SCHOOL ON SYNCHROTRON RADIATION AND APPLICATIONS
In memory of J.C. Fuggle & L. Fonda

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Miramare - Trieste, Italy

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Photoemission from Valence Bands, Dispersion and Fermi Surface Mapping

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Photoemission from Valence Bands, Dispersion and Fermi Surface Mapping

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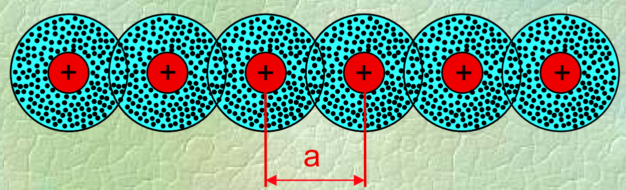
Lecture 1

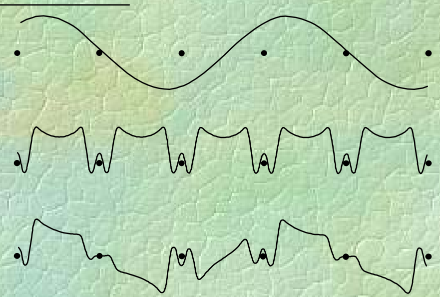
- Electronic Band Structure in 1-3 Dimensions
- Photoemission from a Periodic Potential
- The 3-Step Model
- A 1D Example: p(2x1) O-Cu(110) -> Band Mapping
- A 2D Example: The Shockley Surface State on Cu(111)
- A Few Words about Surface States in General
- Surface States on Stepped Surfaces:
  A Playground for Quantum Mechanics

Electronic Bandstructure in 1 Dimension

chain of atoms:



wave functions:

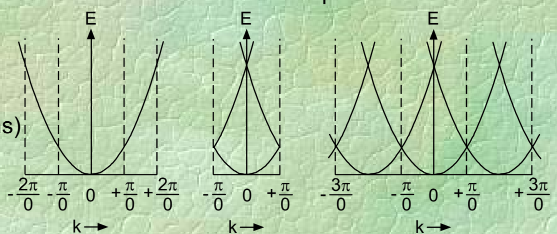


Bloch functions $\psi_k (x) = u_k (x)\, e^{ikx}$

dispersion relation (reciprocal space):

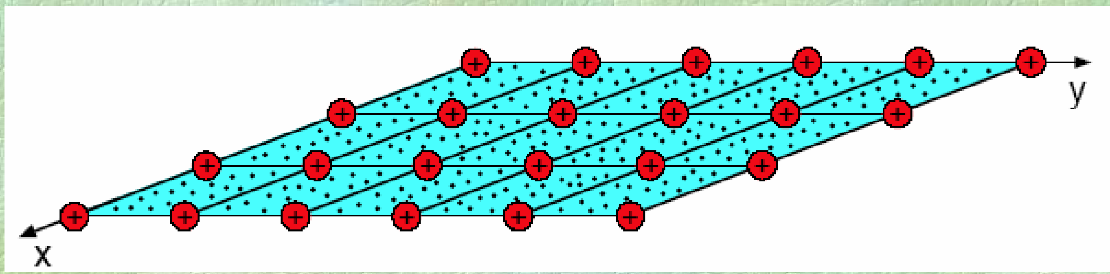
$\varepsilon (k) = \frac{\hbar^2 k^2}{2m}$

(free electrons)

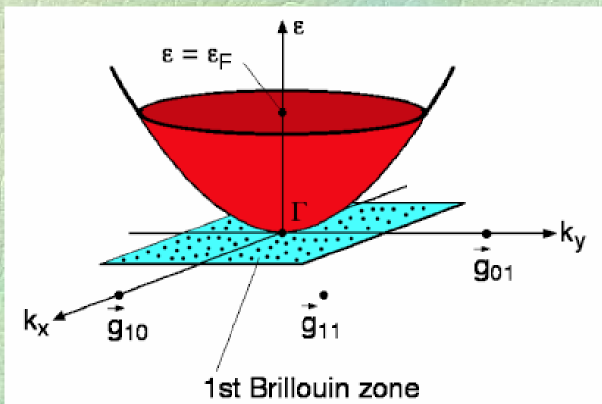


Electronic Structure in 2 Dimensions

(Plane of atoms)



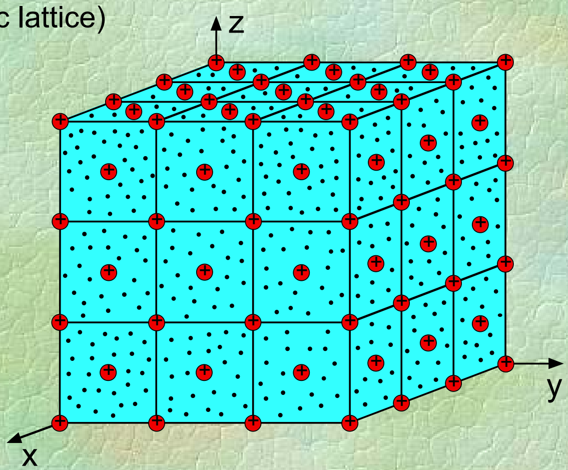
dispersion relation



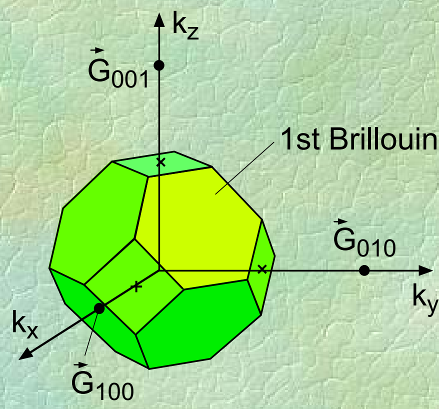
Electronic Structure in 3 Dimensions

real space:

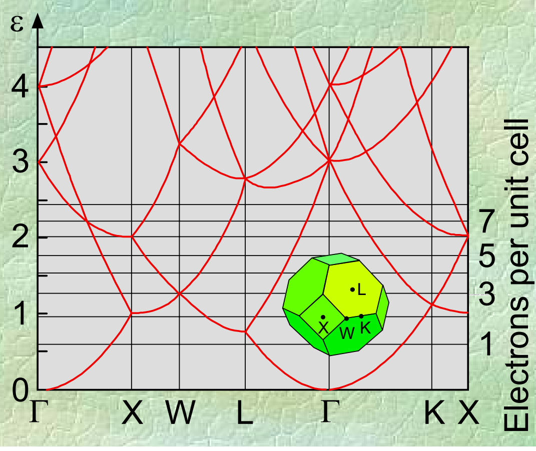
(face-centered cubic lattice)



reciprocal space:



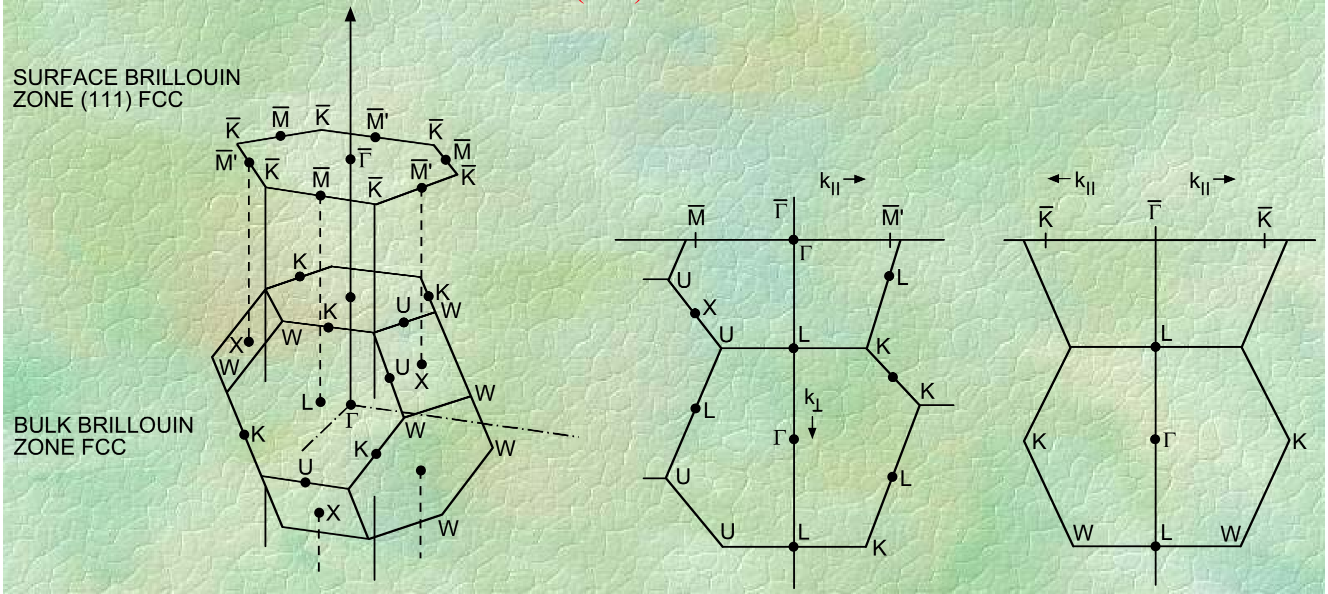
dispersion relation:



The Geography of Reciprocal Space

Surface and Bulk Brillouin Zones for face-centered cubic (fcc) Lattices

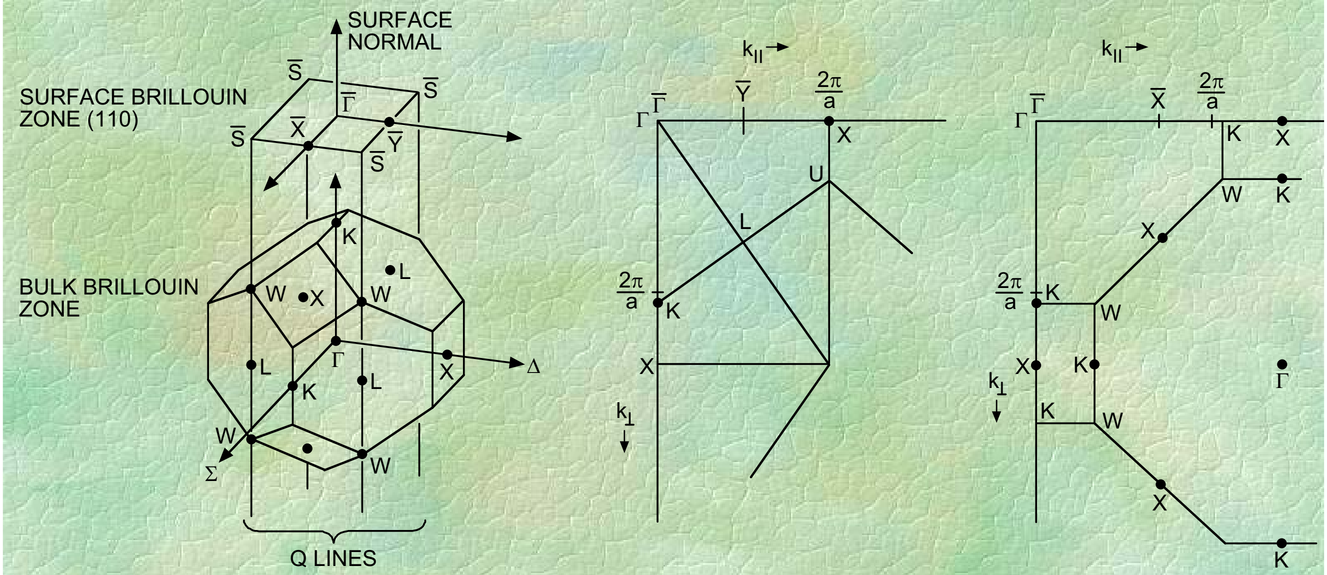
(111) Surface



From E. W. Plummer, W. Eberhardt
Adv. Chem. Phys. 49, 533 (1982)

Surface and Bulk Brillouin Zones for face-centered cubic (fcc) Lattices

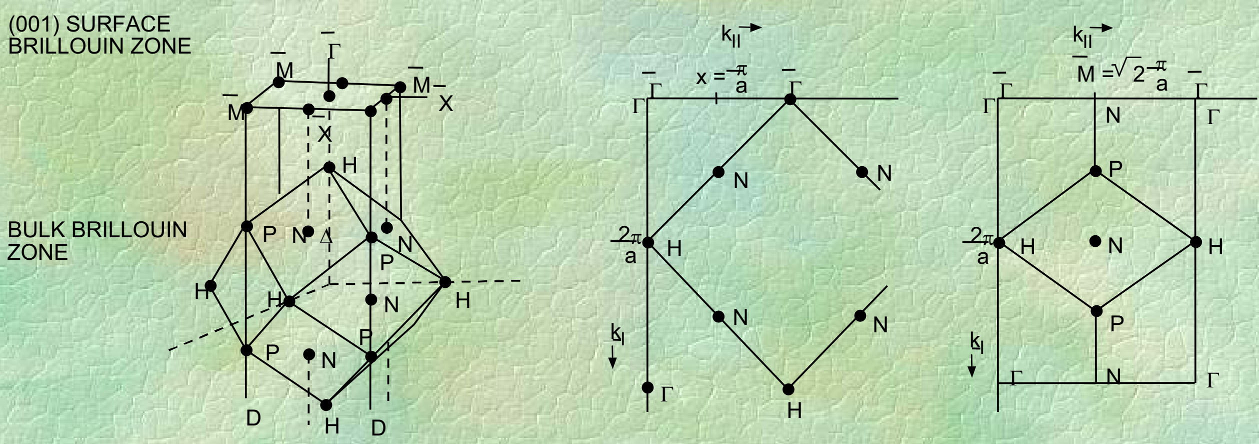
(110) Surface



From E. W. Plummer, W. Eberhardt
Adv. Chem. Phys. 49, 533 (1982)

Surface and Bulk Brillouin Zones for body-centered cubic (bcc) Lattices

(001) Surface



From E. W. Plummer, W. Eberhardt
Adv. Chem. Phys. 49, 533 (1982)

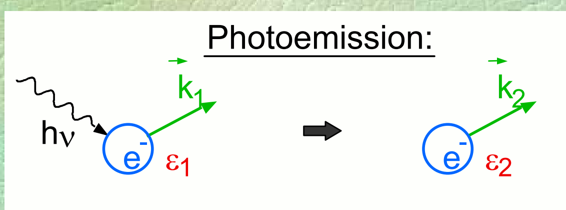
Photoemission of a free electron

	Energy	Momentum
free electron	$\varepsilon(\vec{k}) = \frac{\hbar^2 k^2}{2m}$	$\hbar\vec{k}$
photon ($h\nu$)	$\varepsilon(\vec{k}) = \lvert\hbar\vec{k}\rvert c$	$\hbar\vec{k}$

wave numbers k

e^- : $k = 0.51 \sqrt{\varepsilon\,[\mathrm{eV}]}\ \text{Å}^{-1}$

$h\nu$: $k = 0.51 \cdot \varepsilon\,[\mathrm{eV}] \cdot 10^{-3}\,\text{Å}^{-1}$



Conservation Laws:

$\varepsilon_1 + h\nu = \varepsilon_2$

$\vec{k}_1 + \vec{k}_{h\nu} = \vec{k}_2$

··· cannot be simultaneously fullfilled !
⇨ prozess forbidden

Atoms, Molecules: Recoil
Solids : Recoil (= reciprocal lattice vector)

Photoemission from a Periodic Potential

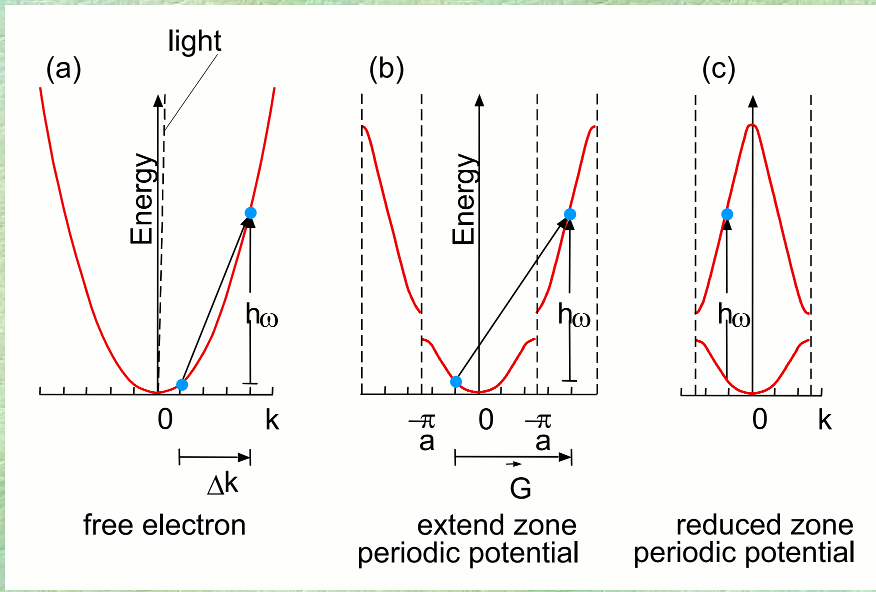
Conservation Laws:

$\varepsilon_i(\vec{k}_i) + h\nu = \varepsilon_f(\vec{k}_f)$

$\vec{k}_i + \vec{k}_{h\nu} + \vec{G} + \vec{g} = \vec{k}_f$

$\vec{k}_{h\nu} \approx 0$

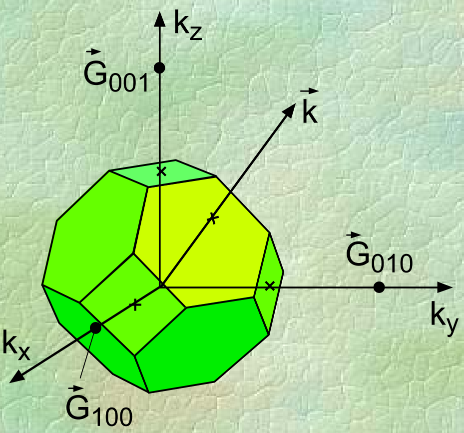
$\vec{g}$: reconstructed surface



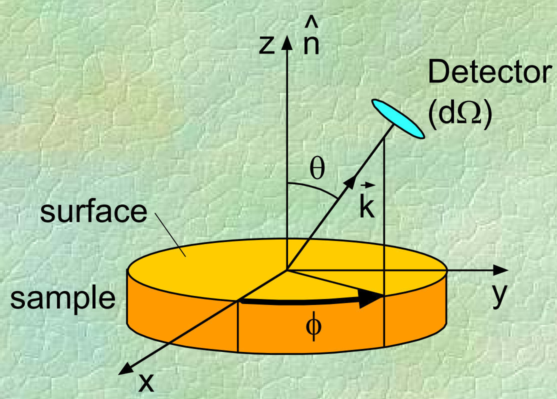
→ Direct Transitions

Measurement of the Photoelectron Momentum

reciprocal space:



real space:



direction: $\hat{k} = \theta, \phi$ (watch for refraction)

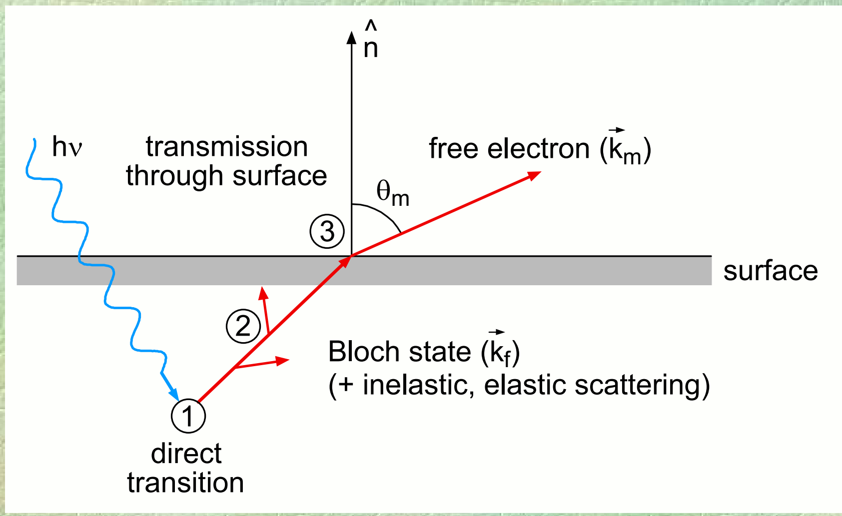
magnitude: from $\varepsilon_f(\vec{k})$ (ε_f is measured)

