Spin-Resolved Fermi Surface Mapping

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Outline

- Electron spin and electron correlations
- Spin-resolved Fermi surface mapping
- Measuring spin polarized bands on Ni(111)
- Measured spin polarization vs. initial state spin polarization
- The spin-splitting of the surface state on Au(111):

  => the first spin-resolved Fermi surface map

- Effectively increased energy resolution by spin-polarization measurement: spin-split surface state on Au(17 11 9)

Spin-Polarized Photoemission at the SLS

Prof. Thomas Greber

Dr. Jorge Lobo-Checa

Dr. Moritz Hoesch

Dr. Matthias Hengsberger

Prof. Vladimir Petro

Dr. Matthias Muntwiler

Andrei Dolocan

Martina Corso

Martin Klöckner

Surfaces/Interfaces: Spectroscopy beamline (SIS)

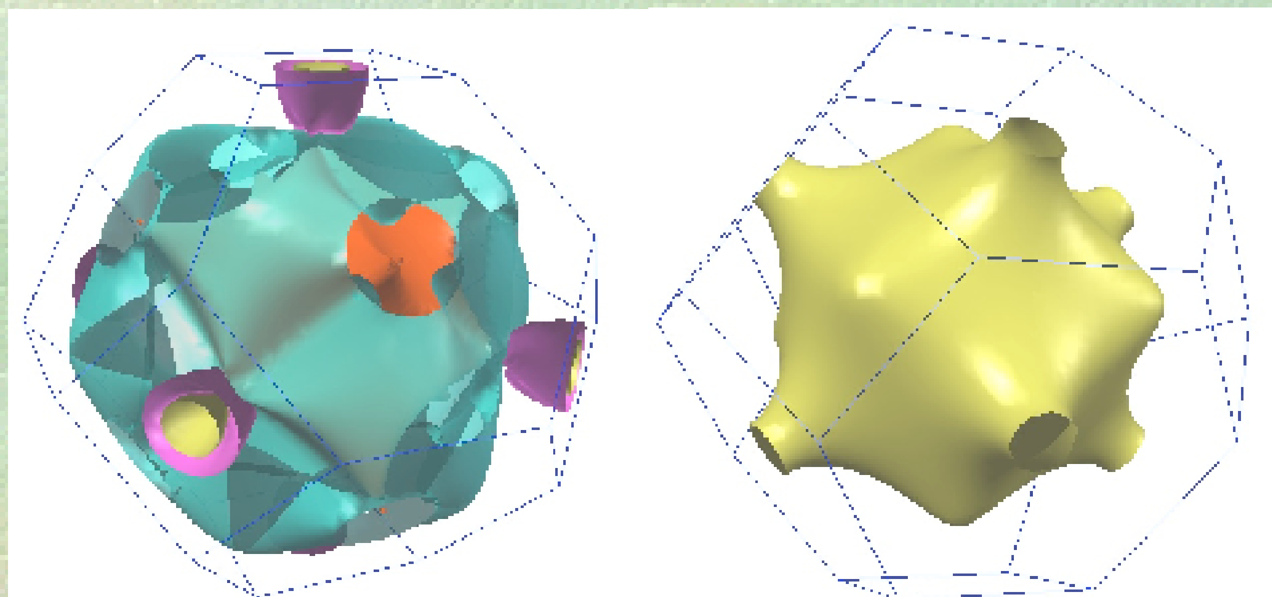
Thanks !

Raphael Abela, Willi Arrigoni, Robin Betemps, ben van den Brandt, Sorin Chiuzbaian, Qianhong Chen, Fritz Dupi, Pascal Erismann, Mihaela Falub, Uwe Fleschig, Karl Gisler, Patrick Hautle, Peter Hottinger, Gerard Ingold, Babak Kalantari, Ueli Kalt, Ton Konter, Andreas Keller, Timo Korhonen, Renata Krempaska, Jurj Krempaski, Luc Patthey, Christoph Quitmann, Martin Rohrer, Thomas Schmidt, Ming Shi, Martin Spielmann, Urs Staub, Christian Vollenweider, Friso van der Veen, Detlef Vermeulen, Peter Winkler, PSI

at the Swiss Light Source

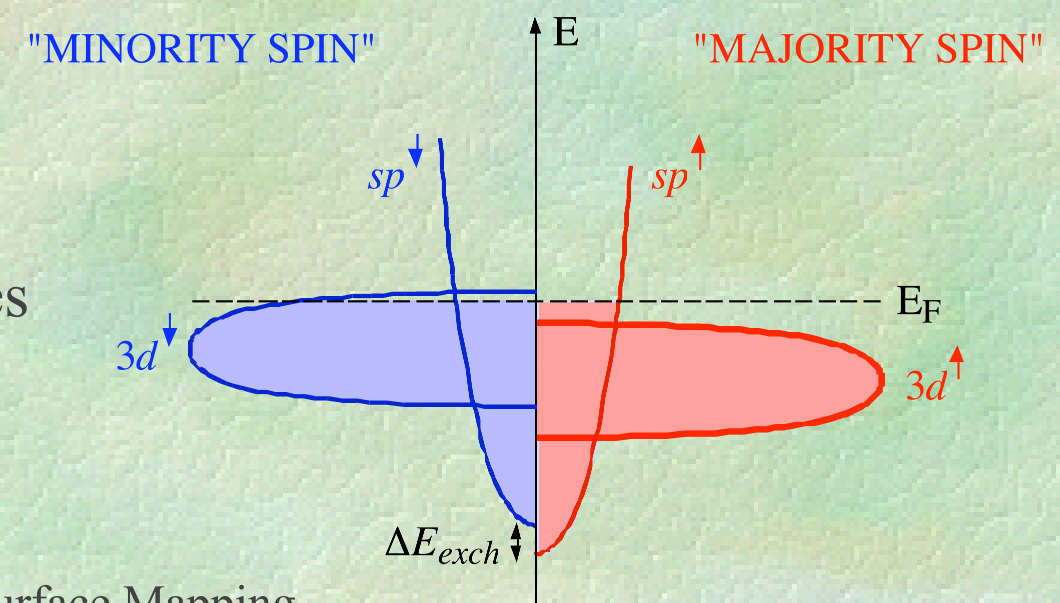
at PSI / Villigen

The Fermi Surface of Nickel Metal

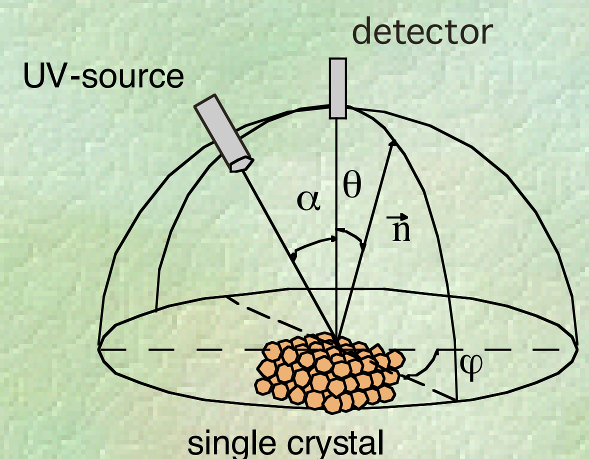


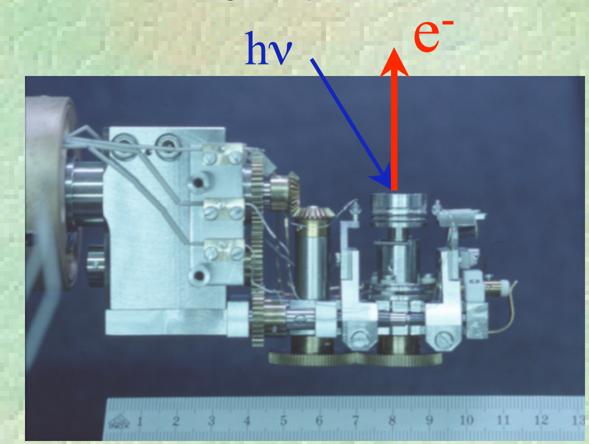
From http://www.phy.tu-dresden.de/~fermisur/

