united nations
educational, scientific
and cultural
organization

international atomic
energy agency

the
abdus salam
international centre for theoretical physics

SMR/1270-35

SCHOOL ON SYNCHROTRON RADIATION

6 November - 8 December 2000

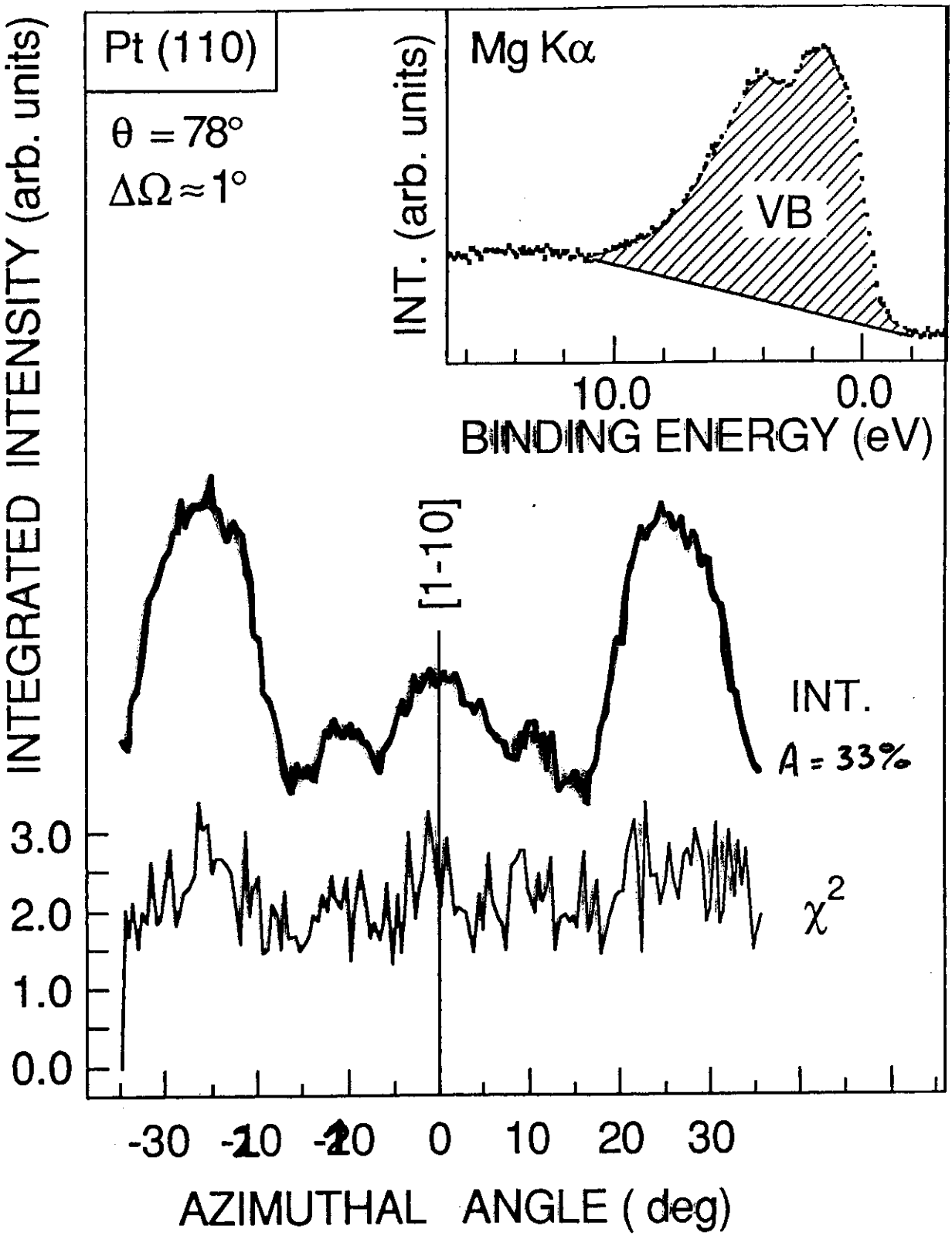