Problem: $\varepsilon_f(\vec{k})$ usually not known

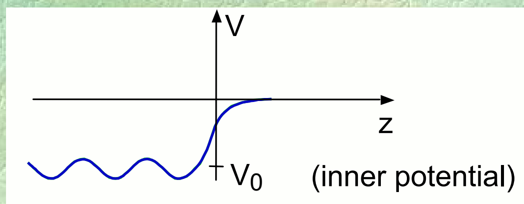
Solution: free electron final state

$$\varepsilon_f(k) = \frac{\hbar^2 k^2}{2m}$$

The 3-Step Model



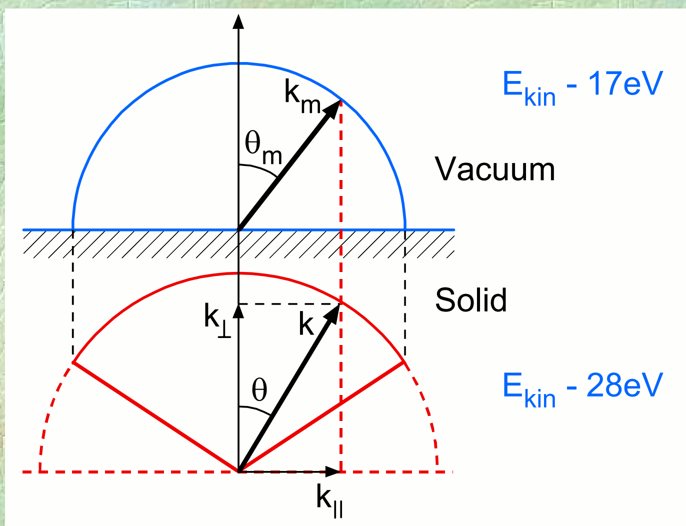
1. Photoexcitation
2. Propagation to surface
3. surface potential step → Refraction



periodicity within surface → $\vec{k}_{f\parallel} = \vec{k}_{m\parallel}$

surface potential step → $\vec{k}_{f\perp} > \vec{k}_{m\perp}$

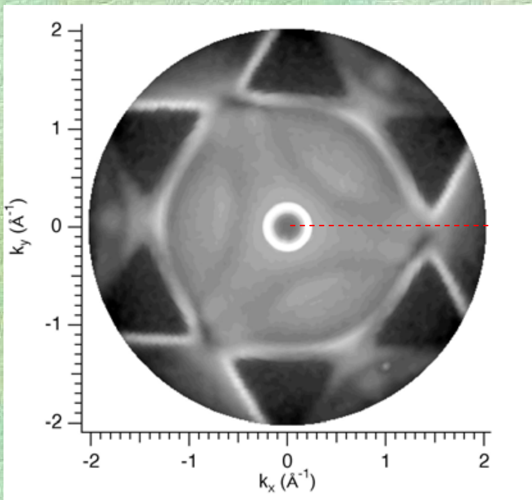
Refraction at the Surface Potential Step

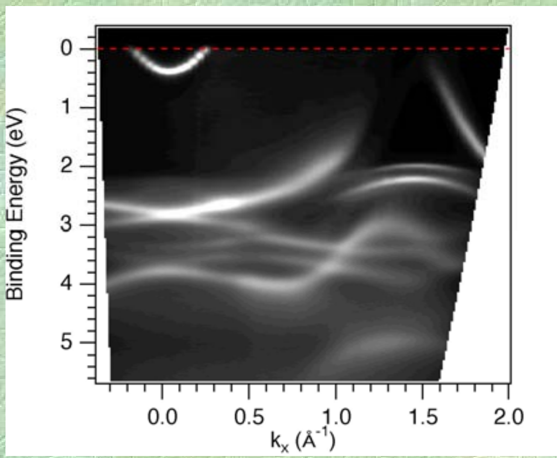


$$\sin\theta = \sin\theta_m \sqrt{\frac{h\nu - \Phi}{h\nu - \Phi + V_0}}$$

Φ : work function
V_0 : inner potential

Angle-Resolved Photoemission from Cu(111)

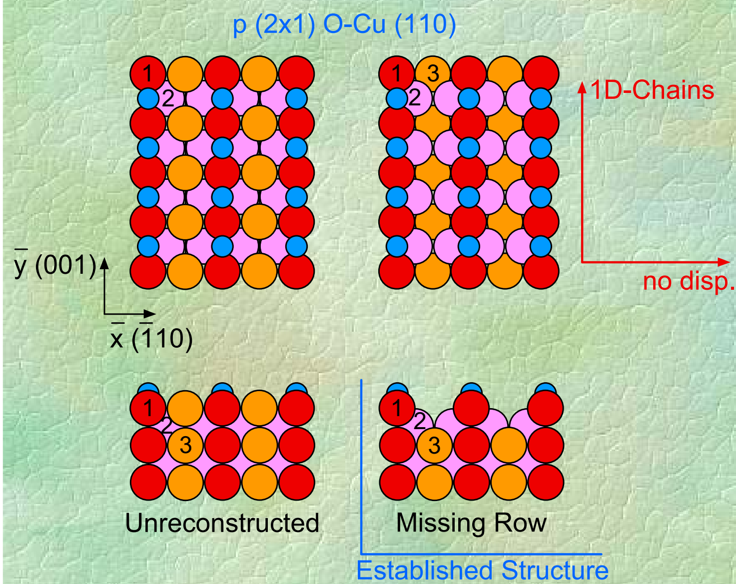


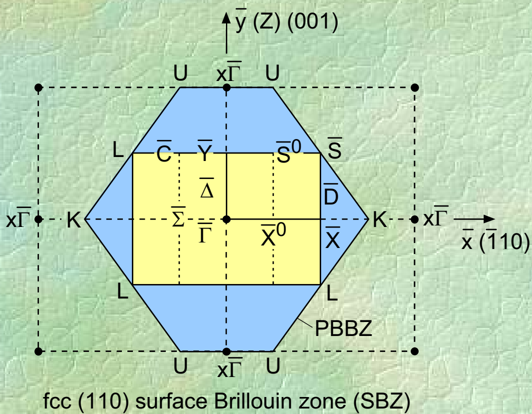


$E_i = E_{fermi}$, scanning of (θ,ϕ):
Cut through the bulk Fermi surface

scanning of E_i *and* θ:
Band structure along curved line in 3D k - space

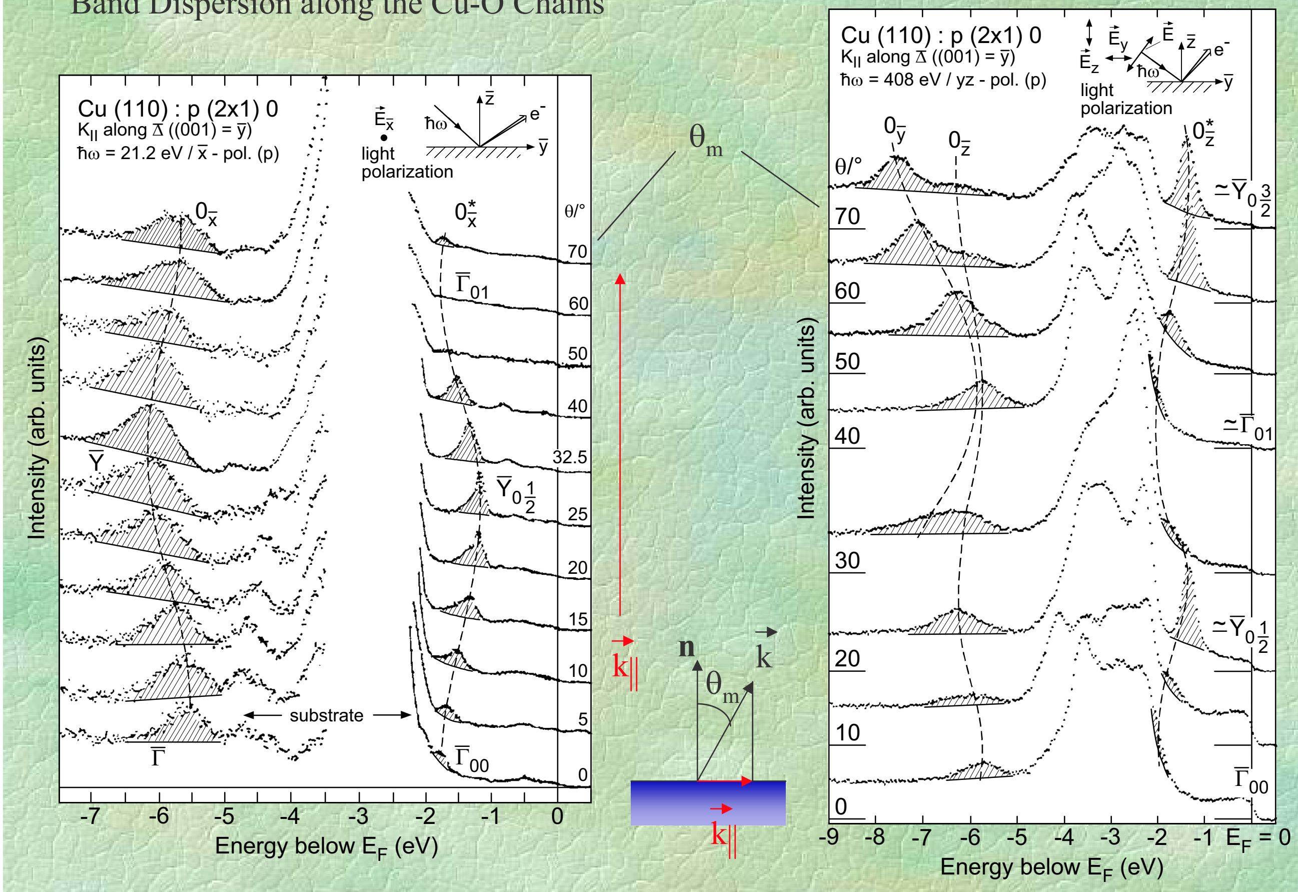
A One-Dimensional Example:





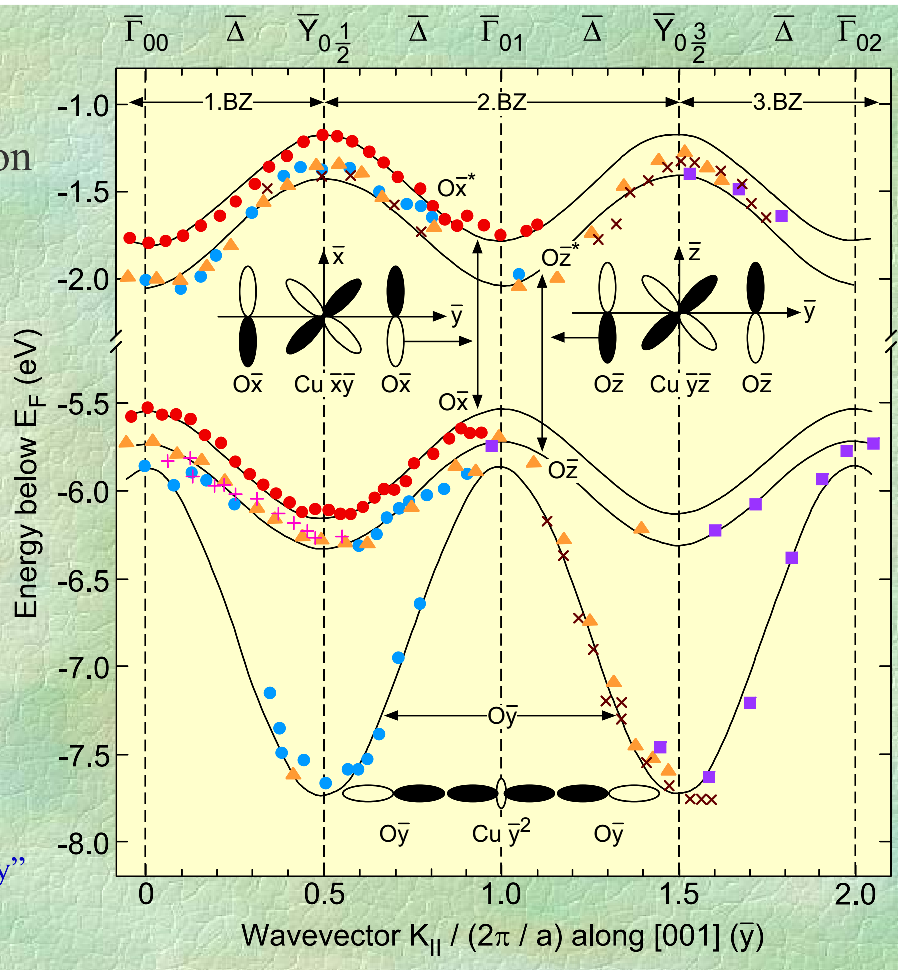
From S.Hüfner, "Photoelectron Spectroscopy" (Springer)

Band Dispersion along the Cu-O Chains



From S.Hüfner, "Photoelectron Spectroscopy" (Springer)

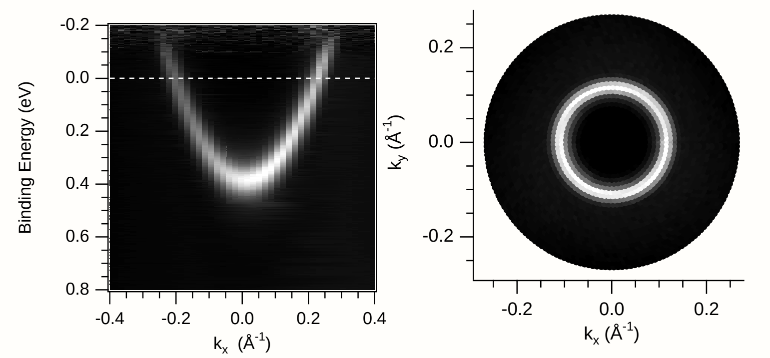
Finding all the States - Interpretation



Often a simple tight binding model works quite well !

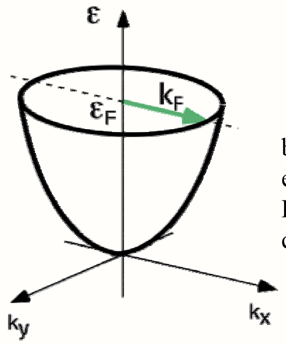
From S.Hüfner, "Photoelectron Spectroscopy" (Springer)

A 2D Example: The Shockley Surface State on Cu(111)



Energy dispersion

Fermi surface



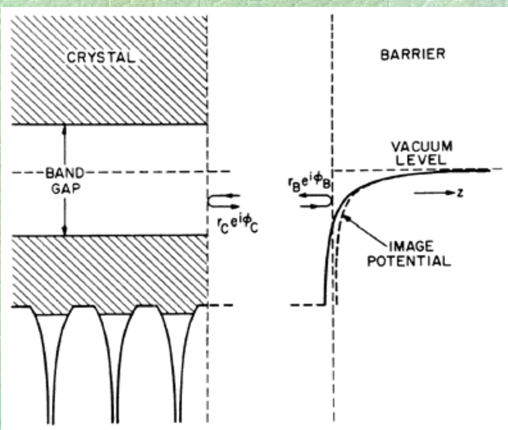
2D free electron gas

binding energy:	390 meV
effective mass:	0.42 m_e
Fermi wave length:	2.9 nm
coherence length:	~ 10 nm (300K)

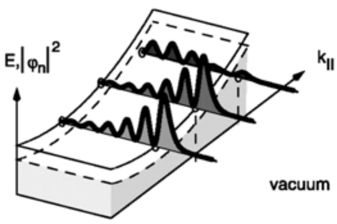
Courtesy F. Baumberger

Multiple reflection model for surface states:

(N.V. Smith, PRB **32**, 3549 (1985))



N.V. Smith, PRB **32**, 3549 (1985)



Surface state wave functions
for different $k_{//}$

(from Kliewer et al. Science 288, 1399 (2000))

$$\phi_c + \phi_b = 2\pi n$$

$$\text{Cu(111)}, \; n = 0: \; E_B = 0.3eV, m^* = 0.5m_e$$

Courtesy F. Baumberger

The Long-Range Image Potential Near a Metal Surface

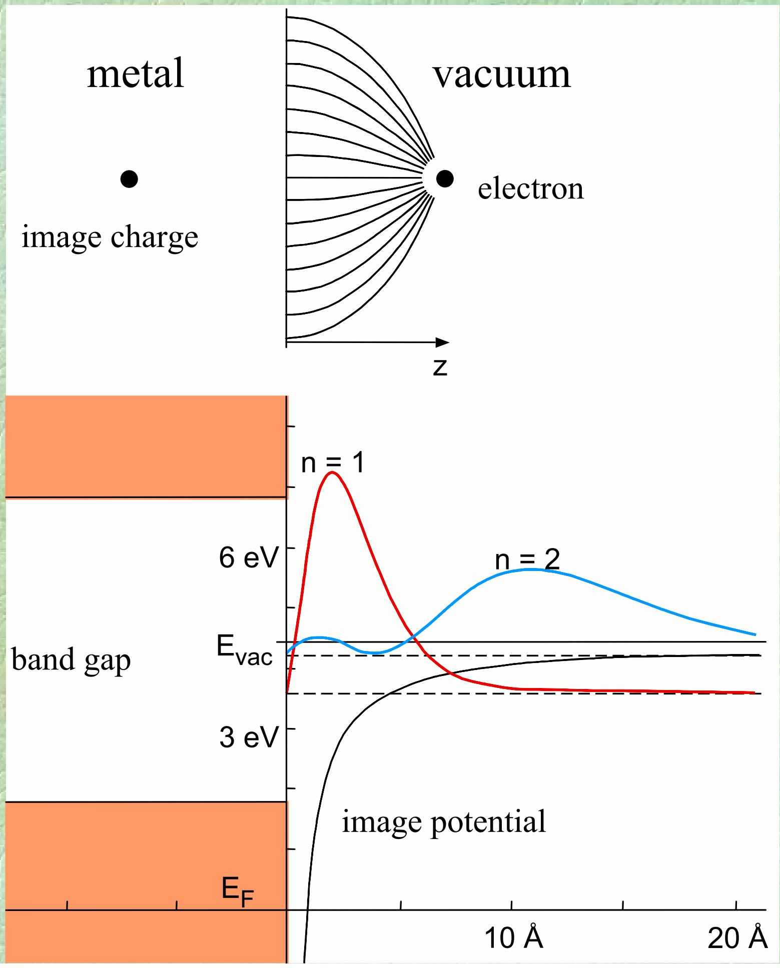


Image Potential States:

$E_B = 0.85 \text{ eV} / (n+a)^2$

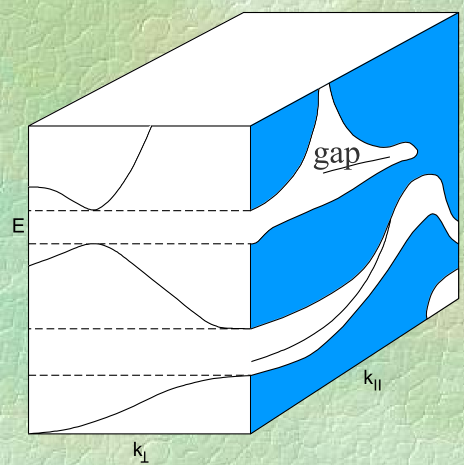
(hydrogen-like Rydberg Series, with 'quantum defect' a accounting for electron reflectivity at The metal surface)

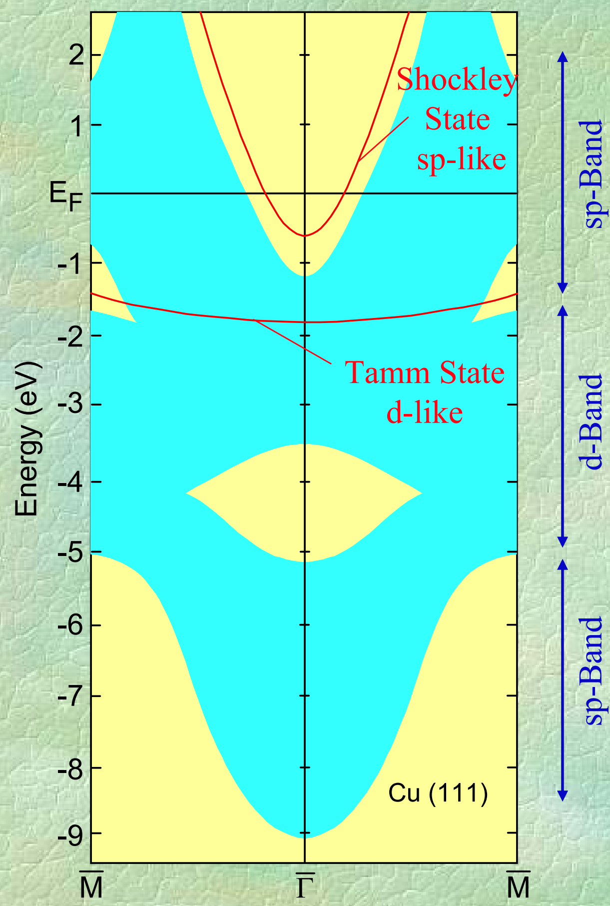
T. Fauster,
Appl. Phys. A 59, 63 (1994)

Where do surface states live in k space?

