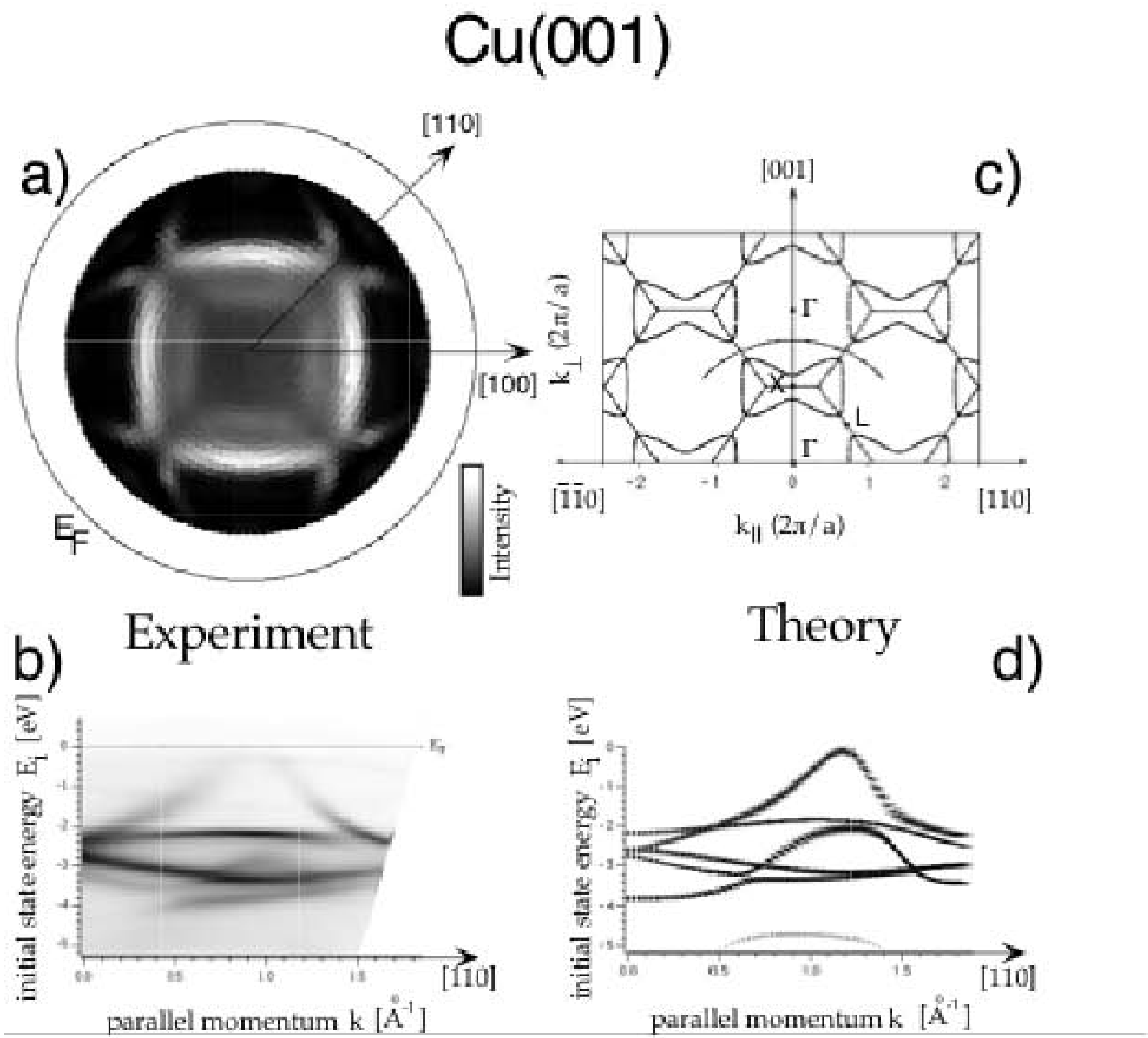
# Photoemission from Valence Bands, Dispersion and Fermi Surface Mapping

*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**

- Electron-Electron Interaction: Weak Effects in Photoemission from Cu
- Electron-Electron Interaction: Strong Effects in Photoemission from Ni and Co
- Electron-Phonon Interaction: Renormalization of Dispersion by Phonons
- Applications: Observation of a Giant Kohn Anomaly on H/Mo(110)
- Applications: Photoemission from High and Low $T_c$ Superconductors
- Laser-Photoemission with Ultrahigh Energy Resolution

# Weak Electron-Electron Interaction Effects in Photoemission from Cu





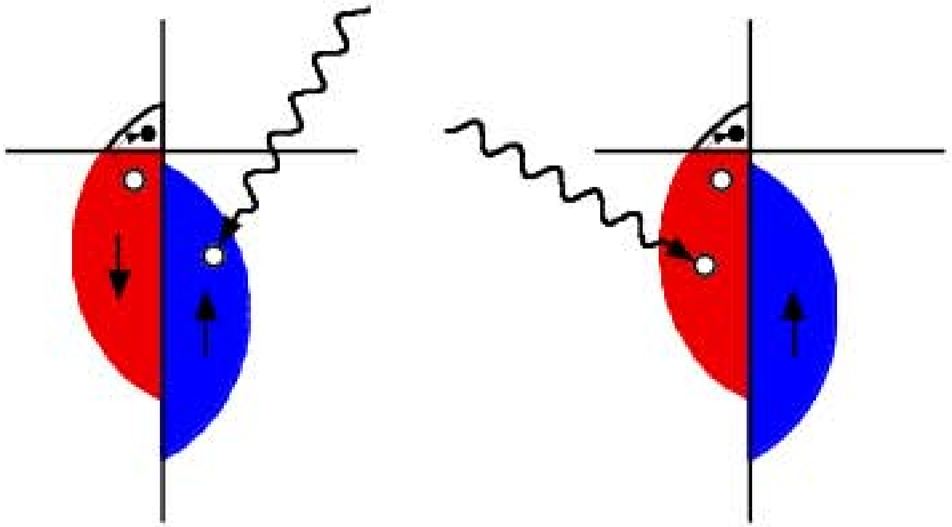



Courtesy P. Aebi, University of Neuchatel

# Valence Photoemission from Ni

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

majority excitation | minority excitation



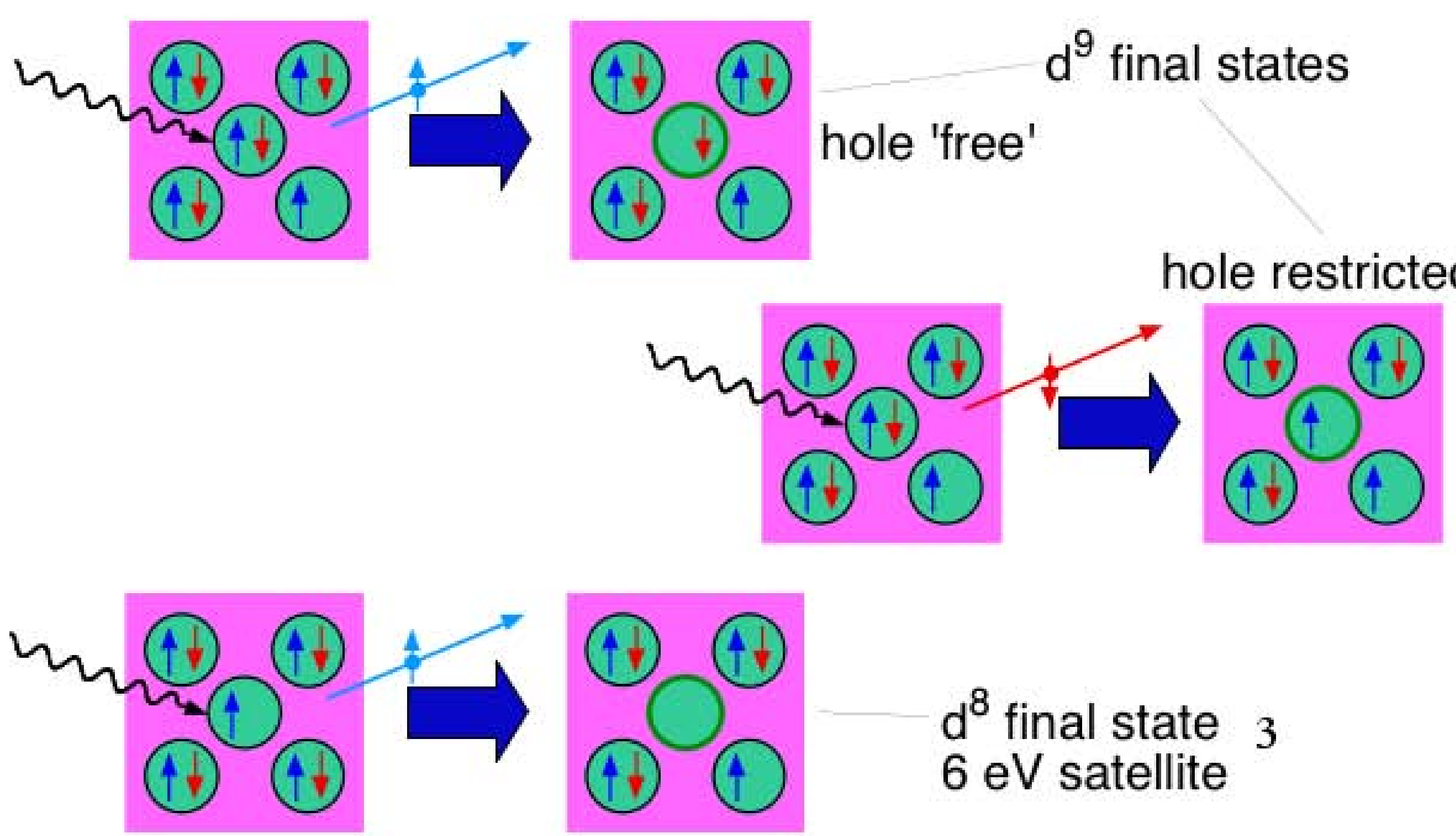
$U_{\alpha\beta}$ | $U_{\alpha\beta} - J_{\alpha\beta}$

"3-body scattering approximation"

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

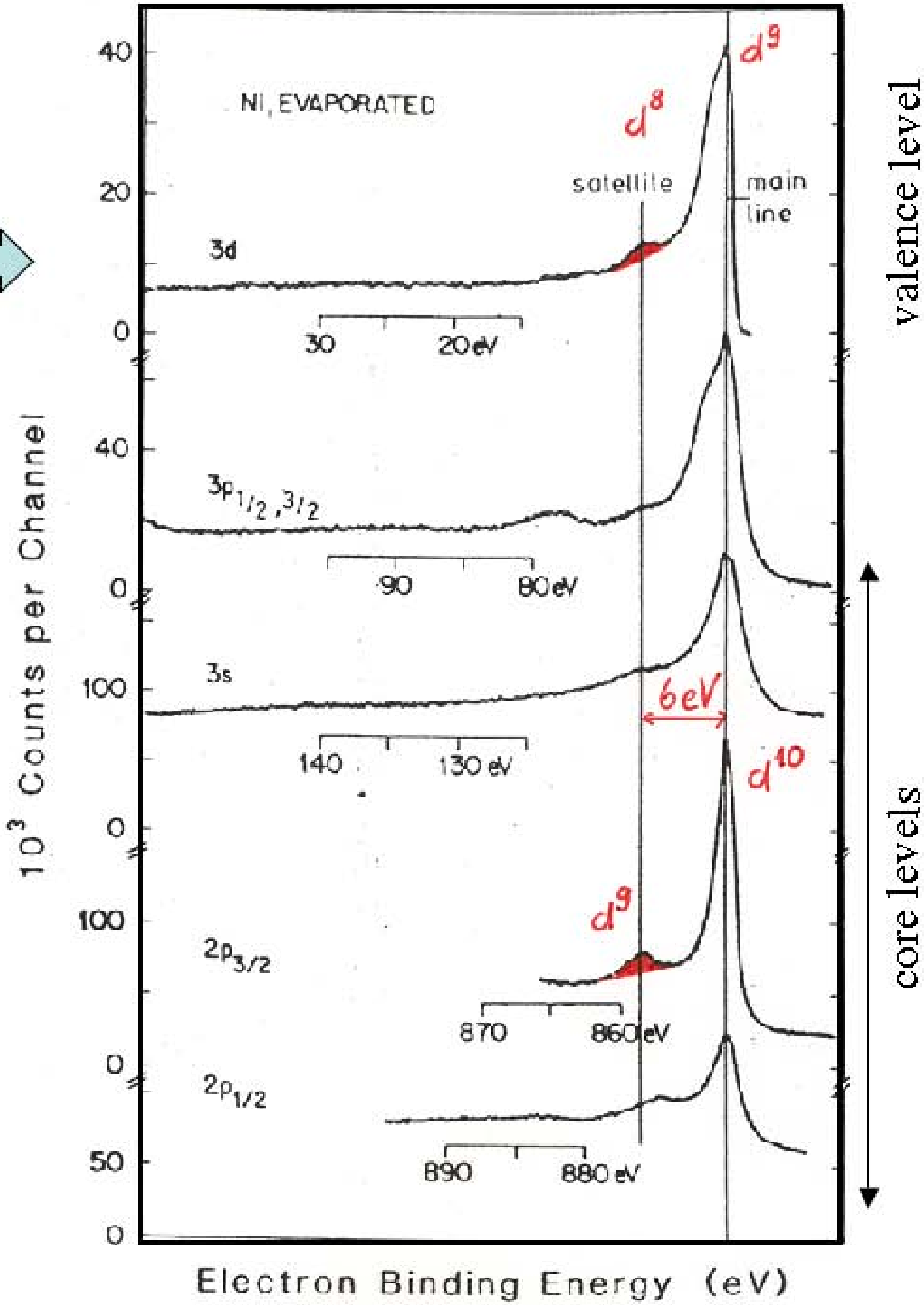
Pictorial:

majority photoelectron | minority photoelectron

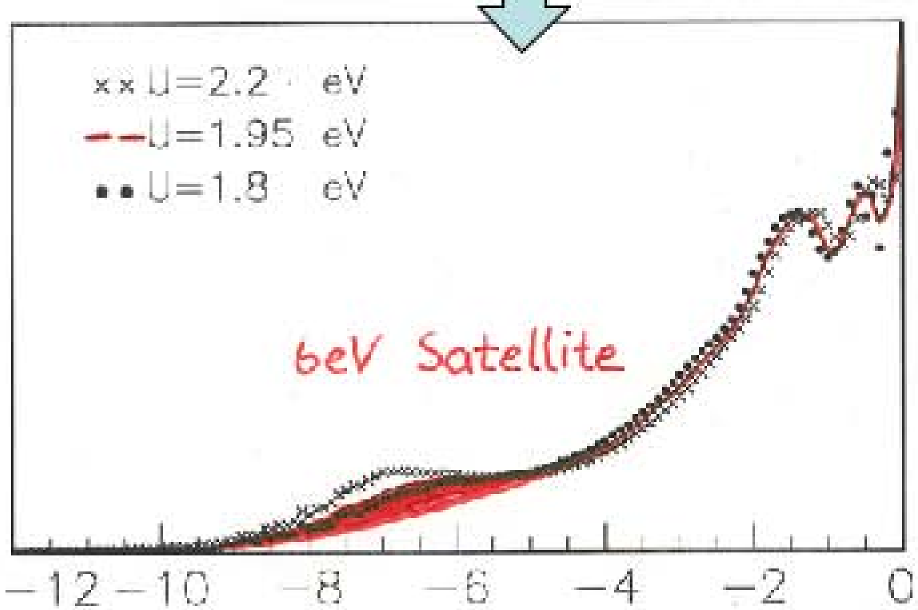


# The 6 eV Satellite in Ni Metal

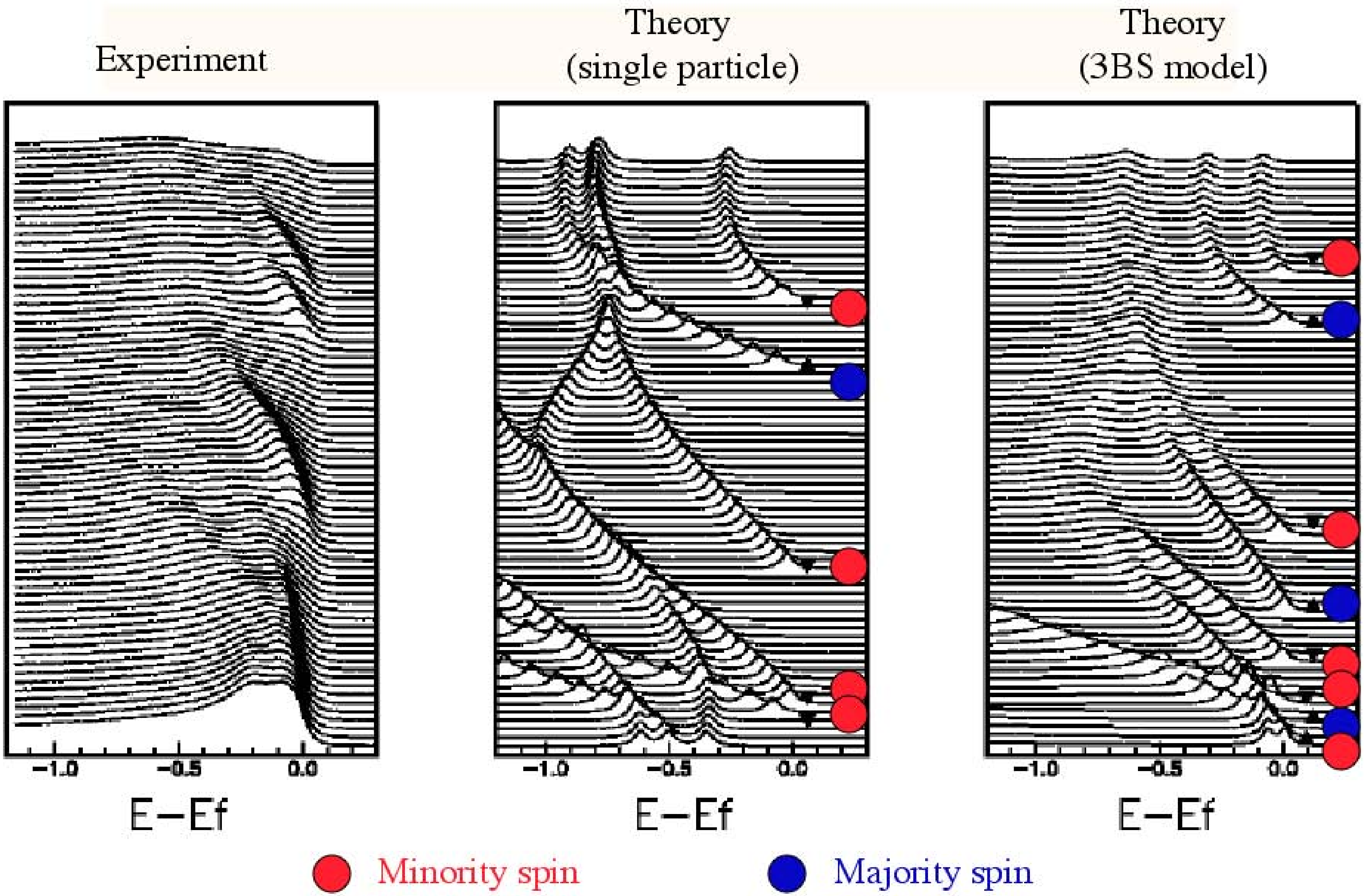
Experiments: Each photohole is accompanied by a 6 eV satellite
(S. Hüfner, Photoelectron Spectroscopy (Springer, Berlin 1995))