Miramare - Trieste, Italy

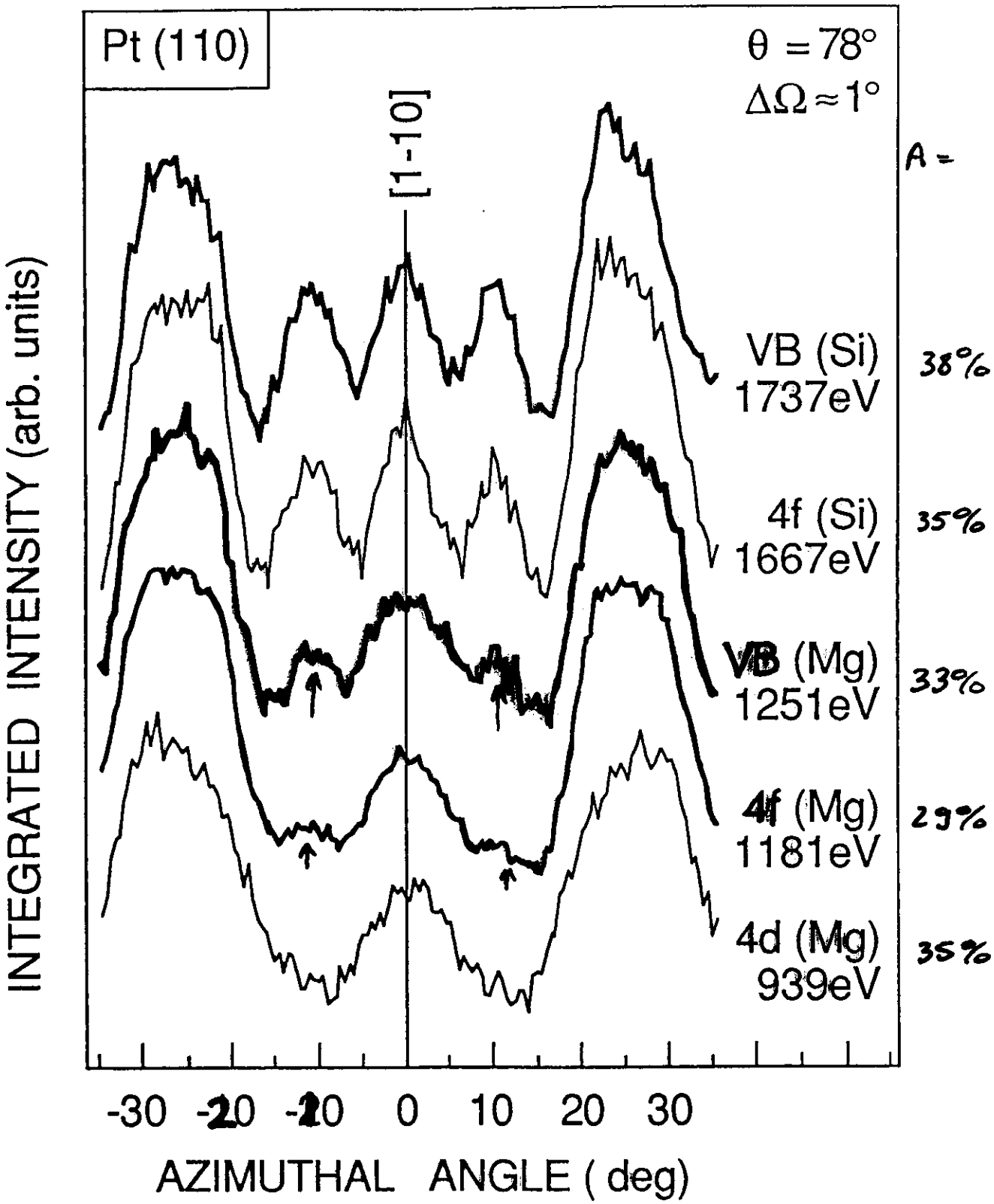
Supported in part by the Italian Ministry of Foreign Affairs in connection with the SESEME project

Co-sponsors: Sincrotrone Trieste, Società Italiana di Luce di Sincrotrone (SILS) and the Arab Fund for Economic and Social Development