Experimental identification:

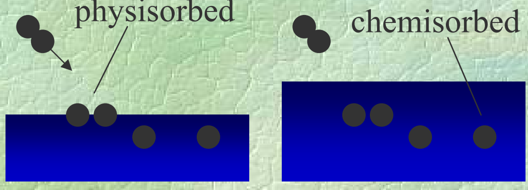
-"crud test" (sensitivity to adsorbates)
-no dispersion in k_{perp} (use synchrotron rad.)
-lives in projected band gap





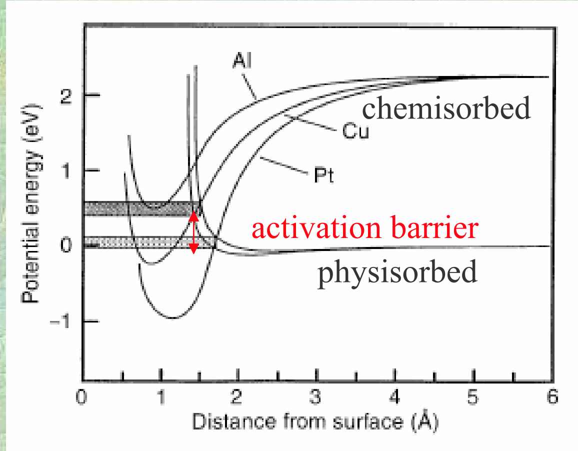
Are Surface States Important at All ?

Dissociative chemisorption:



Without S.S. With S.S.

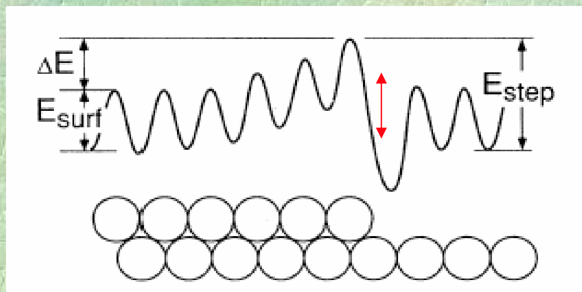
E. Bertel et al.,
Appl. Phys. A 63, 523 (1996)



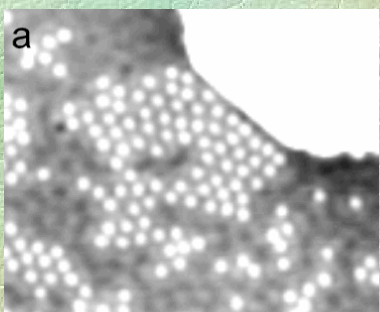
Surface Diffusion:

Schwöbl barrier is reduced by surface state !
⇒Adatoms can move across steps.
⇒Layer-by-layer growth of films

Memmel, Bertel, PRL 75, 485 (1995)

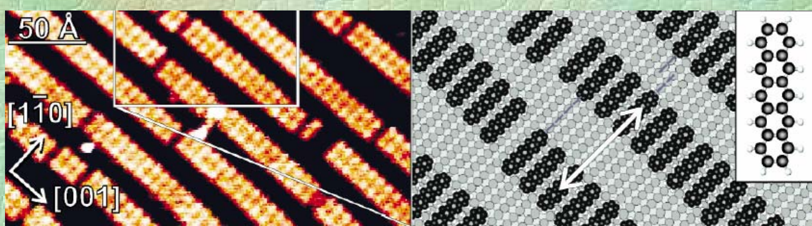


Surface state mediated long range interactions of adatoms and adsorbates



J. Repp *et al.*, PRL **85**, 2981 (2000)

Cu/Cu(111), T=15K:
Oscillatory interaction with $\lambda_F/2$=14Å

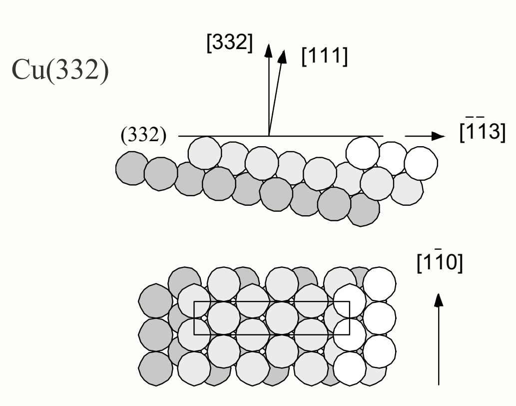


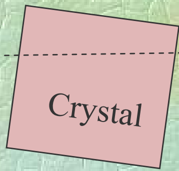
Pentacene, on Cu(110)

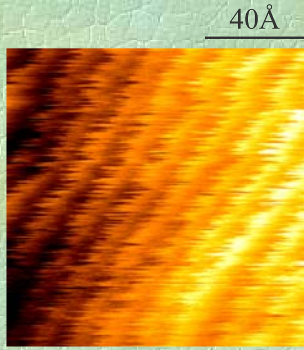
S. Lukas *et al.*, PRL **88**, 028301 (2002)

Courtesy F. Baumberger

Vicinal Cu(111) Surfaces

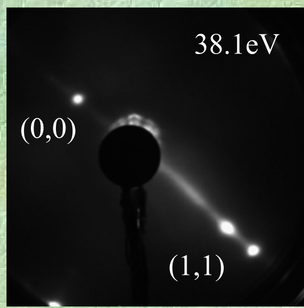






Scanning tunneling microscopy (STM), Cu(332)

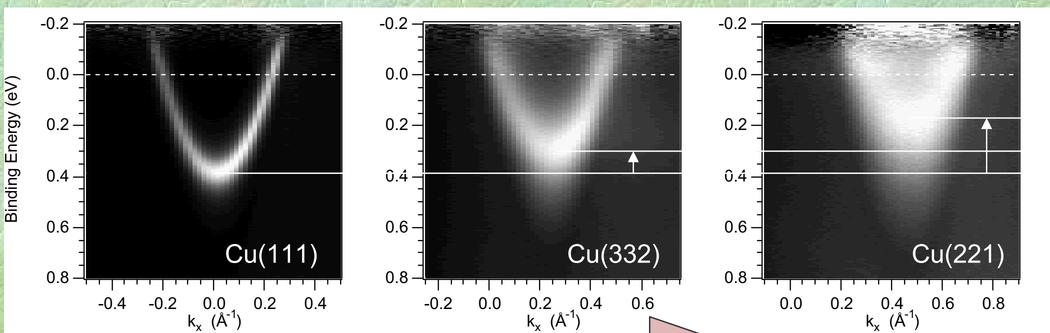
	Cu(112)	Cu(221)	Cu(332)	Cu(443)
α	19.5°	15.8°	10.0°	7.3°
ℓ	6.24Å	7.66Å	12Å	16.3Å
n	3	4	6	8



Low energy electron diffraction (LEED), Cu(332)

Neat way for nanostructuring surfaces !

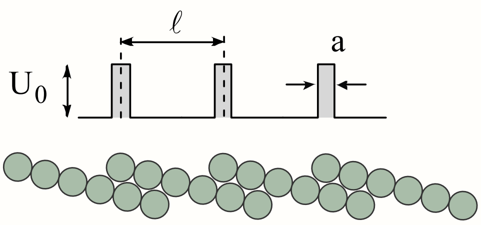
How does the electron gas react to the steps ?



Decreasing terrace width (l)

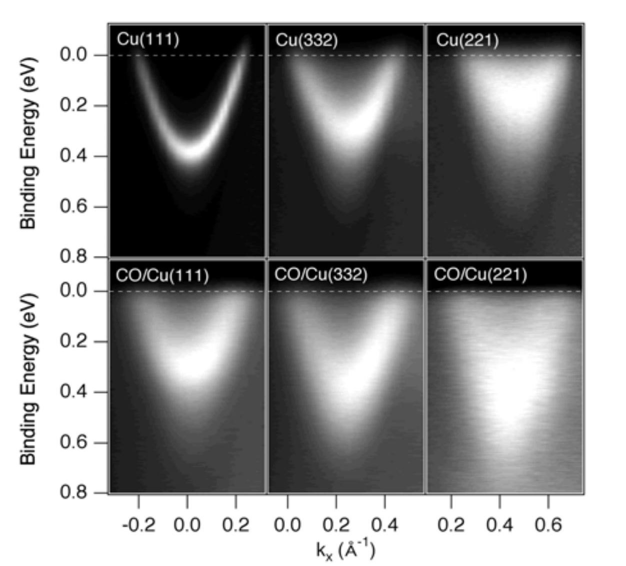
1D periodic potential: $\Delta E_B = \frac{U_0 a}{\ell}$

$U_0 a = 1.3$eVÅ



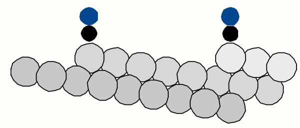
Steps act as potential barriers

Tailoring confining barriers: CO/vicinal Cu(111)

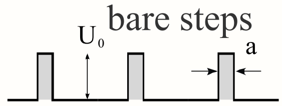


F. Baumberger et al.,
PRL **88**, 237601 (2002)

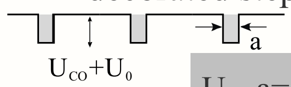
CO molecules decorate steps



bare steps

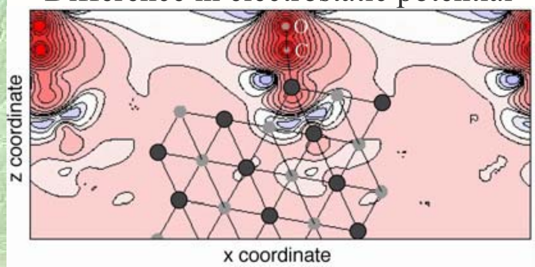


decorated steps

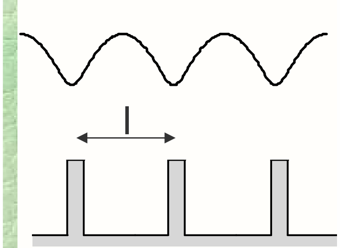


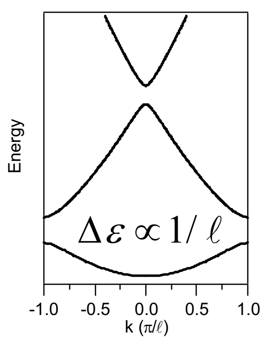
$U_{CO}a$=-2.9eVÅ

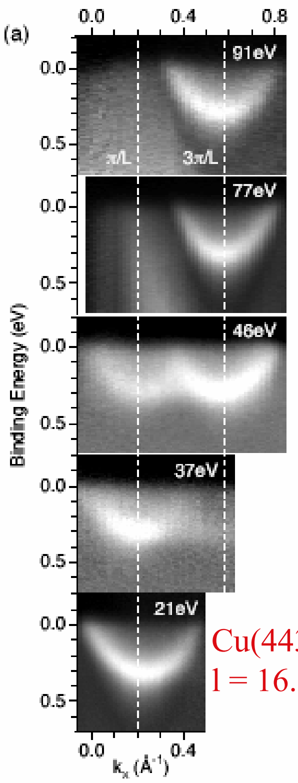
Difference in electrostatic potential



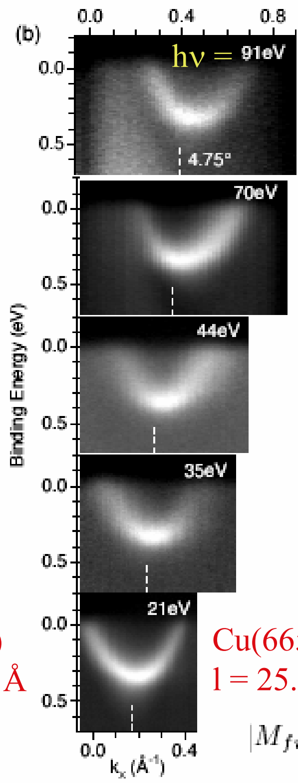
Periodic potential or decoupled quantum wells?



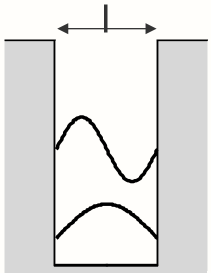


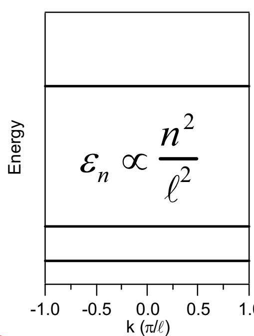


Cu(443)
l = 16.3 Å



Cu(665)
l = 25.2 Å

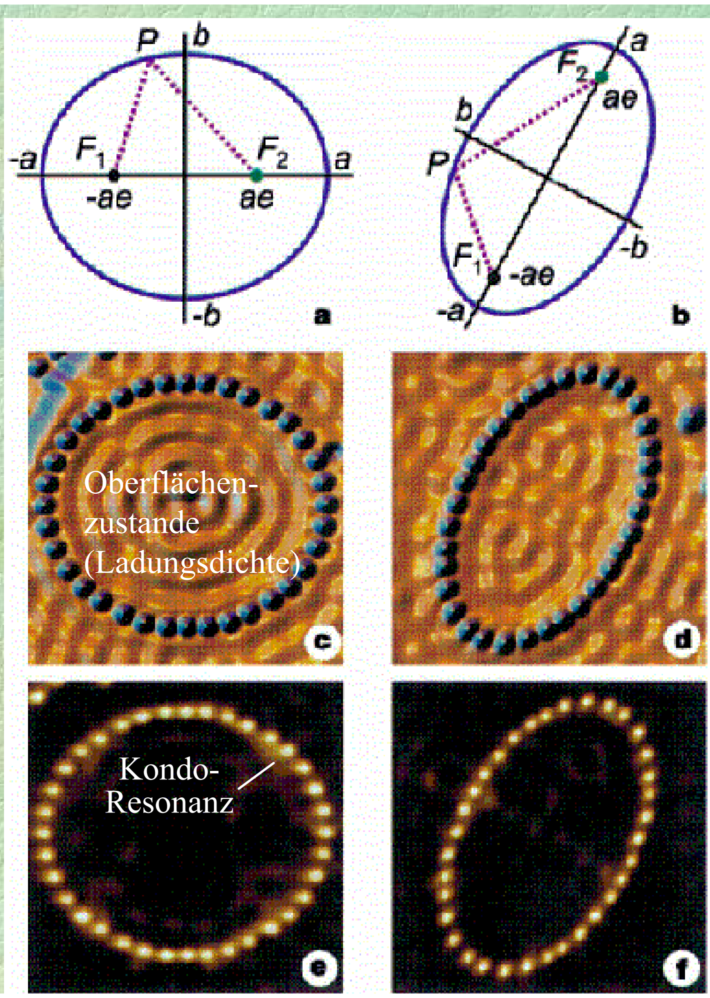




$$|M_{fi}|^2 \propto \frac{N^2}{L^3}\frac{1-(-1)^N\cos(k_x L)}{(k_x^2-(\pi N/L)^2)^2}$$

Photon energy (k_{perp}) dependence can unravel the character of the wave functions

Elliptical
"Quantum Corrals"
Prepared and Imaged
by a 4K STM



H. C. Manoharan, C. P. Lutz,
D. M. Eigler,
Nature 403 (2000) 512

Photoemission from Valence Bands, Dispersion and Fermi Surface Mapping

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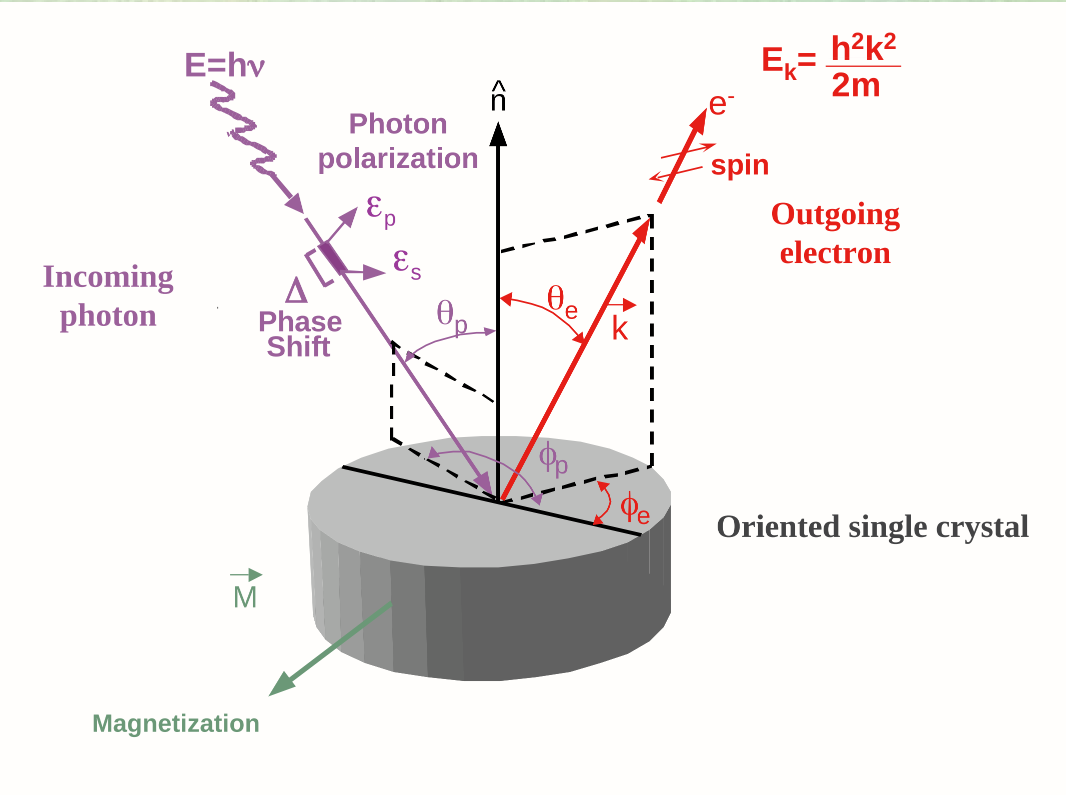
CH-8057 Zürich, Switzerland - osterwal@physik.unizh.ch
http://www.physik.unizh.ch/groups/grouposterwalder/

Lecture 2

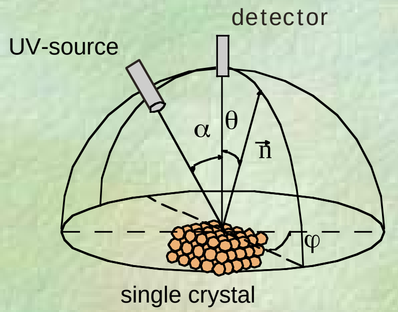
- Constant Energy Mapping in 3D Systems
- A Few Words about the Fermi Surface in General
- 3D Examples for Fermi Surface Mapping: Cu, Al
- The Fermi Surface of Ni: Case of an Itinerant Ferromagnet
- The Magnetic Phase Transition in Ni: More Details

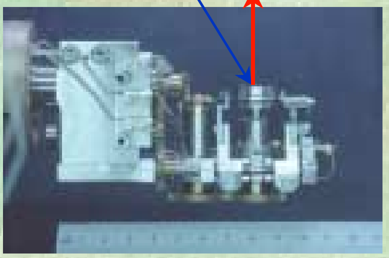
The photoemission experiment

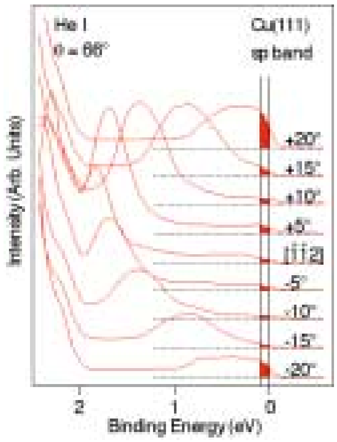


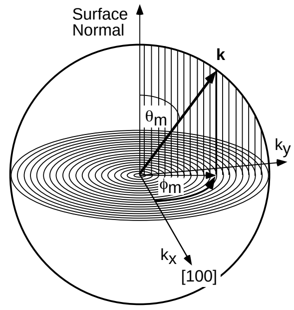
Courtesy G. Paolucci

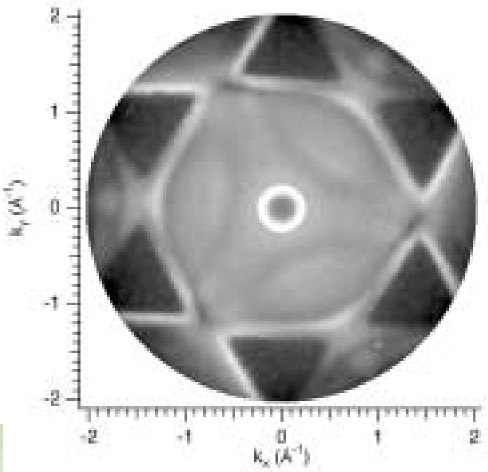
Fermi Surface Mapping by Photoemission



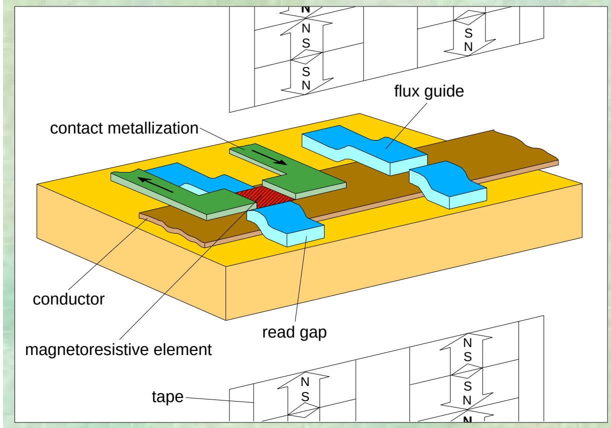








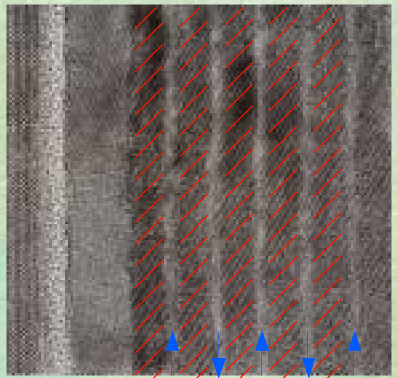
Magnetic Read Heads Based on Giant Magneto-Resistance in Magnetic Multilayers