Theory: 3BS Model
(F. Manghi et al., PRB 59, R10409 (1999))

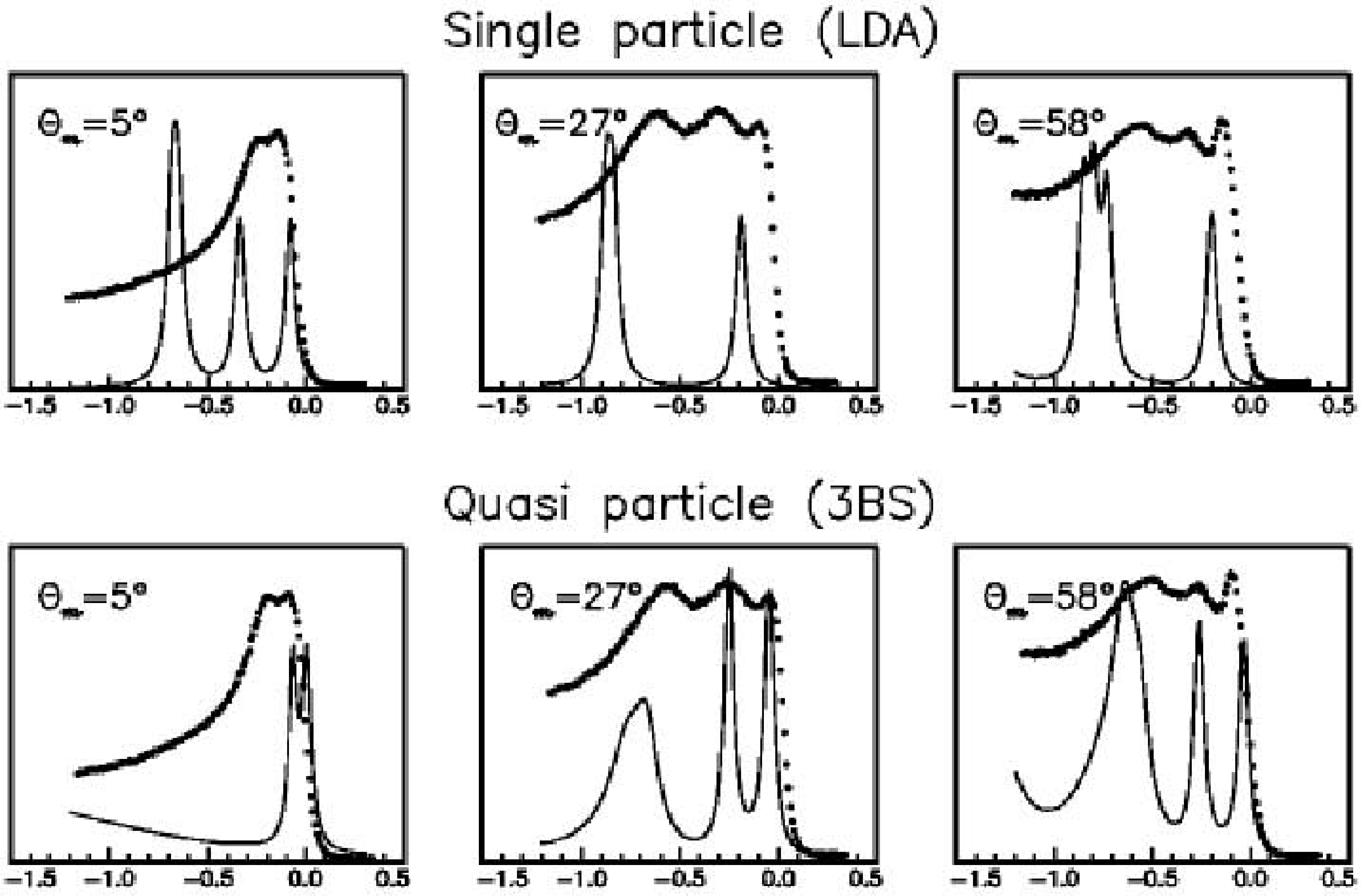


# Renormalization of Band Dispersion by e-e Interaction: Ni




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

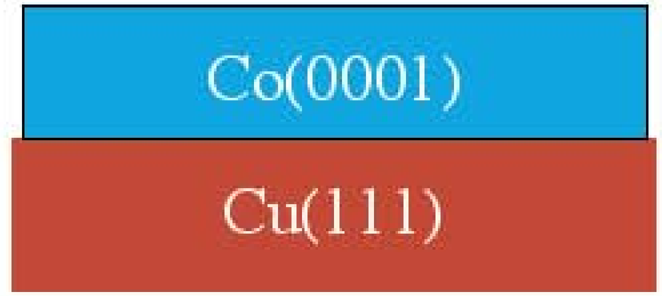
# Quantitative Comparison of e-e Interaction Effects in Ni

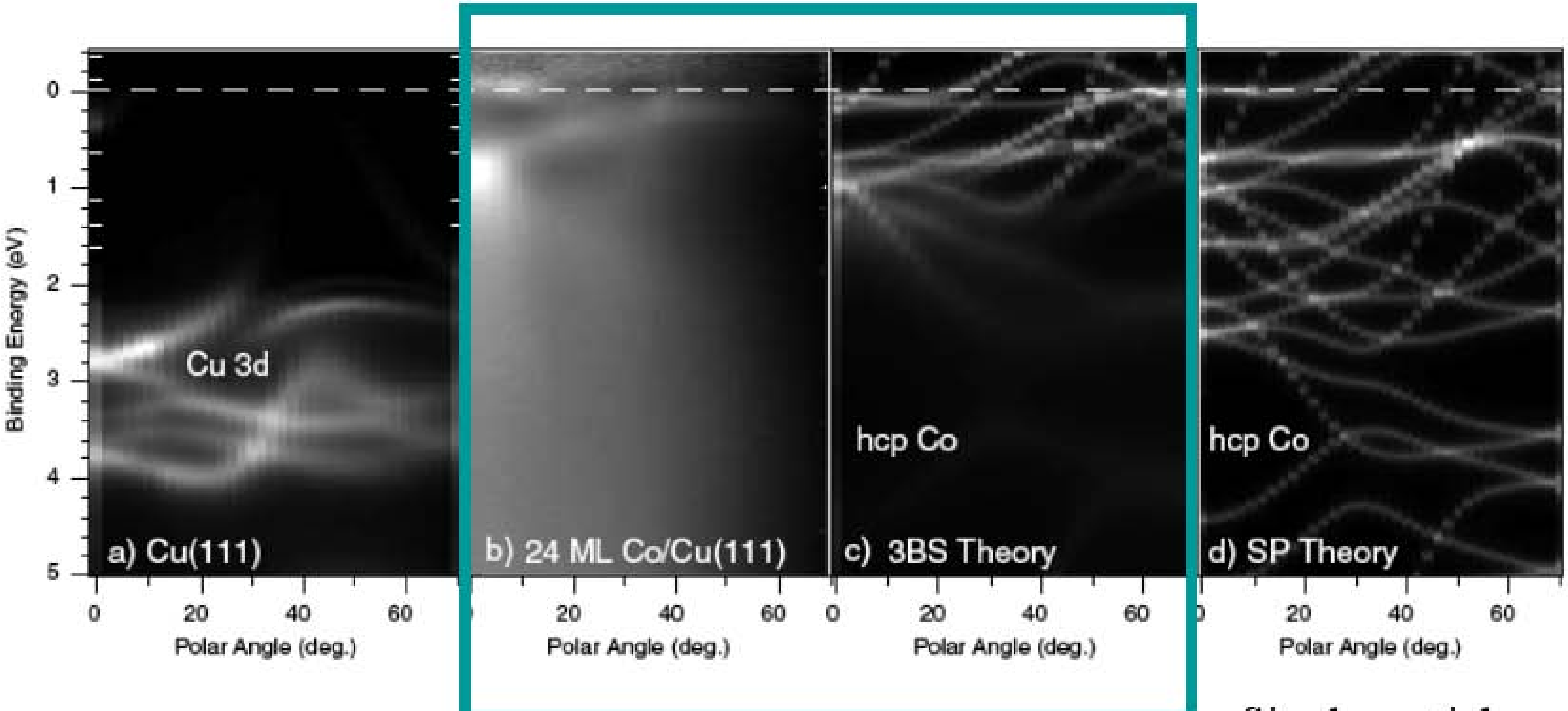



F. Manghi et al., PRB 59, R10409 (1999)

# Even Stronger Renormalization in Cobalt

Sample:



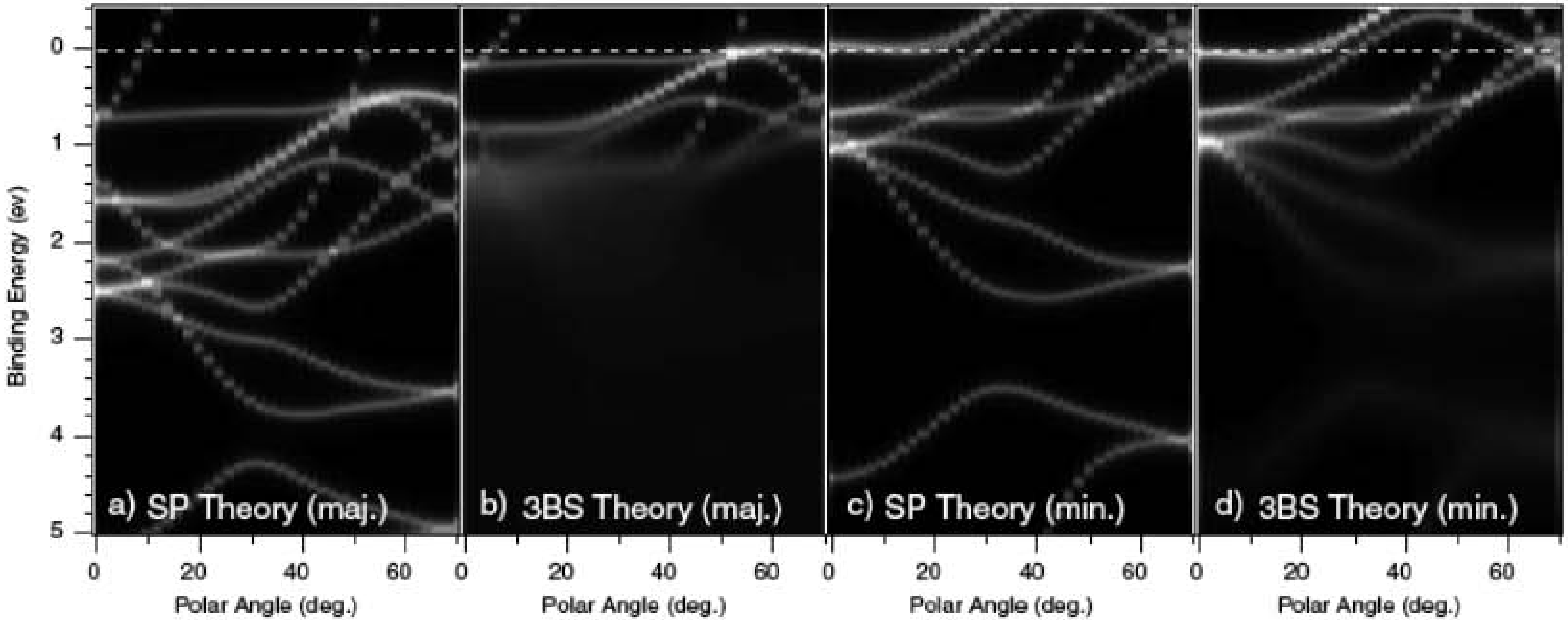

Single particle

Strong many-body effects !



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

# Many-Body Effects are Strongly Spin Dependent




Majority spin

Minority spin





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

# Electron-Phonon Interaction: Renormalization of Dispersion by Phonons

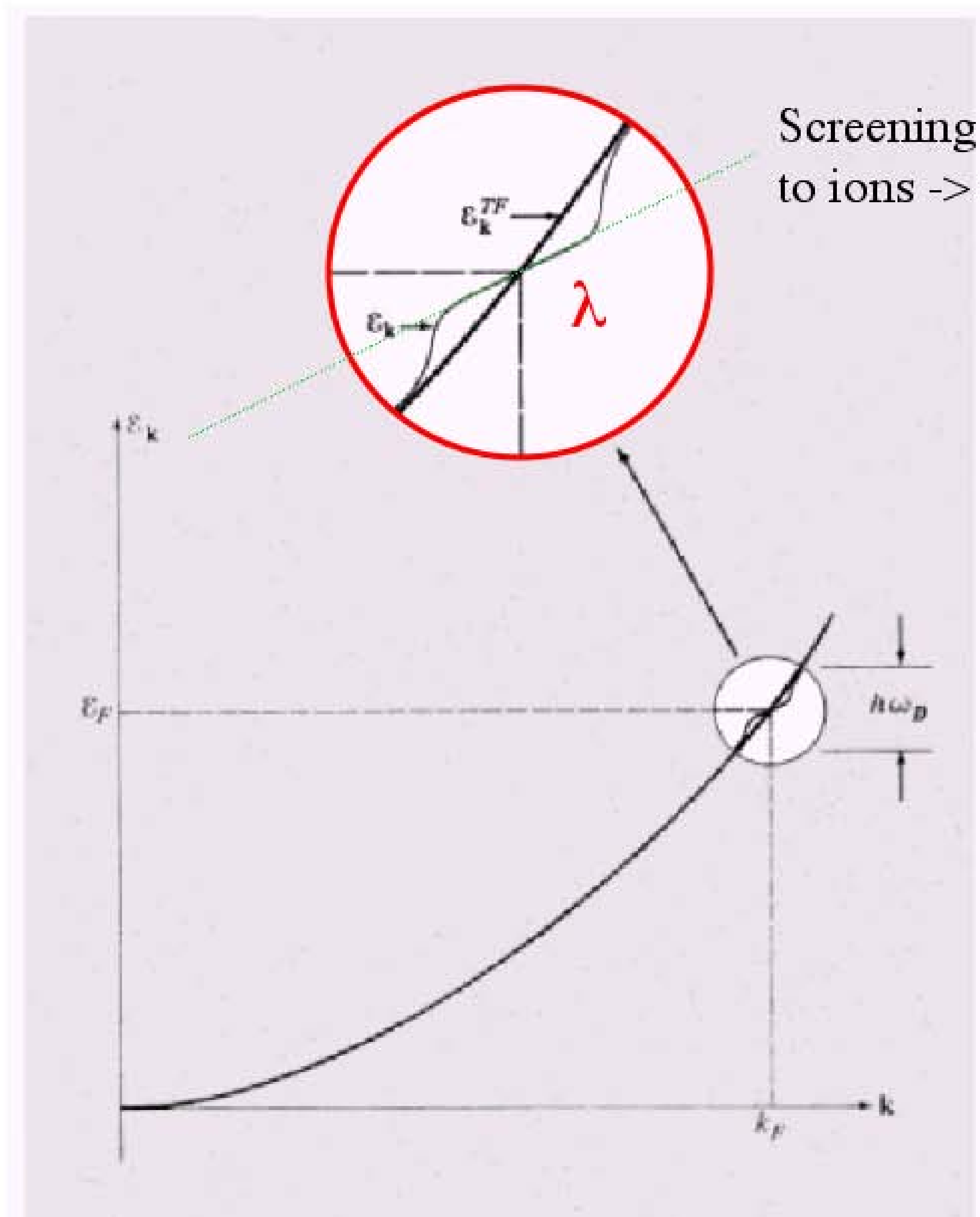
λ
electron-phonon coupling constant

Renormalization of m* by

$Z^{-1} = 1+\lambda$

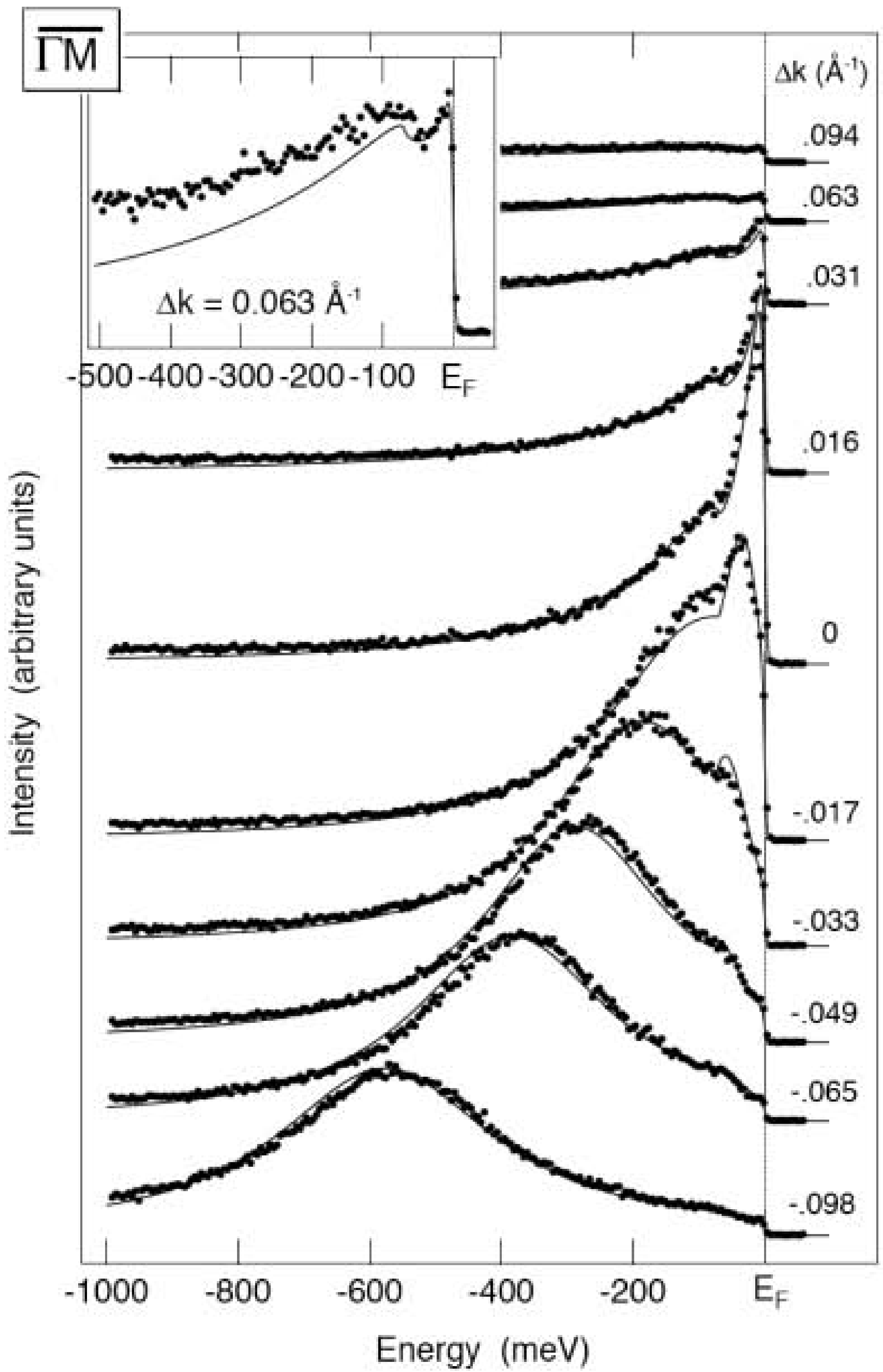
Some values for λ:

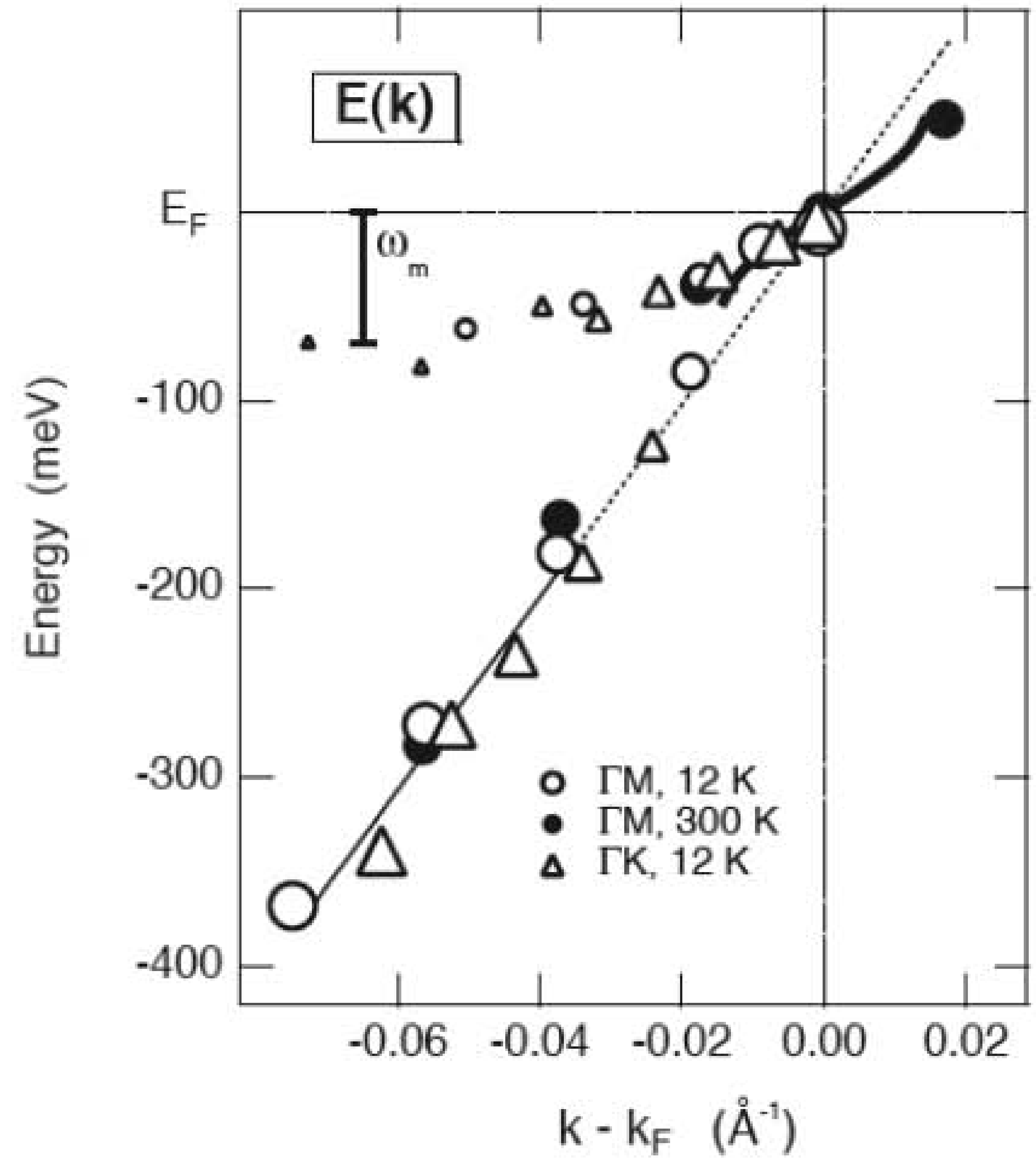
Cu 0.15
Be 0.24
Pb 1.50




Ashcroft, Mermin
*"Solid State Physics"*

# Observation of m* Renormalization in Beryllium

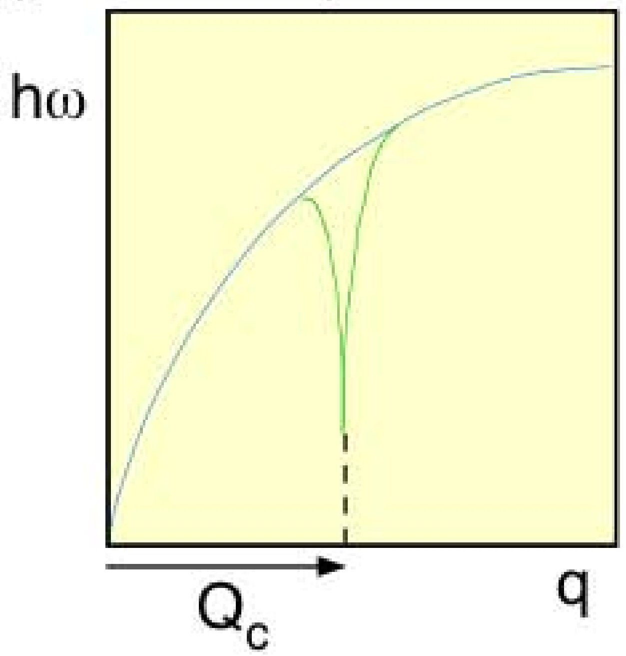


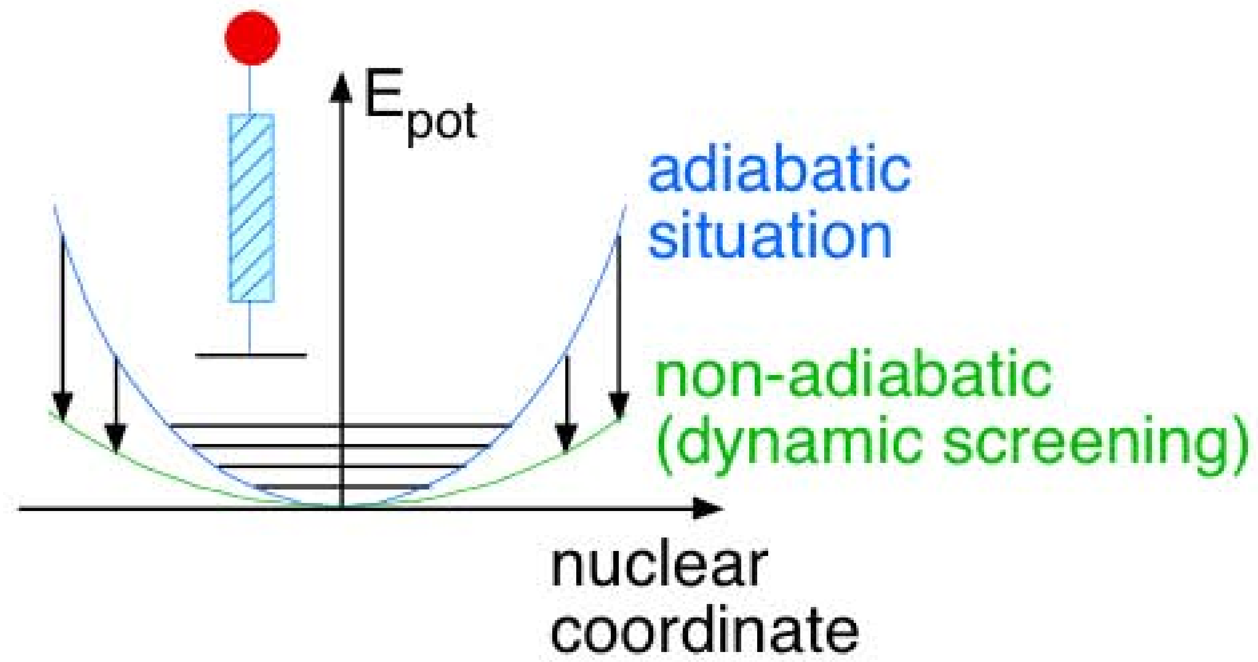




M. Hengsberger et al., PRL 83, 592 (1999).

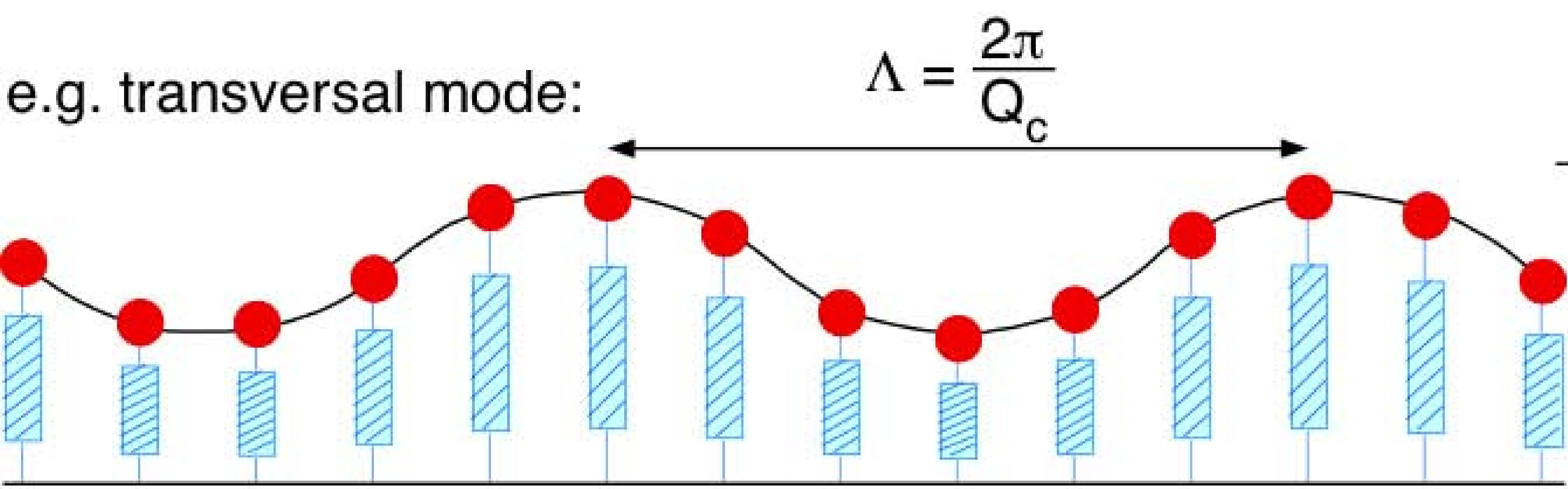
# Giant Kohn Anomaly

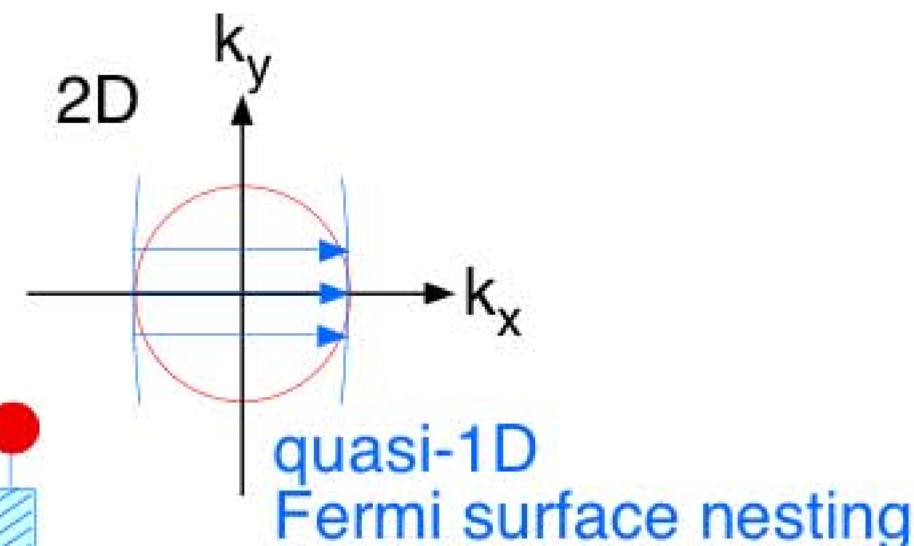
phonon dispersion curve



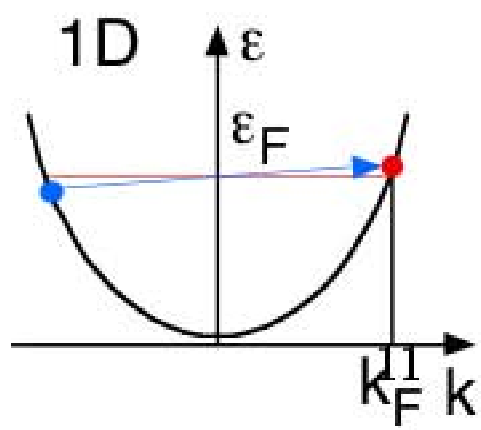

e.g. transversal mode:



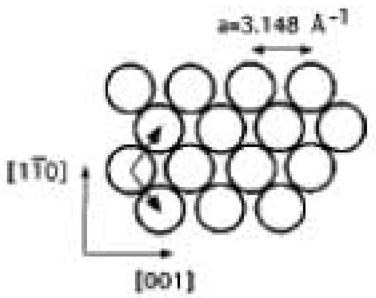




optimum screening:

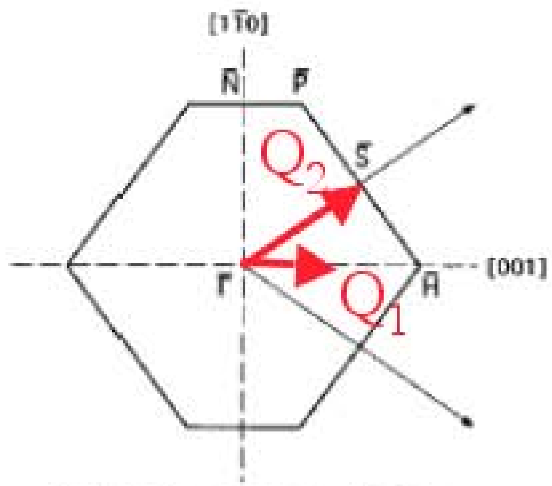
- standing wave with same wave number ($Q_c = 2\ k_F$ !)
- large phase space for $e^-$ - hole pair excitations (low ε / high q)