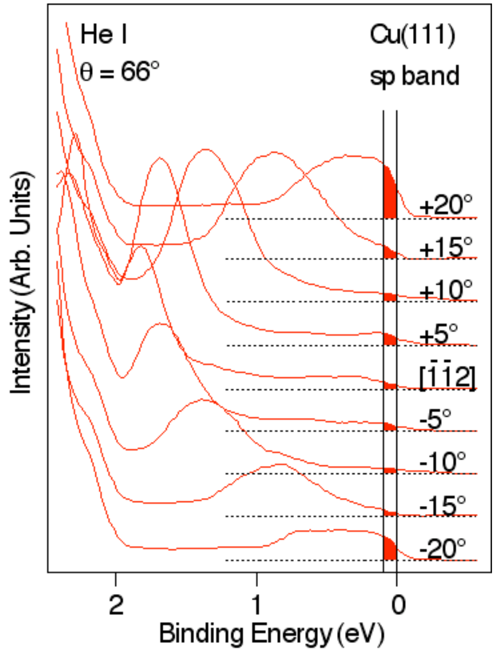
Schematic Density of States

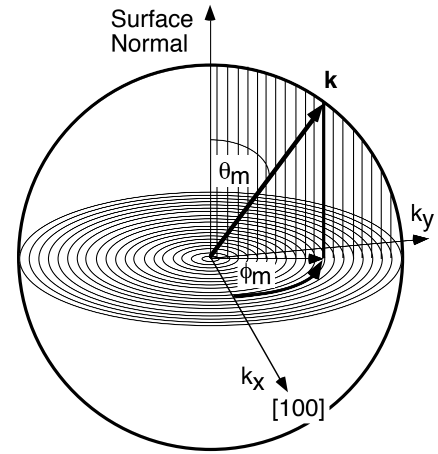


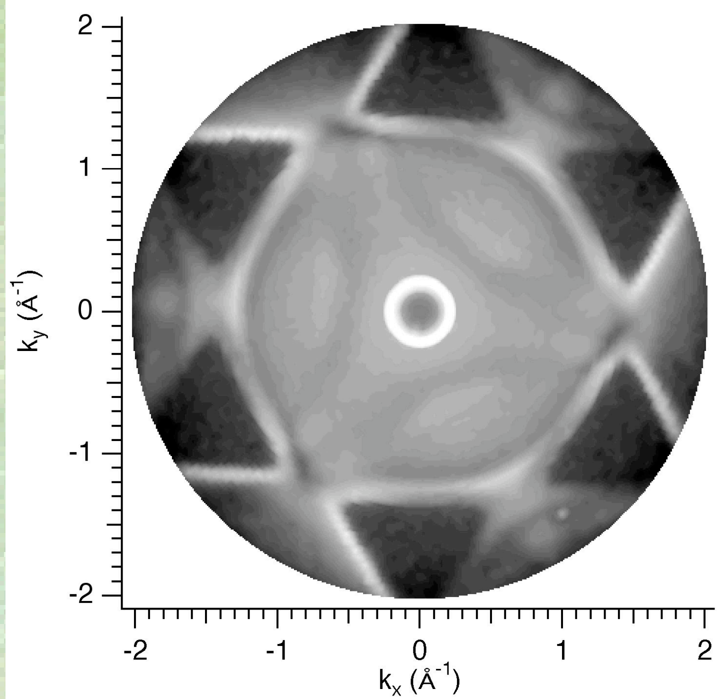
Fermi Surface Mapping by Photoemission



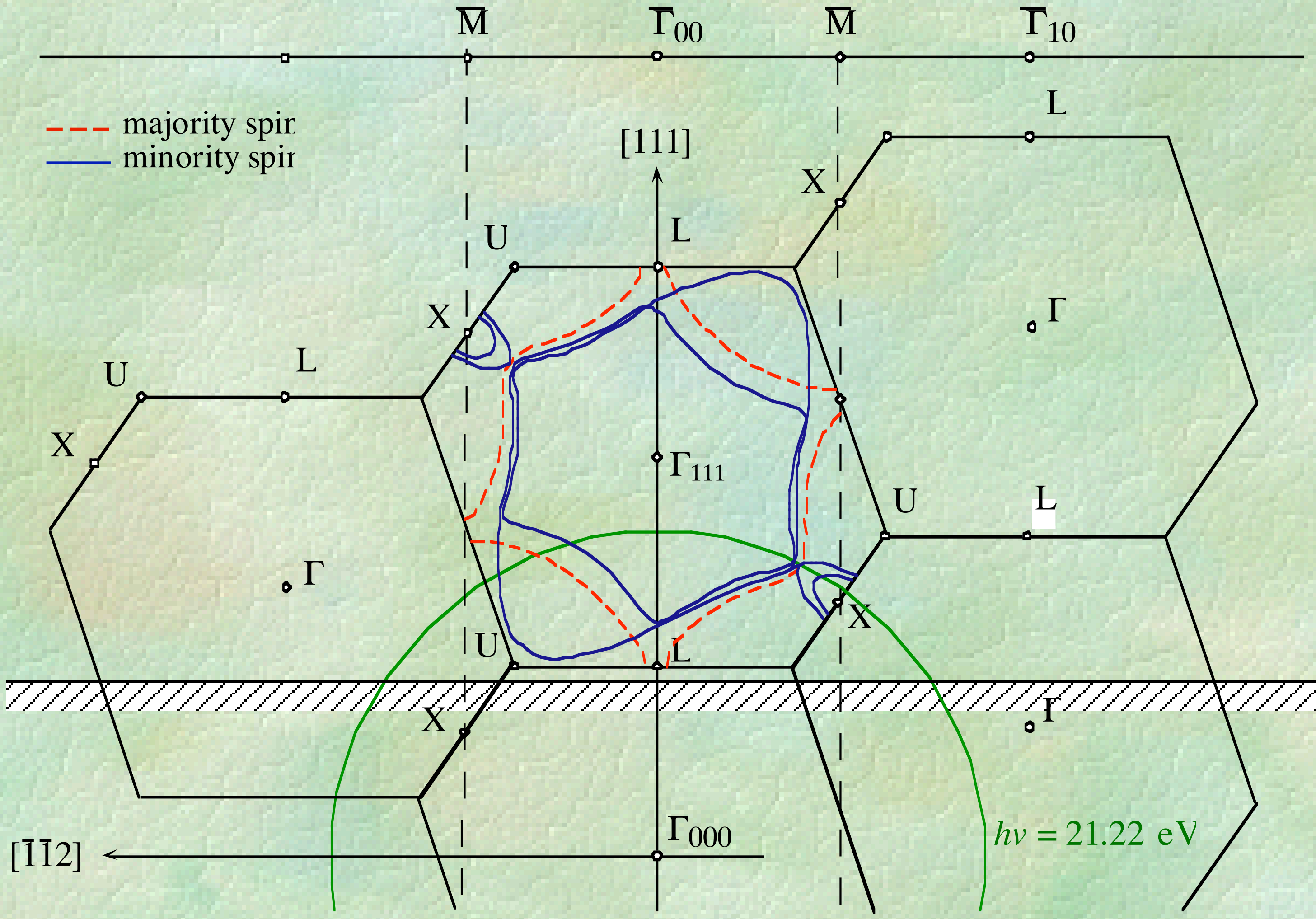






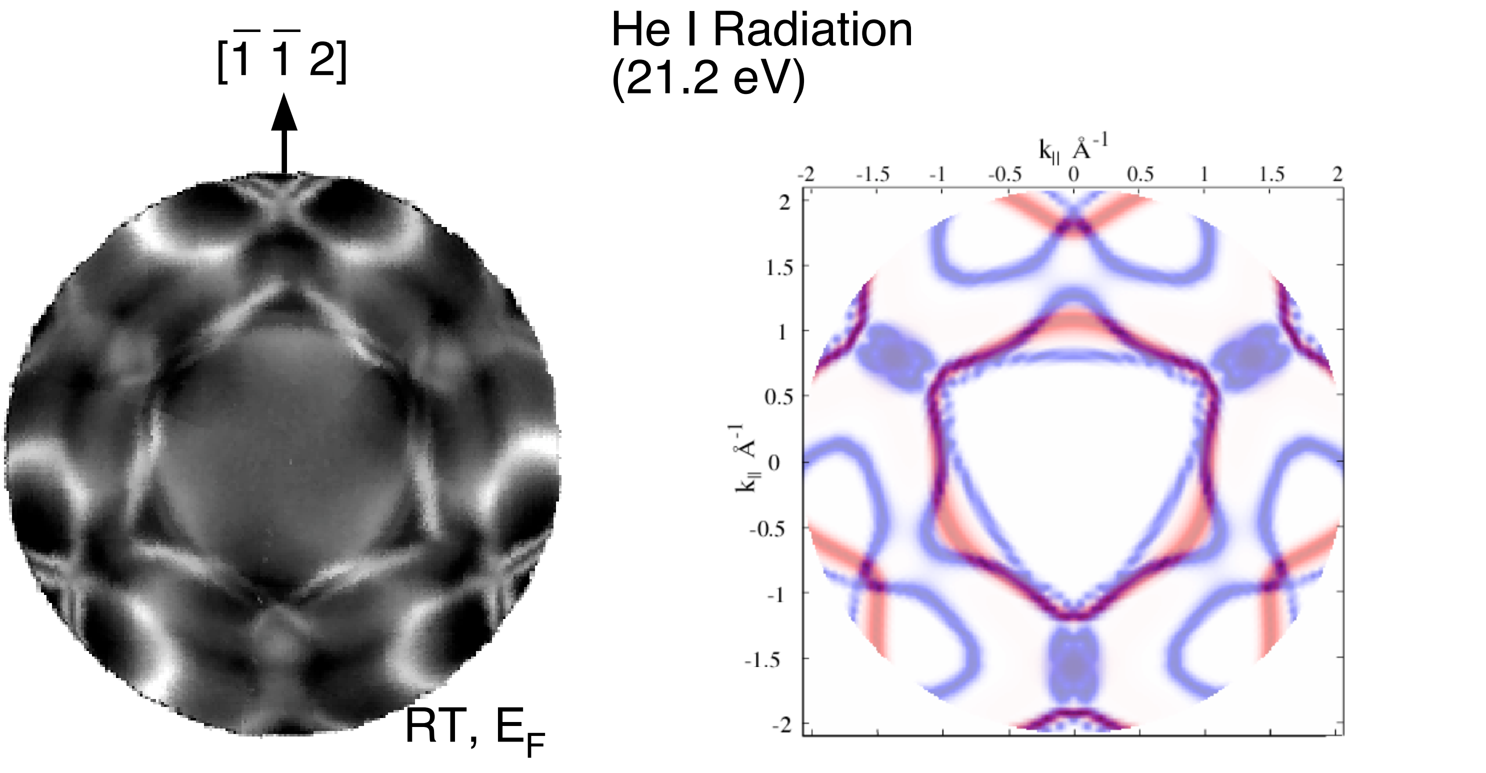


Reciprocal Space on Ni(111)



Fermi surface calculation (density functional theory, Wien 97)

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

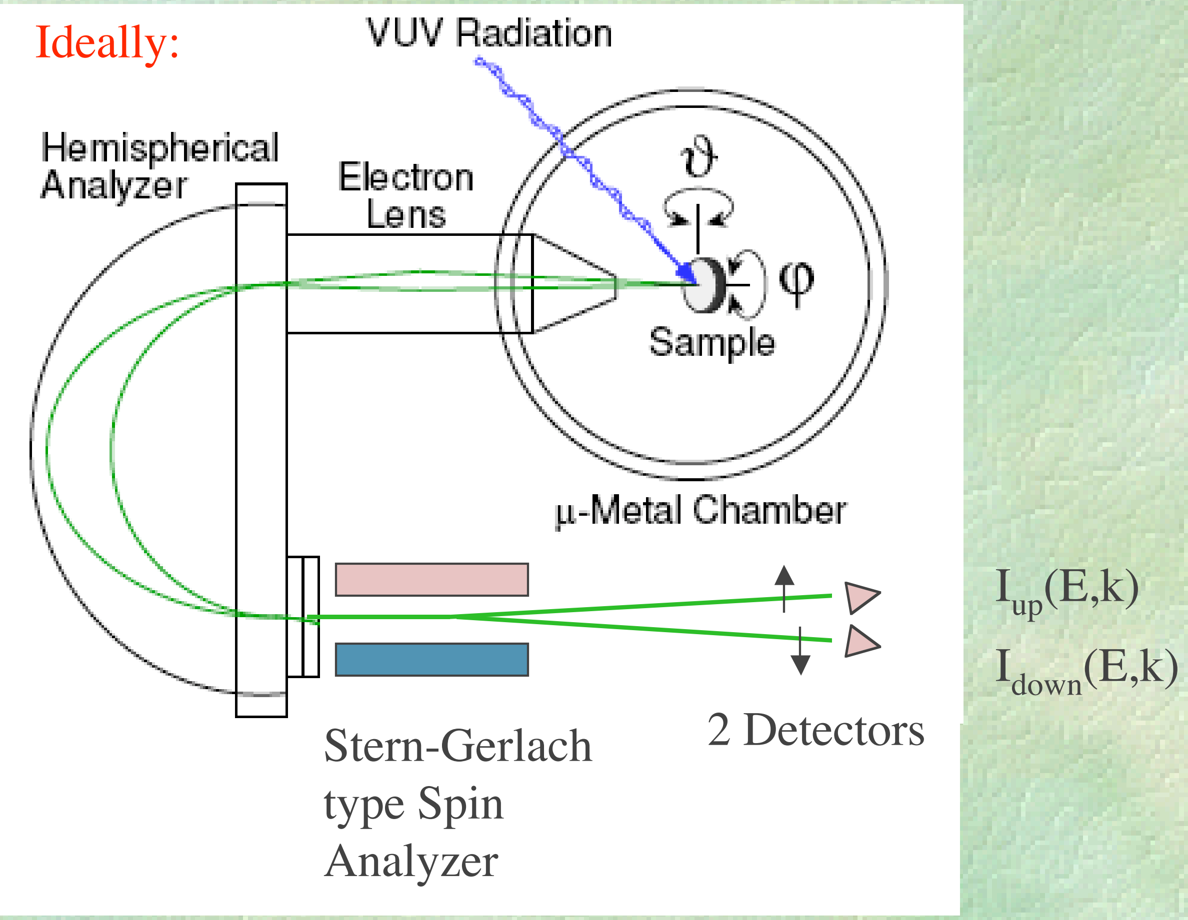


Experiment

DFT theory

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

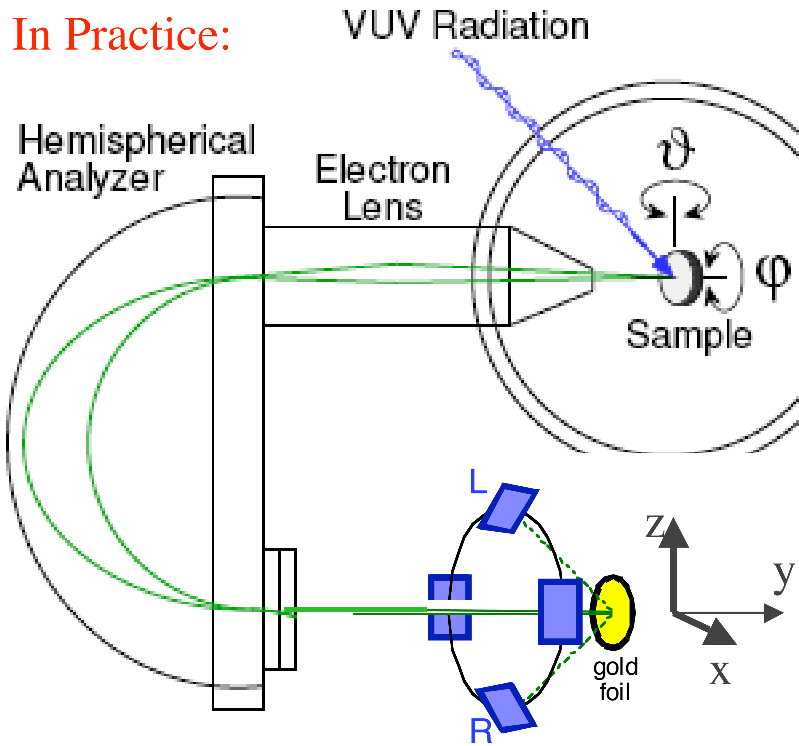
ARPES with Spin Resolution



Does not work! (Lorentz forces & uncertainty principle)

ARPES with Spin Resolution

In Practice:



Mott Scattering
(~ 50 keV)

two orthogonal axes are spanned by two pairs of detectors

4 Detectors

Scattering asymmetry

$$A_x = \frac{(I_L - I_R)}{(I_L + I_R)}$$

Spin Polarization

$$P_x = A_x / S.$$

S: Sherman function

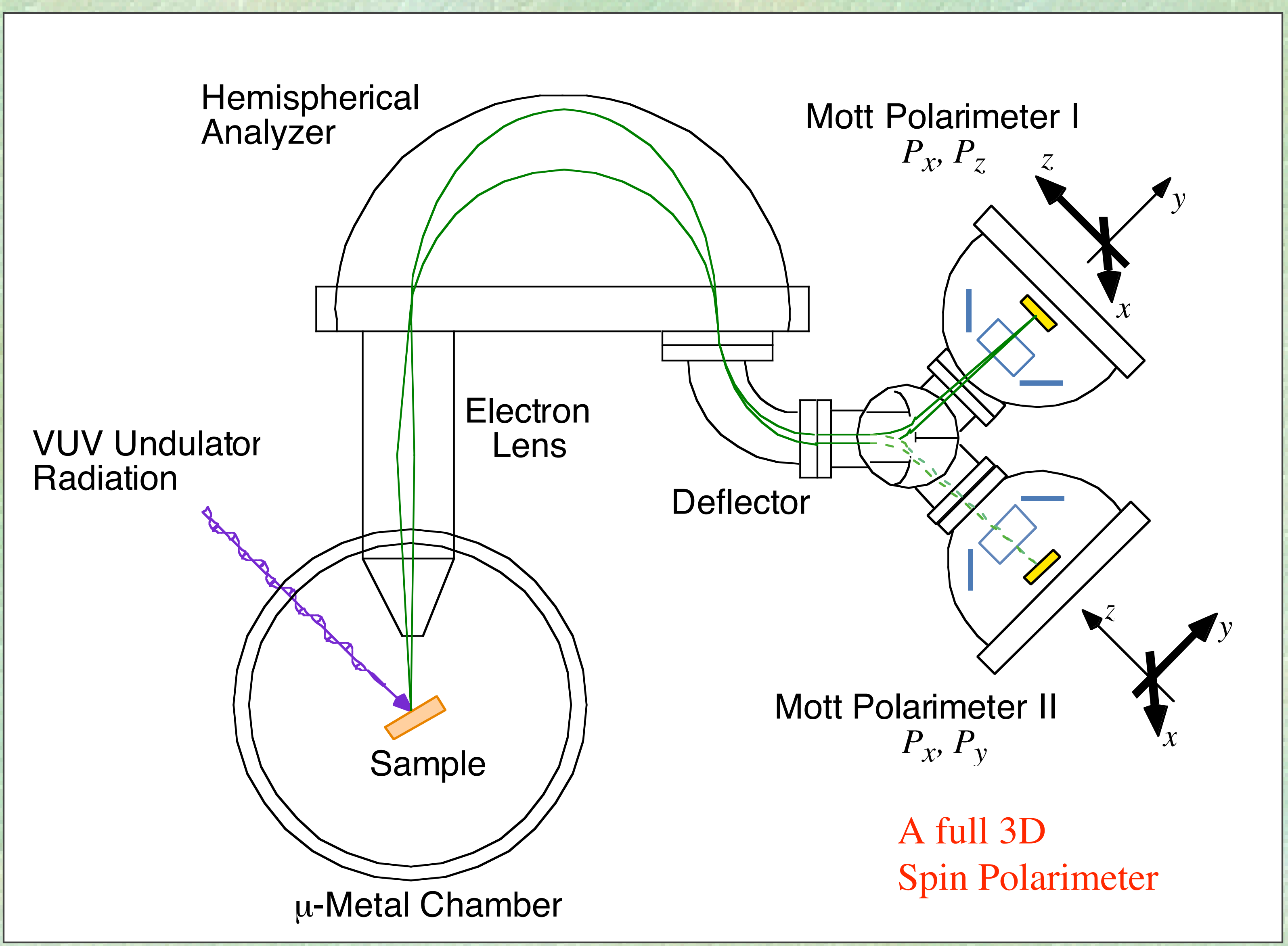
Spin Polarization:

$$P_I(E, \mathbf{k}) = \frac{I_\uparrow(E, \mathbf{k}) - I_\downarrow(E, \mathbf{k})}{I_\uparrow(E, \mathbf{k}) + I_\downarrow(E, \mathbf{k})},$$

Inefficient !

