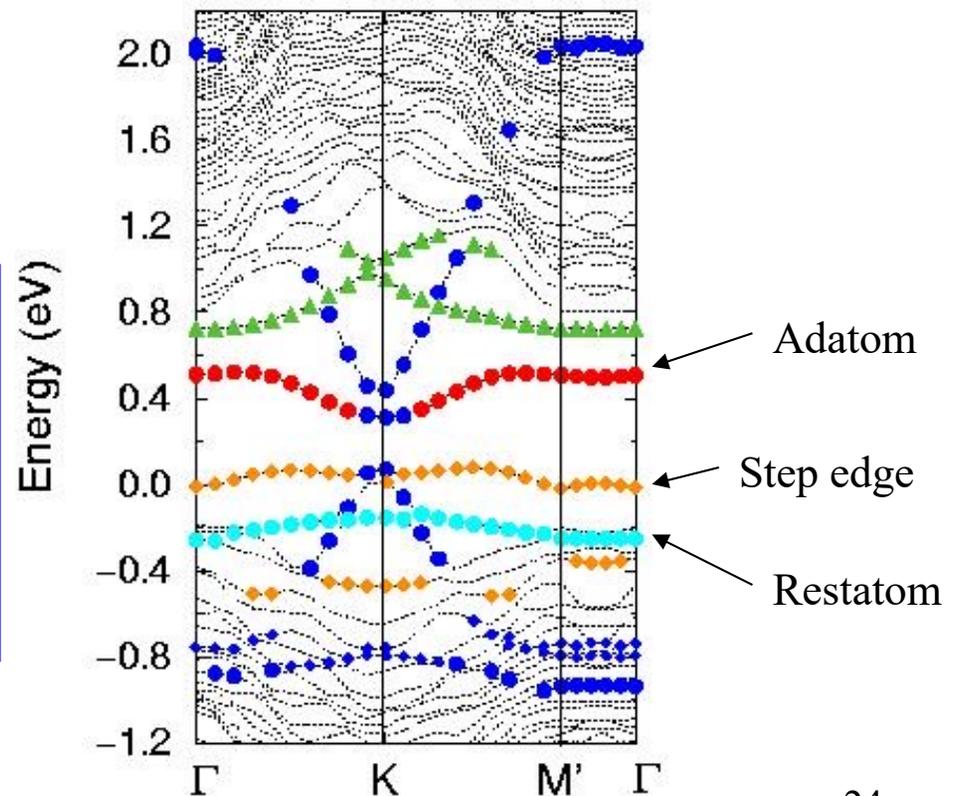
D. Sanchez-Portal et. al. (to be published)

The presence of **one row of adatoms** partially saturating some of the dangling bonds **do not modify** our main conclusions
However it is slightly **favorable energetically**, with a gain of ~ 0.14 eV/Au



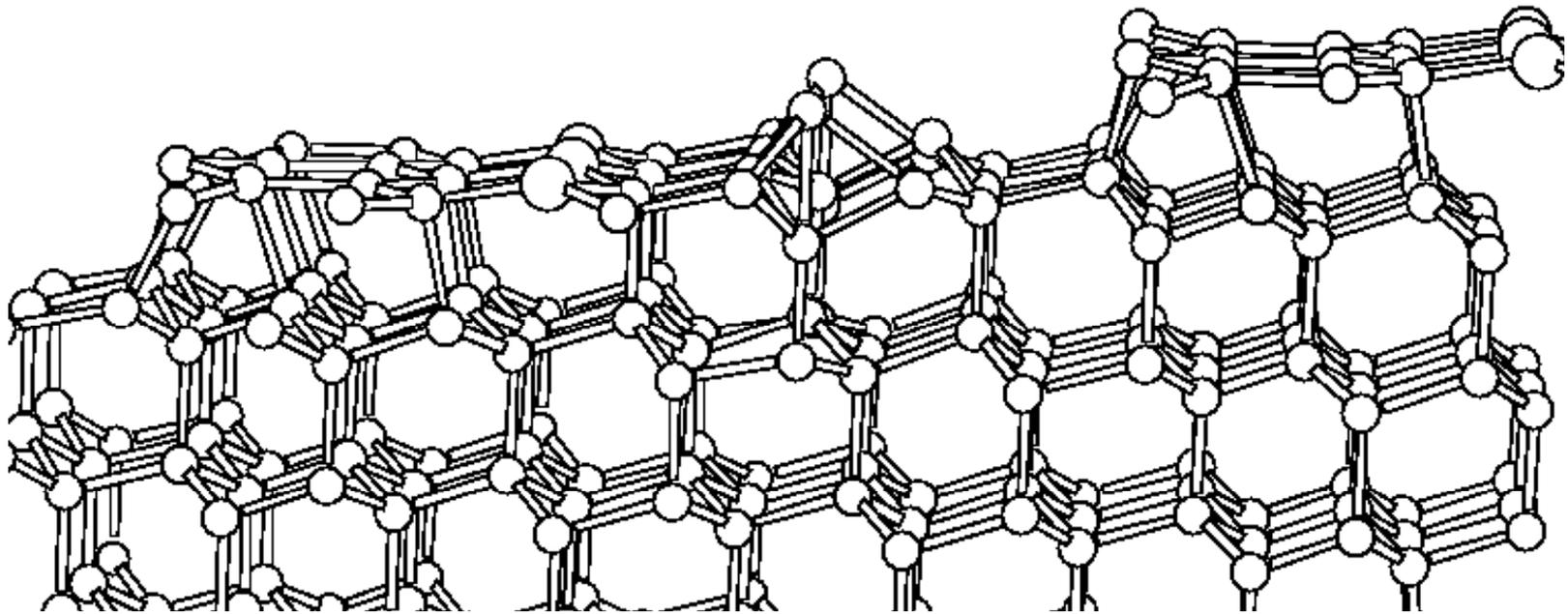
- The **step-edge band** (orange) is located precisely at the Fermi energy
- Still **two bands*** (blue symbols) associated to the gold chain.

*They appear as four bands due to the folding associated to the doubling of the unit cell



Energy-minimized Model of Au/Si(557) 1x2 with Adatom

D. Sanchez-Portal et. al. (to be published)



Conclusions

- Direct imaging of structure containing heavy atom
- Au stabilizes terraced Si(557) substrate
- Au substitutes for Si in **middle** of terrace
- 1D quantum wires seen in photoemission
- Superstructure yet to be resolved