# Surface Phonon Modes for H/Mo(110) - A Giant Kohn Anomaly ?

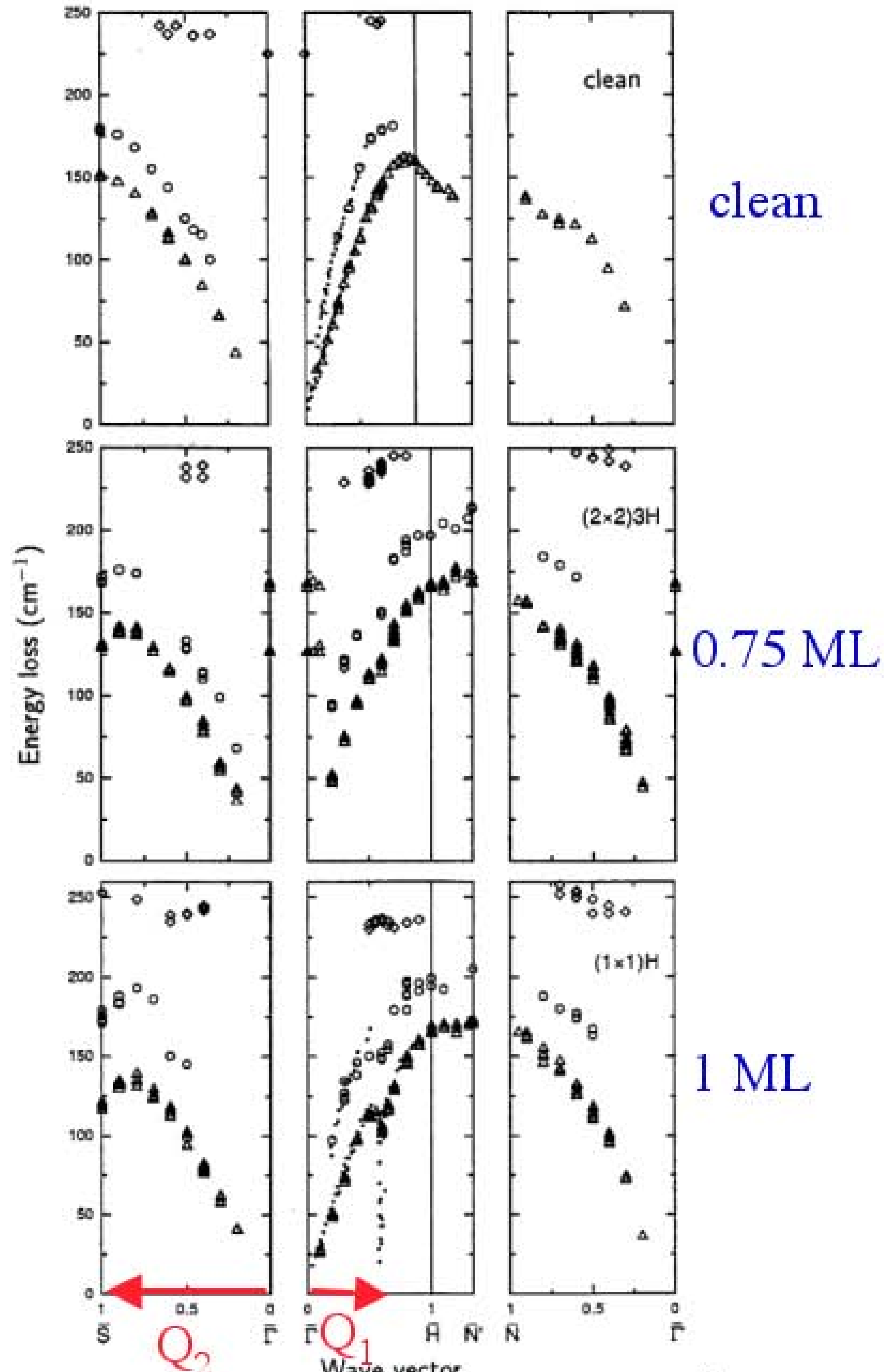



Mo(110)-direct lattice




Mo(110)-reciprocal lattice

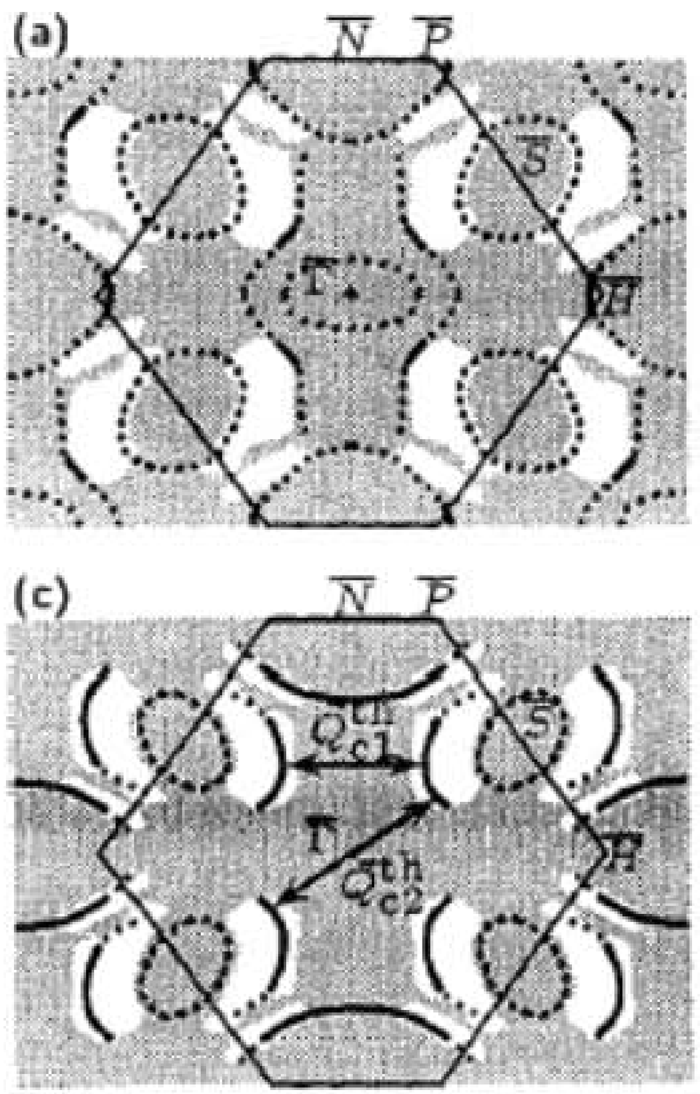
HREELS Data



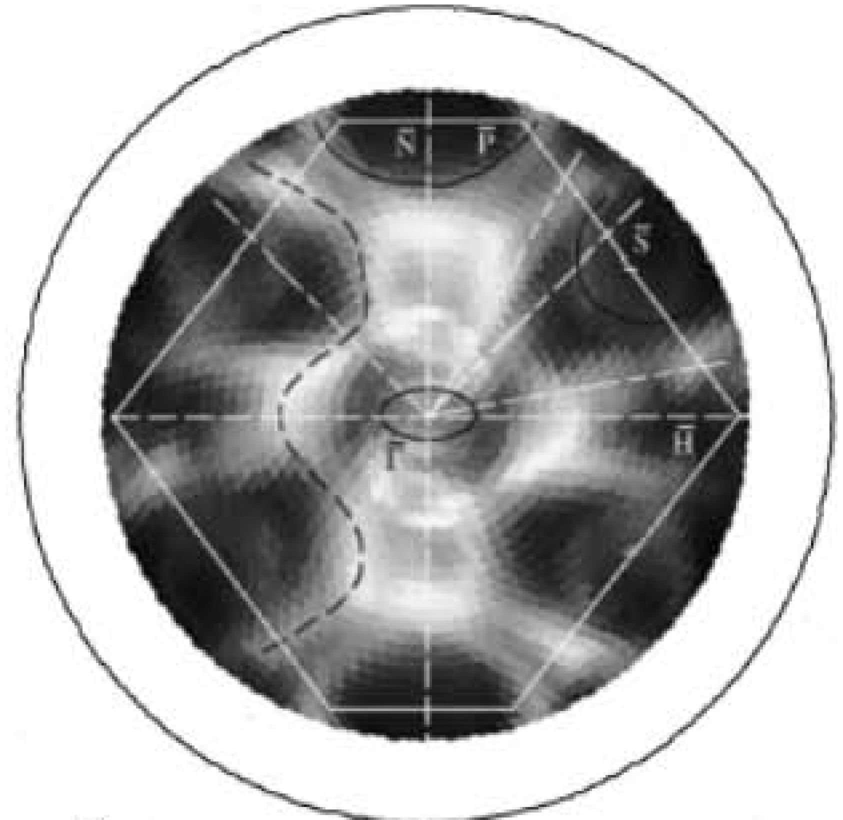

J. Kröger et al., PRB 55, 10895 (1997)

# Fermi Surface Contours of Surface States on Mo(110)

Theory:

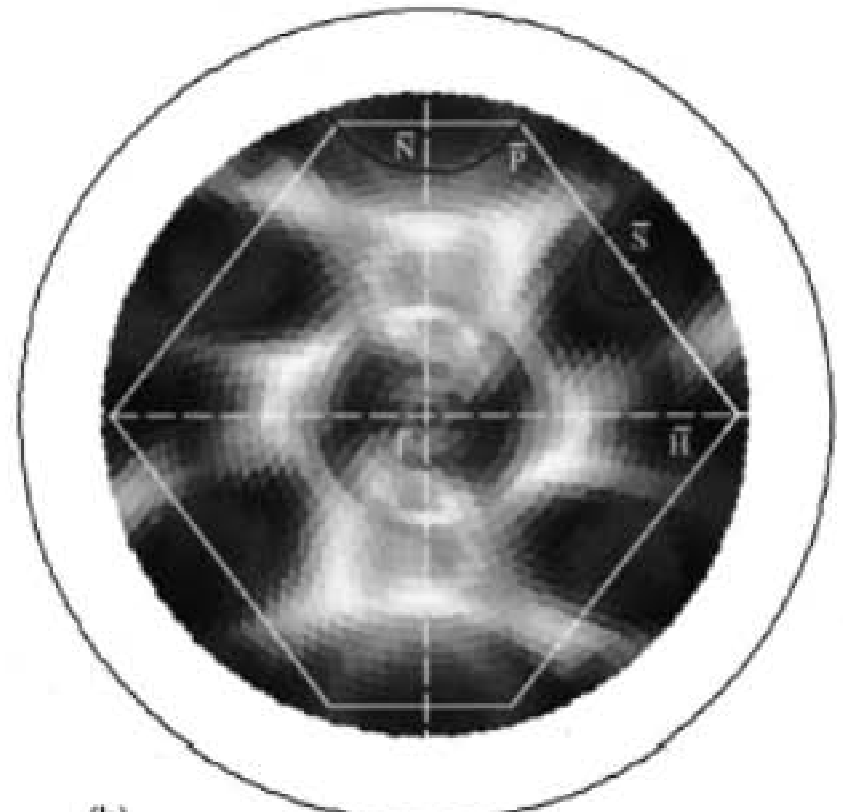



B. Kohler et al., PRL 74, 1387 (1995)




(a)

Clean Mo(110)

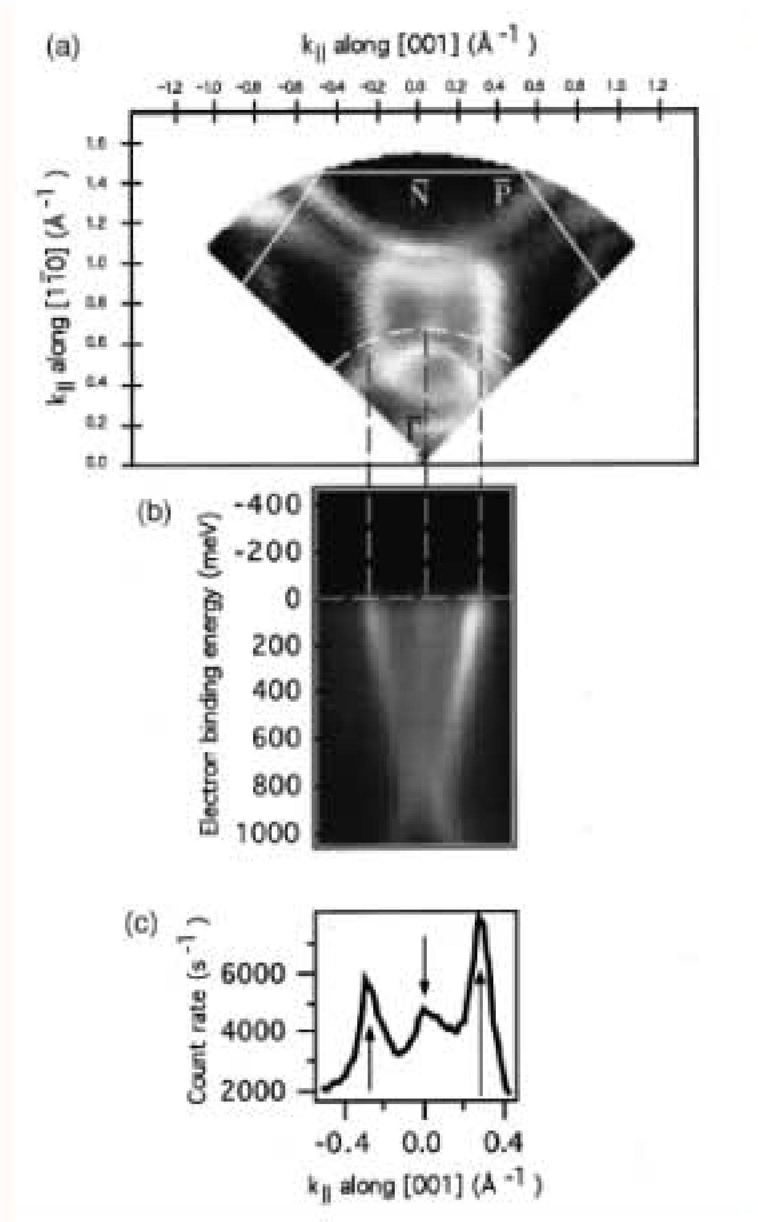


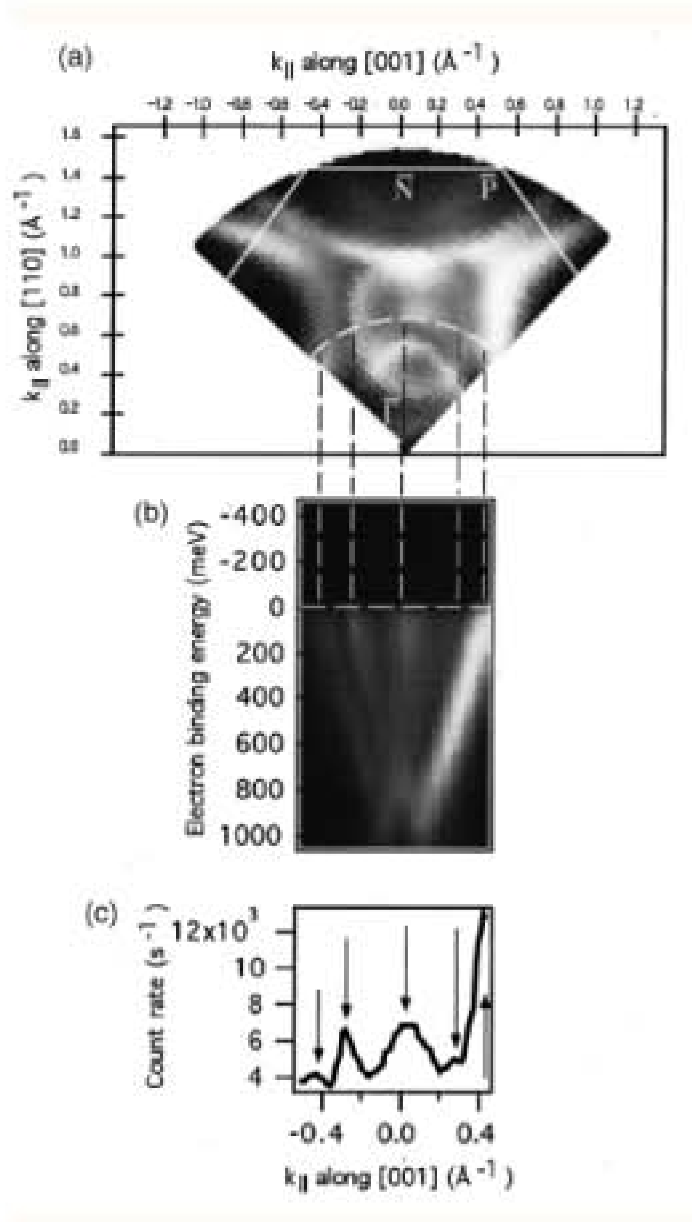

(b)