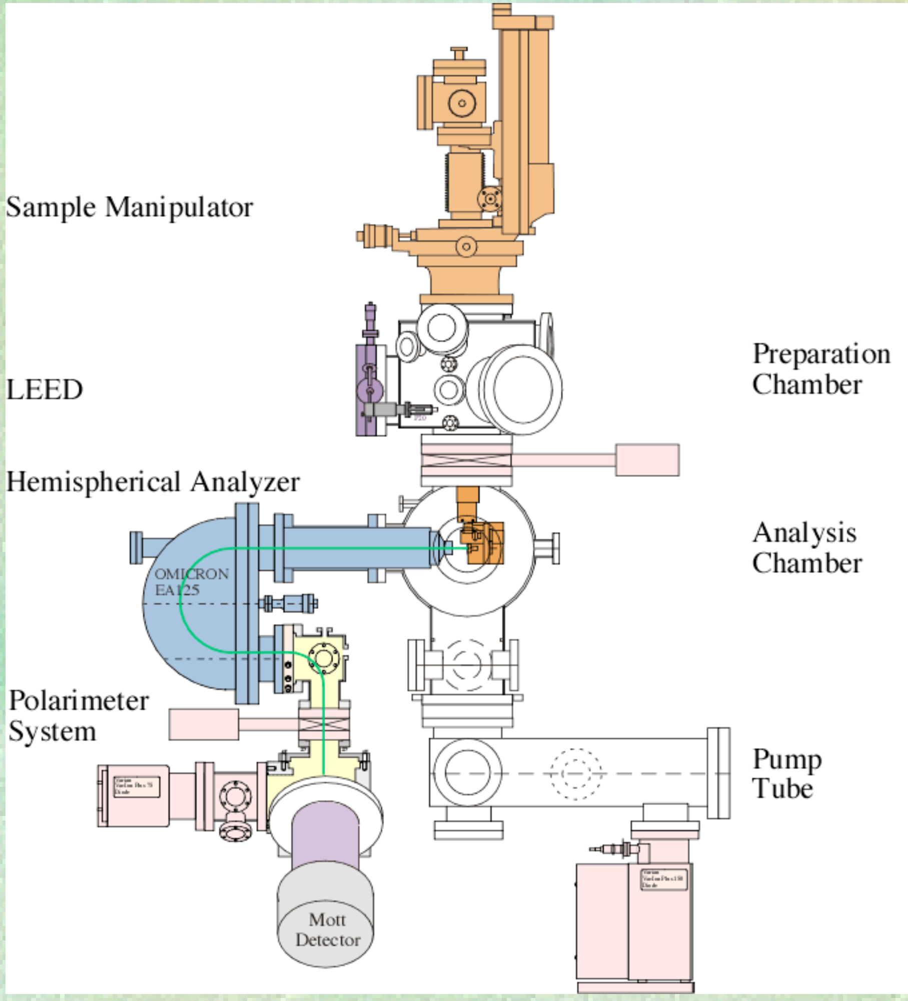
$$I_{\uparrow,\downarrow}(E, \mathbf{k}) = I_M(E, \mathbf{k})(1 \pm P_I(E, \mathbf{k}))/2.$$

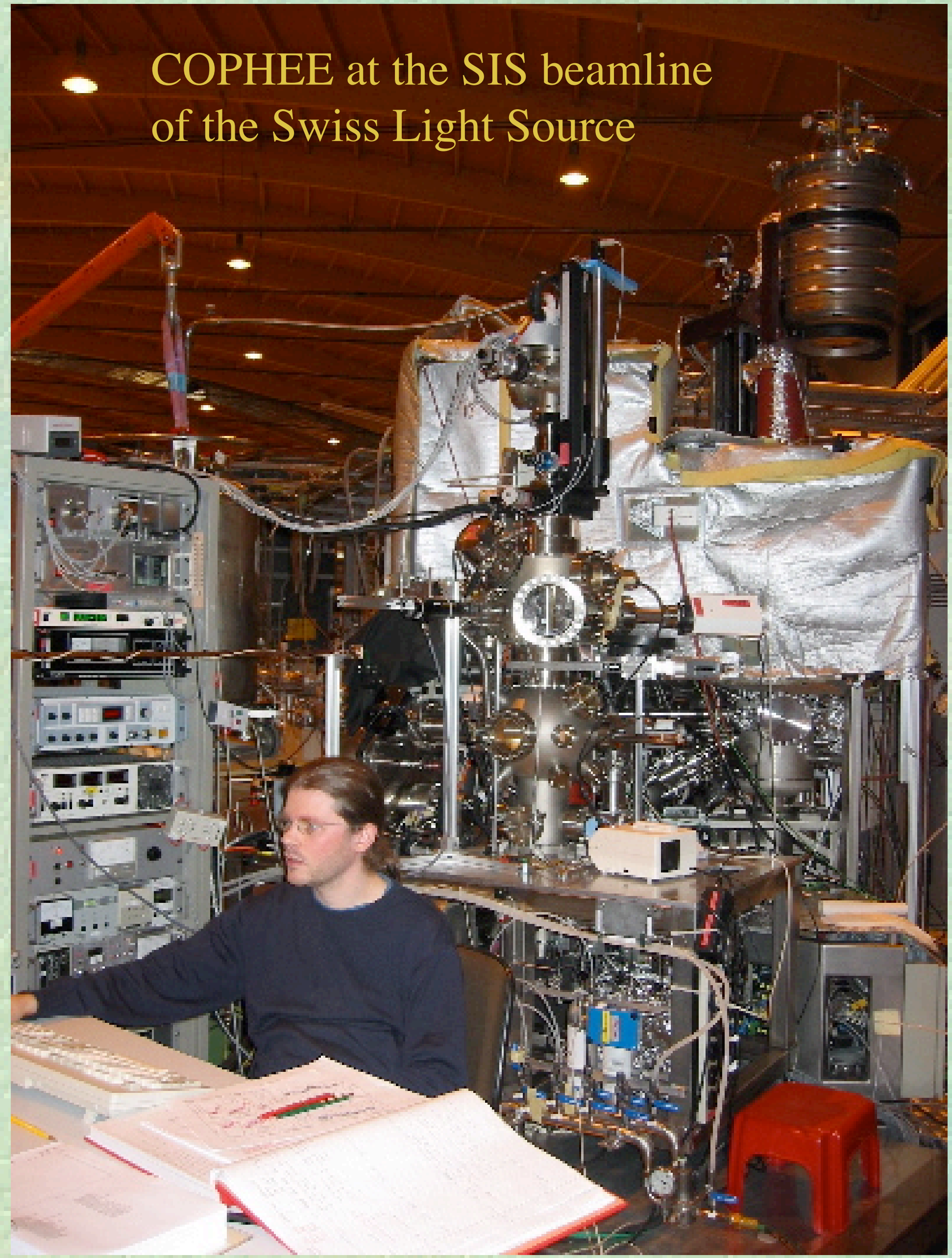
COPHEE - The Complete Photoemission Experiment



M. Hoesch, Ph. D. Thesis, 2002

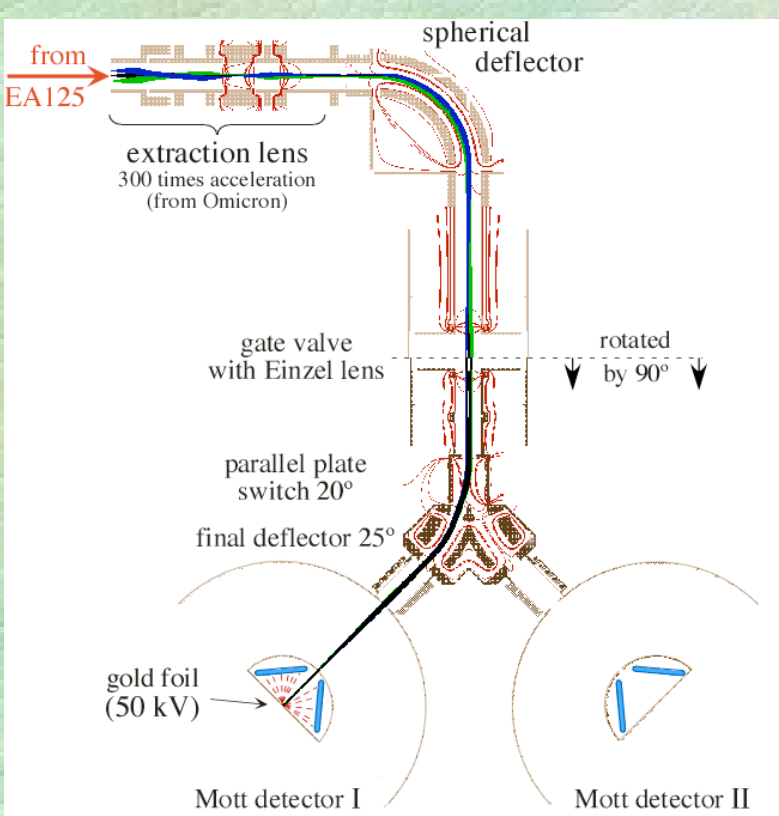
Setup of COPHEE:

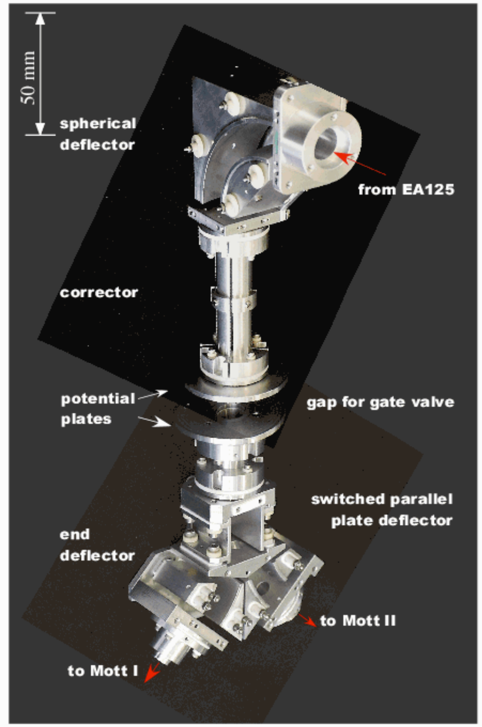




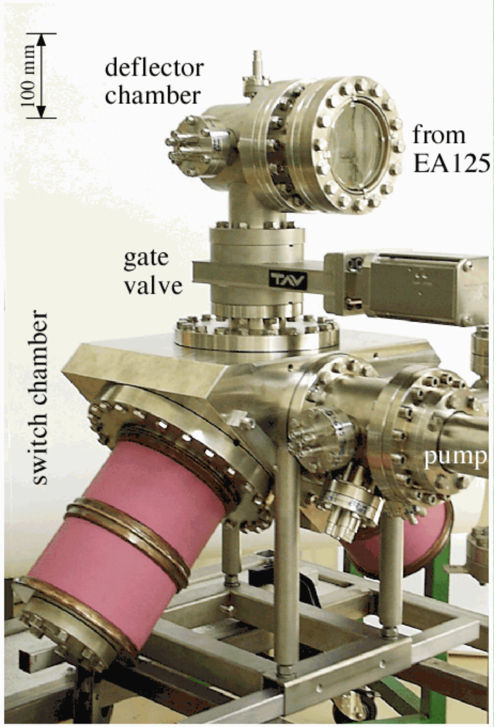
CORPES05
Spin-Resolved Fermi Surface Mapping