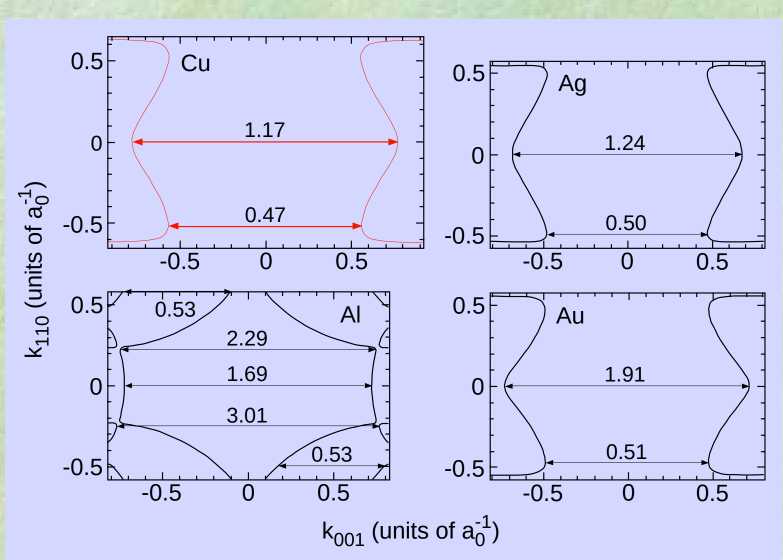


PHYSICAL REVIEW B VOLUME 48, NUMBER 10 1 SEPTEMBER 1993-II

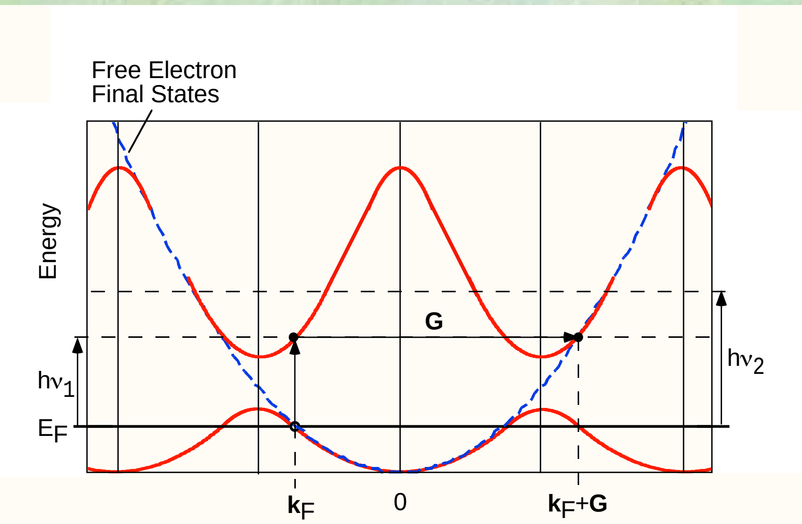
Exchange coupling in magnetic heterostructures

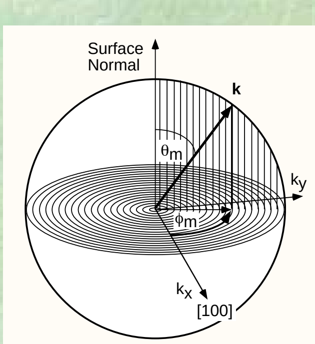
M. D. Stiles
National Institute of Standarts and Technology, Gaithersburg, Maryland 20899
(Received 3 May 1993)





Direct Transitions from the Fermi Surface





$$E_{kin}^{m} = h\nu - \Phi - E_B$$

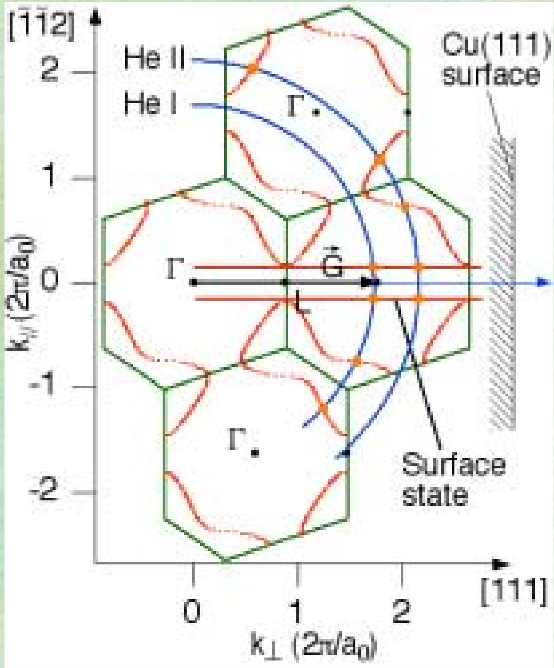
$$|\vec{k}_{||}| = \frac{1}{\hbar}\sqrt{2mE_{kin}^{m}}\sin\theta_m$$

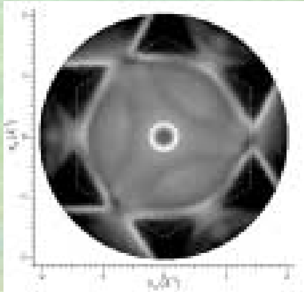
$$k_{\perp} = \frac{1}{\hbar}\sqrt{2m(E_{kin}^{m} + V_0)}\cos\theta_m$$

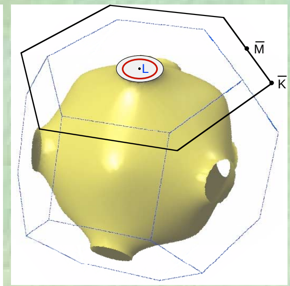
Refraction: $\sin\theta = \sin\theta_m\sqrt{\frac{E_{kin}^{m}}{(E_{kin}^{m}+V_0)}}$

Fermi surface mapping

Section along (1$\bar{1}$0) plane in reciprocal space







In the photoemission process:

Energy conservation:

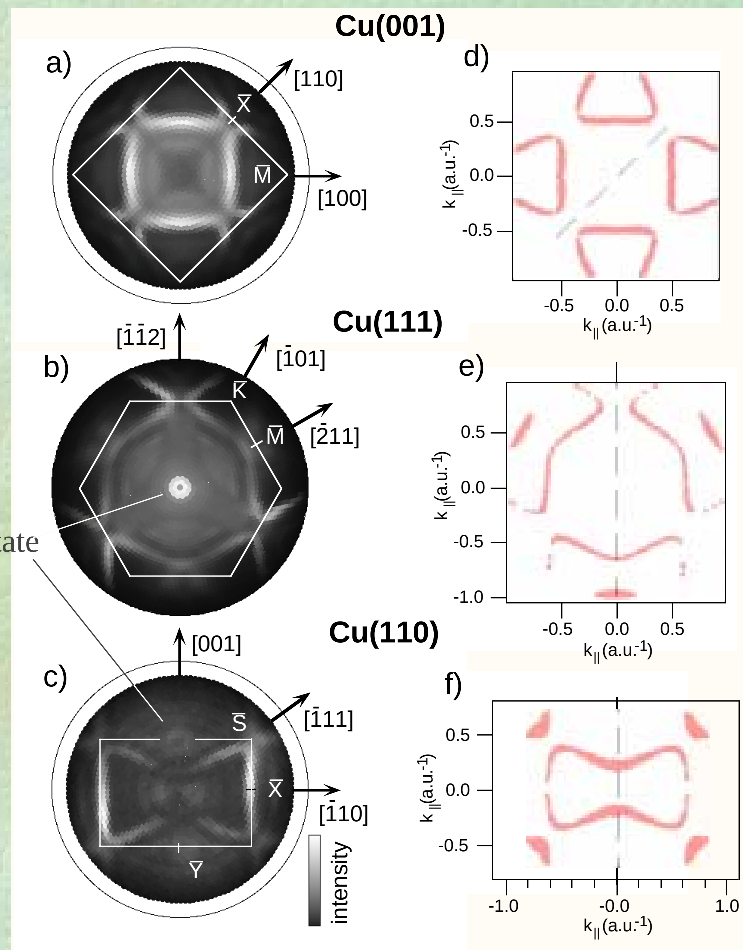
$$E_f = E_i + h\nu$$

Momentum conservation:

$$\vec{k}_f = \vec{k}_i + \vec{G}$$

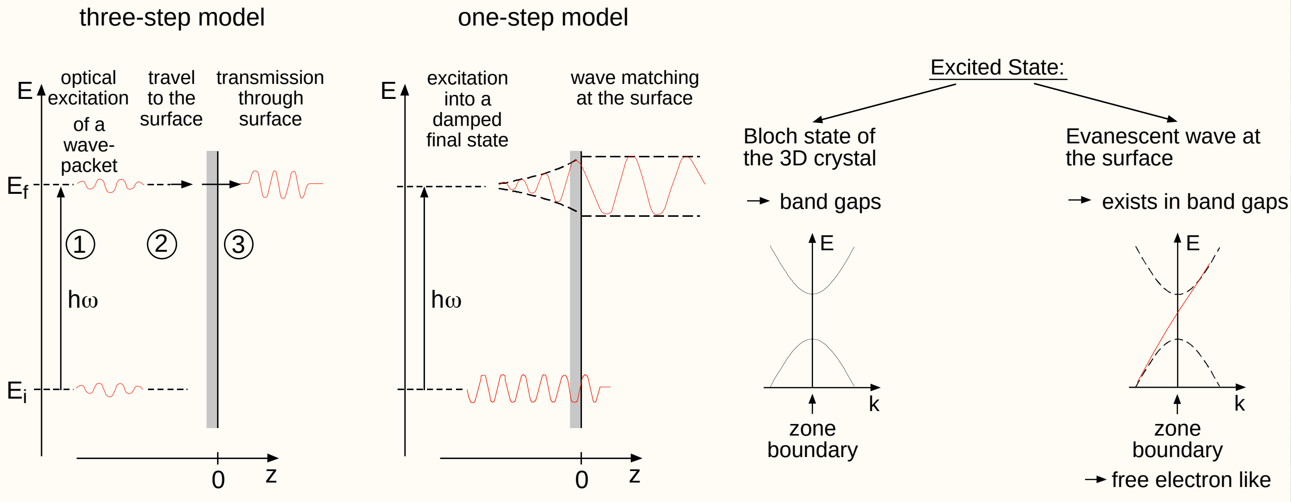
P. Aebi et al. Surf. Sci. 307-309, 917 (199

Comparison of Measured Fermi Surface Maps to Calculaded Fermi Surface Sections

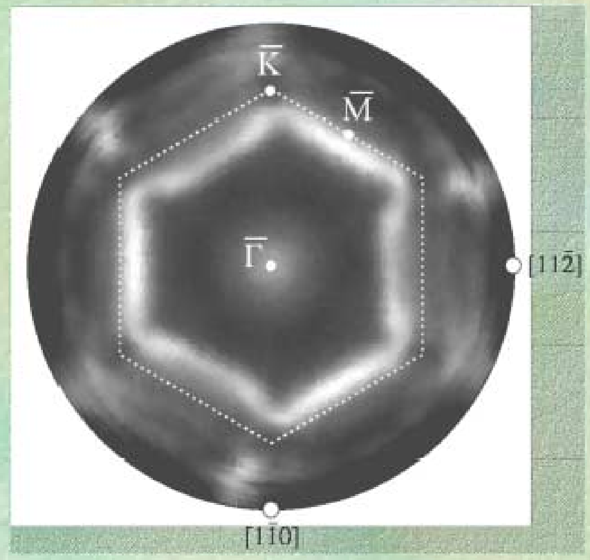


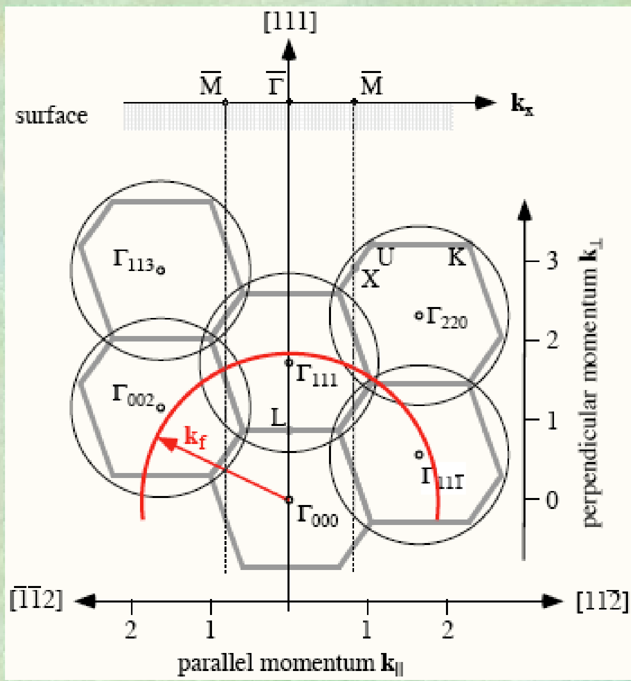
Calculations done with the Wien2k band structure code, assuming the structure of bulk Cu.

Comments on the Free Electron Final State



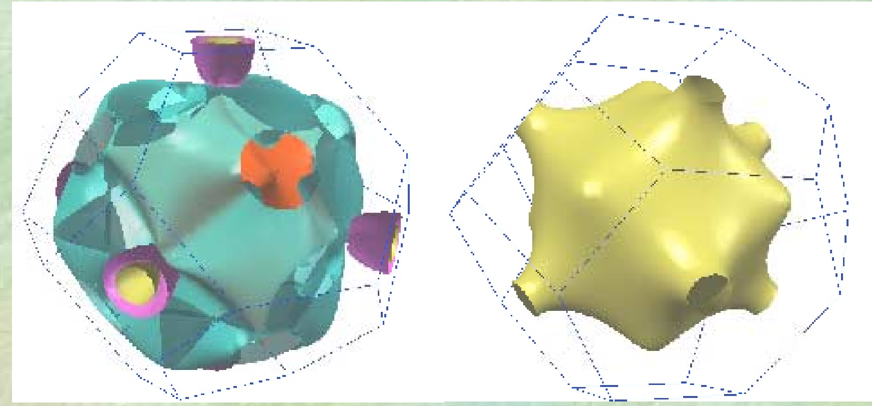
The Fermi Surface of Aluminium

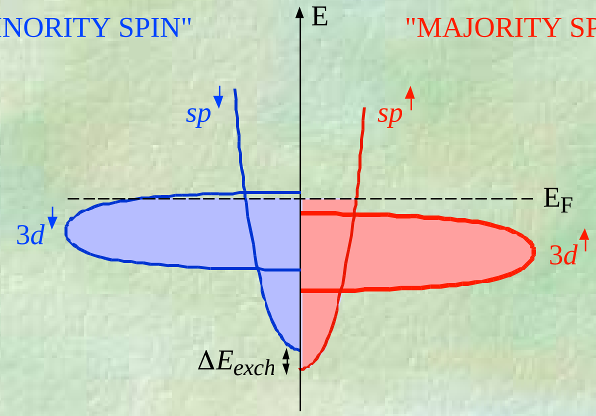




Courtesy R. Fasel

The Two Fermi Surfaces of Nickel Metal





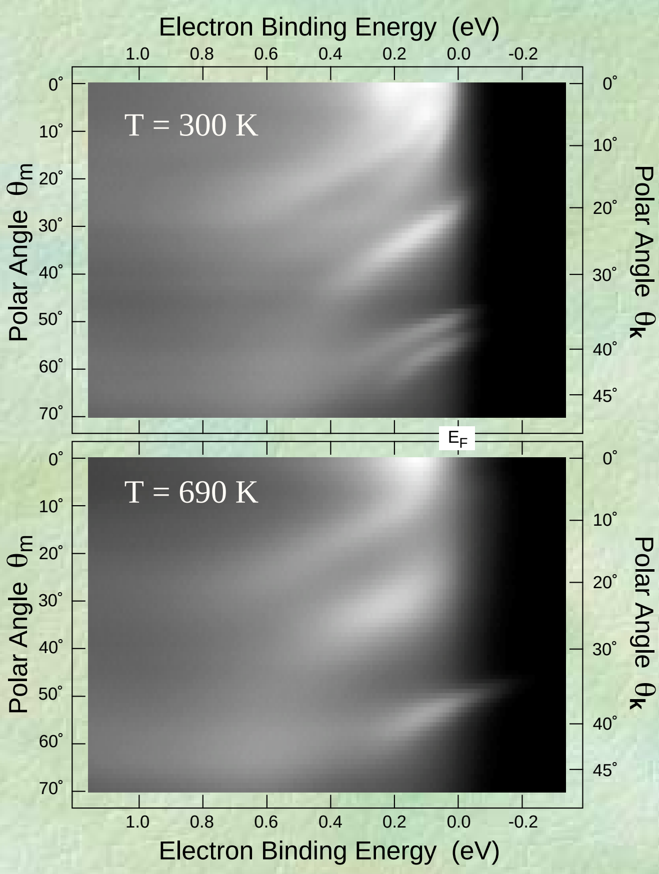
Schematic
Density of States

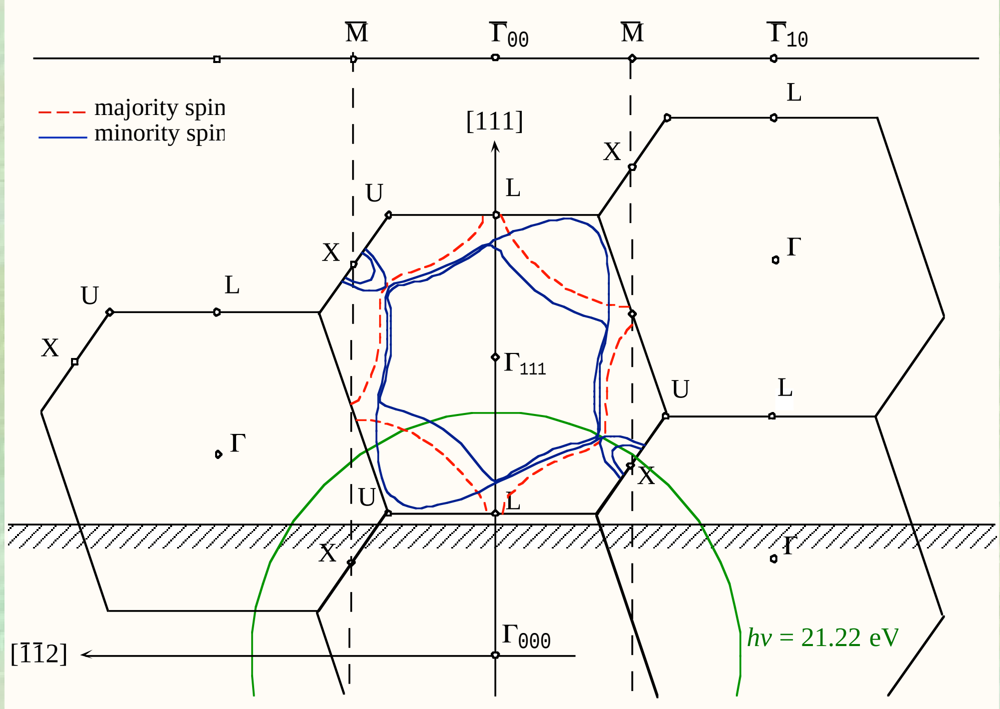
Monitoring the Magnetic Phase Transition

T_c = 631 K

Question:
How does the band structure change when nickel goes from the ferromagnetic to the paramagnetic state ?

