Surface Structure Studies at the PEARL Beamline of the Swiss Light Source

Matthias Muntwiler :: Paul Scherrer Institut, Villigen PSI, Switzerland
Jun Zhang :: Paul Scherrer Institut, Villigen PSI, Switzerland
Roland Stania :: Universität Zürich, Switzerland
Fumihiko Matsui :: Nara Institute of Science and Technology, Nara, Japan
Thilo Glatzel :: Universität Basel, Switzerland
Thomas A. Jung :: Paul Scherrer Institut/Universität Basel, Switzerland
Philipp P. Aebi :: Université de Fribourg, Switzerland
Thomas Greber :: Universität Zürich, Switzerland
Roman Fasel :: Federal Institute for Materials Science and Technology (Empa), Dübendorf, Switzerland

http://www.psi.ch/sls/pearl

PEARL Beamline

PEARL = Photo-Emission and Atomic Resolution Laboratory

scientific case

- structural characterization of local bonding geometry
- molecular adsorbates on metal or semiconductor surfaces
- nanostructured surfaces
- surfaces of complex materials
- structural, electronic, and magnetic properties

methods

- X-ray photoelectron diffraction
  - angle-scanned (XPD)
  - photon energy-scanned (PhD)
- scanning tunneling microscopy (STM) and spectroscopy (STS)
- X-ray absorption spectroscopy (XAS)
- magnetic circular dichroism (XMCD)

Photoelectron Diffraction

chemical state specific emission

$$E_{\mathrm{kin}} = h\nu - E_{\mathrm{B}} - \Phi$$

wave vector / wave length

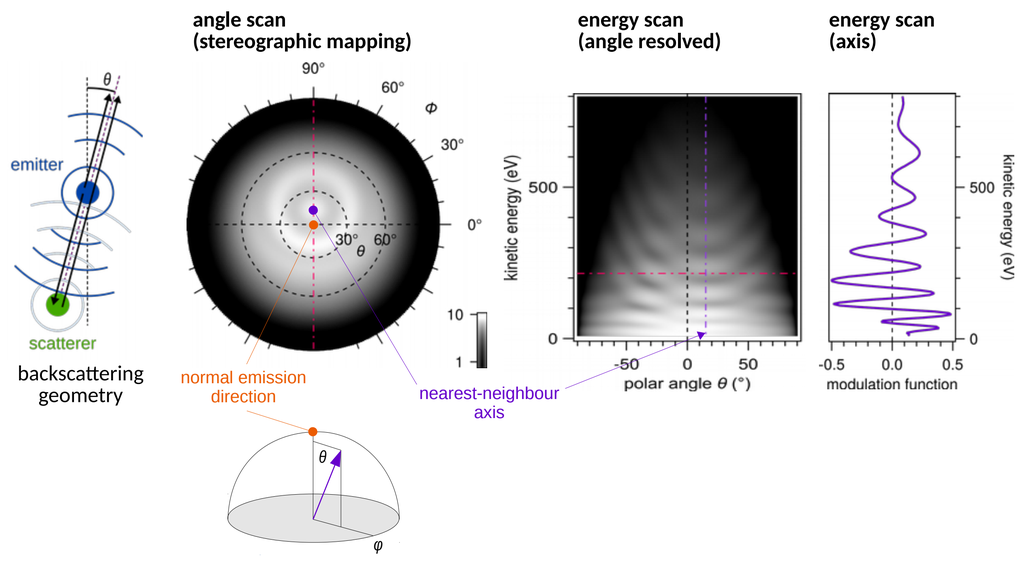
$$\hbar k = \frac{h}{\lambda} = \sqrt{2m_e(E_{\mathrm{kin}} + V_0)}$$

scattering phase shift

$$Rk(1-\cos\theta) + \delta$$

local geometry — atomic scattering

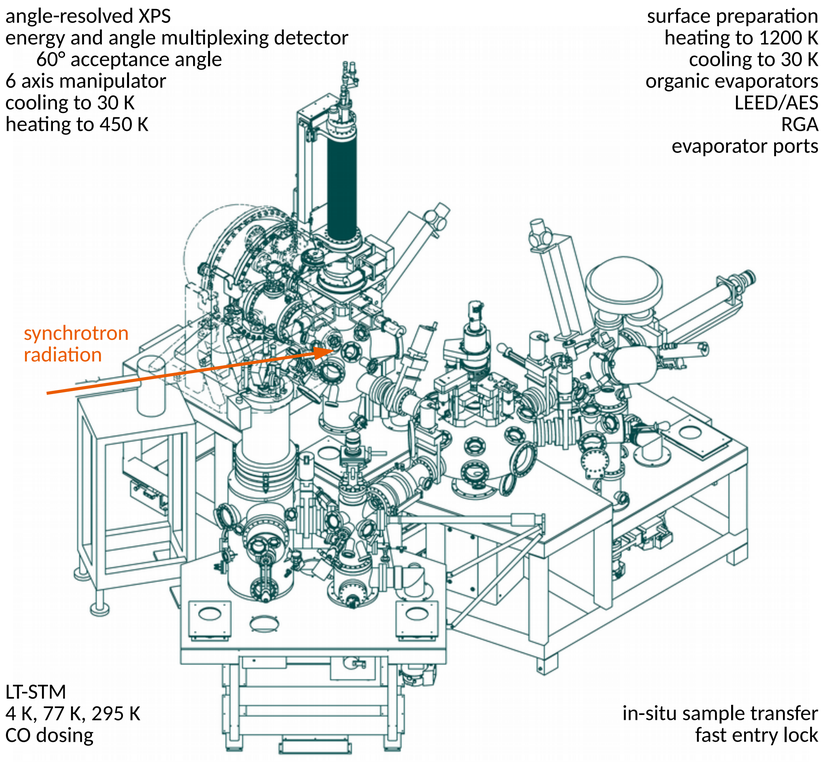
photoelectron diffraction probes local geometry (bond length and bond angle)