The Transfer / Distributor Lens



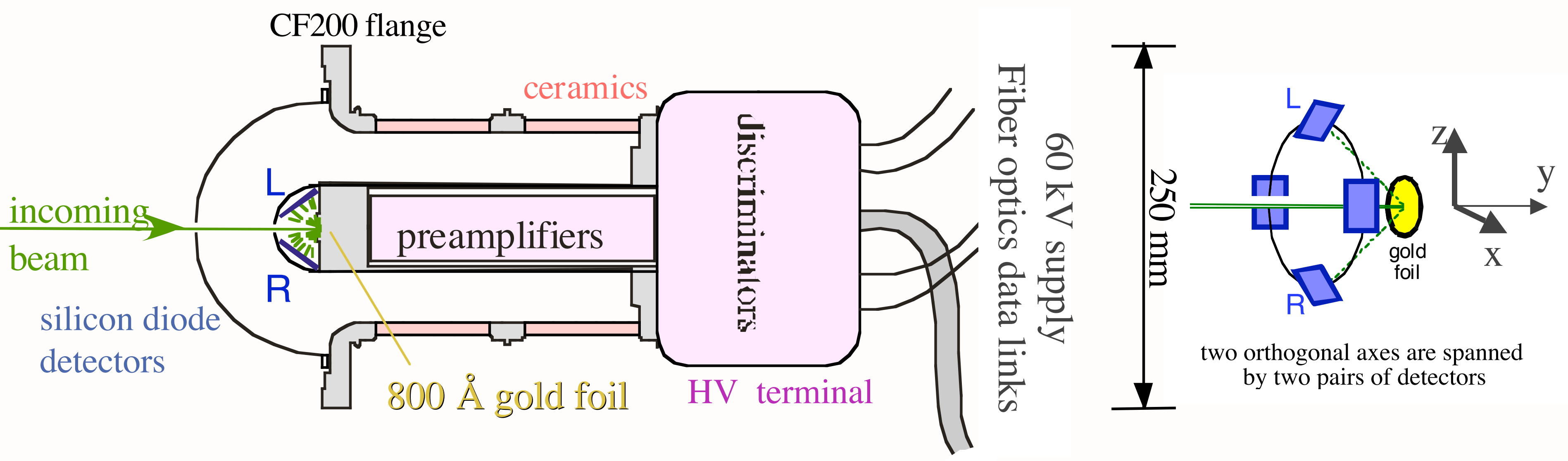


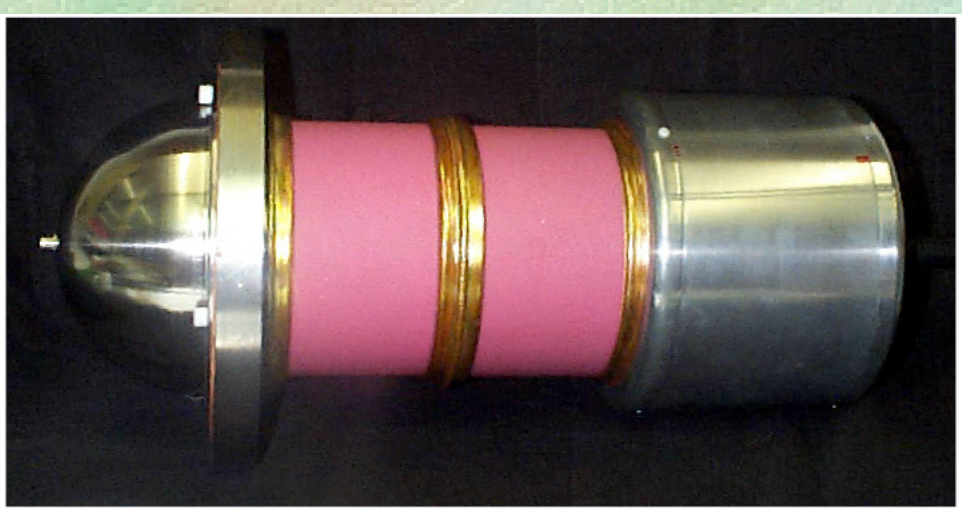
lens electrodes



vacuum envelope

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)

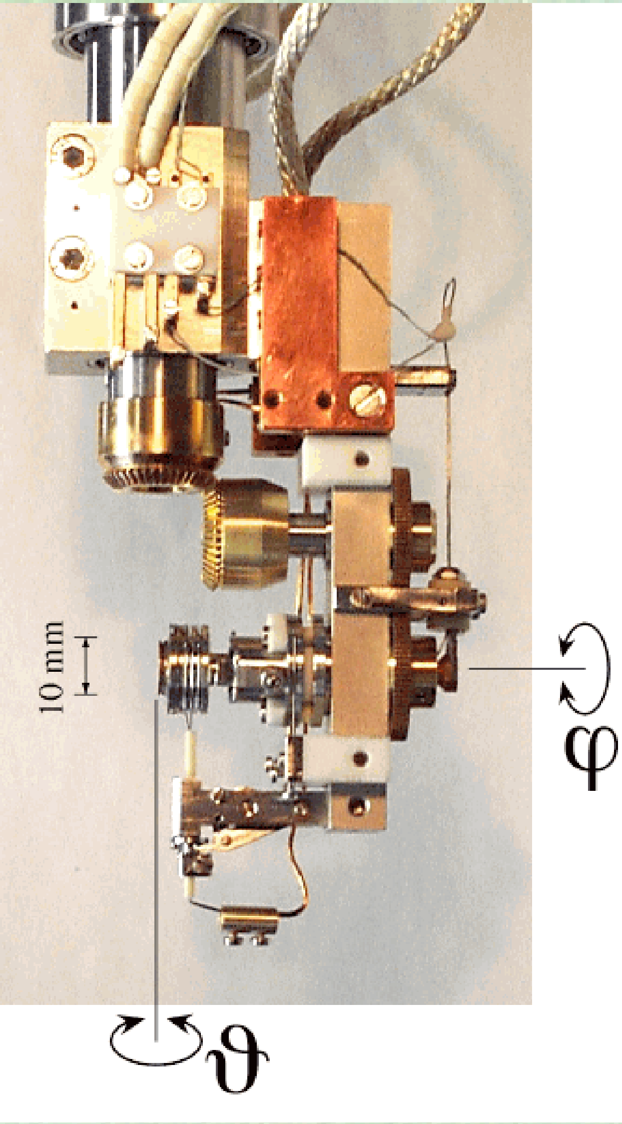
Here:

S ~ 0.15

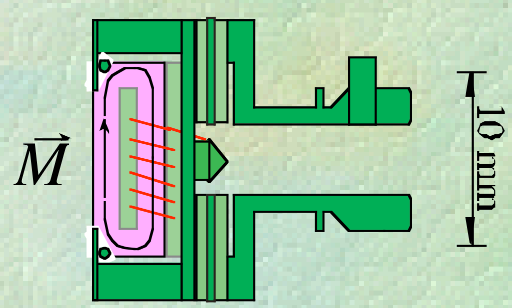
Backscattering at high energies:
Very inefficient process (~10^{-3})

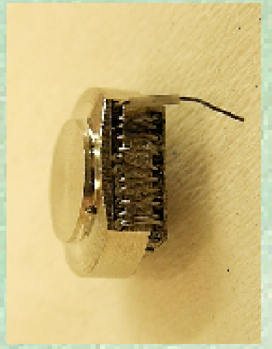
V. N. Petrov et al., RSI 72, 3729 (2001)

Important: Control over the sample magnetization in ARPES !



We need a magnetized sample (ideally a single domain) to measure spin polarized bands !

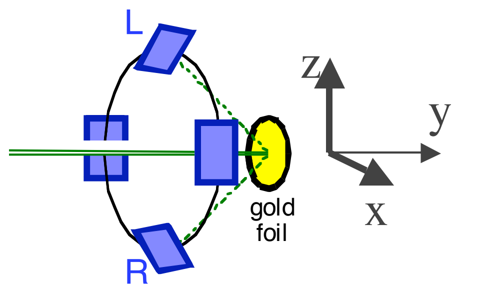




Switching magnetization direction (⊕,⊖)

⇒ Forming cross asymmetries cancels instrumental asymmetries

$$A^{\otimes} = \frac{(I_L^{\oplus} + I_R^{\ominus}) - (I_R^{\oplus} + I_L^{\ominus})}{(I_L^{\oplus} + I_R^{\ominus}) + (I_R^{\oplus} + I_L^{\ominus})}.$$



two orthogonal axes are spanned by two pairs of detectors

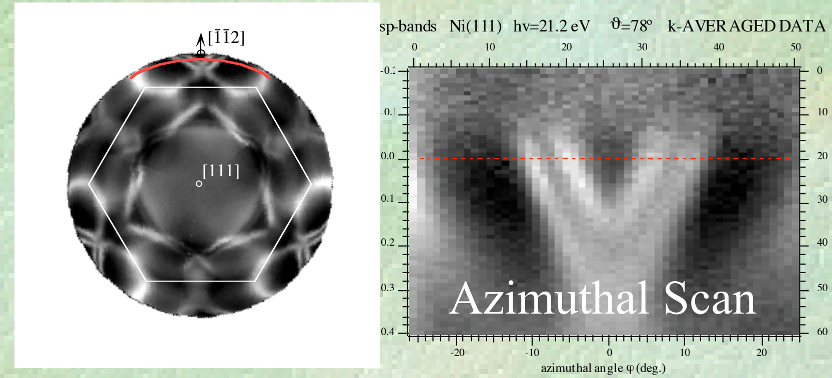
Polarization P = A / S

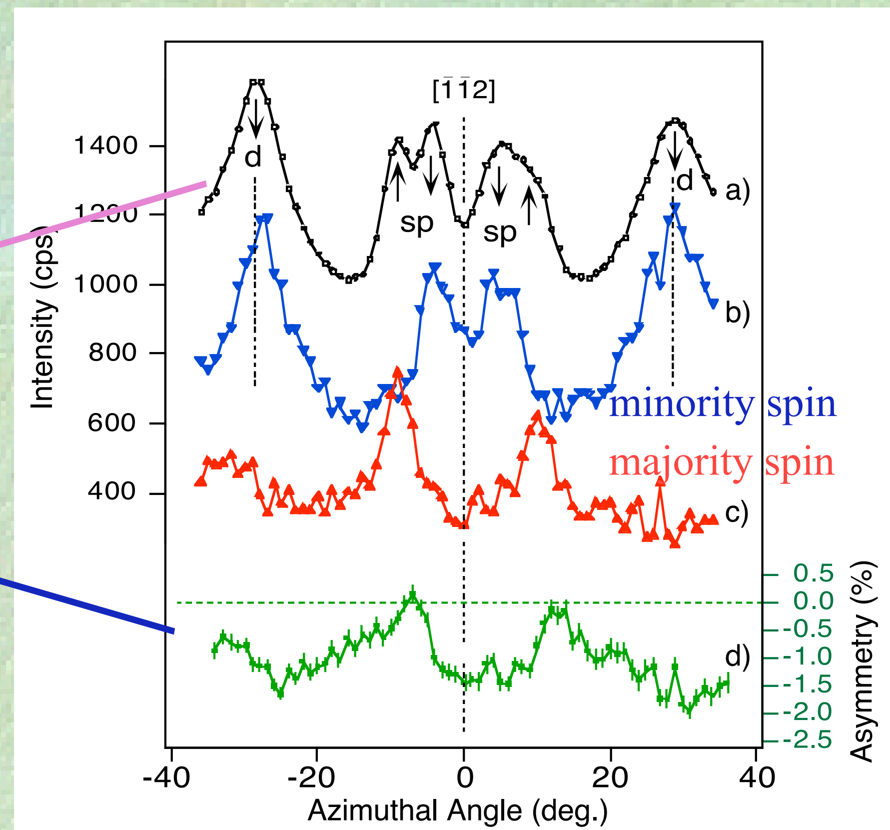
S ~ 0.15, but not precisely known (requires calibration)

⇒ P = 0 is measured exactly !

⇒ P scale is known roughly

Spin-Resolved Momentum Mapping on Ni(111)





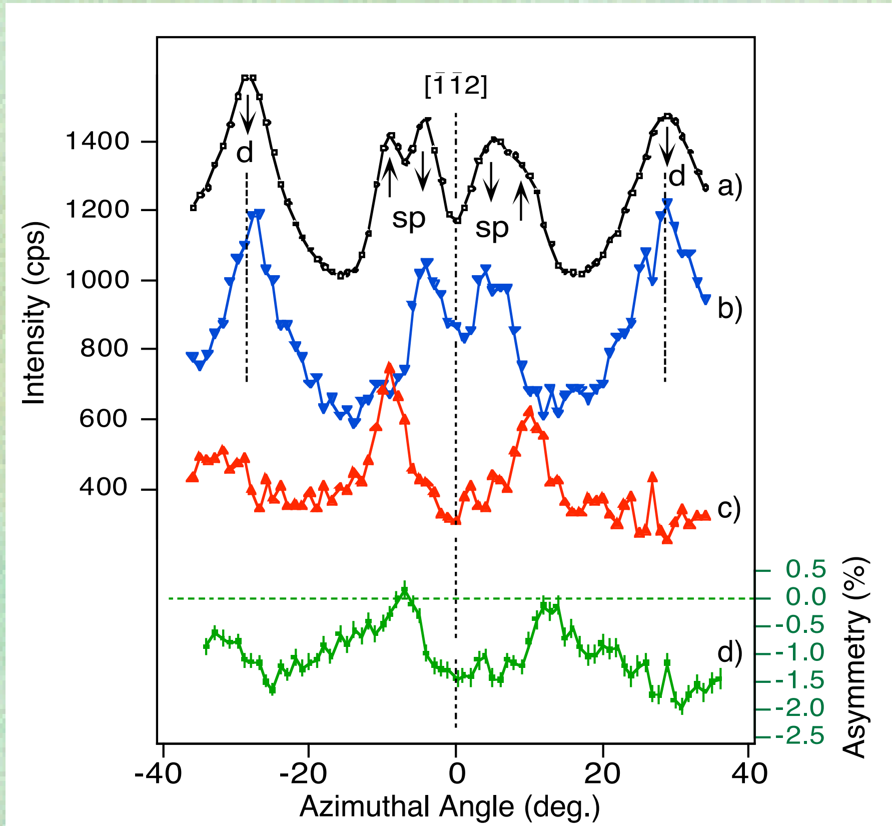
$$I_{\uparrow,\downarrow}(E,\boldsymbol{k}) = \qquad (1 \pm \qquad (E,\boldsymbol{k}))/2.$$

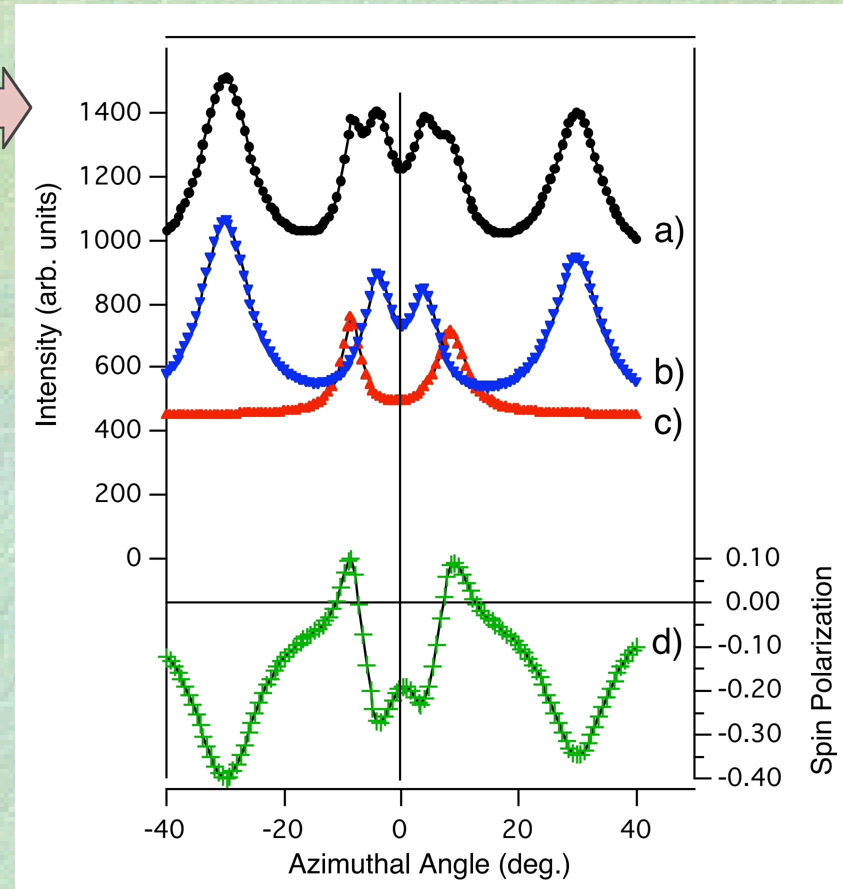
$$P_I(E,\boldsymbol{k}) = \frac{I_\uparrow(E,\boldsymbol{k}) - I_\downarrow(E,\boldsymbol{k})}{I_\uparrow(E,\boldsymbol{k}) + I_\downarrow(E,\boldsymbol{k})}.$$