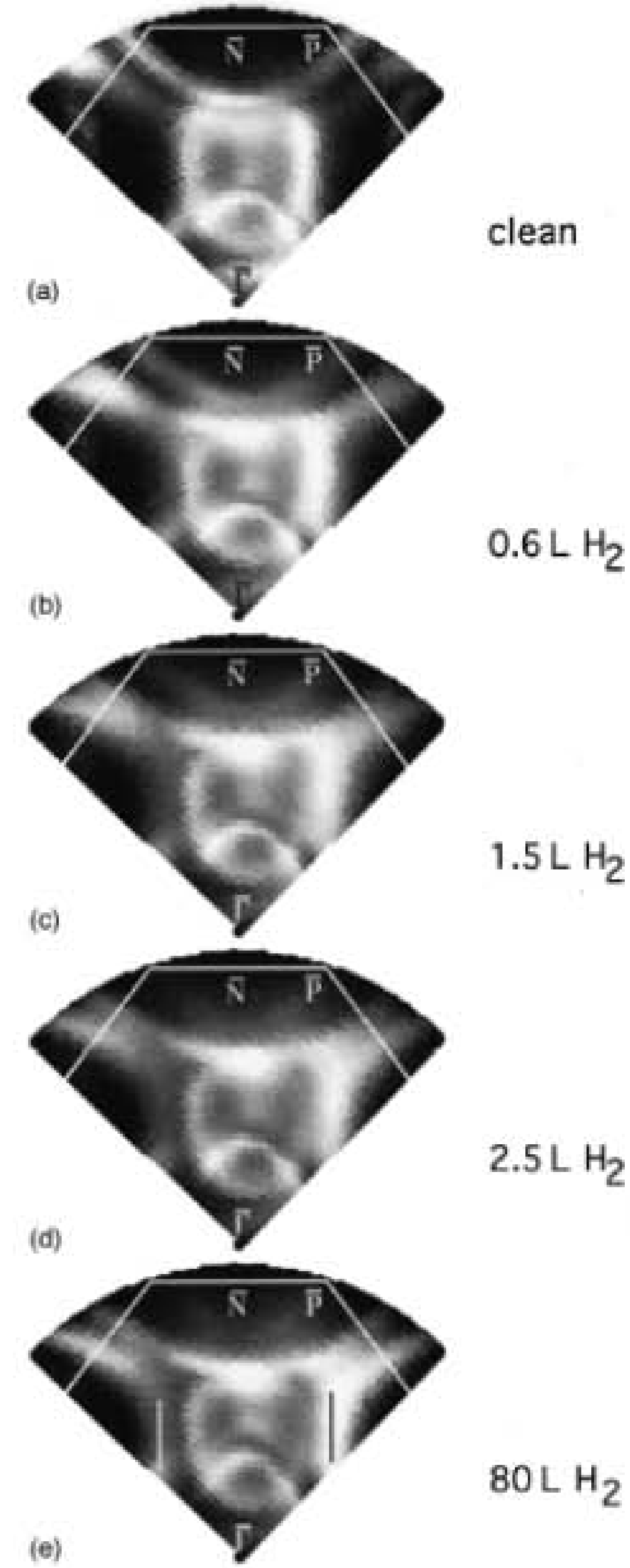
1 ML Hydrogen

J. Kröger et al., PRB 61, 14146 (2000).

# Evolution of Fermi Surface Contours with Hydrogen Coverage



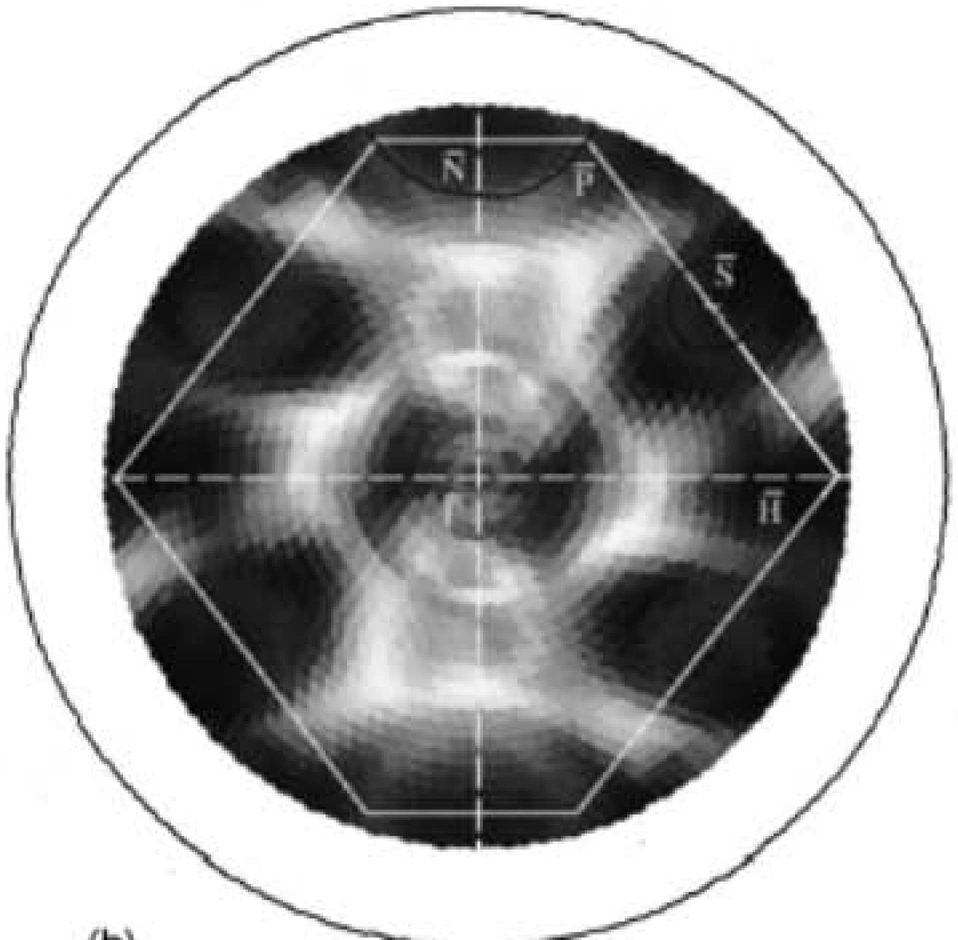




=> H-induced shift of Fermi surface contour

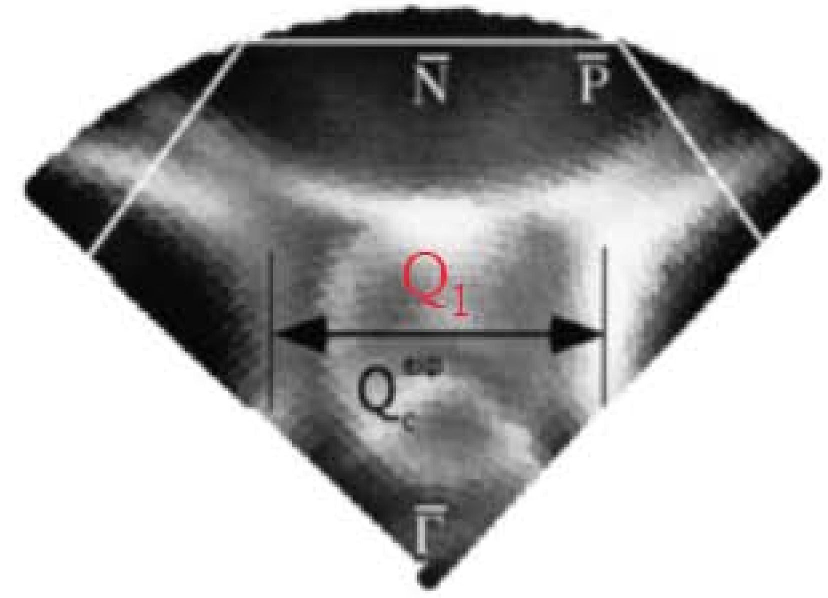


J. Kröger et al., PRB 61, 14146 (2000).

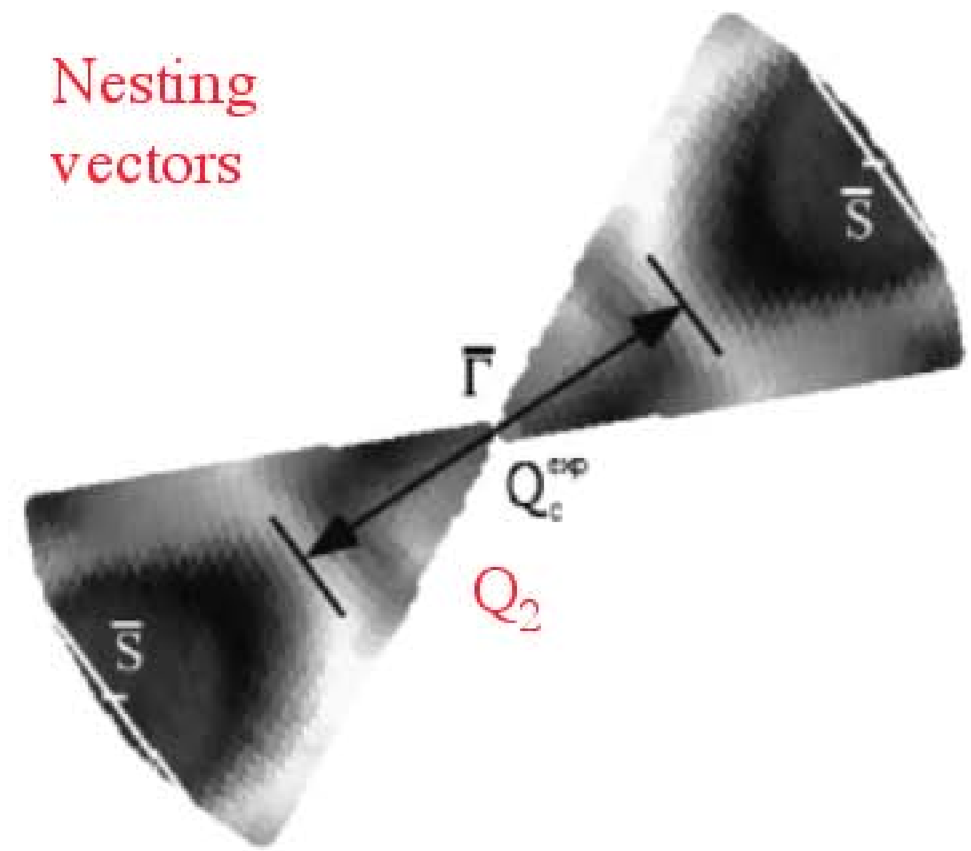
# Fermi Surface Nesting on 1 ML H/Mo(110) Seen by Photoemission




(b)




Nesting vectors

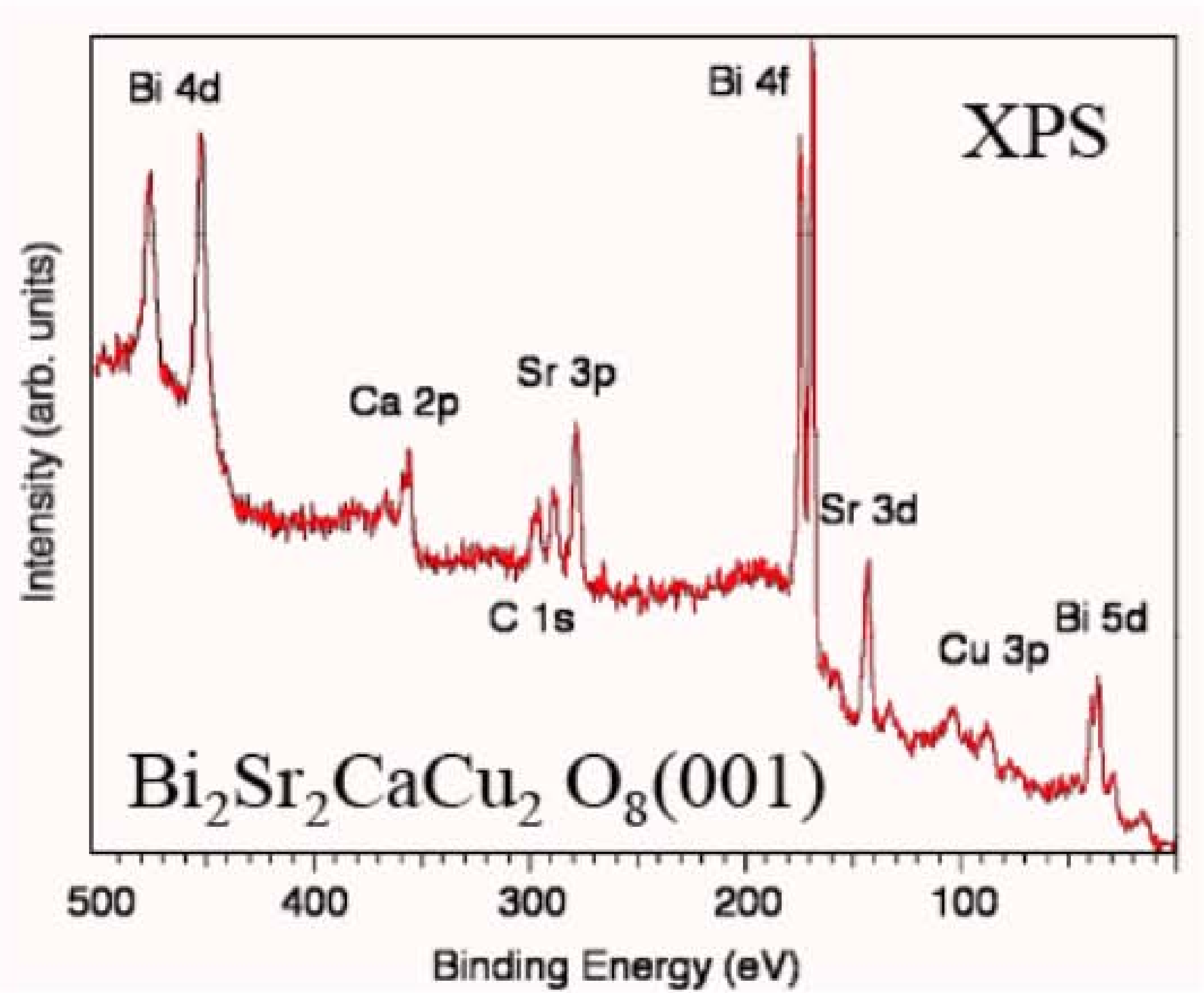


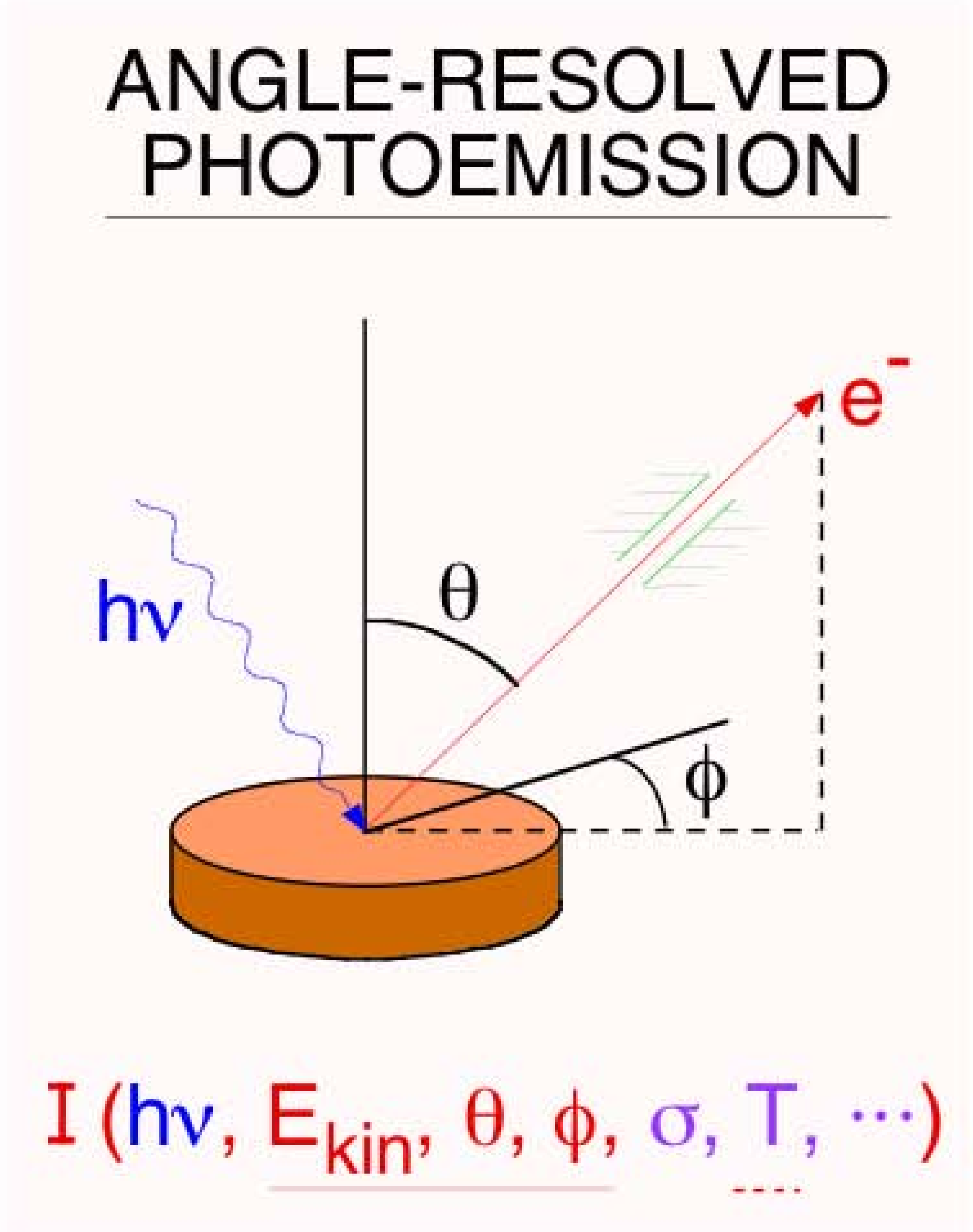

| | $Q_1$(Å$^{-1}$) | $Q_2$(Å$^{-1}$) |
|---|---|---|
| EELS | 0.90 | 1.22 |
| PE | 0.85 | 1.19 |
| DFT | 0.86 | 1.23 |

J. Kröger et al., PRB 61, 14146 (2000).

# Photoemission Studies of High Temperature Superconductors

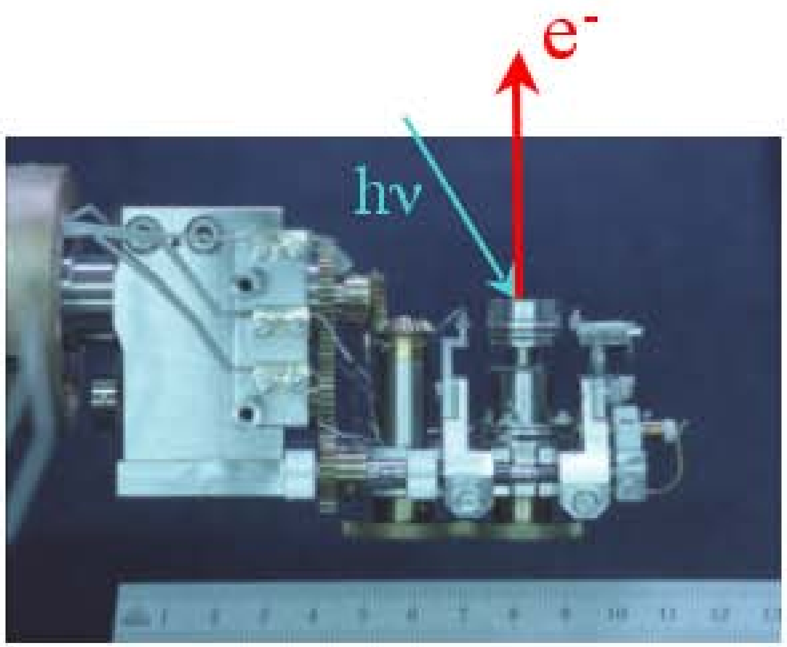
Start with core levels to understand your sample !