Experimental Station

angle-resolved XPS
energy and angle multiplexing detector
60° acceptance angle
6 axis manipulator
cooling to 30 K
heating to 450 K

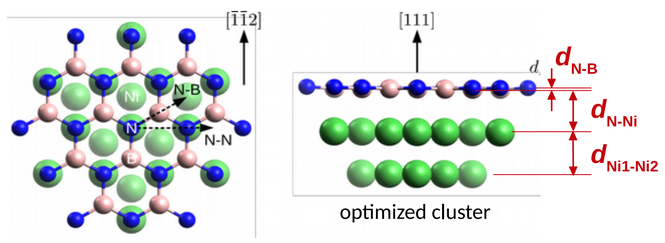
surface preparation
heating to 1200 K
cooling to 30 K
organic evaporators
LEED/AES
RGA
evaporator ports



LT-STM
4 K, 77 K, 295 K
CO dosing

in-situ sample transfer
fast entry lock

Hexagonal Boron Nitride on Ni(111) – Photoelectron Diffraction

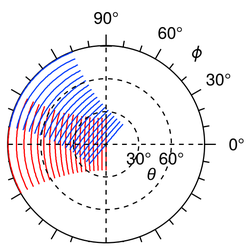


structural parameters

	LEED [4]	XPD [2,3]	DFT [4]	PhD [this]
registry (N,B)	(top,fcc)	(top,fcc)	(top,fcc)	
corrugation $d_{N\text{-}B}$	0.18 Å	0.07 Å	0.11 Å	
$d_{N\text{-}Ni}$	2.22 Å	1.95 Å	2.19 Å	2.11 Å
$d_{Ni1\text{-}Ni2}$	1.98 Å		2.03 Å	1.99 Å

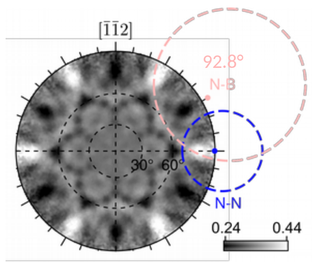
Angle-Scanned Photoelectron Diffraction (XPD)

scanning scheme



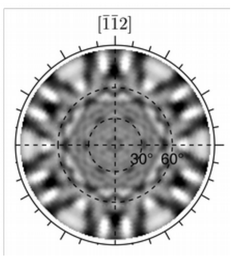
θ step 1°
Φ step 15°
2184 angle settings
stereographic projection

experiment



N 1s
E_{kin} = 399 eV
(α,θ)-normalized
three-fold average

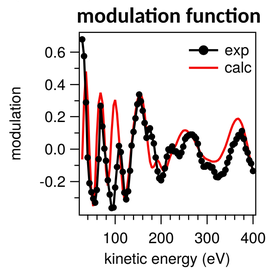
multiple scattering calculation



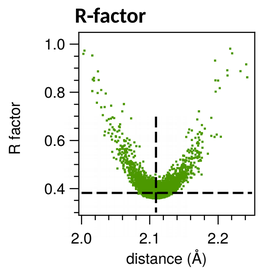
θ-normalized
two-fold average

Energy-Scanned Photoelectron Diffraction (PhD)