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

Quantitative Aspects of Spin Polarization Measurements

Modelling Spin Polarization:
6 Lorentzians (2 up, 4 down)
+ constant background (S/B~0.6)

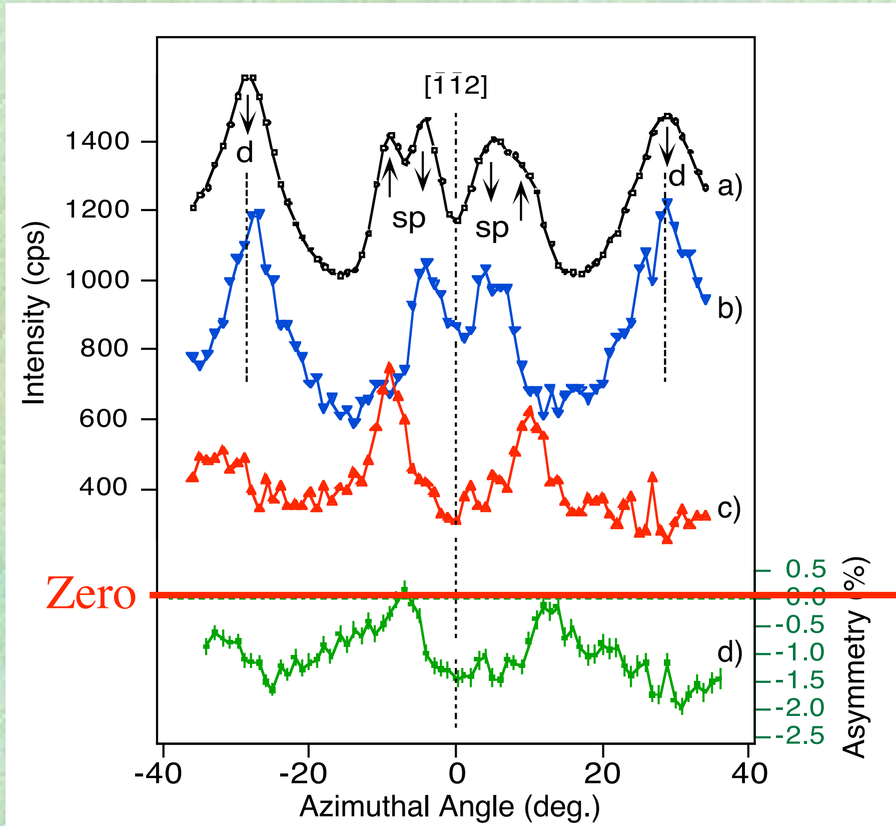


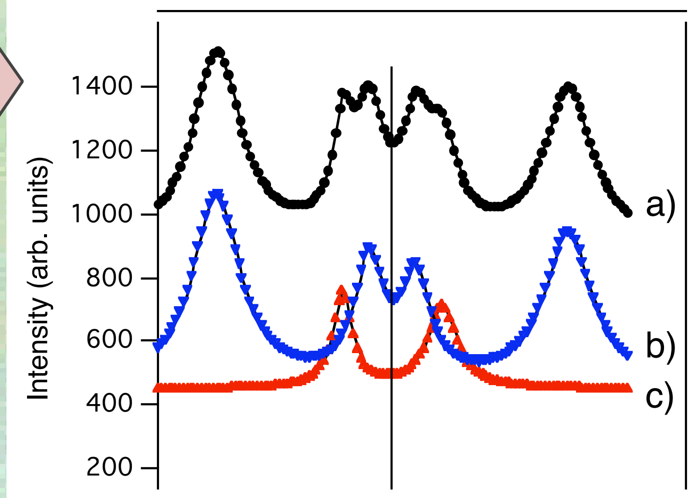


=> We can understand these asymmetry curves !

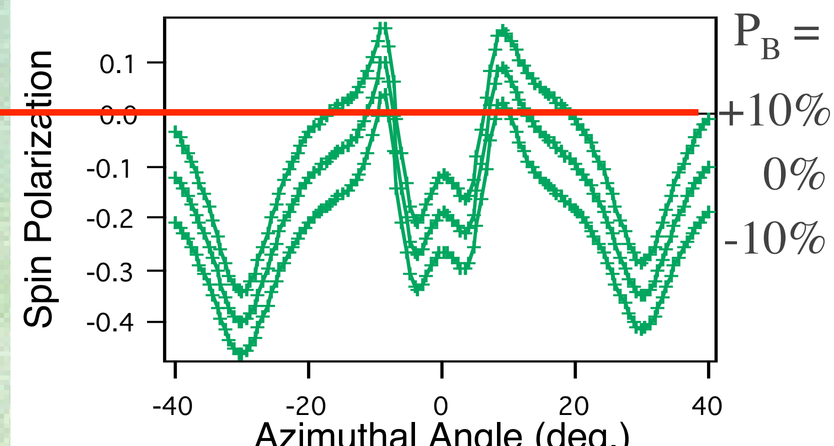
Quantitative Aspects of Spin Polarization Measurements

Modelling Spin Polarization:
6 Lorentzians (2 up, 4 down)
+ constant background (S/B~0.6)





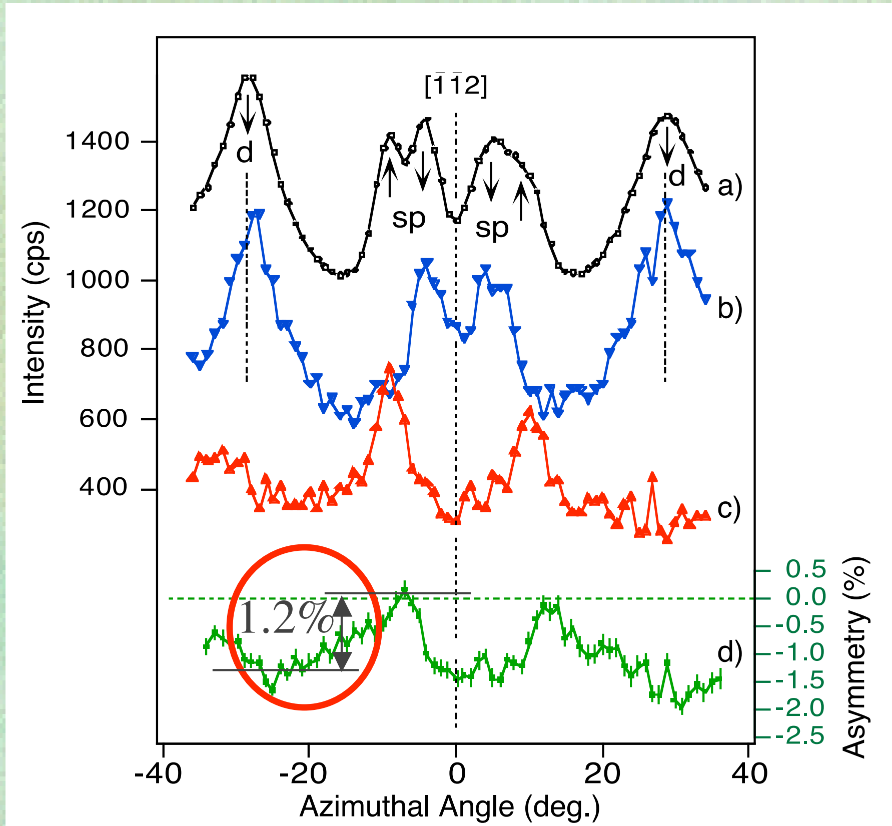
Vary polarization P_B of Background:

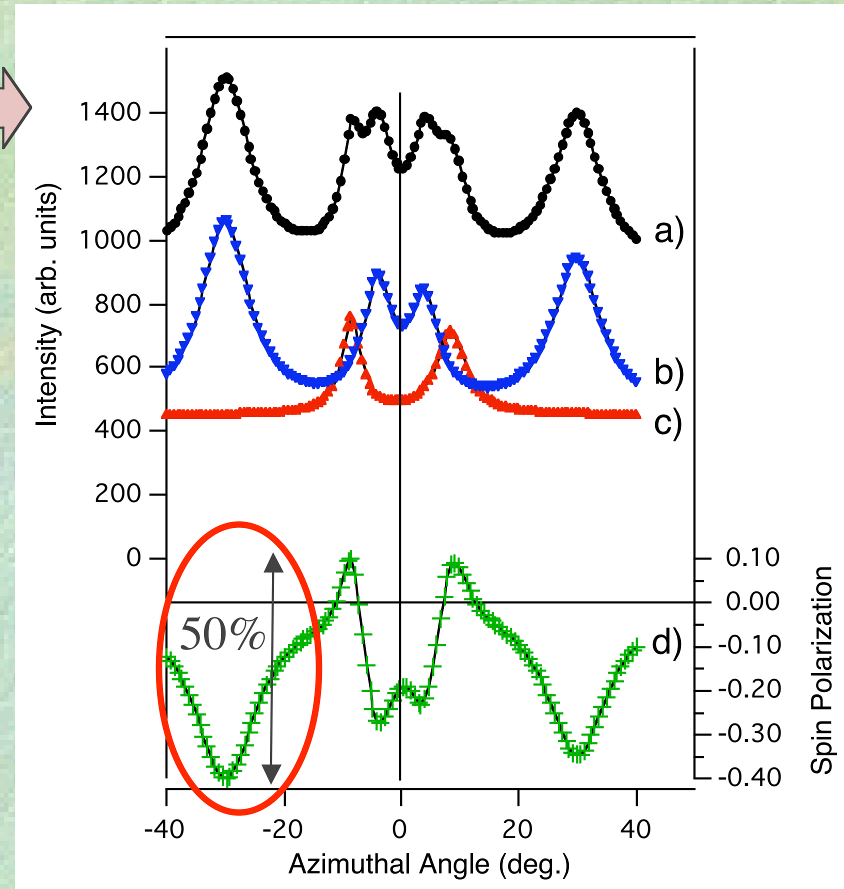


Background is ~ unpolarized !

Quantitative Aspects of Spin Polarization Measurements

Modelling Spin Polarization:
6 Lorentzians (2 up, 4 down)
+ constant background (S/B~0.6)





Polarization P = A / S
S ~ 0.15, but not precisely

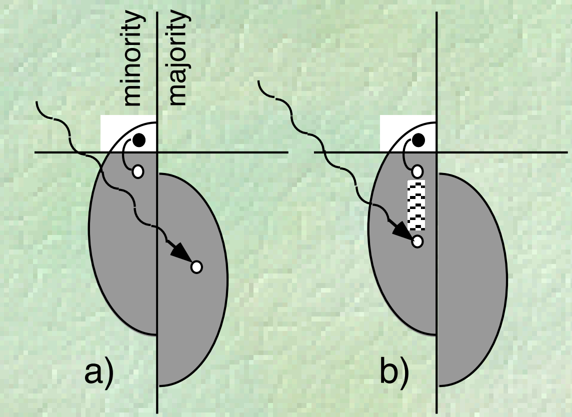
Here: S_{eff} = A / P ~ 0.03

⇒Sample poorly magnetized
$M / M_S \sim 0.15$

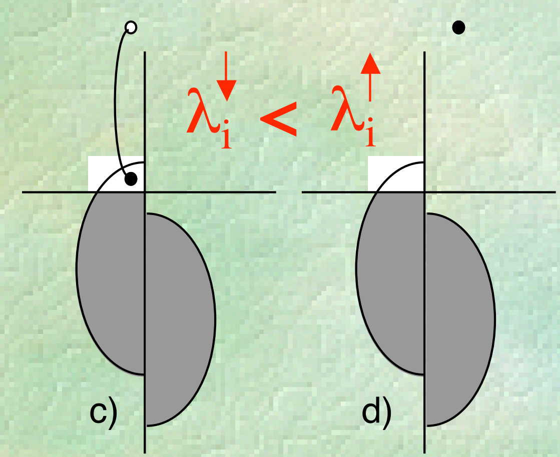
Effects That Can Influence the Measured Spin Polarization

- Spin polarization can be introduced by the photoexcitation process
  Example: Photoemission from GaAs using circularly polarized light
  (optical pumping of spin-orbit split states)
  => spin-polarized electron source !

- Electron correlation effects in the hole state:
  => Spin-dependent self-energies !