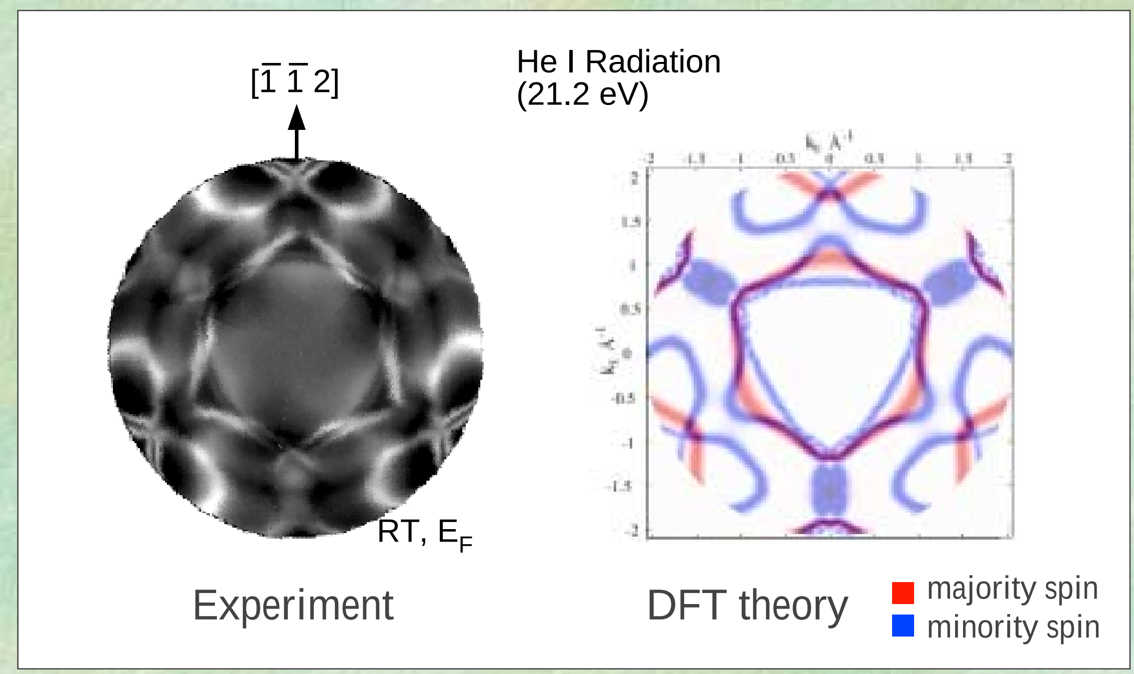
Answer:
Magnetic exchange splittings disappear

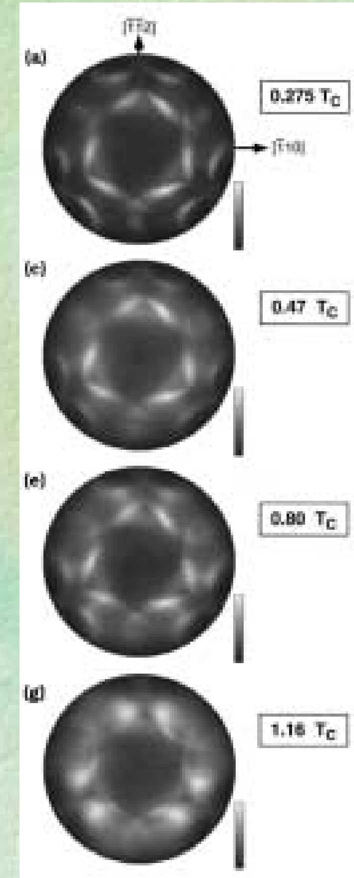




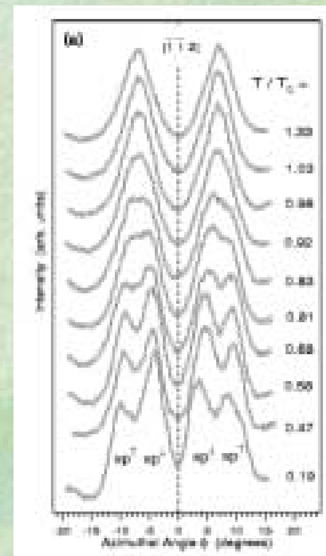
Fermi surface calculation (density functional theory, Wien 97)

FermiSurface of Ni as Seen Through the Ni(111) Surface

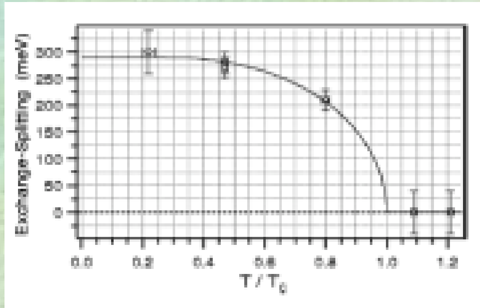




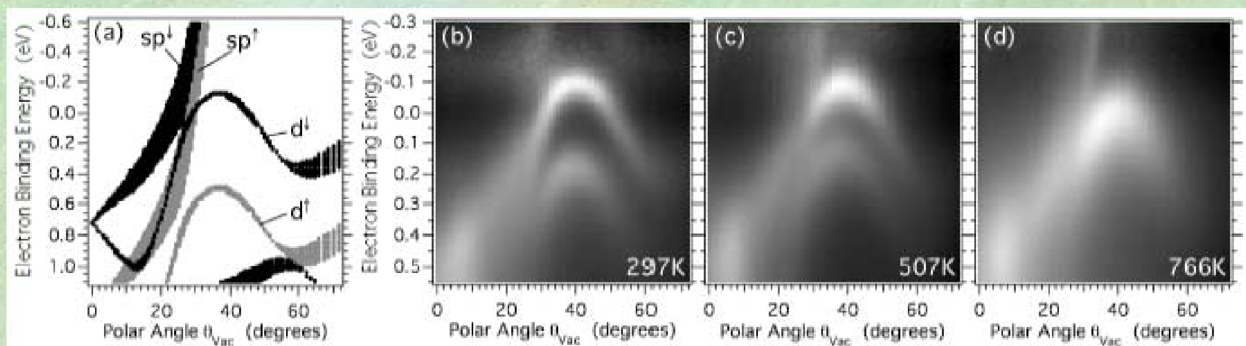
Evolution of the Fermi Surface During the Phase Transition



… and quantifying the exchange splitting:

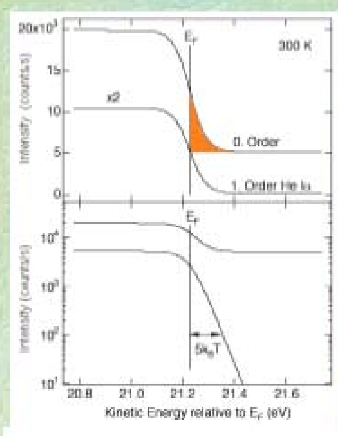


Observing the Magnetic Exchange Splitting in the d Band

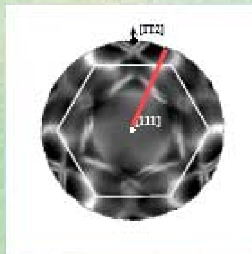


Photoemission above the Fermi Level ?

T. Greber et al., PRL 79, 4465 (1997)

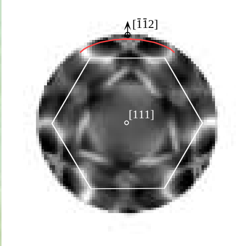


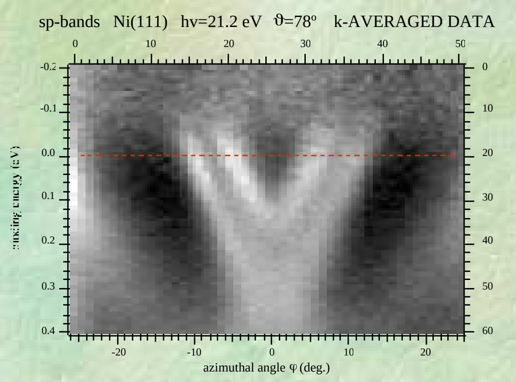
Polar Scan

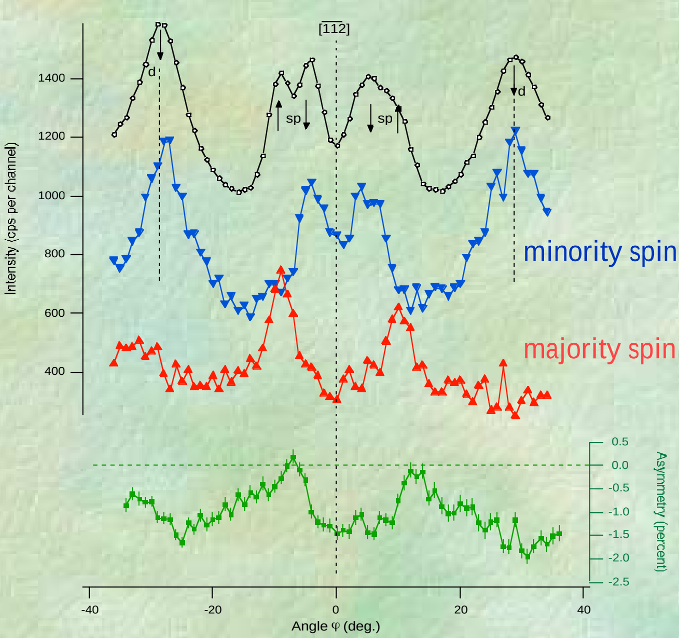


Spin-Resolved Fermi Surface Mapping

Azimuthal Scan







... a new, spin-resolved spectrometer

M. Hoesch et al., JES 124, 263 (2002)

School on Synchrotron Radiation and Applications, ICTP Trieste, May 3-6, 2004

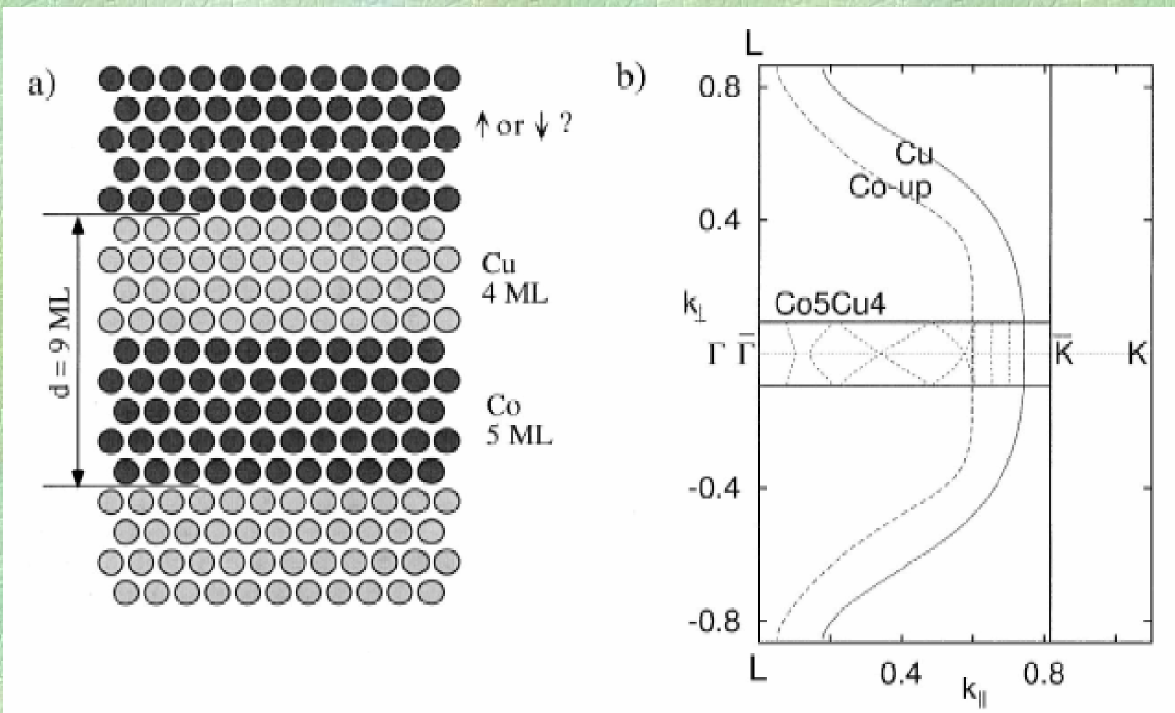
Photoemission from Valence Bands, Dispersion and Fermi Surface Mapping

Jürg Osterwalder
Physik-Institut, Unversität Zürich, Winterthurerstr. 190,
CH-8057 Zürich, Switzerland - osterwal@physik.unizh.ch
http://www.physik.unizh.ch/groups/grouposterwalder/

Lecture 3

- Fermi Surface Mapping with Spin Resolution: Design of a New Spectrometer
- Spin-Resolved Fermi Surface Contours in Nickel
- Spin-Orbit-Split Surface State on Au(111)
- Ultrathin Films of Ni on Cu(001)
- Intensities in Valence Photoemission: Polarization Effects
- Intensities in Valence Photoemission: Atomic Effects
- Intensities in Valence Photoemission: Diffraction Effects

Magnetic Bandstructure in Multilayered Films



Band folding along k_{perp} leads to a multitude of bands!

Spin-Resolved Fermi Surface Mapping

Problem:
Sample rotation over 2π => rotation of the magnetization over 2π

=> need a 3D spin polarimeter !

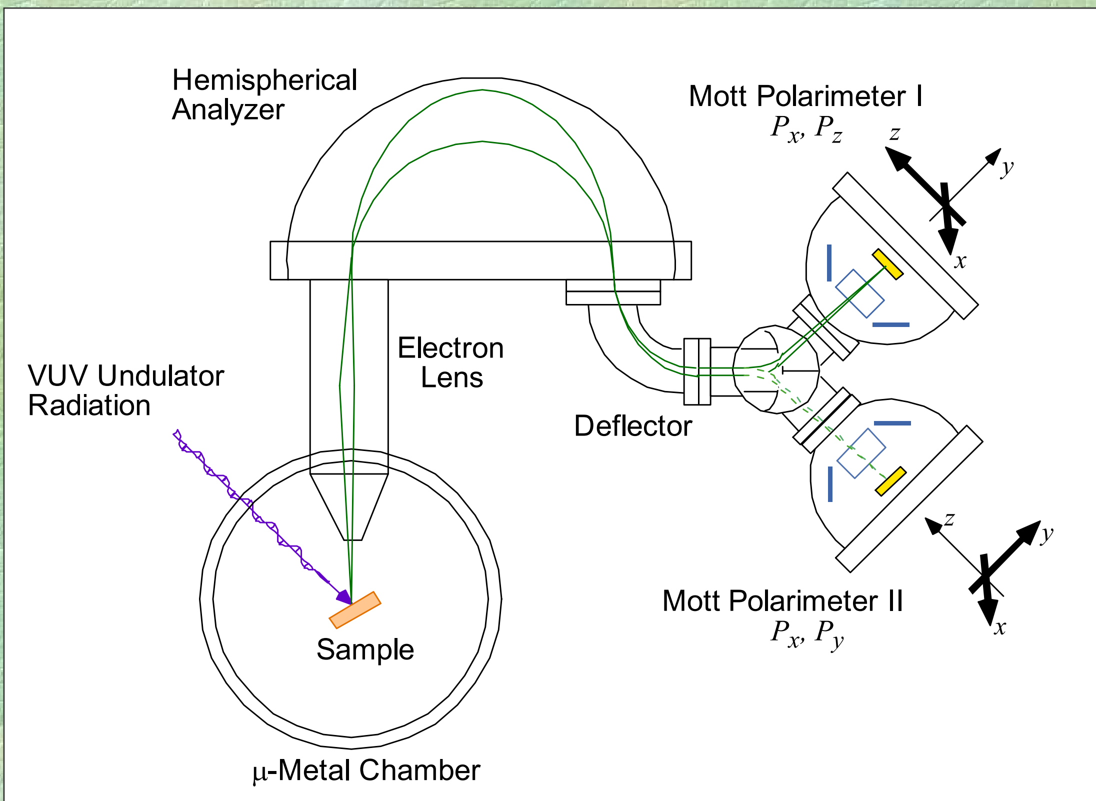
COPHEE: the complete photoemission experiment

...measures all properties of the photoelectron:

- energy
- momentum (~ 3D, at the SLS !)
- spin (3D)

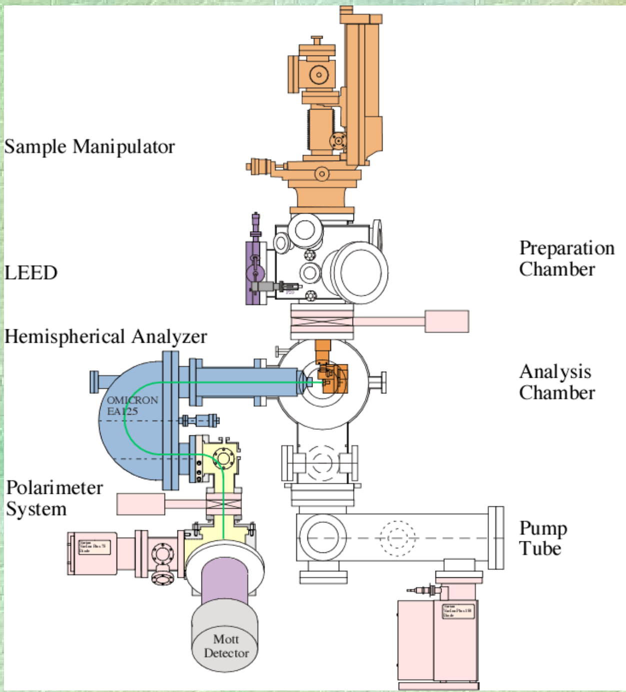
... controlled by CROISSANT software !

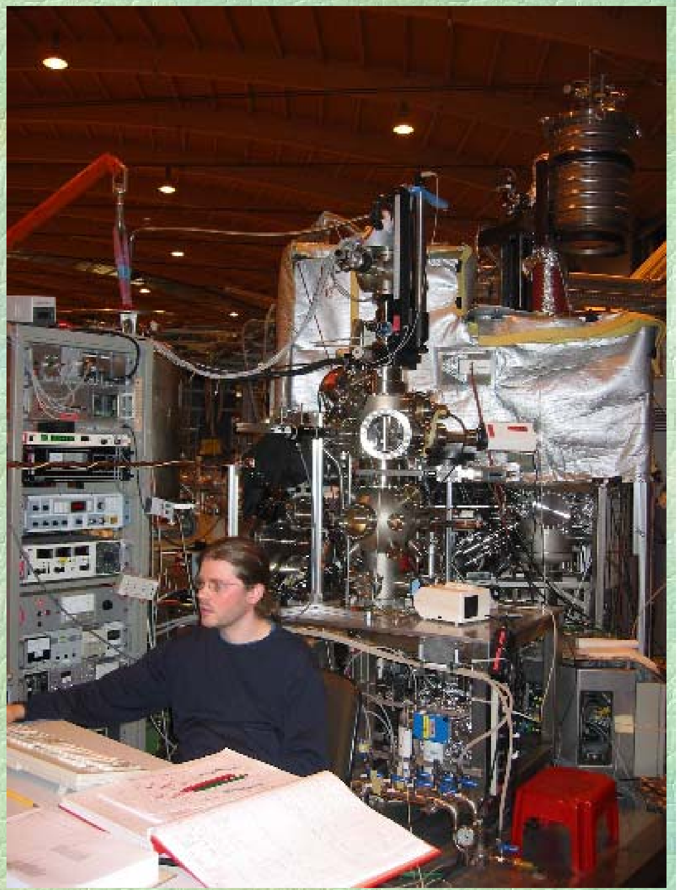
COPHEE - The Complete Photoemission Experiment



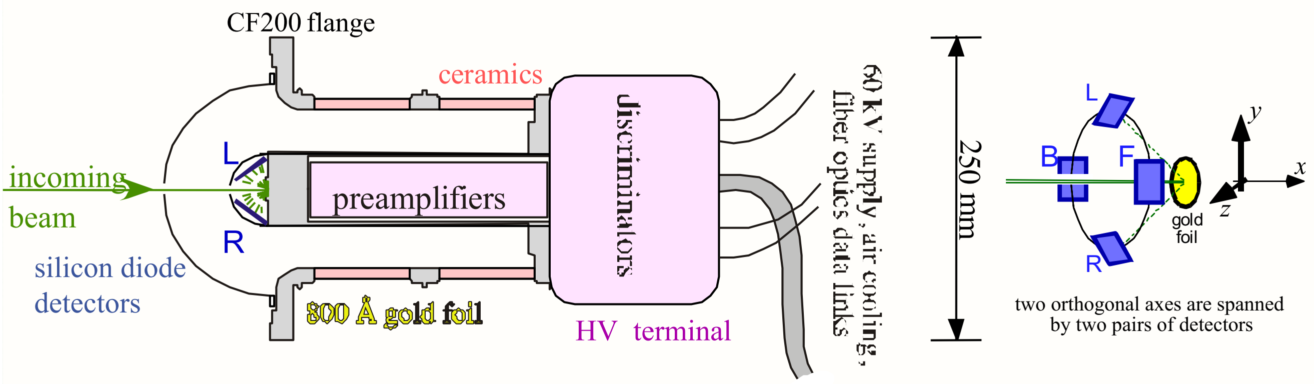
M. Hoesch, Ph. D. Thesis, 2002

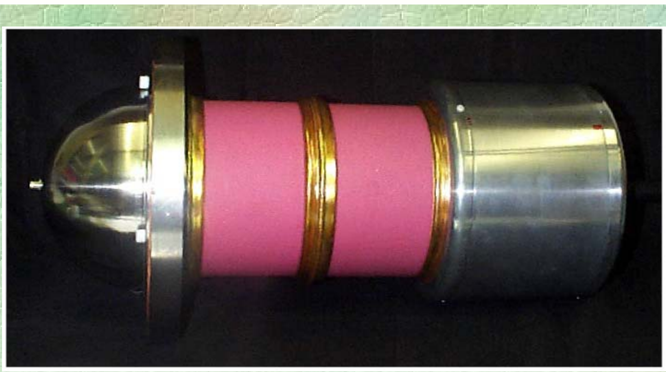
Setup of COPHEE:





The 60 keV Mott Detector





asymmetry $A = \frac{(N_L - N_R)}{(N_L + N_R)}$

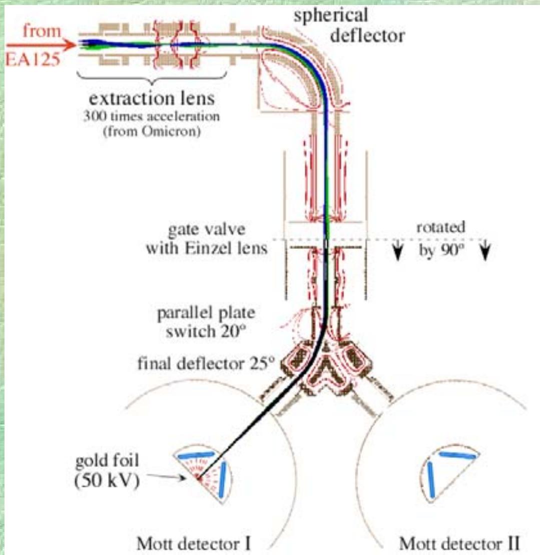
electron polarization $P = \frac{A}{S}$

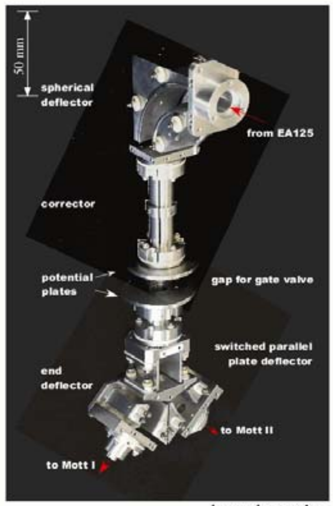
S = "Sherman function" (analyzing power)

Backscattering at high energies:
Very inefficient process (~10^{-3})

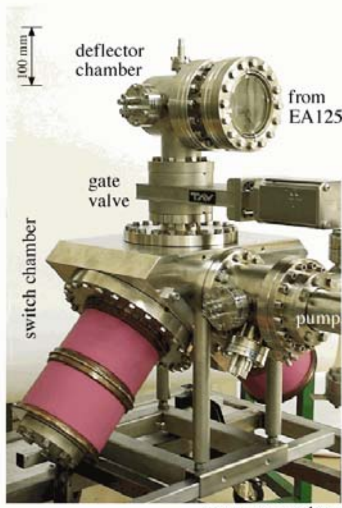
V. N. Petrov et al., RSI 72, 3729 (2001)

The Transfer / Distributor Lens





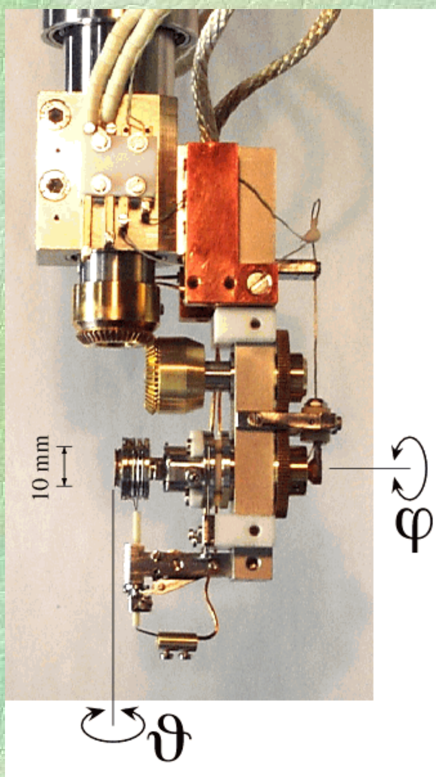
lens electrodes



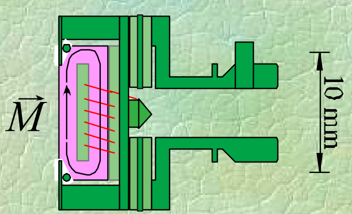
vacuum envelope

M. Hoesch et al., JES 124, 263 (2002)

Goniometer Head of the Sample Manipulator



- 2 axis rotation
- liquid He cooling (60 K)
- contacts for heating and magnetizing
- sample transfer to preparation facilities



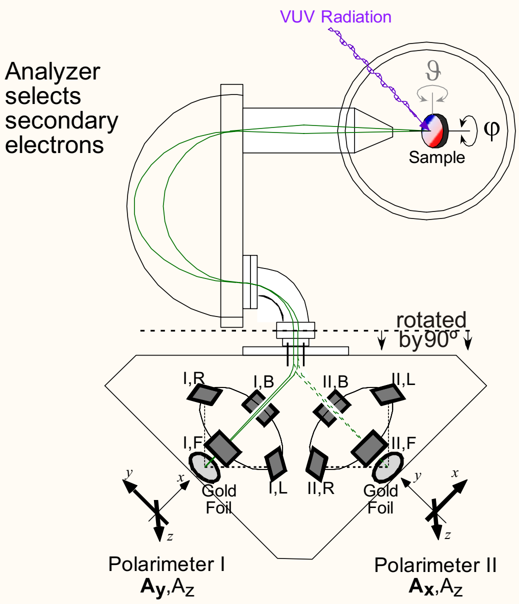
Swiss Stub sample holder with picture frame sample

Nickel sample with the filament for DC resistive heating and pulsed current magnetising remanence ~30%

Secondary electron polarimetry

Courtesy M. Hoesch

secondary electrons from a magnetized sample are polarized along the magnetization direction (M. Landolt *et al.* 1985)



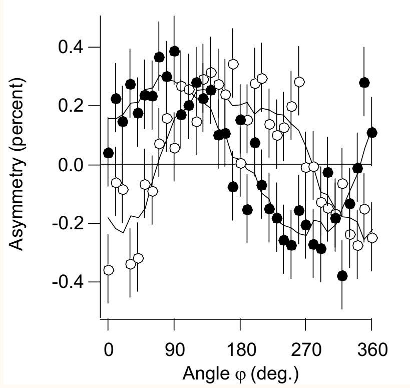
$A_x^{(S)} = \frac{1}{\sqrt{2}} [(\cos\varphi - \sin\varphi) A_x - (\cos\varphi + \sin\varphi) A_y]$

$A_y^{(S)} = \frac{1}{\sqrt{2}} [(\cos\varphi + \sin\varphi) A_x - (\cos\varphi - \sin\varphi) A_y]$

Measured asymmetries

$A_x = \circ$, $A_y = \bullet$

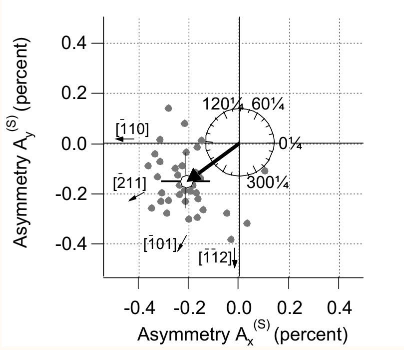
(detector coordinates)



Reconstructed asymmetries

$(A_x^{(S)}, A_y^{(S)})$ = ⬢

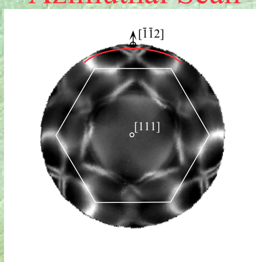
(sample coordinates)

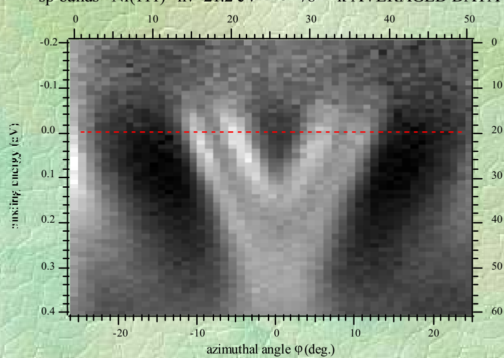


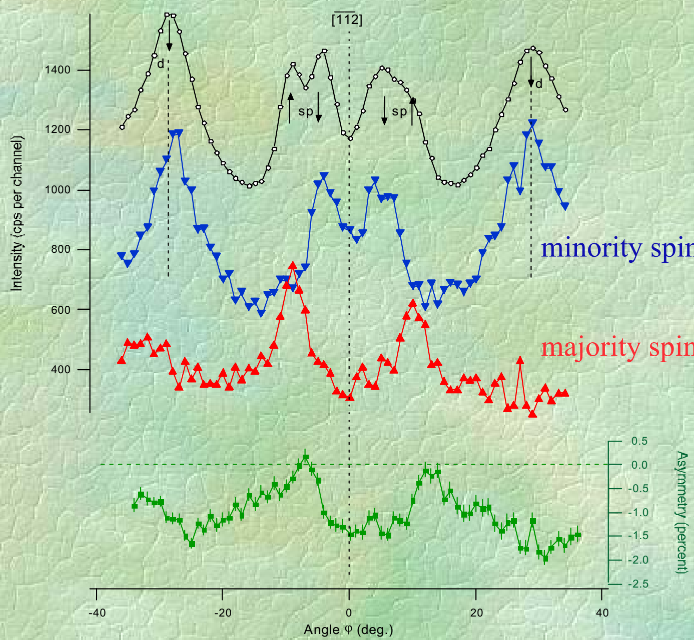
=> vectorial sensitivity !

Spin-Resolved Fermi Surface Mapping

Azimuthal Scan





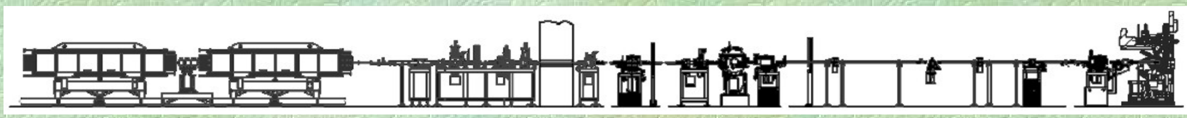


... a new, spin-resolved spectrometer

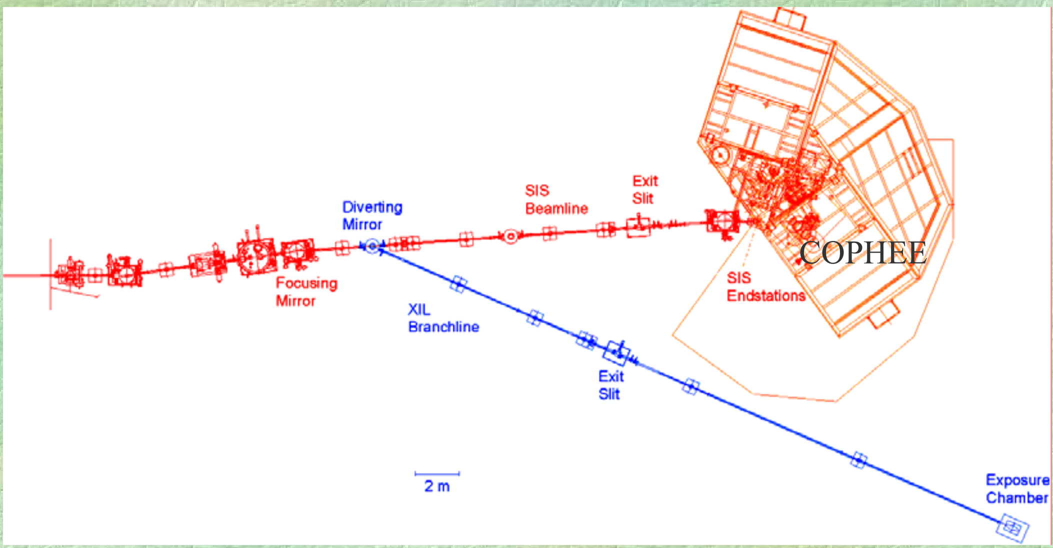
M. Hoesch et al., JES 124, 263 (2002)

Surfaces/Interfaces: Spectroscopy beamline (SIS) at the Swiss Light Source (SLS)

Side view:



Twin UE212 Optics Spectrometers



Courtesy L. Patthey / SLS

COPHEE at the SIS beamline

⇒ Access to very interesting photon beam properties

- small light spot on sample => high energy resolution with Omicron EA125 !
- photon energy range: k-space mapping (ARPES) and also core level spectroscopy (incl. XPD)
- fast polarization switching (future) => dichroism with spin detection
- clean photons (low background in quasiperiodic mode) => photoemission of thermally excited electrons

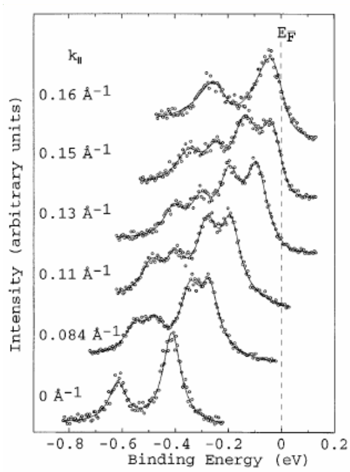
First taste: the surface state on Au(111)

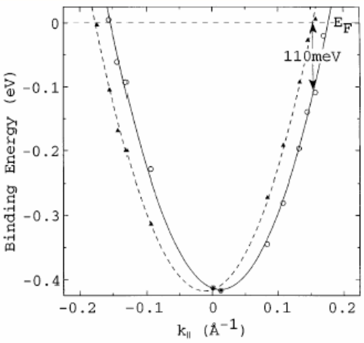
The Spin-Orbit Split Surface State on Au(111)

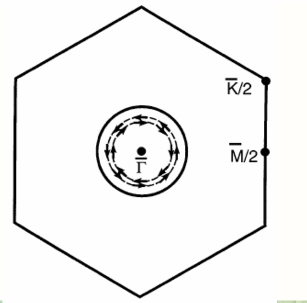
VOLUME 77, NUMBER 16 PHYSICAL REVIEW LETTERS 14 OCTOBER 1996

Spin Splitting of an Au(111) Surface State Band Observed with Angle Resolved Photoelectron Spectroscopy

S. LaShell, B. A. McDougall, and E. Jensen
Physics Department, Brandeis University, Waltham, Massachusetts 02254
(Received 19 July 1996)





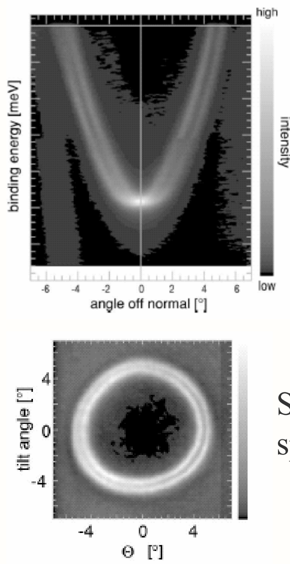


hν=11.62eV

PHYSICAL REVIEW B, VOLUME 63, 115415

Direct measurements of the *L*-gap surface states on the (111) face of noble metals by photoelectron spectroscopy

F. Reinert,* G. Nicolay, S. Schmidt, D. Ehm, and S. Hüfner
Fachrichtung Experimentalphysik, Universität des Saarlandes, 66041 Saarbrücken, Germany
(Received 6 October 2000; published 1 March 2001)



Scienta 2002 spectrometer

hν=21.21eV

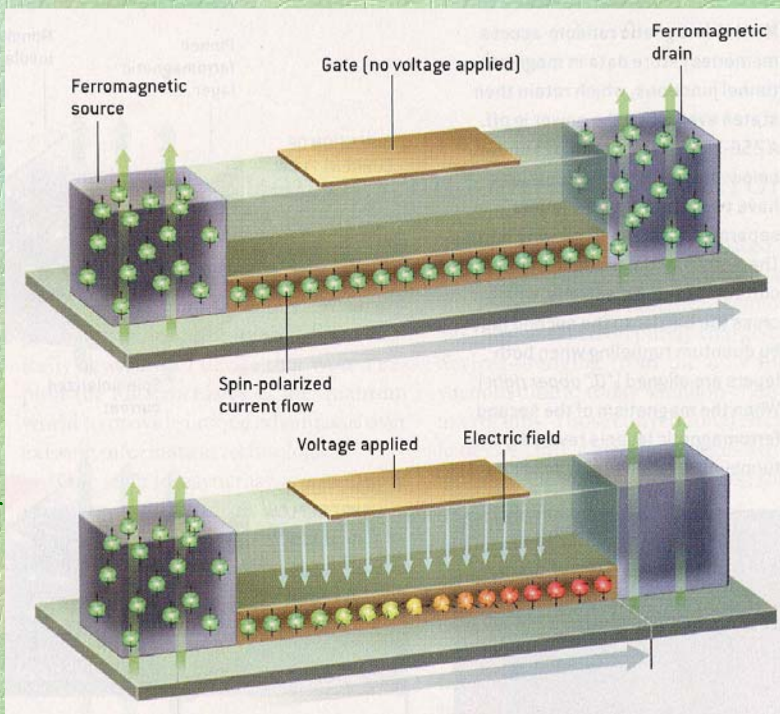
=> spin-resolution is a challenging task

The Spin Field Effect Transitor (spin FET)

Principle – electric field from gate causes spins to precess. Channel impedance depends of extent of spin rotation

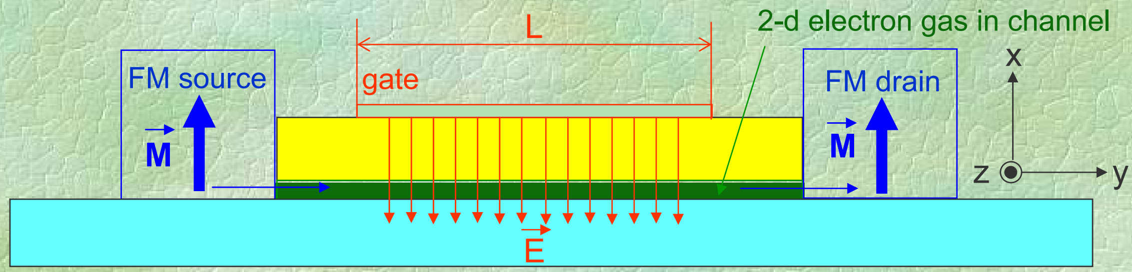
Advantage – much less energy and time required to flip spins than to depopulate channel

Problem – has yet to be built due to lack of suitable spin injectors for III-Vs and Si. Ferromagnetic semiconductors are best due to conductivity match. Need high T_c DMS materials!



S. Datta & B. Das,
Appl. Phys. Lett. 56, 665 (1990)

Spin precession in an electric field (?)



Spin-orbit interaction: $\boldsymbol{H}_{SO} \sim (\vec{E} \times \vec{k}) \bullet \vec{\sigma}$ (Rashba term)

In the channel: $\boldsymbol{H}_{SO} \sim k_y \sigma_z$

Source: injects spins with $|s_x\rangle = |-1/2\rangle$

In rotated frame: $|s_z\rangle = 1/\sqrt{2}\,|-1/2\rangle + 1/\sqrt{2}\,|+1/2\rangle$

$E(|+1/2\rangle) = E_{kin} + \alpha\, k_y$
$E(|-1/2\rangle) = E_{kin} - \alpha\, k_y$

$E = E_F \Rightarrow k_{F(\Uparrow)} - k_{F(\Downarrow)} = 2m^*\alpha/\hbar^2$

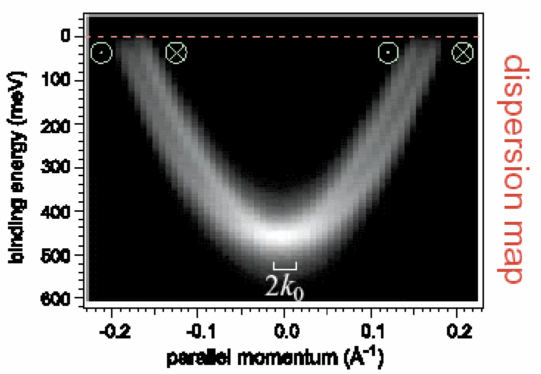
$\Rightarrow$ Phase shift $\Delta\phi = (k_{F(\Uparrow)} - k_{F(\Downarrow)})L = (2m^*\alpha/\hbar^2)L$

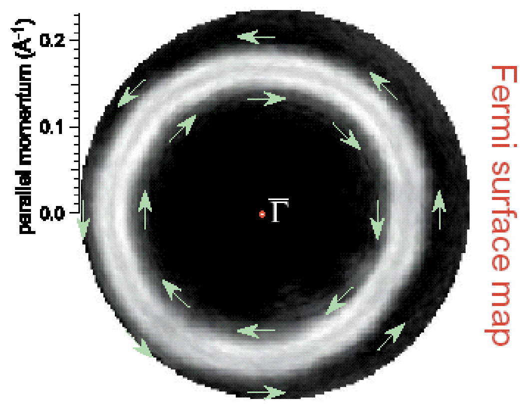
$\Rightarrow$ Spin precession around z axis !