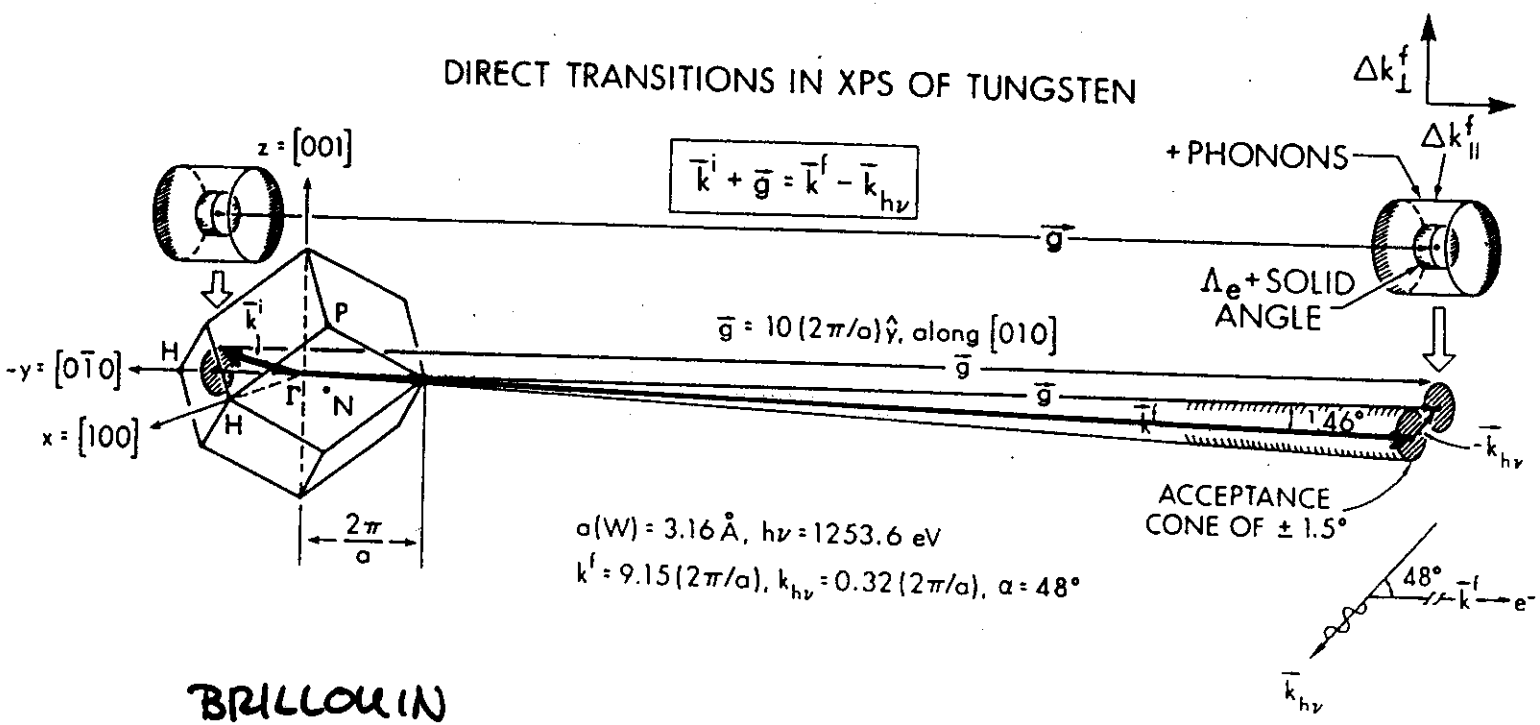
X-Ray Excited Valence Photoemission - Highest Resolution Photoemission

Juerg Osterwalder
Universitaet Zuerich-Irchel


Pt (110)
θ = 78°
ΔΩ ≈ 1°
Mg Kα
INT. (arb. units)
VB
10.0
0.0
BINDING ENERGY (eV)
INTEGRATED INTENSITY (arb. units)
[1-10]
INT.
A = 33%
3.0
2.0
1.0
0.0
χ²
-30
-20
0
10
20
30
AZIMUTHAL ANGLE (deg)


Pt (110)
θ = 78°
ΔΩ ≈ 1°
[1-10]
A =
VB (Si)
1737eV
38%
4f (Si)
1667eV
35%
VB (Mg)
1251eV
33%
4f (Mg)
1181eV
29%
4d (Mg)
939eV
35%
INTEGRATED INTENSITY (arb. units)
-30 -20 -10 0 10 20 30
AZIMUTHAL ANGLE (deg)