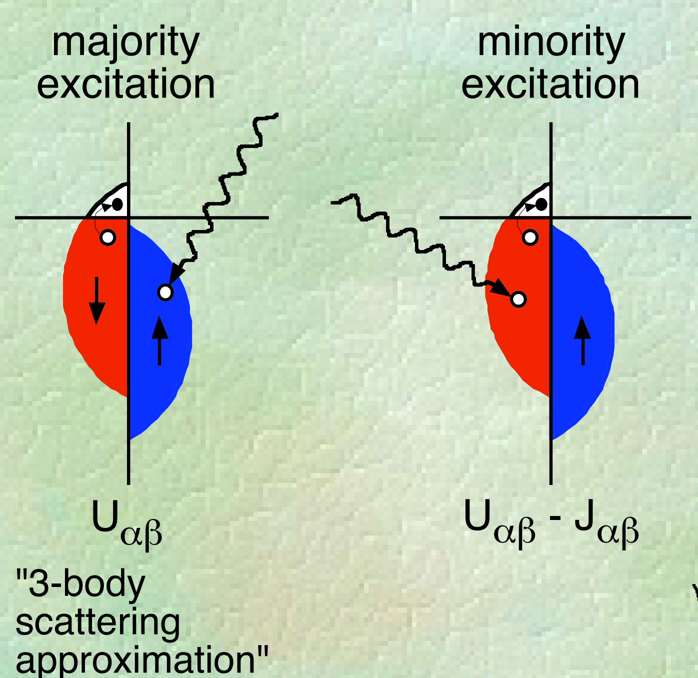
- Spin-dependent photoelectron transport to and through the surface
  => Spin-filter effect !
  and
  => Spin-polarized photoelectron diffraction (exchange scattering, spin-orbit)



Inelastic Mean Free Path λ_i is spin dependent !

Spin-Dependent Self-Energy Effects in Valence Photoemission from Ni

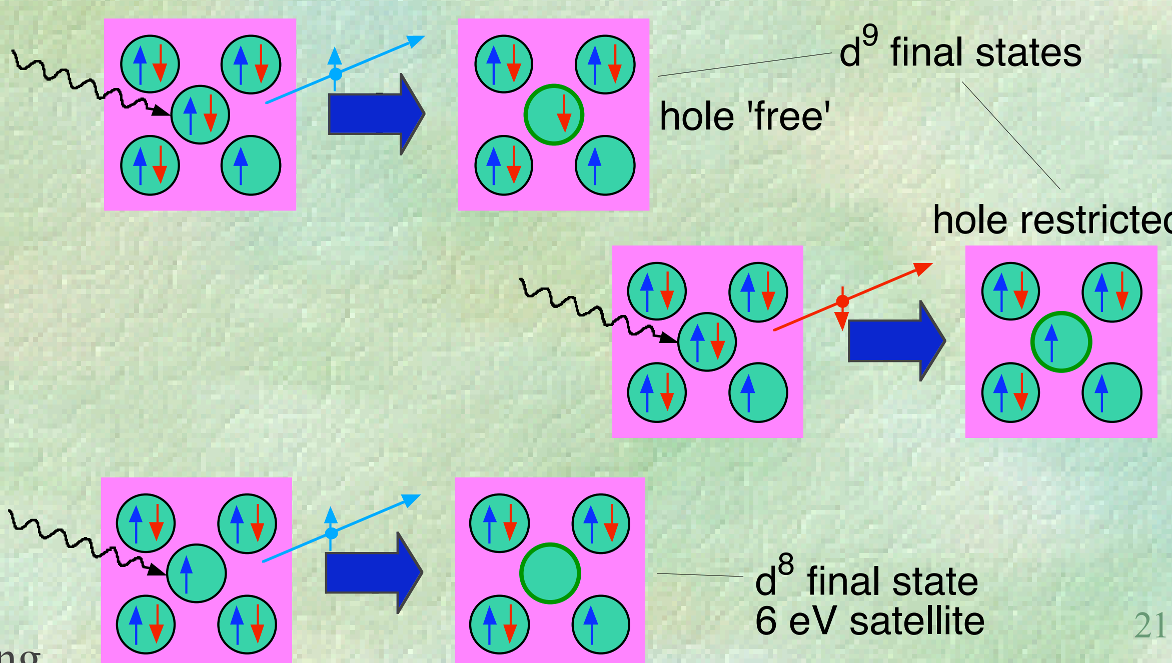
$3d^{9.4}$ → correlation effects in the 3d channel



Pictorial:

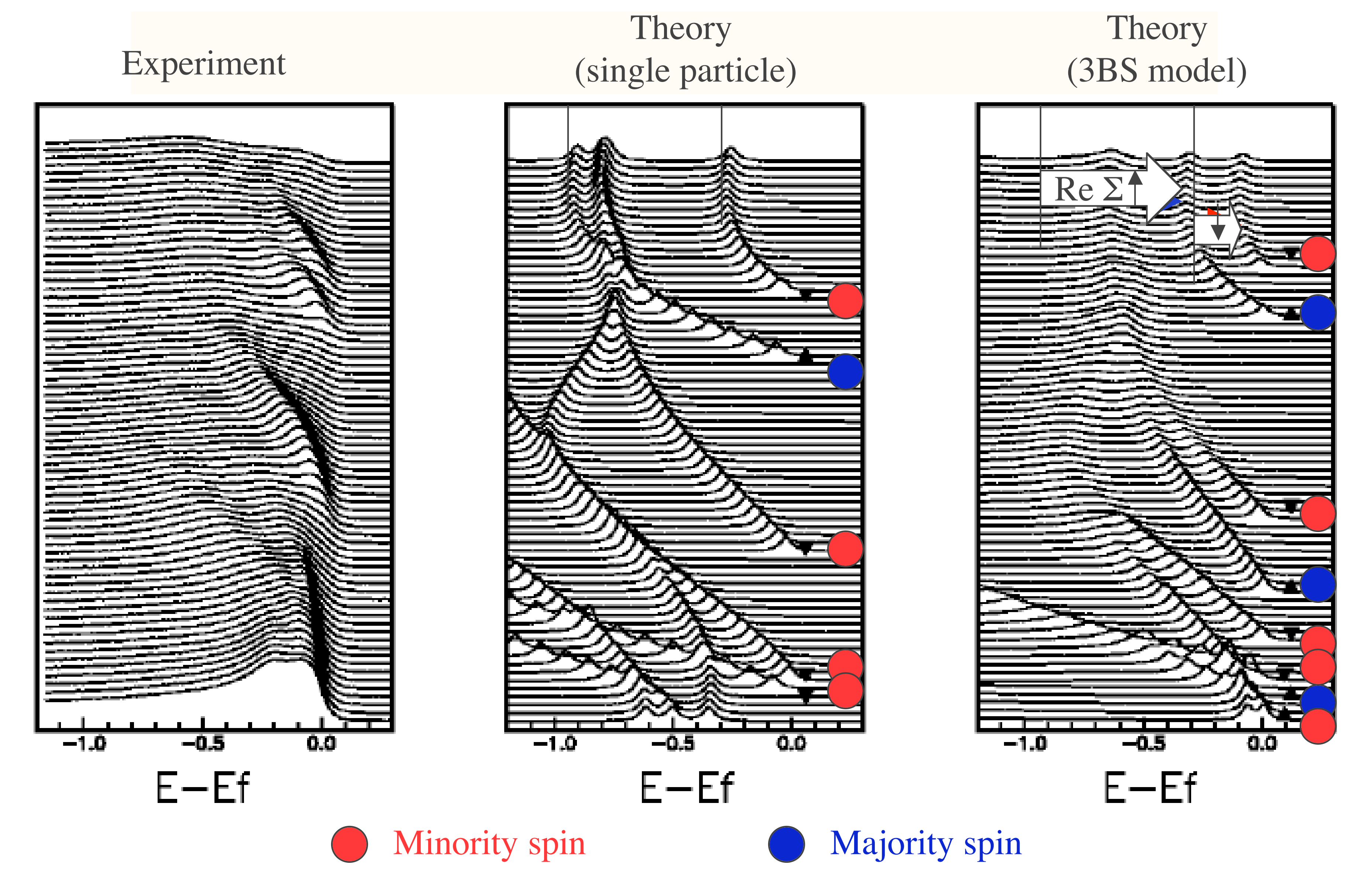
majority photoelectron

minority photoelectron



F. Manghi et al.,
PRL 73, 3129 (1994).

Renormalization of Band Dispersion by e-e Interaction: Ni



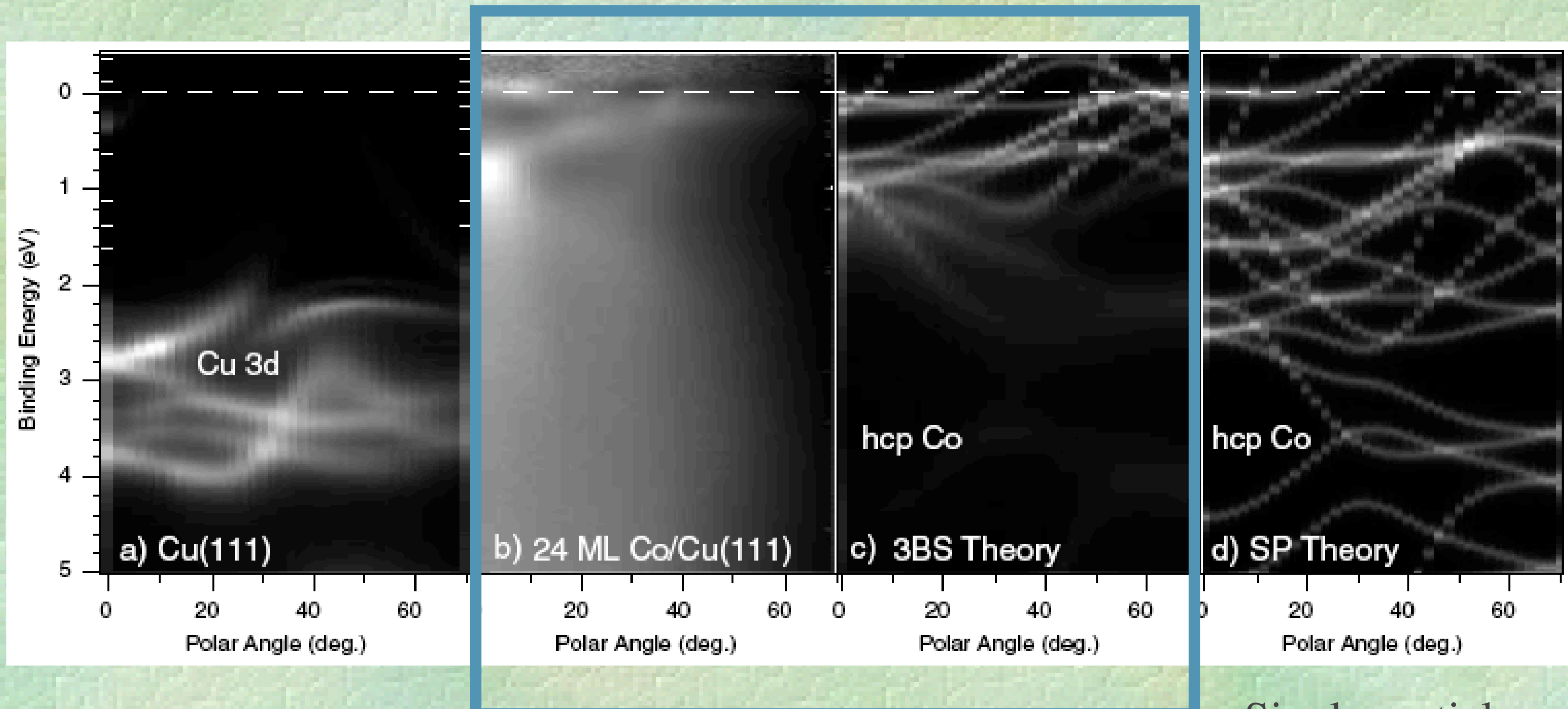
F. Manghi et al., PRB 59, R10409 (1999)

Even Stronger Renormalization in Cobalt

Sample:

Co(0001)

Cu(111)

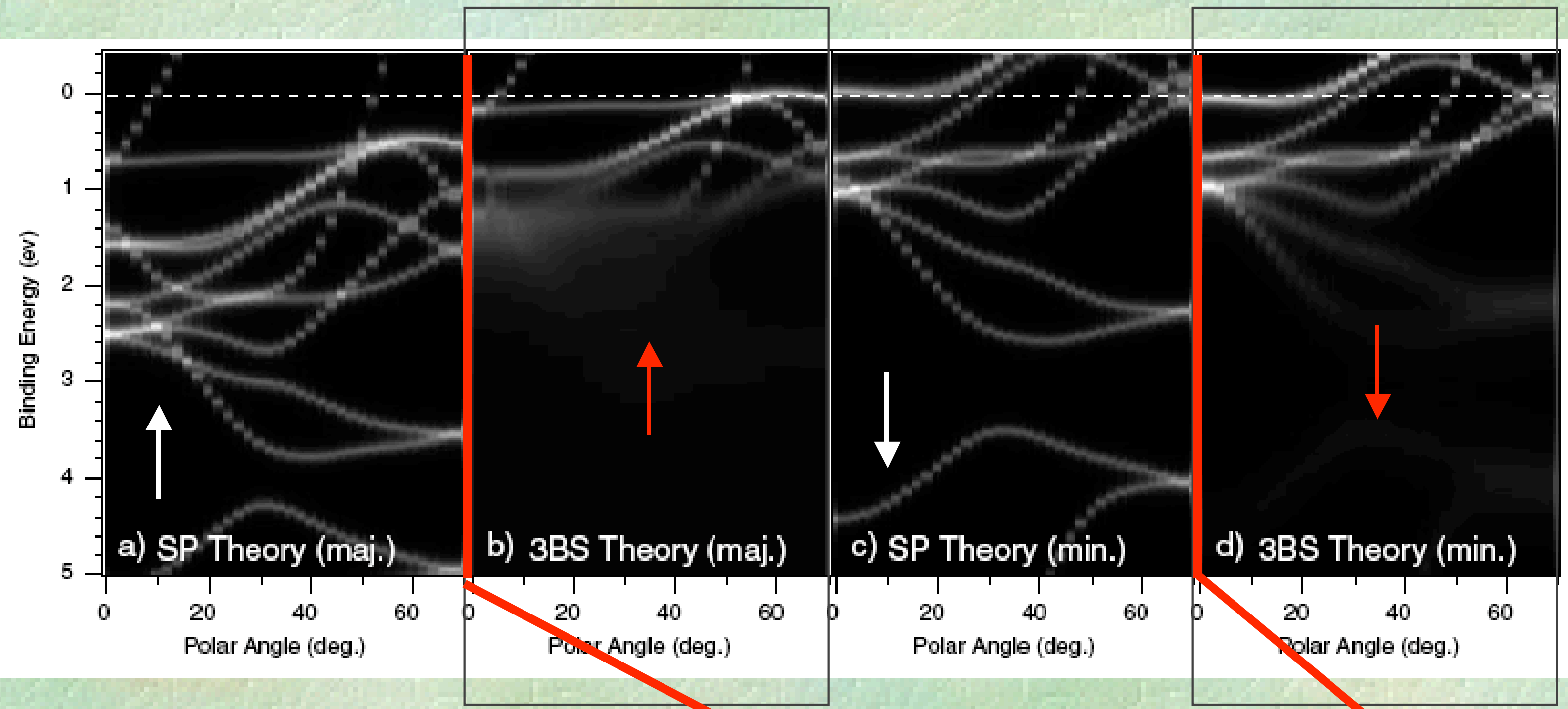


Single particle

Strong many-body effects !