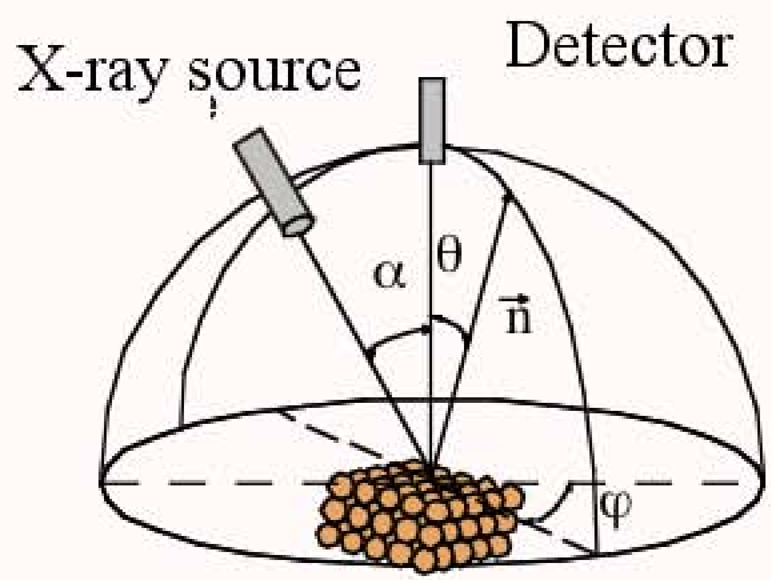




=> Photoelectron diffraction

# Full-hemispherical (2π) XPD patterns



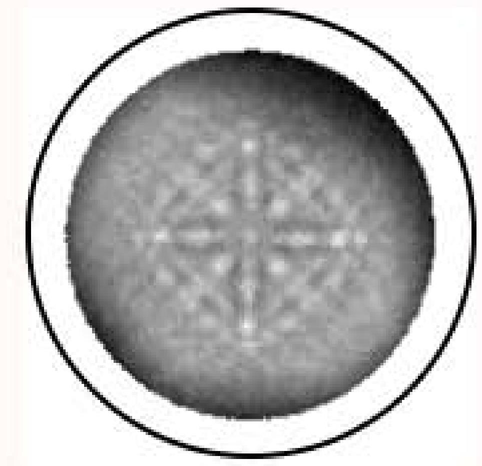

Fully automated two-axis sample goniometer (Fadley type)




Single Crystal

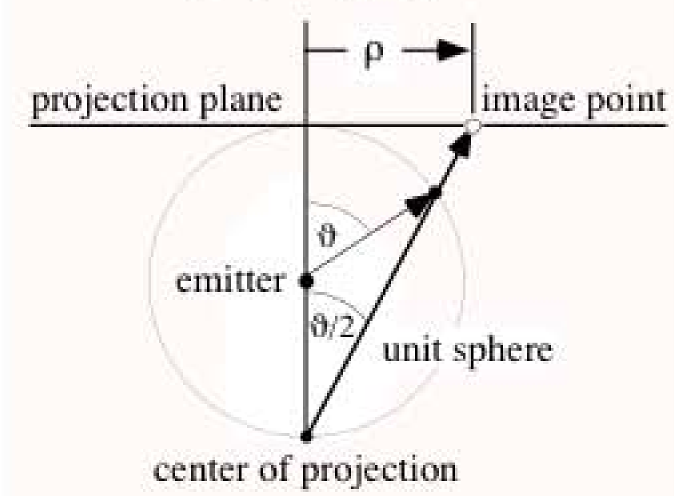
Sequential measurement of core level intensities at ca. 4000 angular settings

e.g. Bi 4f



Intensities in grey scale, stereographic projection

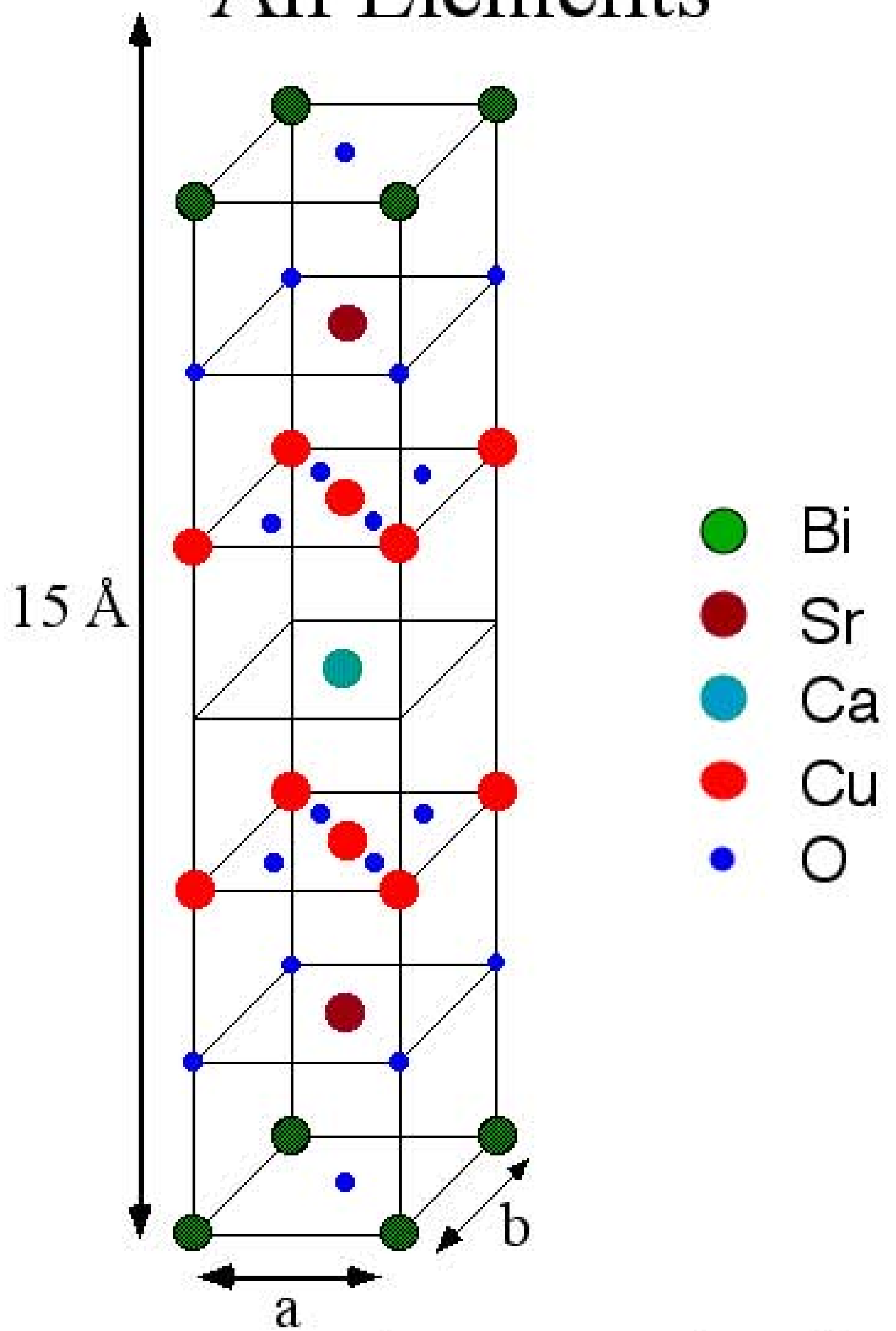
stereographic projection



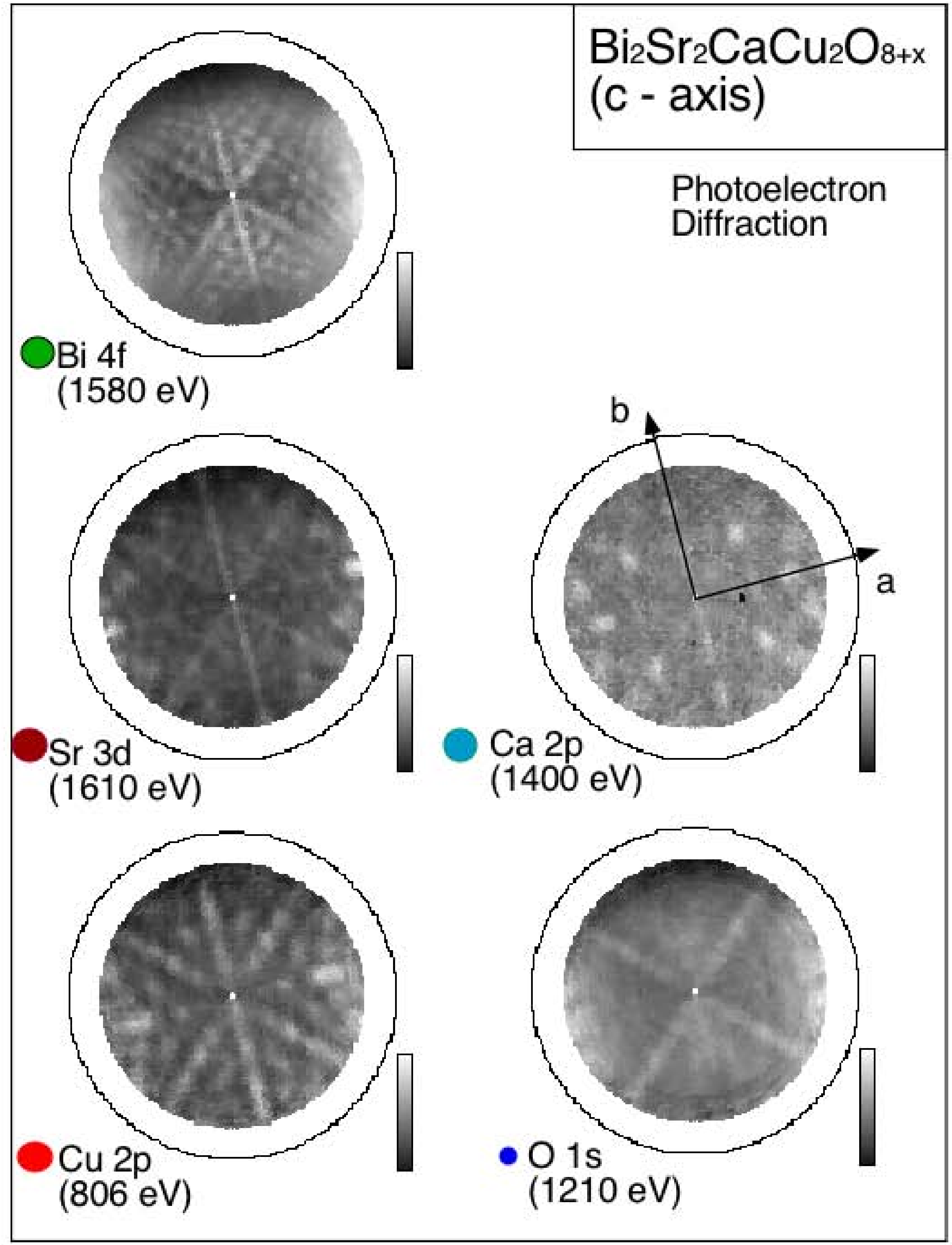

$\rho = 2\tan(\vartheta/2)$

Measuring times for full 2π XPD pattern:
1 hour to 24 hours
(depending on count rates **and** on anisotropies)

# XPD Patterns of All Elements



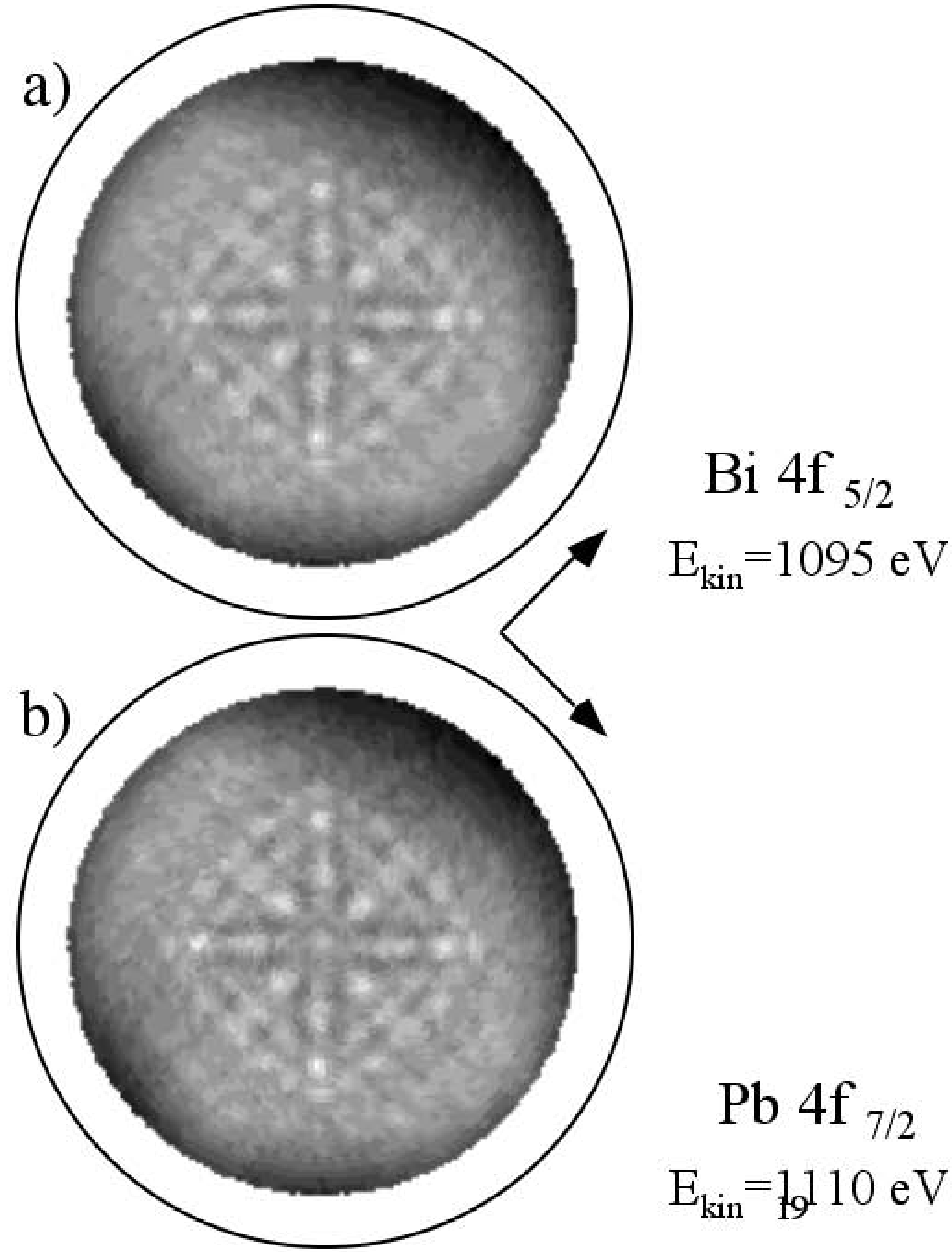

=> Surface Termination




M. Shimoda et al., Physica C 196 (1992) 236

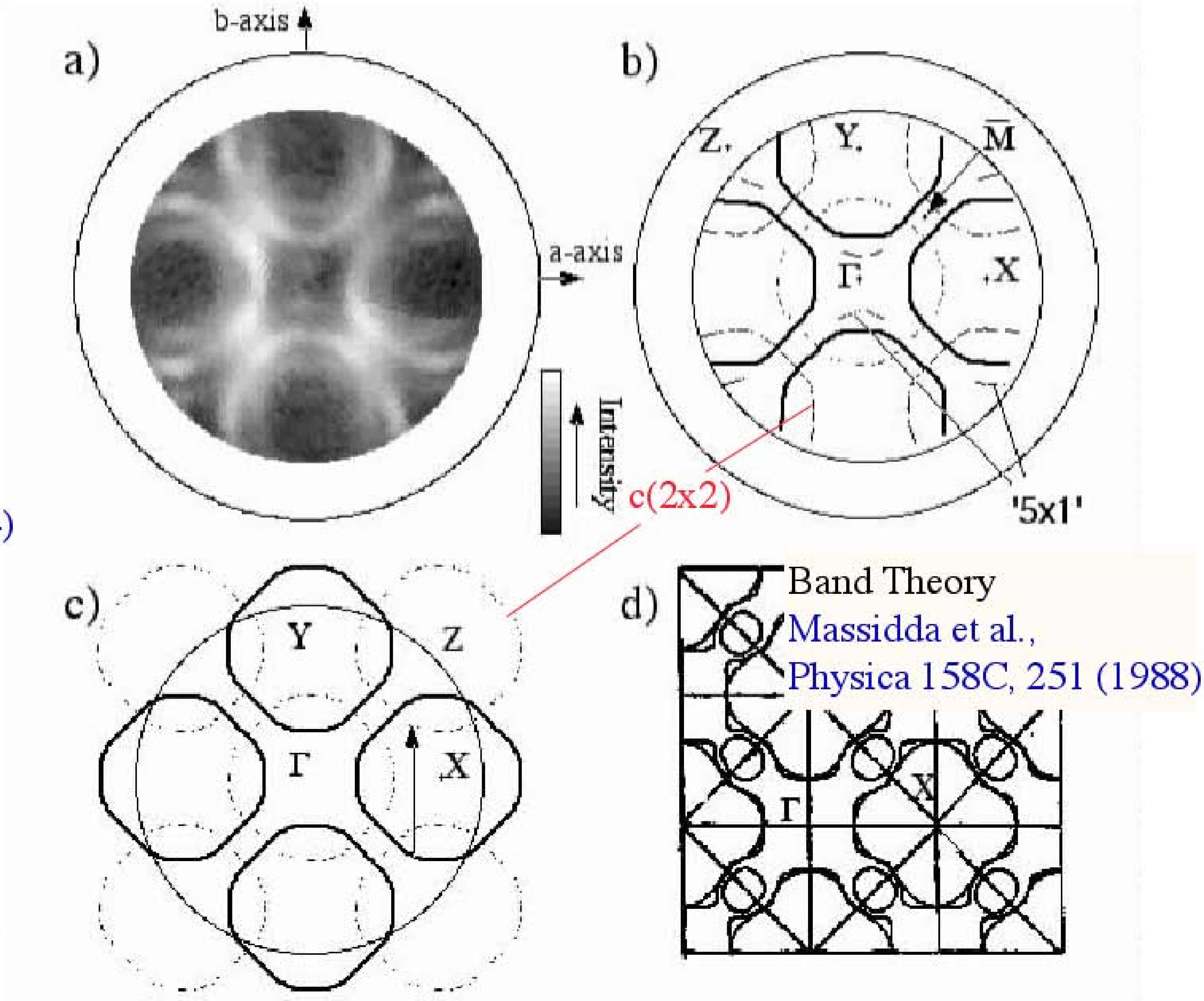
# Determination of Dopant Sites

$Pb_{0.4}Bi_{1.6}Sr_2CaCu_2\,O_8(001)$




P. Schwaller et al., JES 76 (1995) 127

# Fermi Surface Mapping on a High Temperature Superconductor: $Bi_2Sr_2CaCu_2O_{8+\delta}$ (001)

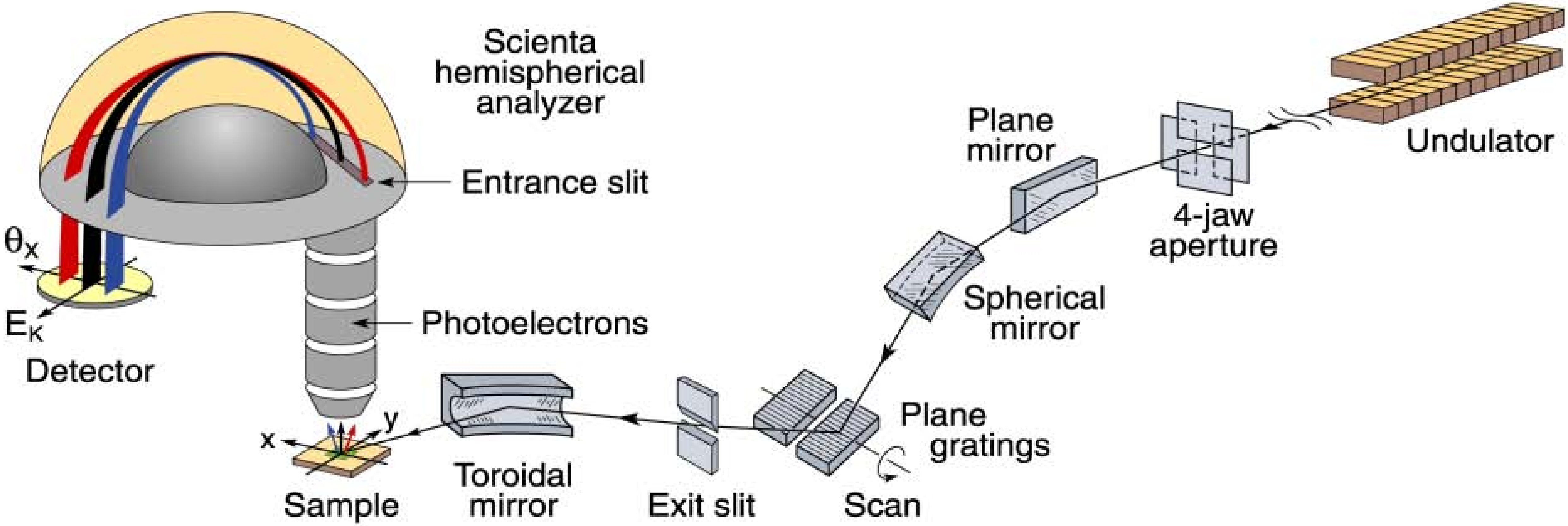



P. Aebi et al.,
PRL 72, 2757 (1994)

Band Theory
Massidda et al.,
Physica 158C, 251 (1988)