modulation function



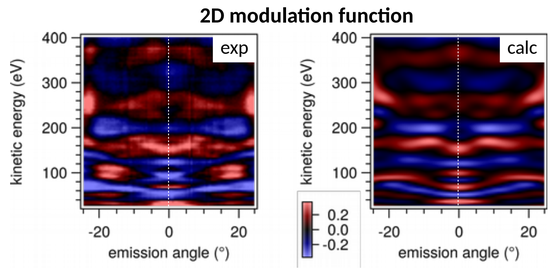
R-factor

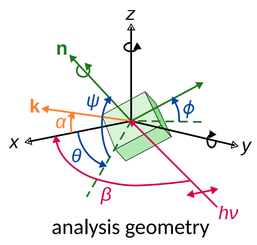


multi-dimensional cluster optimization
7 parameters
13700 configurations

$d_{N\text{-}Ni}$ = 2.11 ± 0.02 Å

2D modulation function

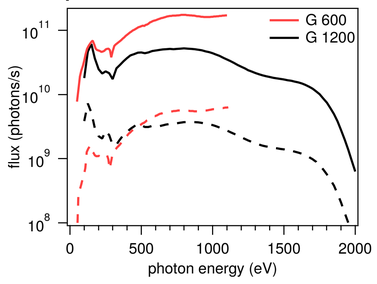




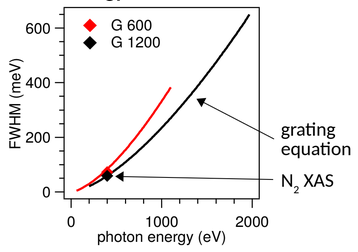
analysis geometry

Beamline Performance

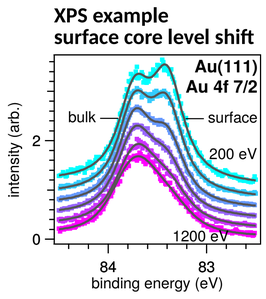
photon flux



energy resolution



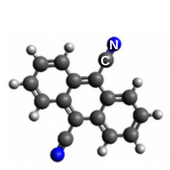
XPS example surface core level shift

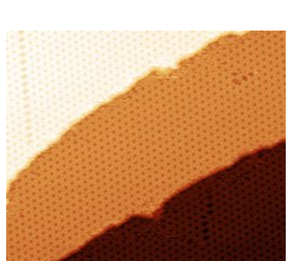


photon energy	60 – 1100, 200 – 2000 eV
ultimate energy resolution	< 0.1 eV (E < 1000 eV)
polarization	linear horizontal circular +/- (< 70%)
spot size	200 µm x 70 µm (H x V, FWHM) 1000 µm x 1000 µm

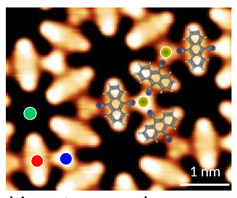
Metal-Organic Network – Scanning Tunnelling Spectroscopy

9,10-dicyanoanthracene (DCA) on Cu(111)

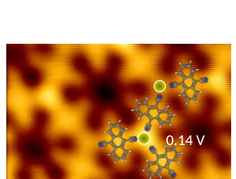




STM topography

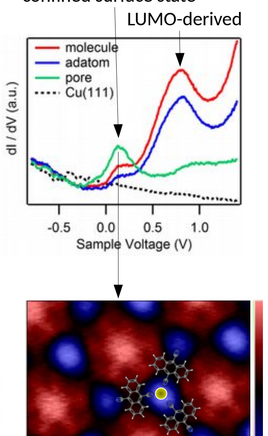


hi-res topography



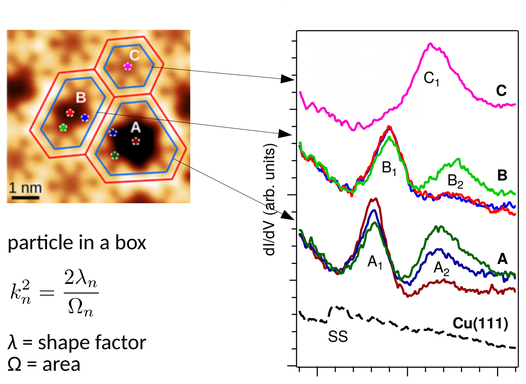
topography

confined surface state



dI/dV map
(local density of states)

confinement of surface state: quantum well states



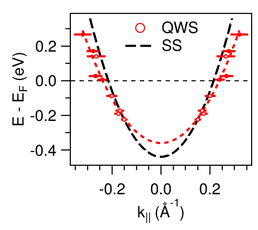
particle in a box

$$k_n^2 = \frac{2\lambda_n}{\Omega_n}$$

λ = shape factor
Ω = area

surface state

$$E(k) = \frac{\hbar^2 k^2}{2m^\star} + E_0$$



Acknowledgements

We thank all scientists, engineers, and technicians involved in the design and construction of PEARL, in particular
U. Staub, F. Nolting, J. Raabe, L. Patthey, V. Strokov, C. Piamonteze, O. Gröning,
R. Wullschleger, Q. Chen, J. Krempasky, A. Jaggi
P. Ascher, C. Hess, B. Sarafimov, M. Schmidt, L. Rotach, T. Kälin,
M. Mühlebach, A. Keller, S. Maag, J. Welte, D. Birchmeier
P. Müller, C. Lüscher, D. Armstrong, B. Marolt, A. Lüdeke
P. Huber, E. Zehnder, K. Dreyer, G. Kaeslin, H. Deppeler, J. Hadobas
and many more …

References

1 C. S. Fadley, Prog Surf Sci 16, 275 (1984)
2 D. P. Woodruff, Surf Sci Rep 62, 1 (2007)
3 F. J. García de Abajo et al., Phys Rev B 63, 75404 (2001)
4 Y. Gamou et al., Sci Rep RITU A 44, 421 (1997)
5 W. Auwärter et al., Surf Sci 429, 229 (1999)
6 M. Muntwiler et al., Surf Sci 472, 125 (2001)
7 G. Grad et al., Phys Rev B 68, 85404 (2003)
8 J. Zhang et al., Chem Commun 50, 12289 (2014)
9 M. Muntwiler et al., in preparation

2017-07-05