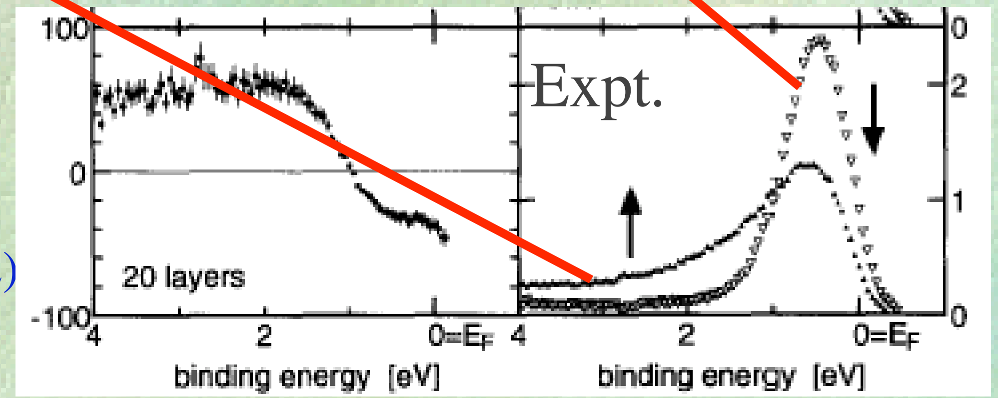
S. Monastra et al., PRL 88, 236402 (2002)

Many-Body Effects are Strongly Spin Dependent



⇒ Measured spin-polarization in Co should be much smaller than expected from band structure calculations !

S. Monastra et al., PRL 88, 236402 (2002)



M. Getzlaff et al., JMMM 161, 70 (1996)

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

VOLUME 77, NUMBER 16 PHYSICAL REVIEW LETTERS 14 OCTOBER 1996

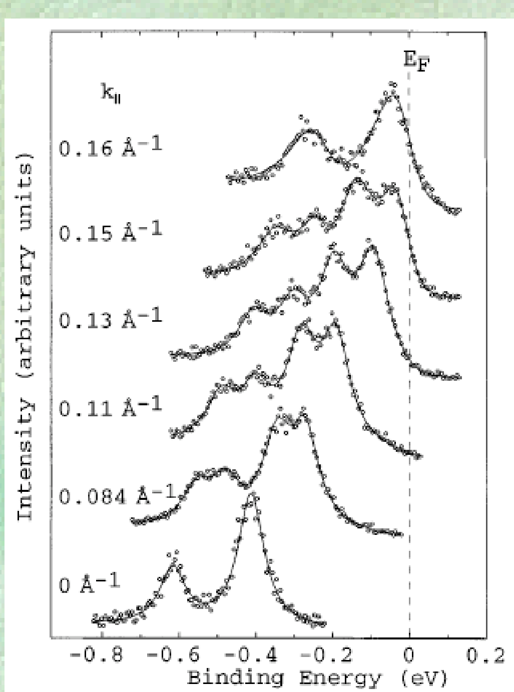
Spin Splitting of an Au(111) Surface State Band Observed with Angle Resolved Photoelectron Spectroscopy

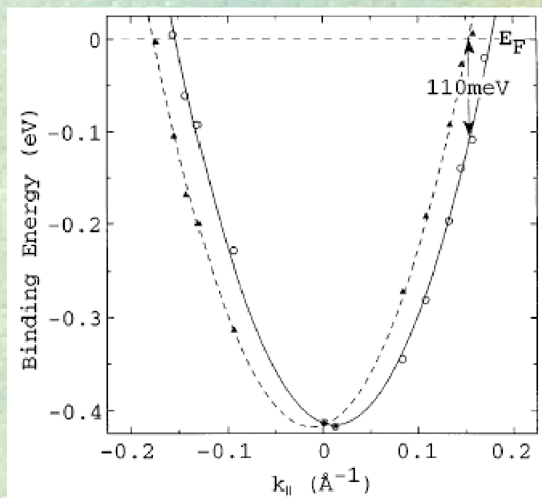
S. LaShell, B. A. McDougall, and E. Jensen
Physics Department, Brandeis University, Waltham, Massachusetts 02254
(Received 19 July 1996)

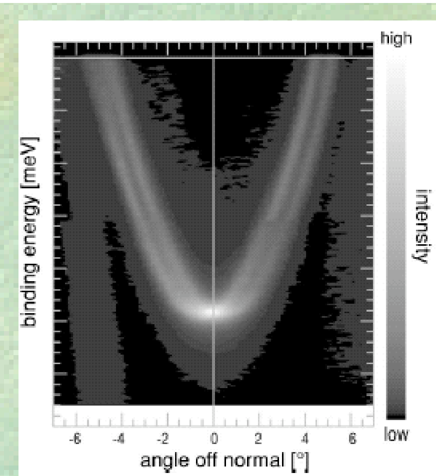
PHYSICAL REVIEW B, VOLUME 63, 115415

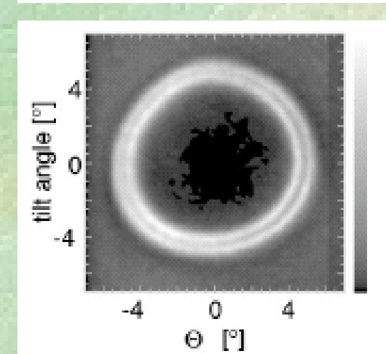
Direct measurements of the *L*-gap surface states on the (111) face of noble metals by photoelectron spectroscopy

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)





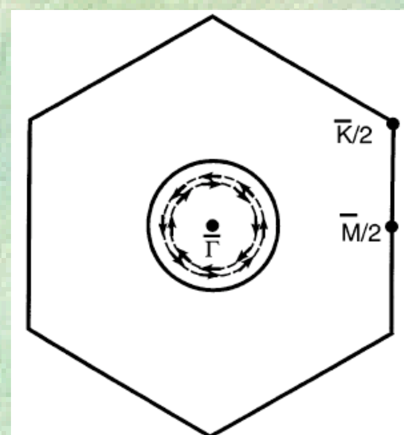




Scienta 2002 spectrometer

hν=21.21eV

hν=11.62eV

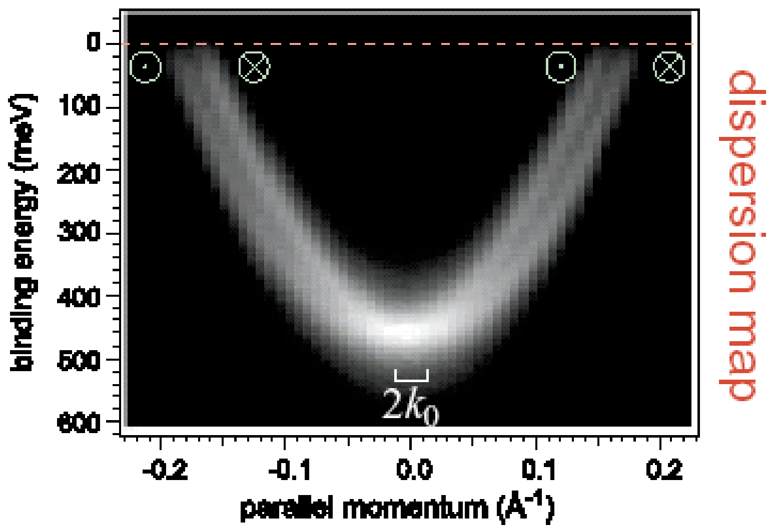


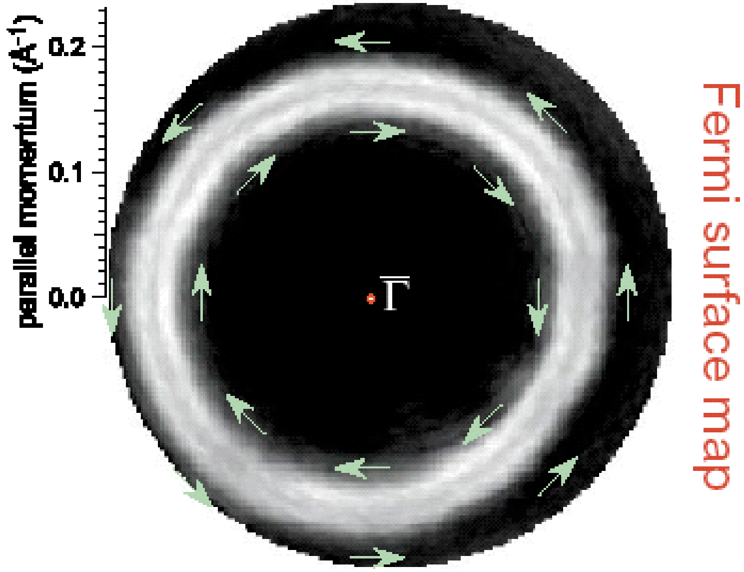
=> spin-resolution is a challenging task

The Shockley surface state on Au(111)

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

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





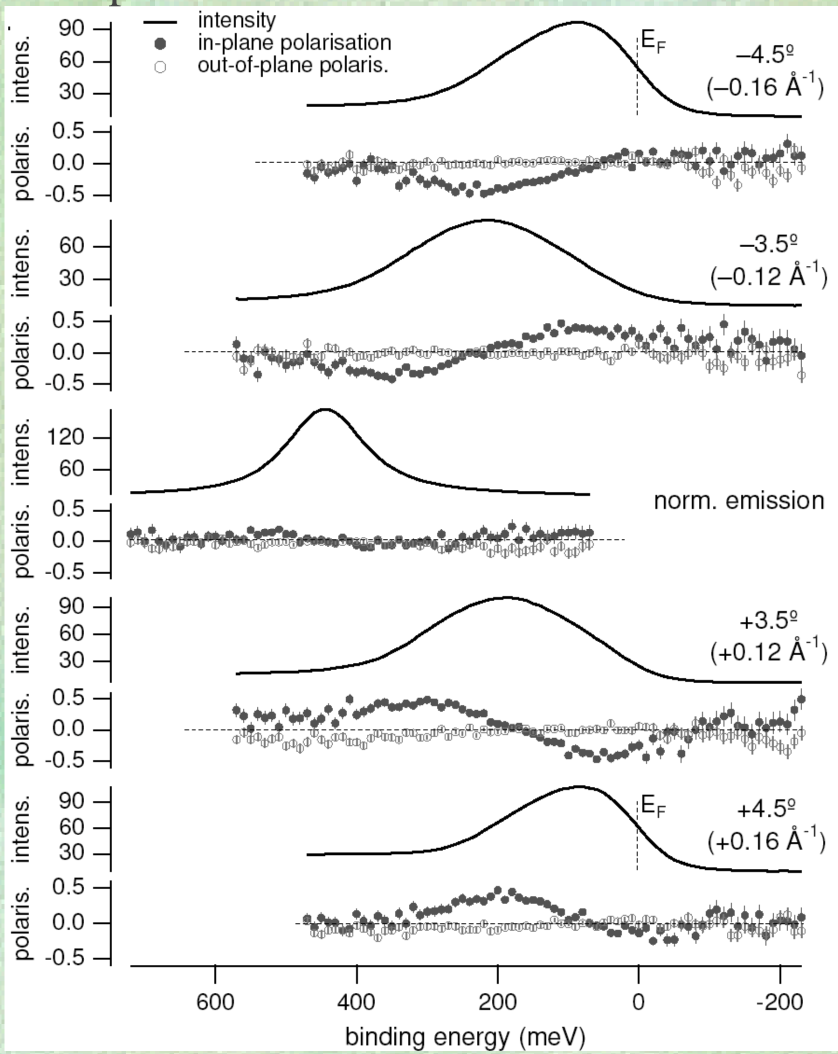
$2k_0 = 0.026$ Å^{-1}	$E_B = 470$ meV	$k_F = 0.173$ Å$^{-1} \pm k_0$	$m^* = 0.24\, m_e$

Theory: spin-orbit coupling

$$H_{SOC} = \frac{\mu_B}{2c^2}(\vec{v} \times \vec{E}) \cdot \vec{\sigma} \qquad E^{\uparrow\downarrow}(k) = E_0 + \frac{(k \pm k_0)^2}{2m^*}$$

Quantitative Spin Polarimetry on the Au(111) Surface State

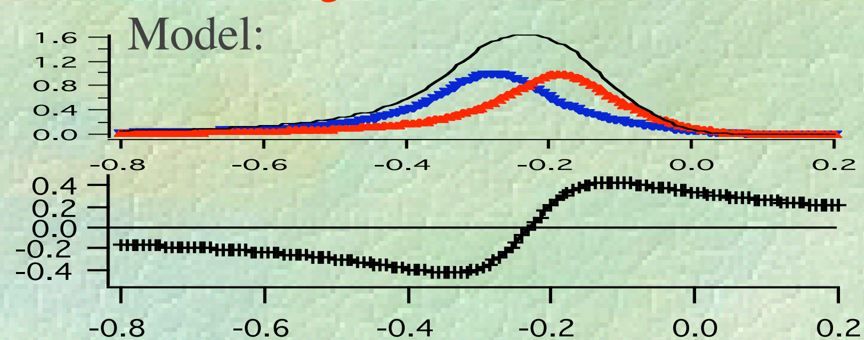
Experimen:



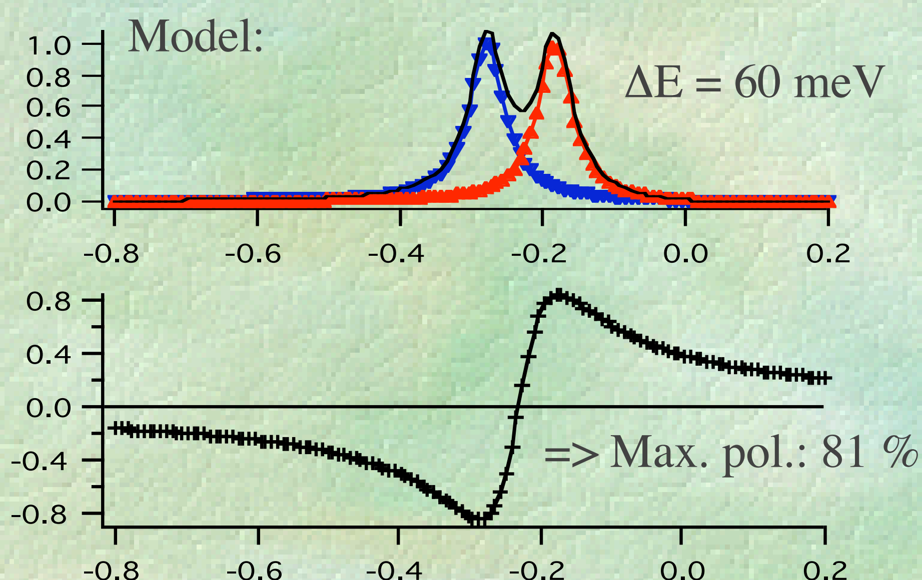
Spin-resolved experiment:

Energy resolution = 120 meV

Angular resolution = 1.2°



=> Max. polarization: 40 %

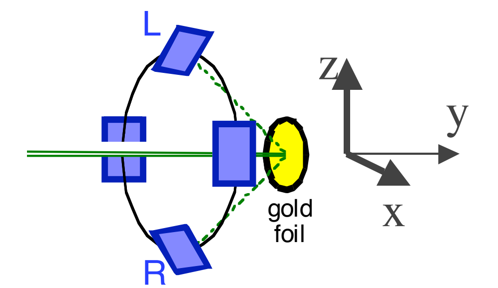


… and Recovering the Spin-Resolved Spectra

Here, sample is not magnetized !
=> Cross asymmetries cannot me obtained !

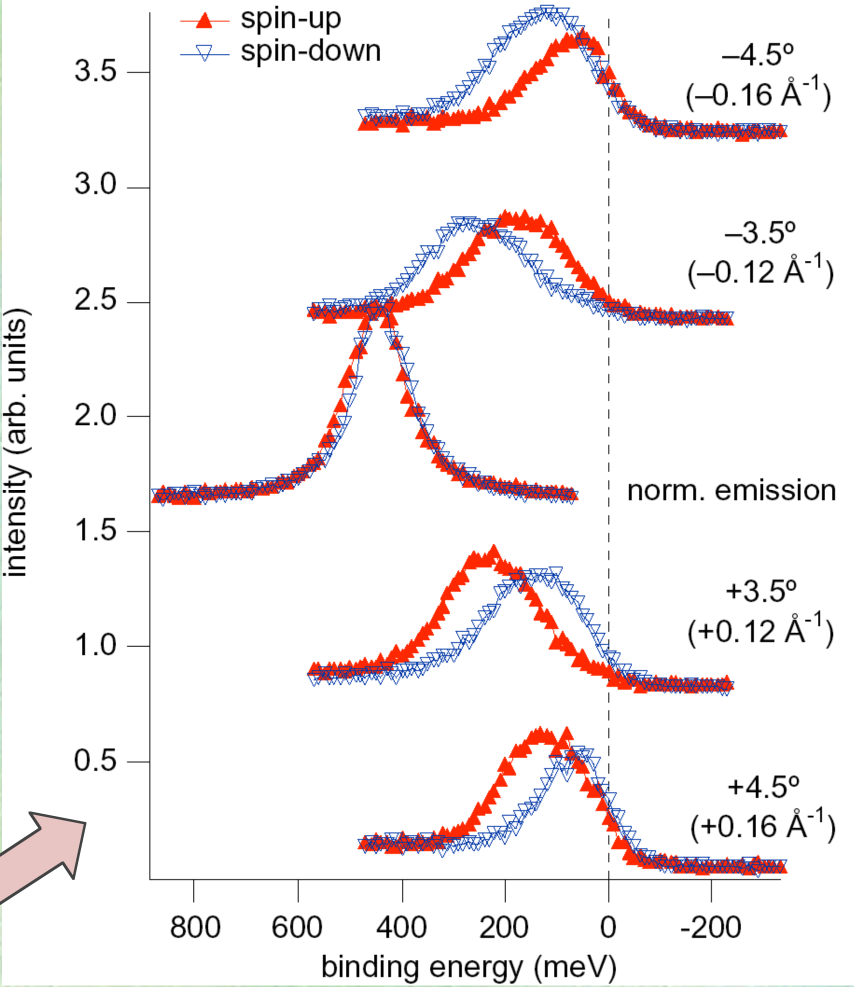
$$P = \frac{1}{S_{eff}} \frac{(I_L - \eta I_R)}{(I_L + \eta I_R)}$$

Use empirical sensitivity factors η
to remove instrumental asymmetries

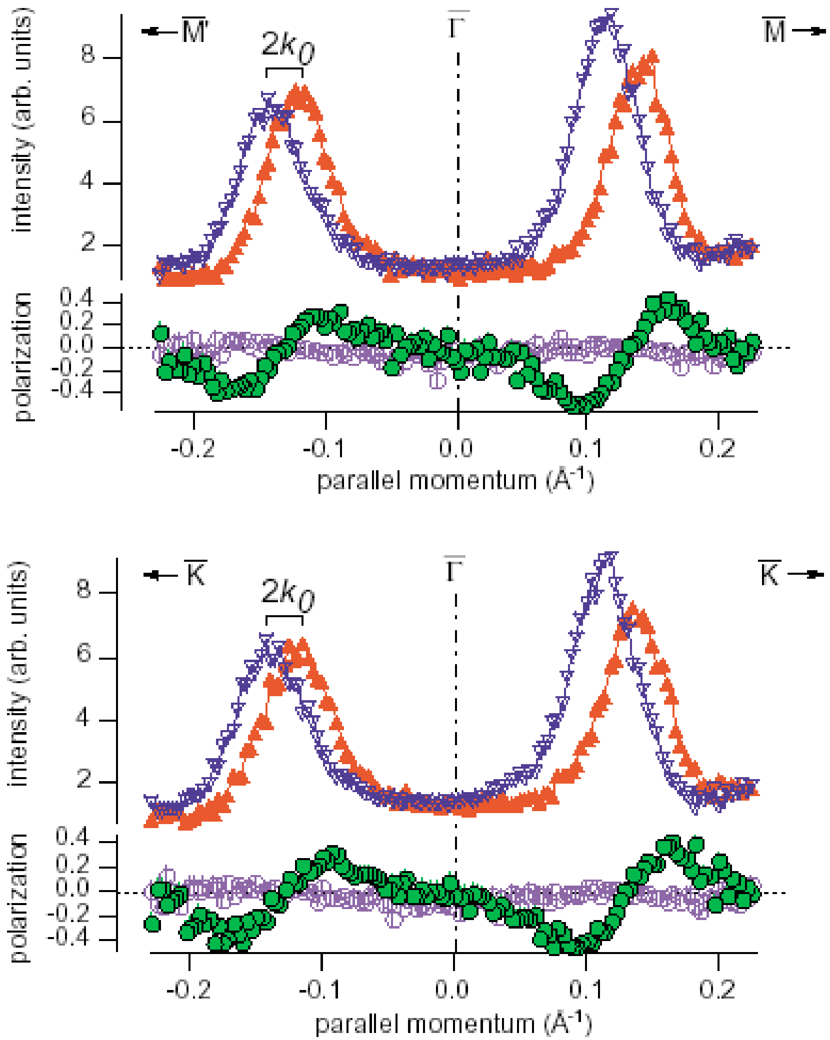


two orthogonal axes are spanned
by two pairs of detectors

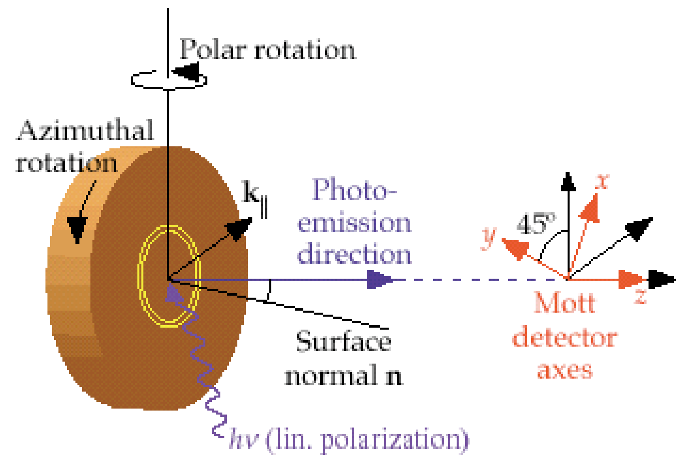
$$I_{\uparrow,\downarrow}(E,\boldsymbol{k}) = I_M(1 \pm P_I(E,\boldsymbol{k}))/2.$$

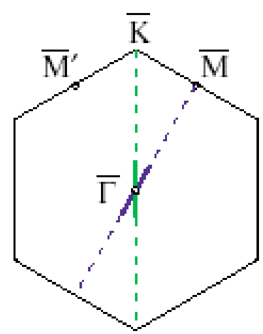


Spin-resolved momentum distribution curves of the surface state on Au(111)



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

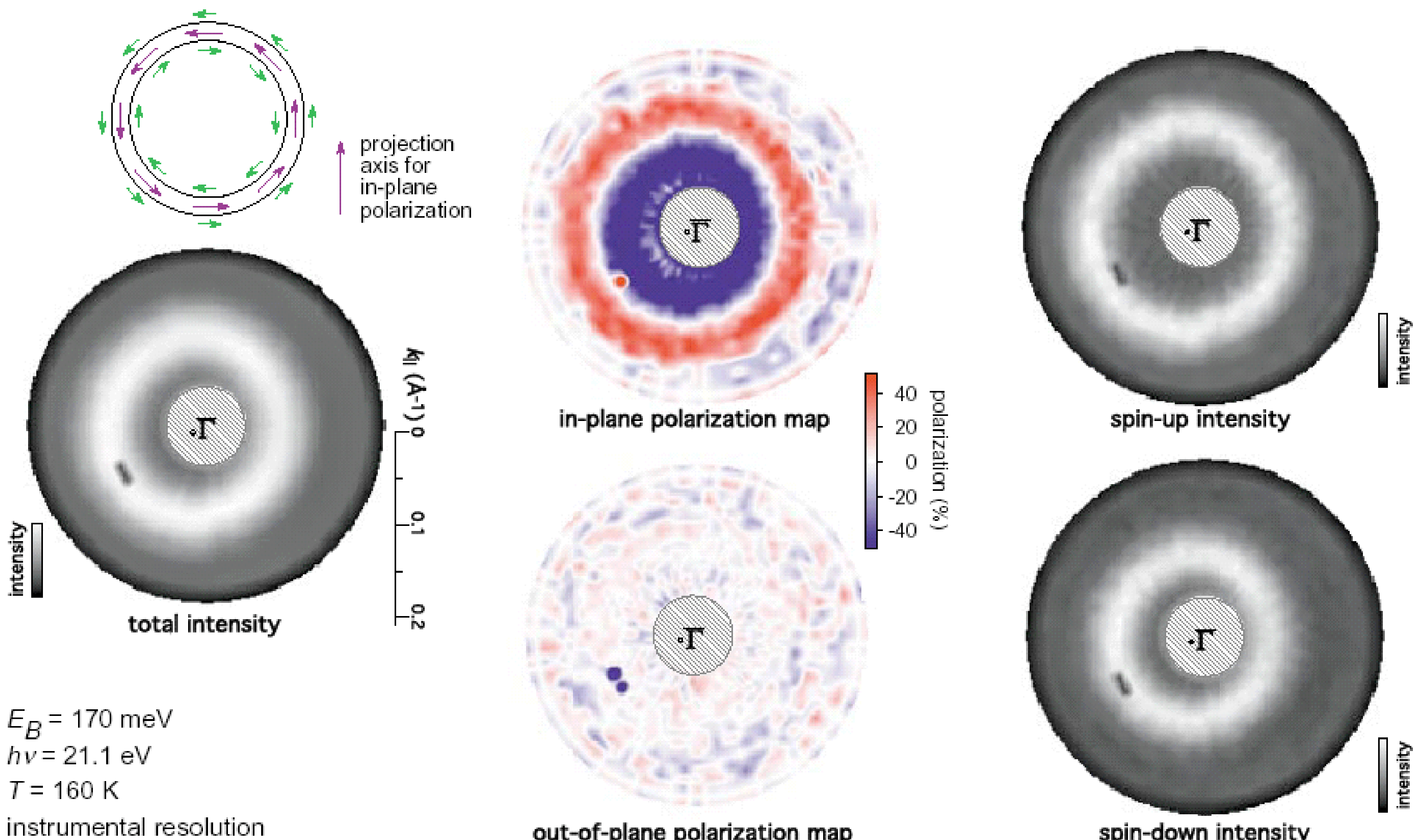




Surface Brillouin zone

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

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



E_B = 170 meV
$h\nu$ = 21.1 eV
T = 160 K
instrumental resolution
ΔE=120 meV, Δϑ=1.8° (FWHM)

=> First spin-resolved "Fermi surface" map

Conclusions

- Spin-polarized photoemission is still a tedious experiment !
  (ca. 10^3 times slower than ARPES)

  Is it worth the effort ?

  Yes !
- Spin-resolution can give definite answers to difficult questions
  (e.g. spin-orbit character in the Au(111) surface state
  and its detailed spin structure)
- Spin resolution can markedly enhance the effective energy resolution for spin-split peaks, even if there individual peaks are broad.
- The interpretation of absolute spin polarization values needs to take into account various effects that can enhance / reduce spin polarization.