# High-Resolution Photoemission

A state-of-the-art photoemission beamline at Stanford (SSRL)




## Highest resolution in energy and momentum

~ 2 meV in energy

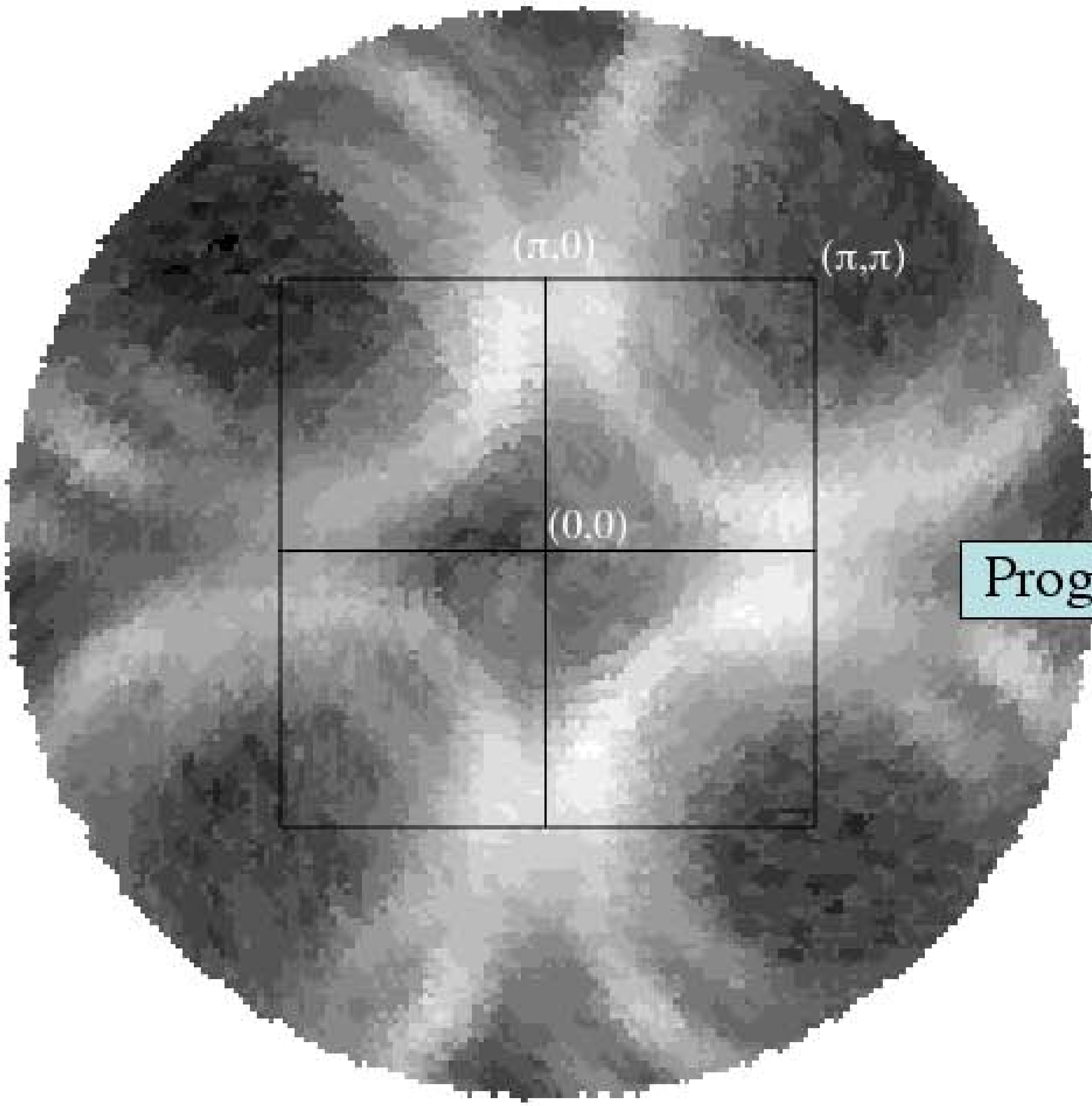
~ 0.005 Å$^{-1}$ in momentum



Courtesy Z.-X. Shen, Stanford University

Bi2212:
First Fermi surface mapping,
superstructure contours

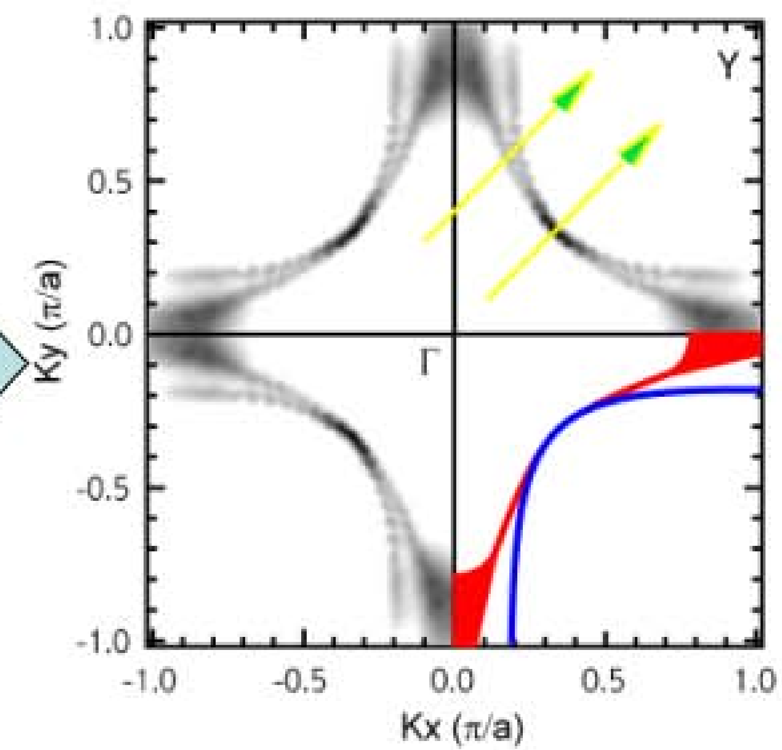
Pb-doped Bi2212:
Bi-layer splitting




P. Aebi et al., Phys. Rev. Lett. 72, 2757 (1994).

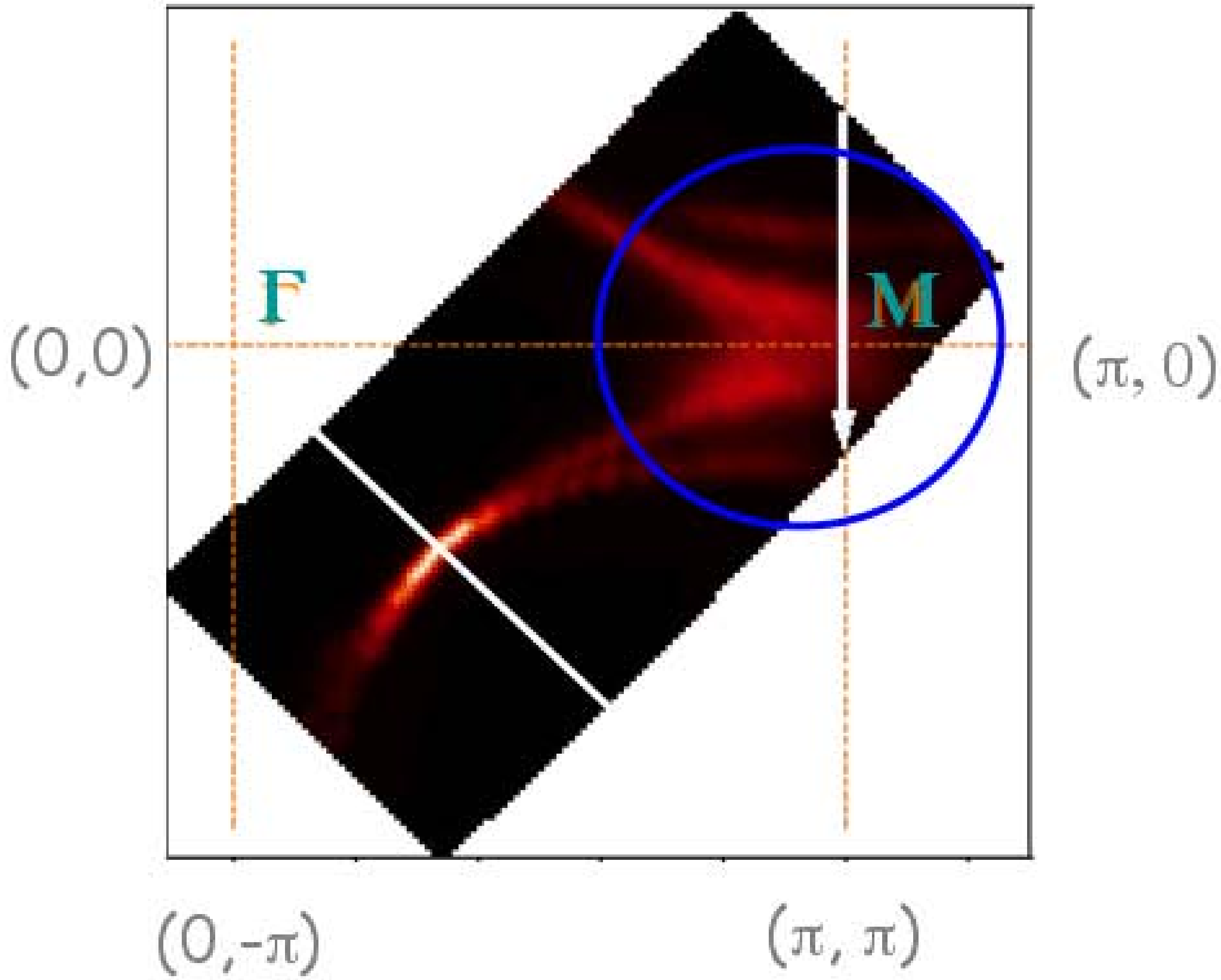
Progress

Two CuO layers
per unit cell




Bogdanov et al.,
Phys. Rev. B 64, 180505 (2001)

# Details on the Fermi Surface of BSCCO



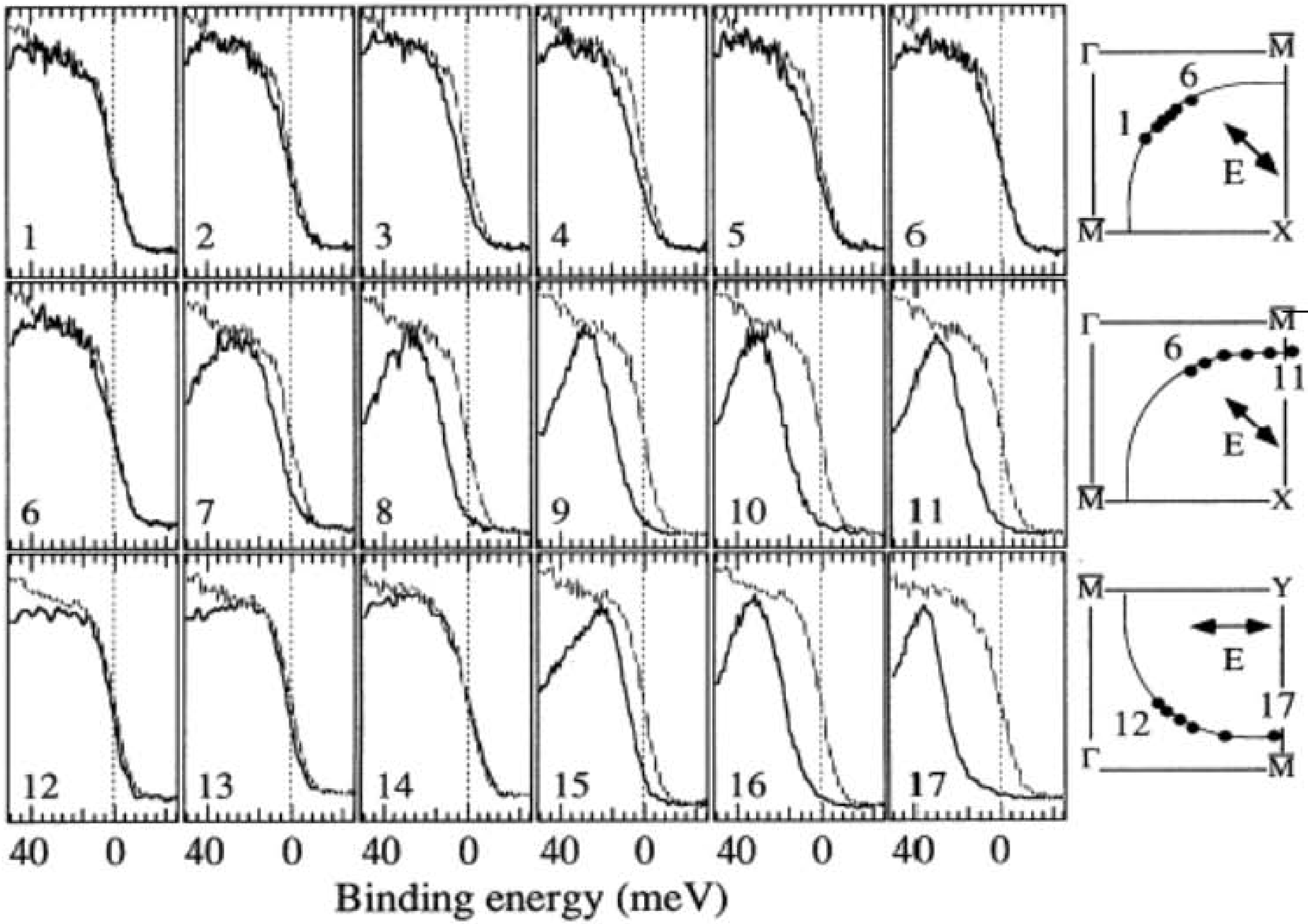

- Superstructure
- Superconducting Gap
- Bilayer Splitting

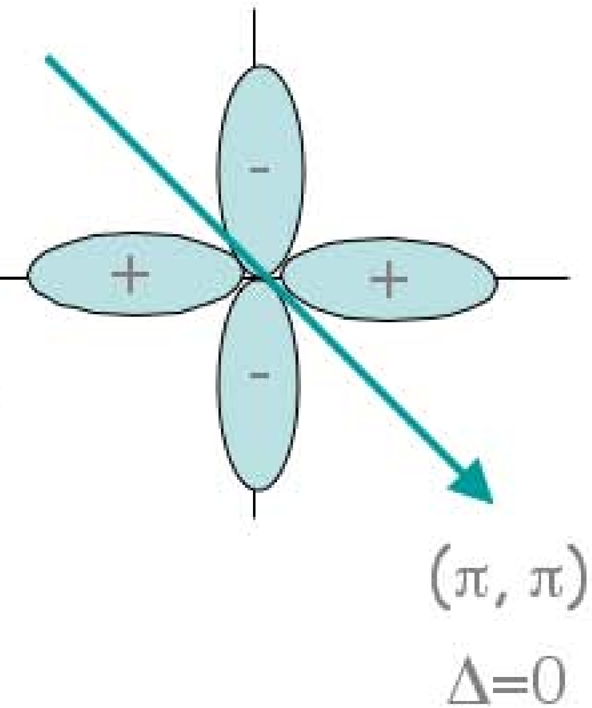


Courtesy Z.-X. Shen, Stanford University

# Anisotropy of the Superconducting Gap in BSCCO

… need to measure spectra exactly on the Fermi surface !