The Shockley surface state on Au(111)

spin-integrated photoemission at $h\nu$ = 21.1 eV, T = 160 K

instrumental resolution
ΔE = 25 meV, $\Delta\vartheta$ = 0.5° (FWHM)





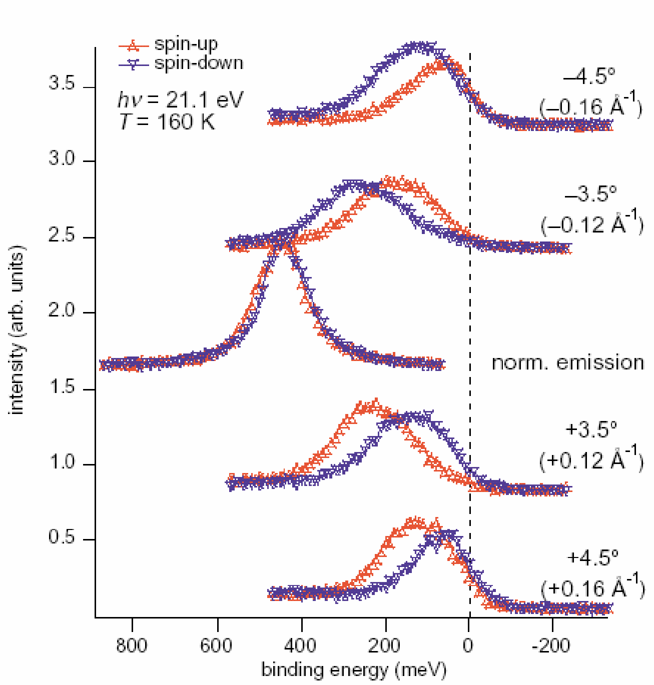
$2k_0 = 0.026$ Å^{-1}	$E_B = 470$ meV	$k_F = 0.173$ Å$^{-1} \pm k_0$	$m^* = 0.24\, m_e$

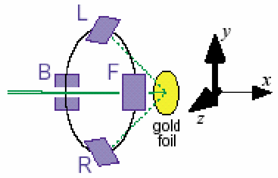
Theory: spin-orbit coupling

$$H_{SOC} = \frac{\mu_B}{2c^2}(\vec{v} \times \vec{E}) \cdot \vec{\sigma}$$

$$E^{\uparrow\downarrow}(k) = E_0 + \frac{(k \pm k_0)^2}{2m^*}$$

Spin-resolved spectra of the surface state on Au(111)





Mott scattering spin detector

asymmetry $A = \frac{(N_L - \eta \cdot N_R)}{(N_L + \eta \cdot N_R)}$

electron polarization $P = \frac{A}{S}$

Intensities $I^{\uparrow\downarrow} = I_0 \cdot (1 \pm P)$

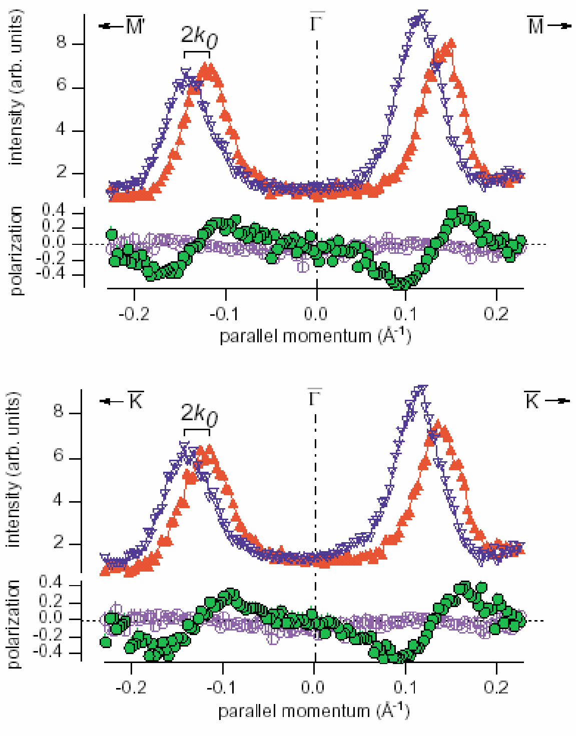
parameters for analysis:

η = Correction of detection efficiency (instrumental asymmetry)

S = "Sherman function" (analyzing power)

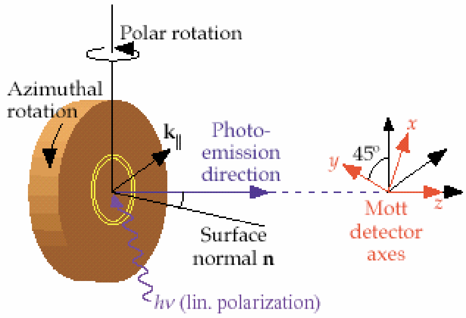
instrumental resolution
ΔE=120 meV, Δϑ=1.8° (FWHM)

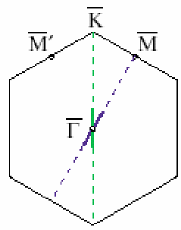
Spin-resolved momentum distribution curves of the surface state on Au(111)



spin-up intensity
spin-down intensity
in-plane polarization
out-of-plane polarization

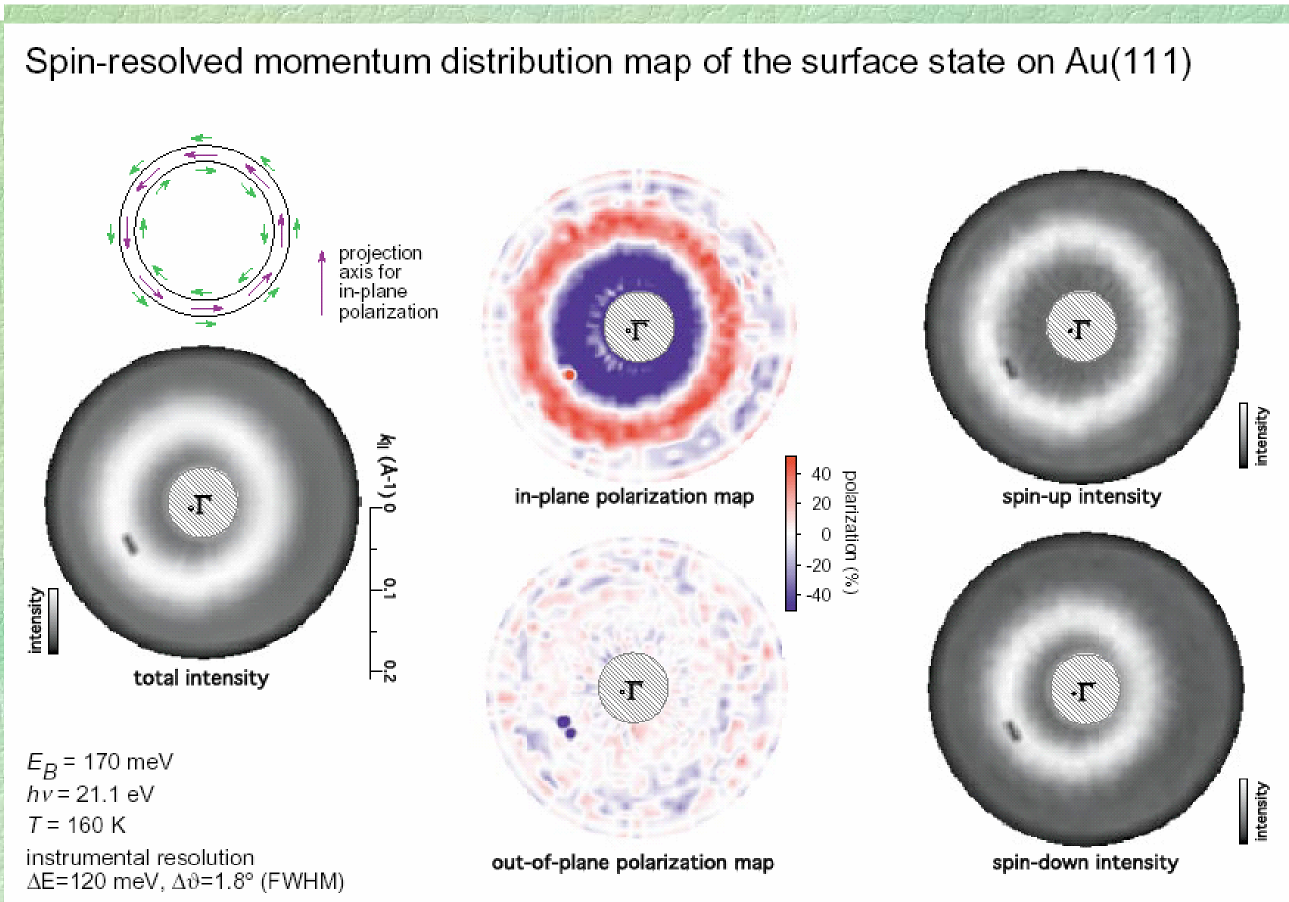
E_B = 170 meV
$h\nu$ = 21.1 eV
T = 160 K





Surface Brillouin zone

instrumental resolution
ΔE=120 meV, Δϑ=1.8° (FWHM)



=> First spin-resolved "Fermi surface" map

Ultrathin Films of Ni on Cu(001)

- grows epitaxially
- well ordered films
- T_c depends on film thickness
- bulk-like Fermi surface already at 1 ML (G. J. Mankey et al., PRL 78, 1146 (1997))
- Full 3d magnetic moment reached only at 6 ML (P. Srivastava et al., PRB 56, R4398 (1997))

Universität Zürich
Physik-Institut

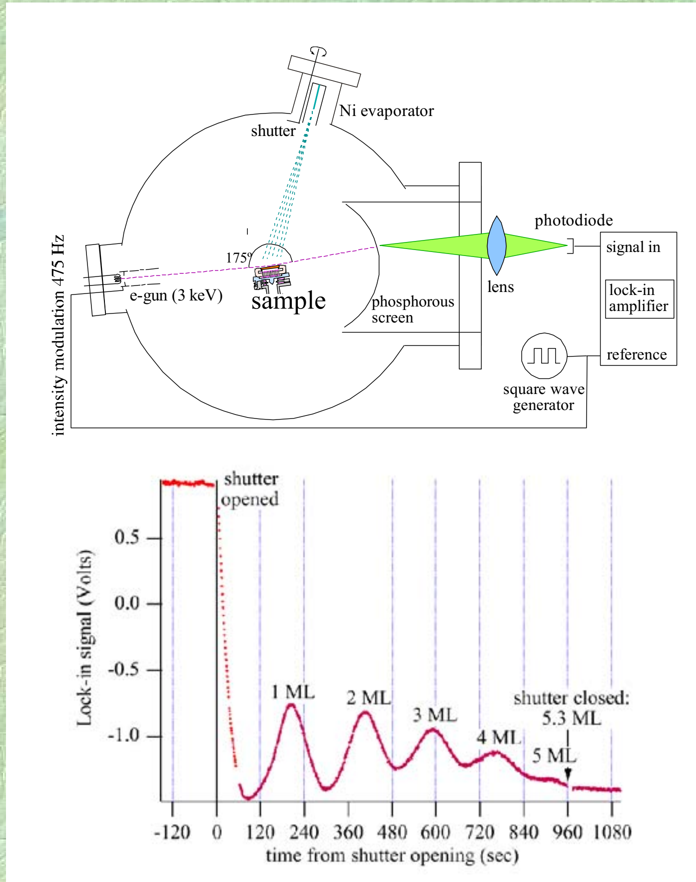
M. Hoesch, Ph. D. Thesis, 2002

Preparation of Monolayer Films of Ni on Cu(001)

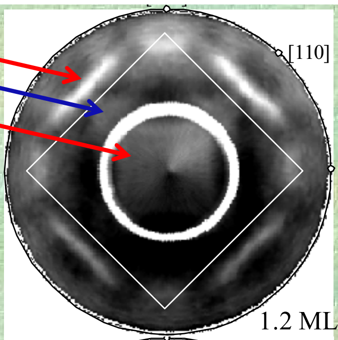
Ni deposited from e-beam heated rod at 0.33 ML/min.onto clean Cu(001)

Annealing to 420 K.

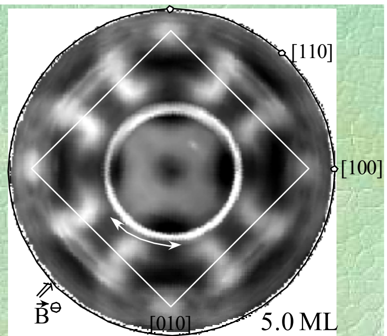
Cooling to 150 K (liquid N_2).



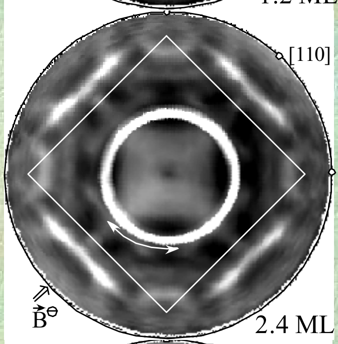
1.2 ML
Ni/Cu(001)
$T_C < 100$ K



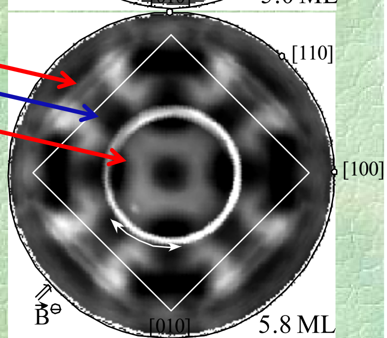
5.0 ML
Ni/Cu(001)
$T_C = 260$ K



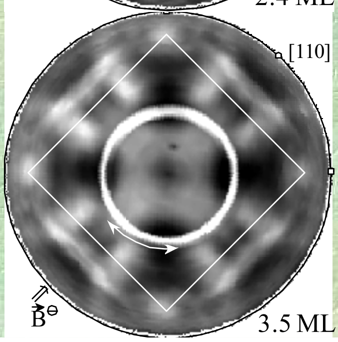
2.4 ML
Ni/Cu(001)
$T_C = 100$ K



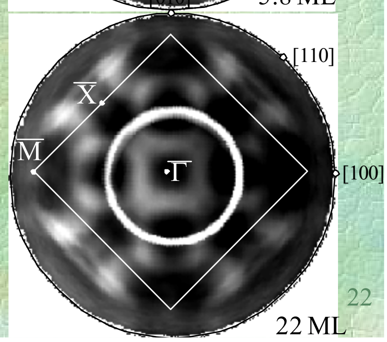
5.8 ML
Ni/Cu(001)
$T_C = 330$ K



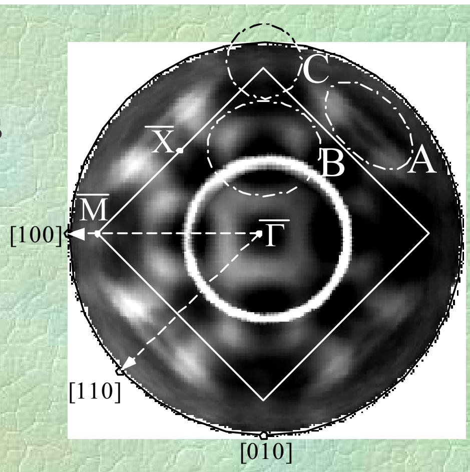
3.5 ML
Ni/Cu(001)
$T_C = 180$ K



22 ML
Ni/Cu(001)
$T_C = 627$ K
equivalent
bulk Ni(001)



Band Character of Fermi Surface Contours (thick film ~ bulk-like)



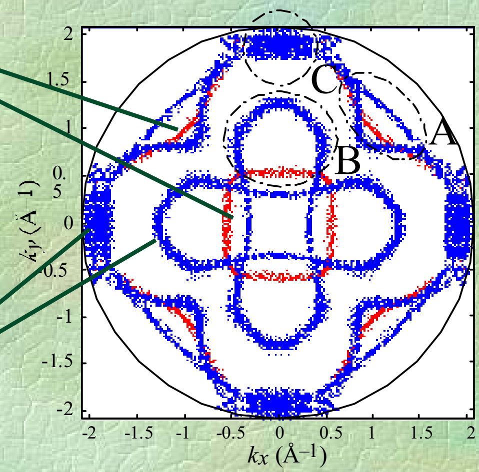
data from 22 ML Ni/Cu(001)

$h\nu$ = 21.22 eV

equivalent bulk Ni(001)

sp band

d band



Fermi surface calculation

free electron final state approximation

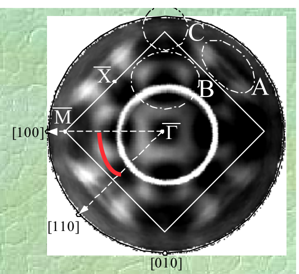
$h\nu$ = 21.22 eV

Φ = 5.2 eV

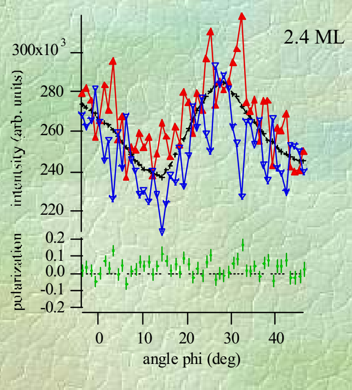
V_0 = 10.2 eV

Ni/Cu(001) azimuthal scans at E_F, ϑ = 28°, $h\nu$ = 21.22 eV, T = 150 K

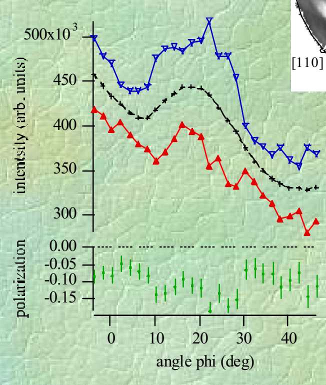
d band



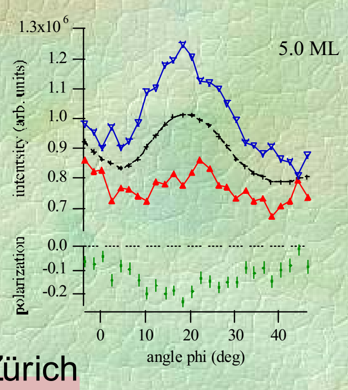
2.4 ML Ni/Cu(001) T_C = 100 K



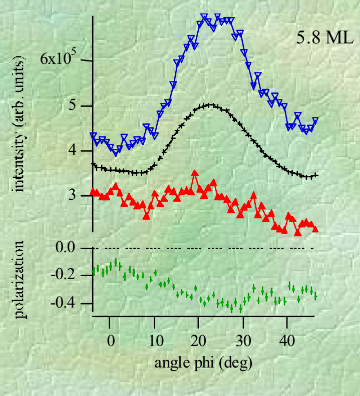
3.5 ML Ni/Cu(001) T_C = 180 K



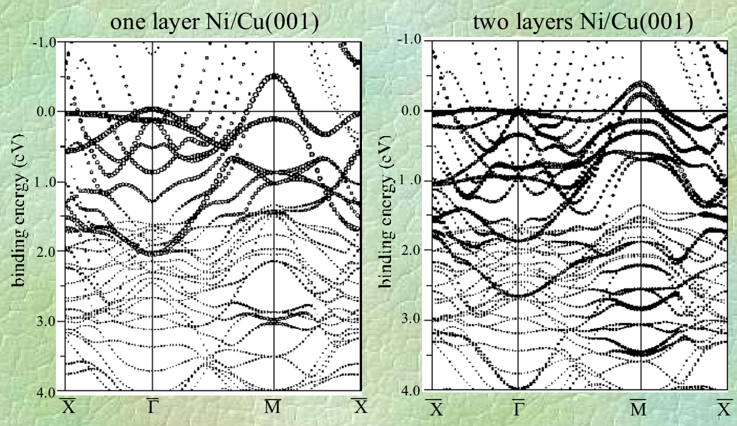
5.0 ML Ni/Cu(001) T_C = 260 K

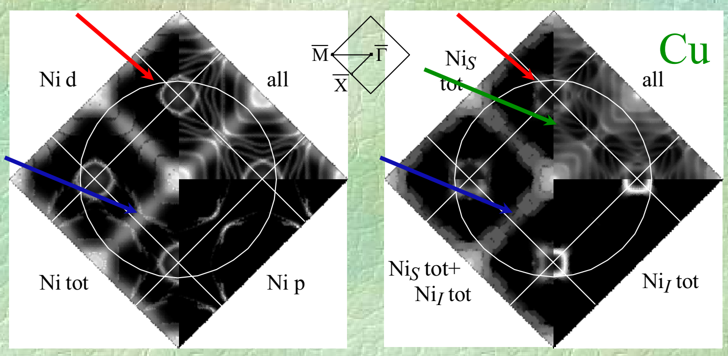


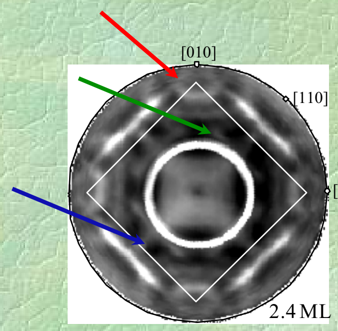
5.8 ML Ni/Cu(001) T_C = 330 K



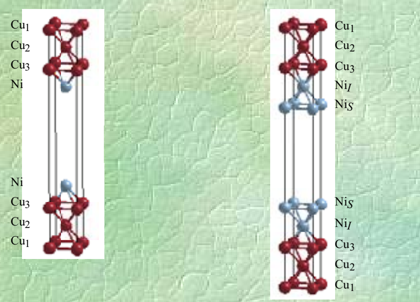
Ni/Cu(001) Slab Calculations







data from
2.4 ML Ni/Cu(001)
hv = 21.22 eV

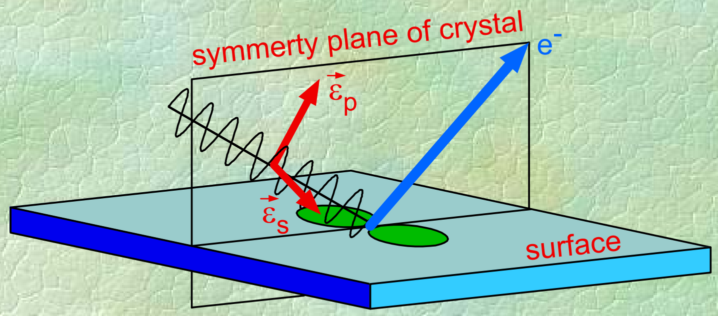


1 ML Ni/5 ML Cu/1 ML Ni   2 ML Ni/5 ML Cu/2 ML Ni

Ultrathin films of Ni on Cu(001)

- < 3 ML: paramagnetic interface band structure
- Around 3 ML two things happen:
  - $T_c > T_{meas}$ => Exchange splitting appears
  - Band structure becomes bulk-like (3D)
- The sp bands are bulk-like already at ~1 ML
- The d bands form interface states for < 3 ML

Intensities in Valence Photoemission - Symmetry Effects



$\vec{\varepsilon}_p$ photon polarization in...