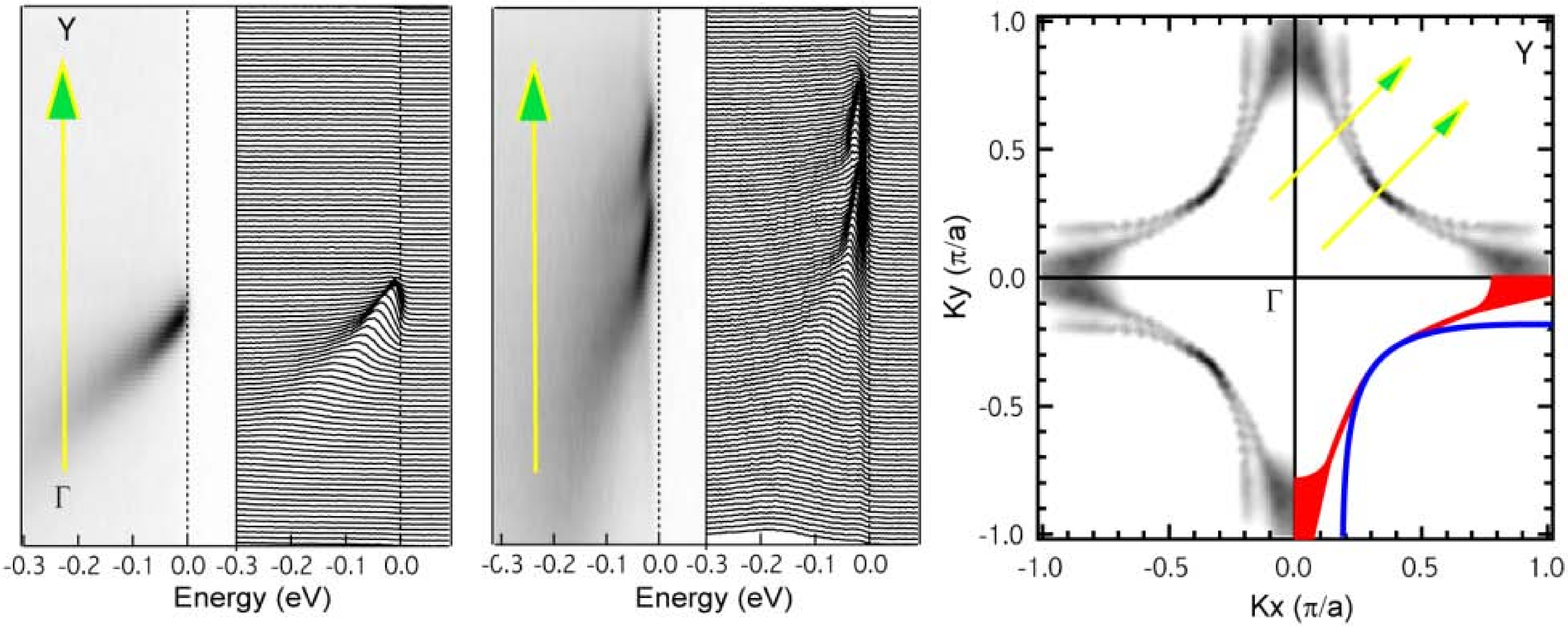

=> d-wave superconductor





H. Ding et al., PRL 74, 2784 (1995)

# Pb-doped Bi2212: Bi-layer splitting




High energy and momentum resolution combined with improved sample enables the clear observation of bilayer splitting

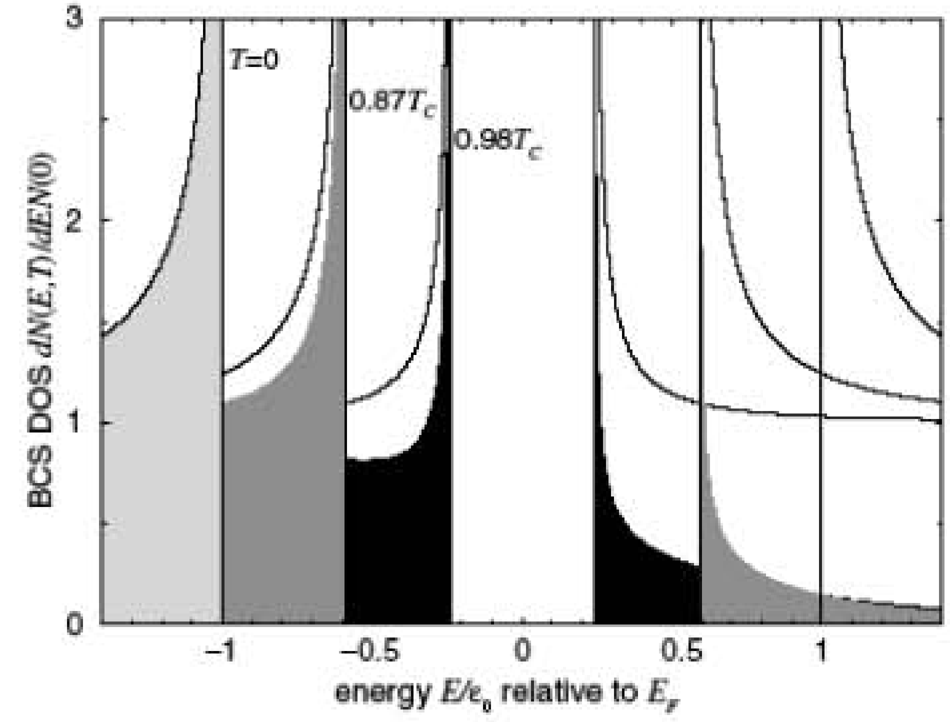




Bogdanov et al. Phys. Rev. B 64, 180505 (2001)

# In Conventional Superconductors it is Much Harder to See the Gap !

Density of states near $E_F$ in the superconducting state: BCS model for different temperatures



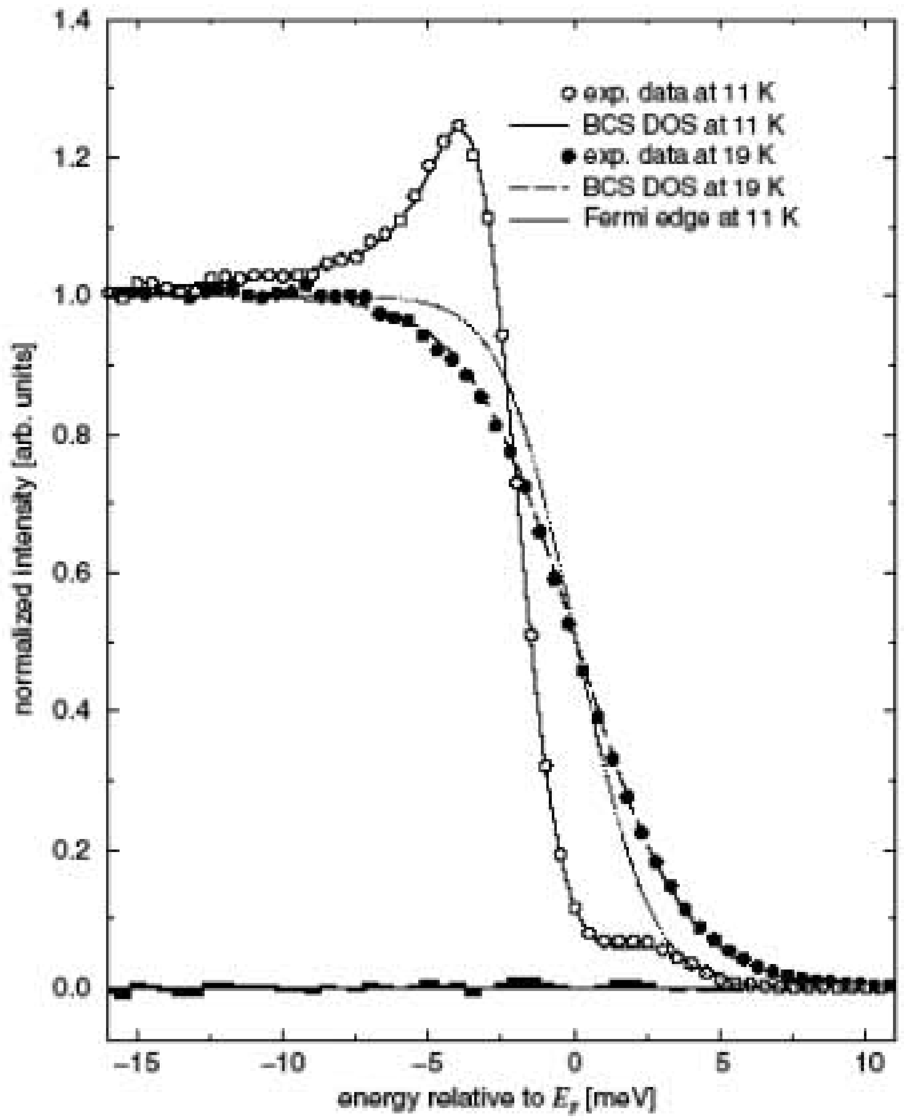

Sample:

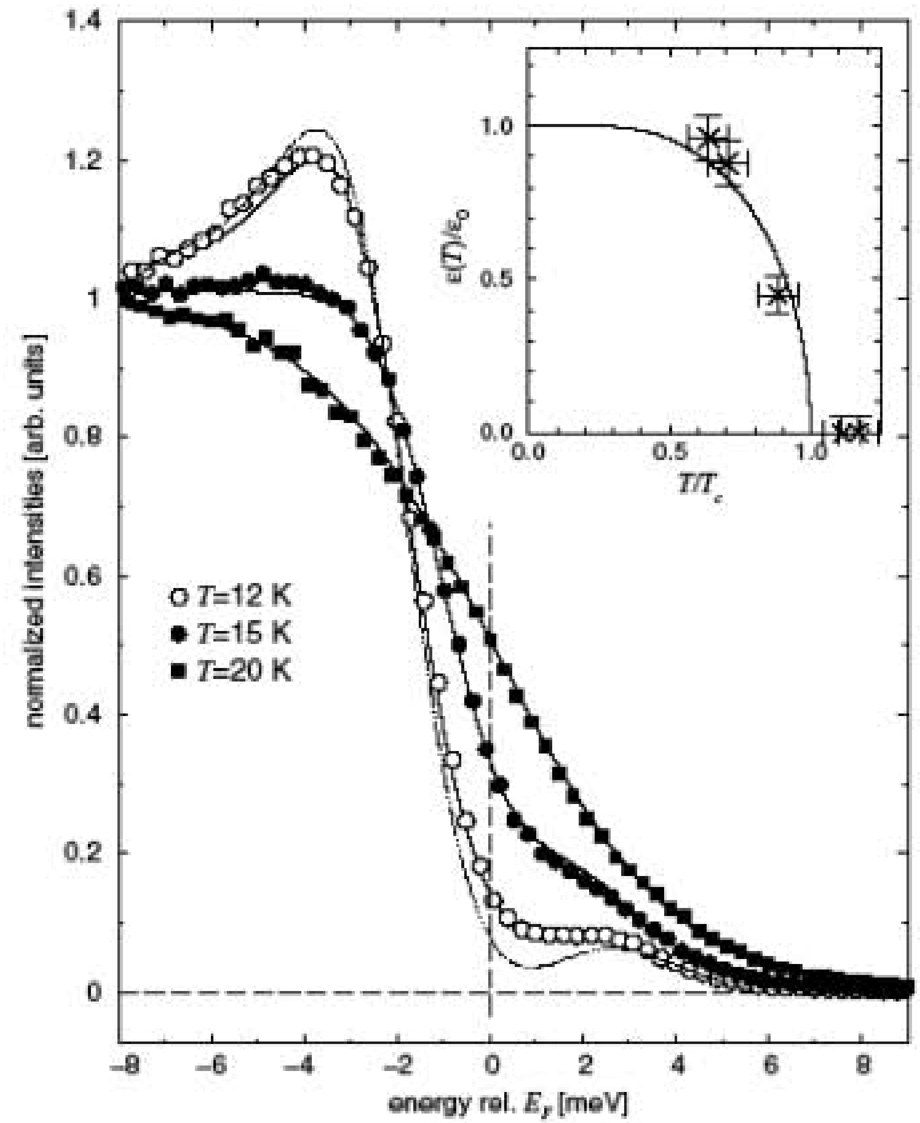
$V_3Si$

$T_c = 17$ K
$\Delta_{gap} = 5$ meV

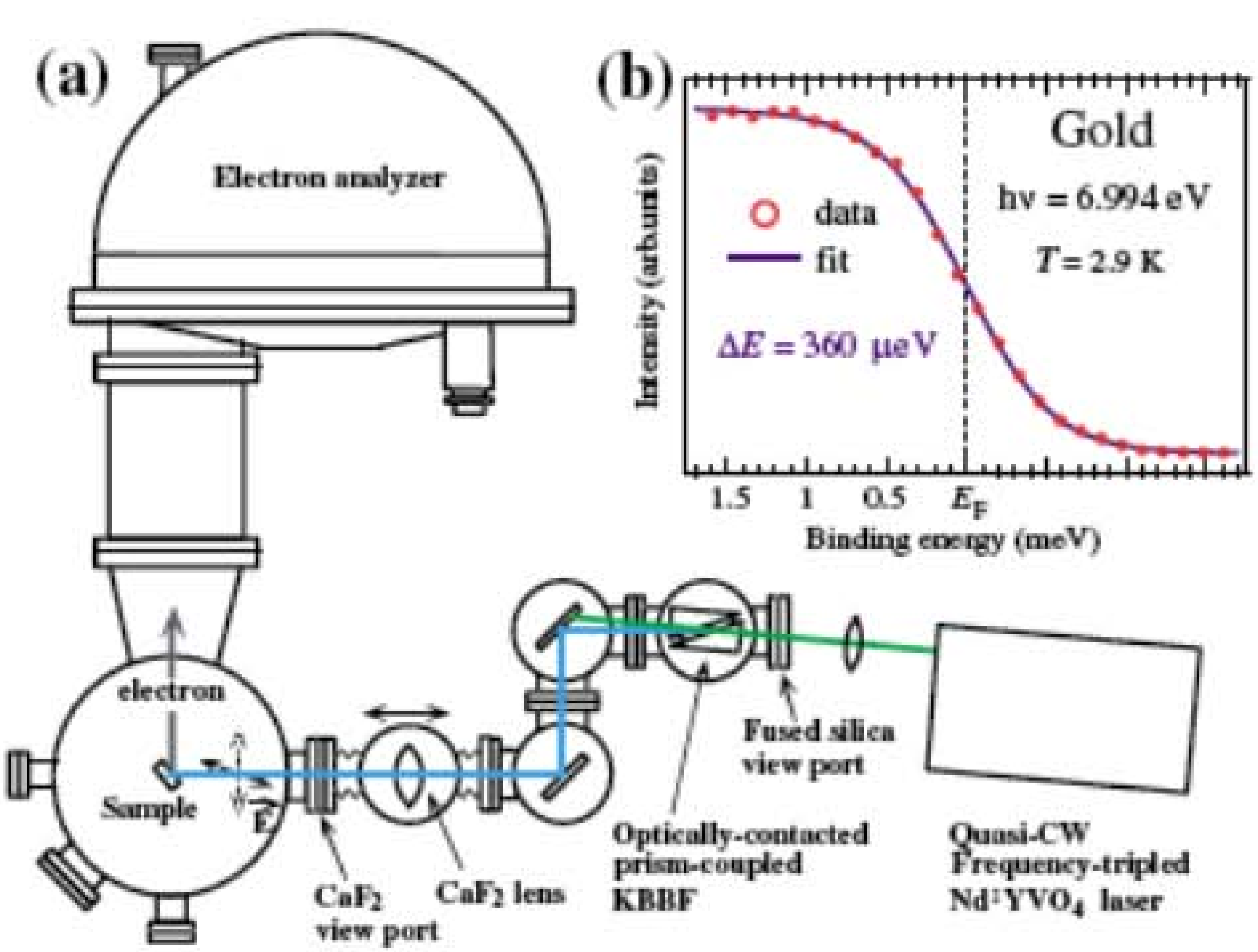
Instr. Res. 2.9 meV !

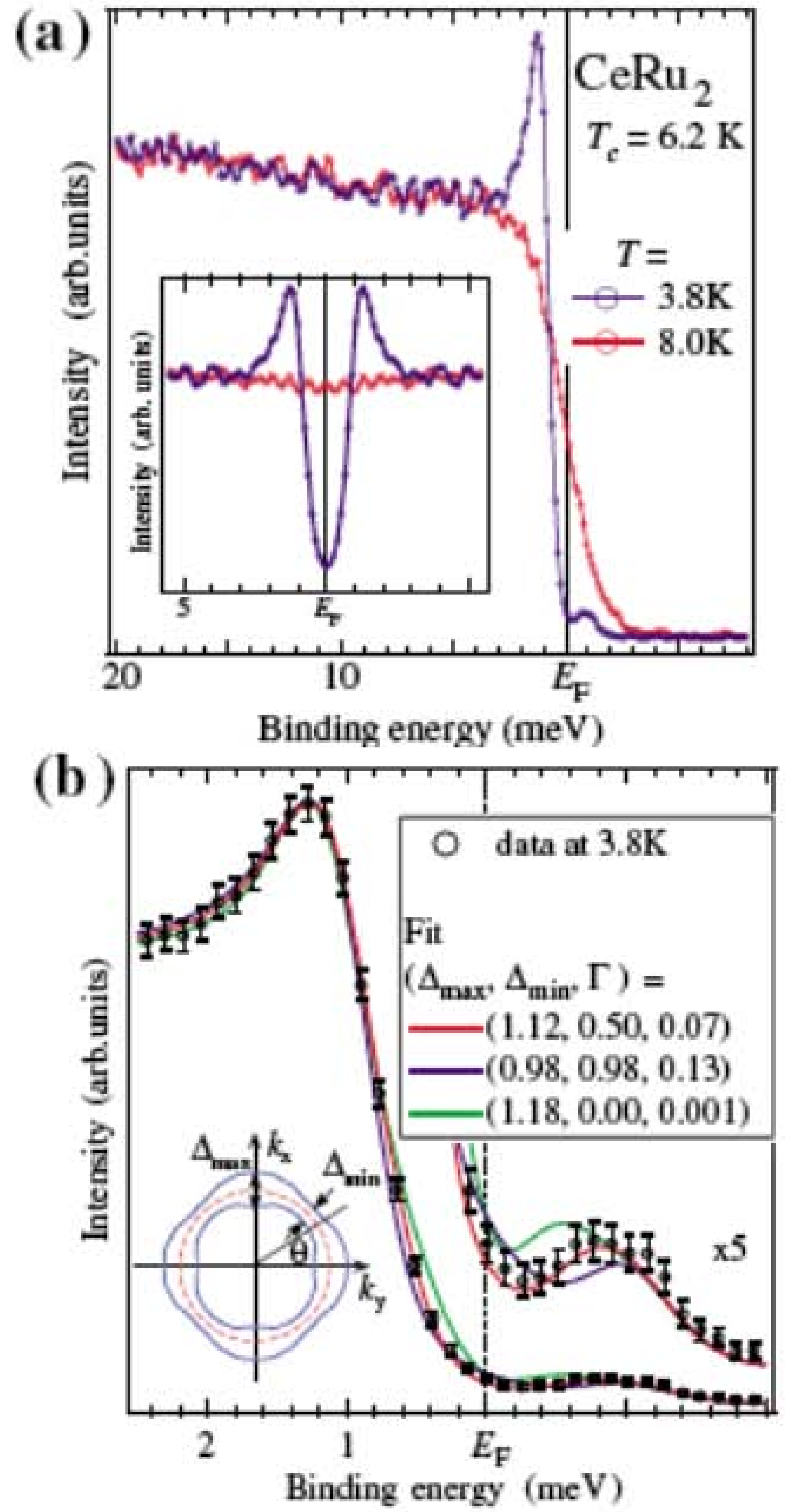
F. Reinert et al.,
PRL 85, 3930 (2000)



# Ultimate Energy Resolution (Feb. 2005)




⇒ Measuring the gap anisotropy
in an f-electron superconductor !

T. Kiss, S. Shin et al.,
Phys. Rev. Lett. 94, 057001 (2005)