$\vec{\varepsilon}_s$ ...perpendicular ("senkrecht") to...scattering plane

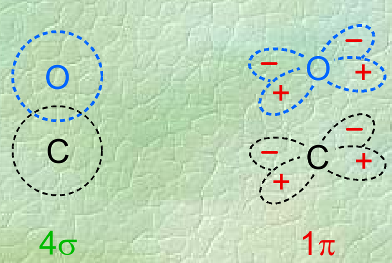
mirror reflection symmetries:

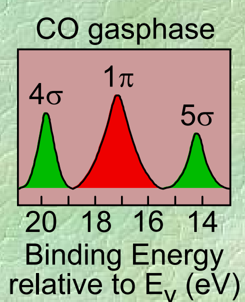
p - pol.	+1	+1	-1	0
	+1	+1	+1	max.
s - pol.	+1	-1	-1	max.
	+1	-1	+1	0

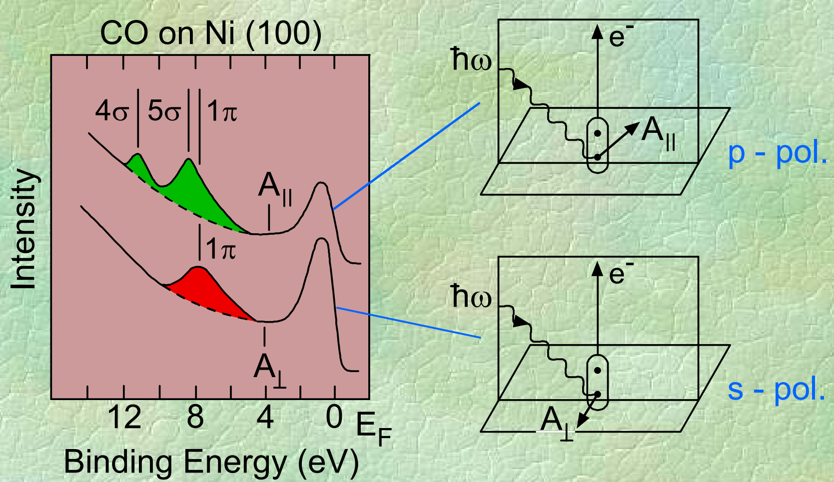
photoemission matrix element:

$$\left| \langle \phi_{f,kin} \,|\, \vec{r}_k \cdot \vec{\varepsilon} \,|\, \phi_{i,k(\vec{r}_k)} \rangle \right|^2 \rightarrow \text{Intensity}$$

CO Molecular Orbitals







from Hüfner

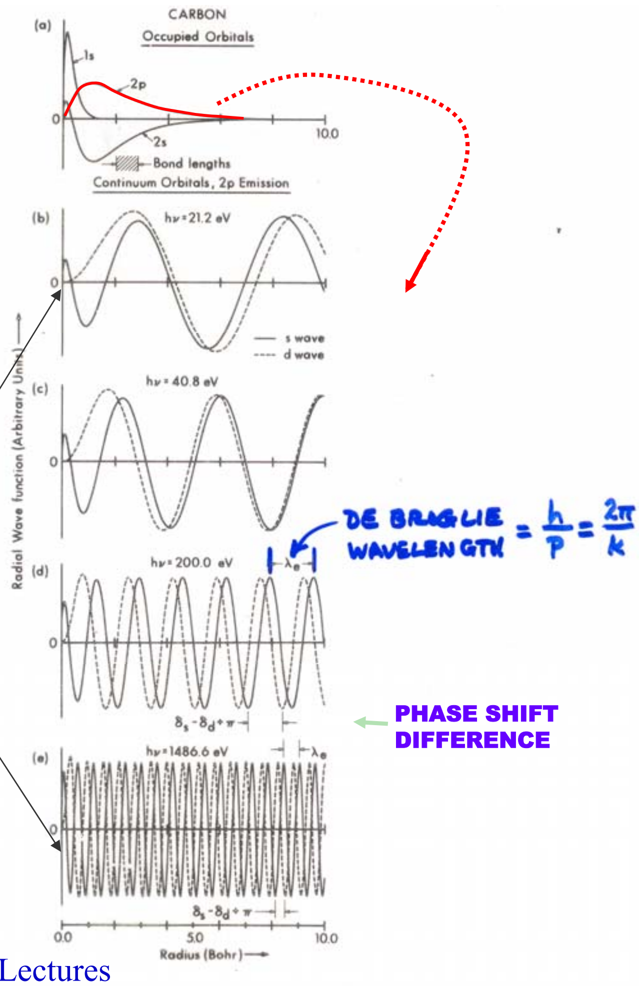
Intensities in Valence Photoemission - Atomic Effects

$m_{i,f} \sim \langle \phi_{f,kin} | \vec{r} \cdot \vec{\varepsilon} | \phi_{i,k} \rangle$

as for core levels

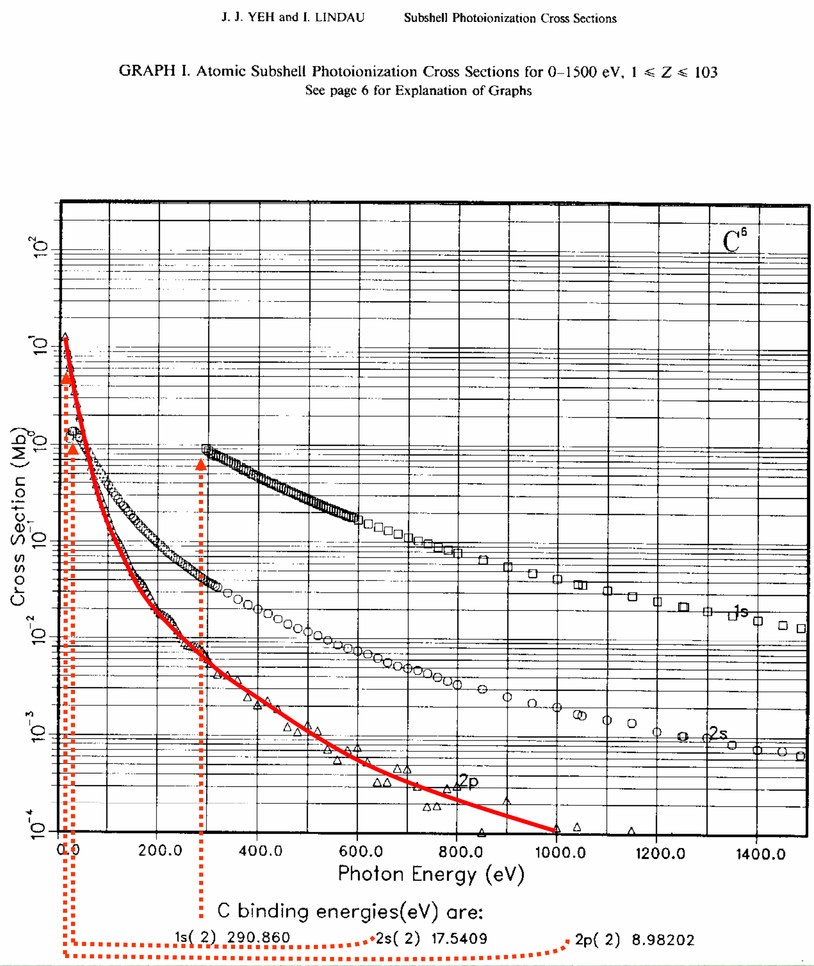
RADIAL MATRIX ELEMENTS TO $\ell \pm 1$ = s and d CHANNELS:

… for various energies



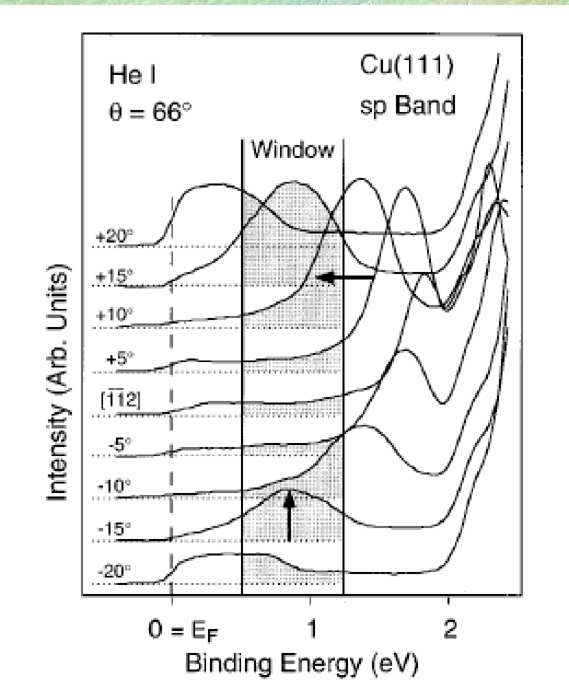
From C. S. Fadley's Lectures

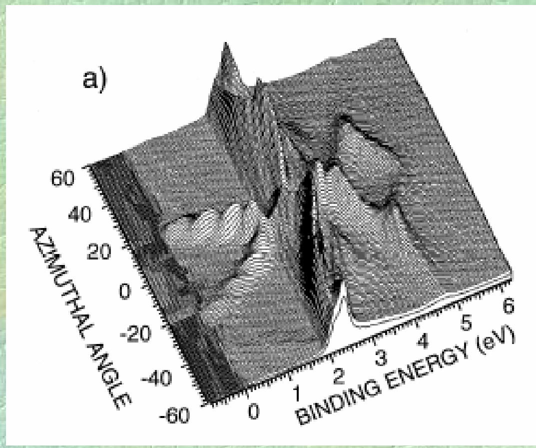
Plus other Examples from Yeh and Lindau in Sec. 1.5 of X-Ray Data Booklet, and plots for all elements at: http:// ulisse.elettra. trieste.it/ elements/ WebElements. html

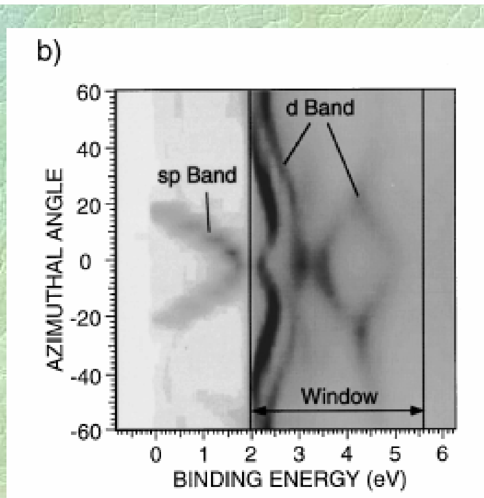


From C. S. Fadley's Lectures

Intensities in Valence Photoemission - Diffraction Effects

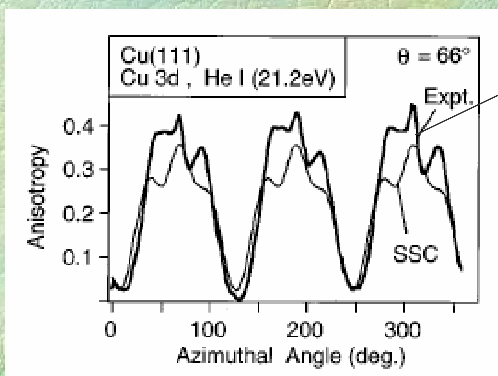






Integration of Intensities over the Entire d-Band Region

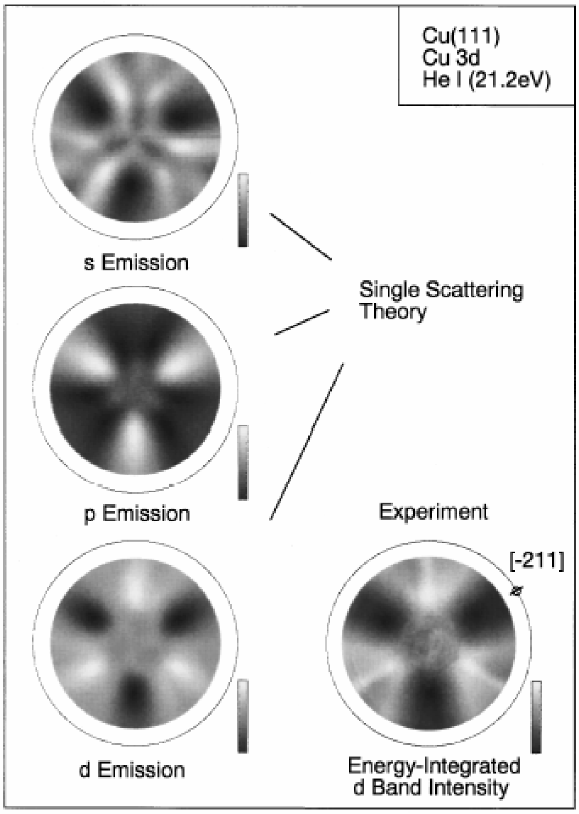
Choose energy window large enough so the d-band peak never leaves the window => the intensity variation of the peaks can be monitored

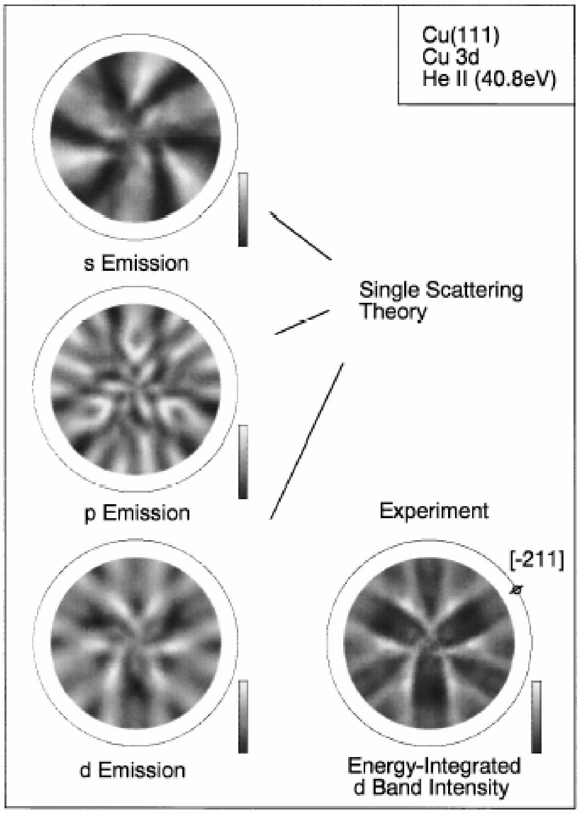


Theoretical curve: Single Scattering Cluster (SSC) calculation for a cluster representing a Cu(111) surface from a localized full d shell (like in x-ray photoelectron diffraction (XPD), hence

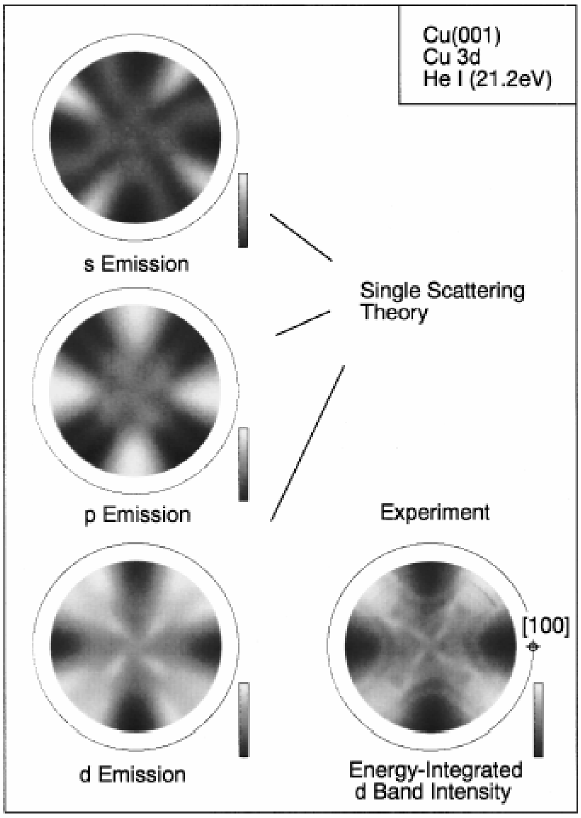
ultraviolet photoelectron diffraction (UPD)

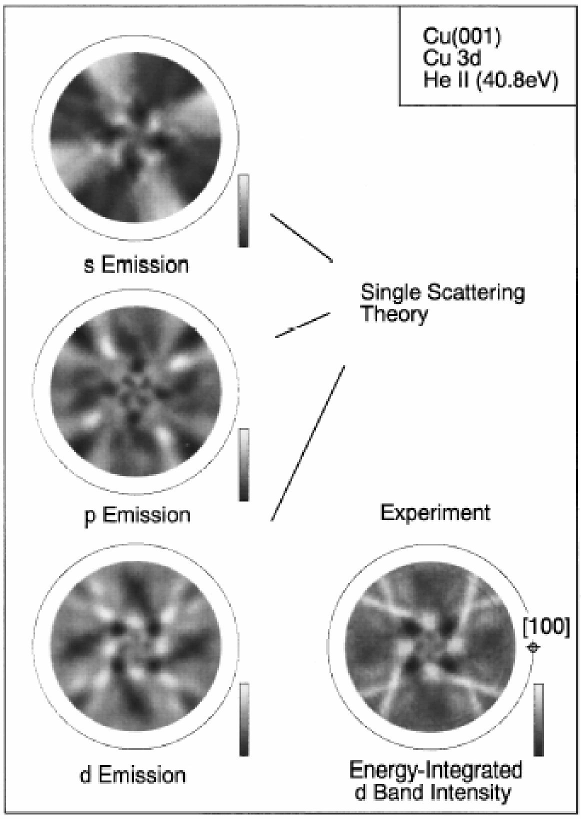
J. Osterwalder et al., PRB 53, 10209 (1996)





J. Osterwalder et al., PRB 53, 10209 (1996)

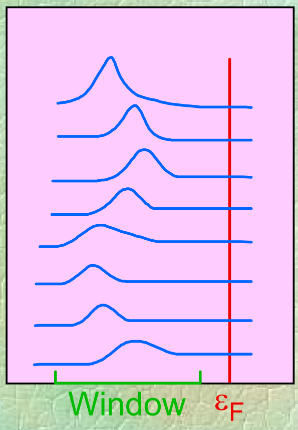




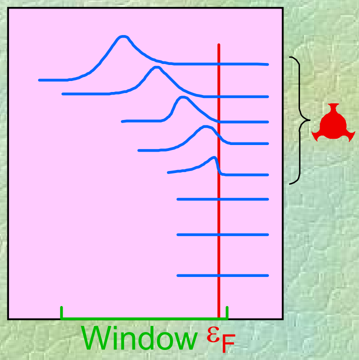
J. Osterwalder et al., PRB 53, 10209 (1996)

UPD and Photoemission Intensities

filled shells:



unfilled shells: ?



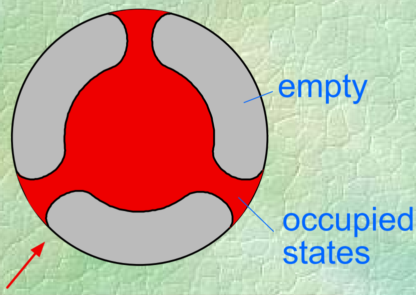
direct transition
is lost at Fermi surface.

direct transition
never disperses
out of measurement
window (e.g. Cu 3d).

⇩

UPD describes overall band intensities !

(sum rule over
several subbands)



But: Must know angular momentum compos.
of occupied (cristal field) states !

UPD may describe intens. in occupied $\vec{k}$-Region