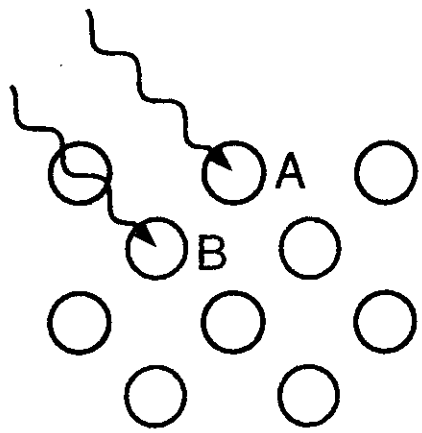
X-RAY EXCITATION



BRILLOUIN ZONE AVERAGING

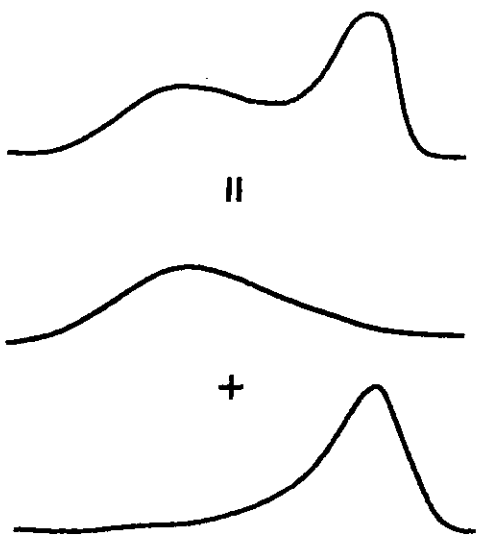
Application to Binary Systems

Localization:



Photoemission
(VB) localized at Atom A
or at Atom B

→ XP valence band spectrum.....



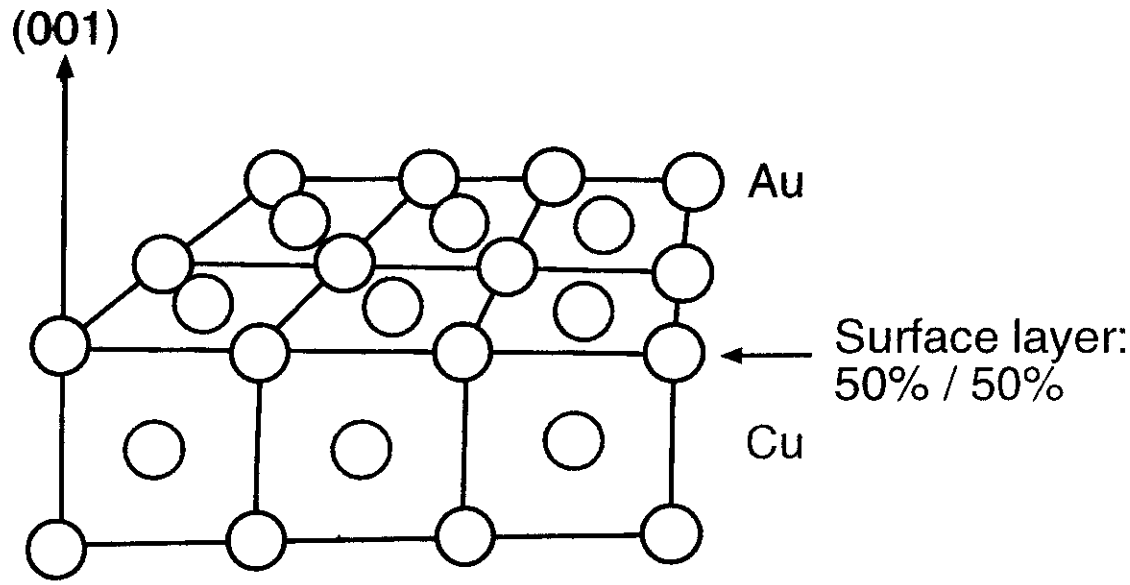
Local DOS
around atom A

.....
around atom B

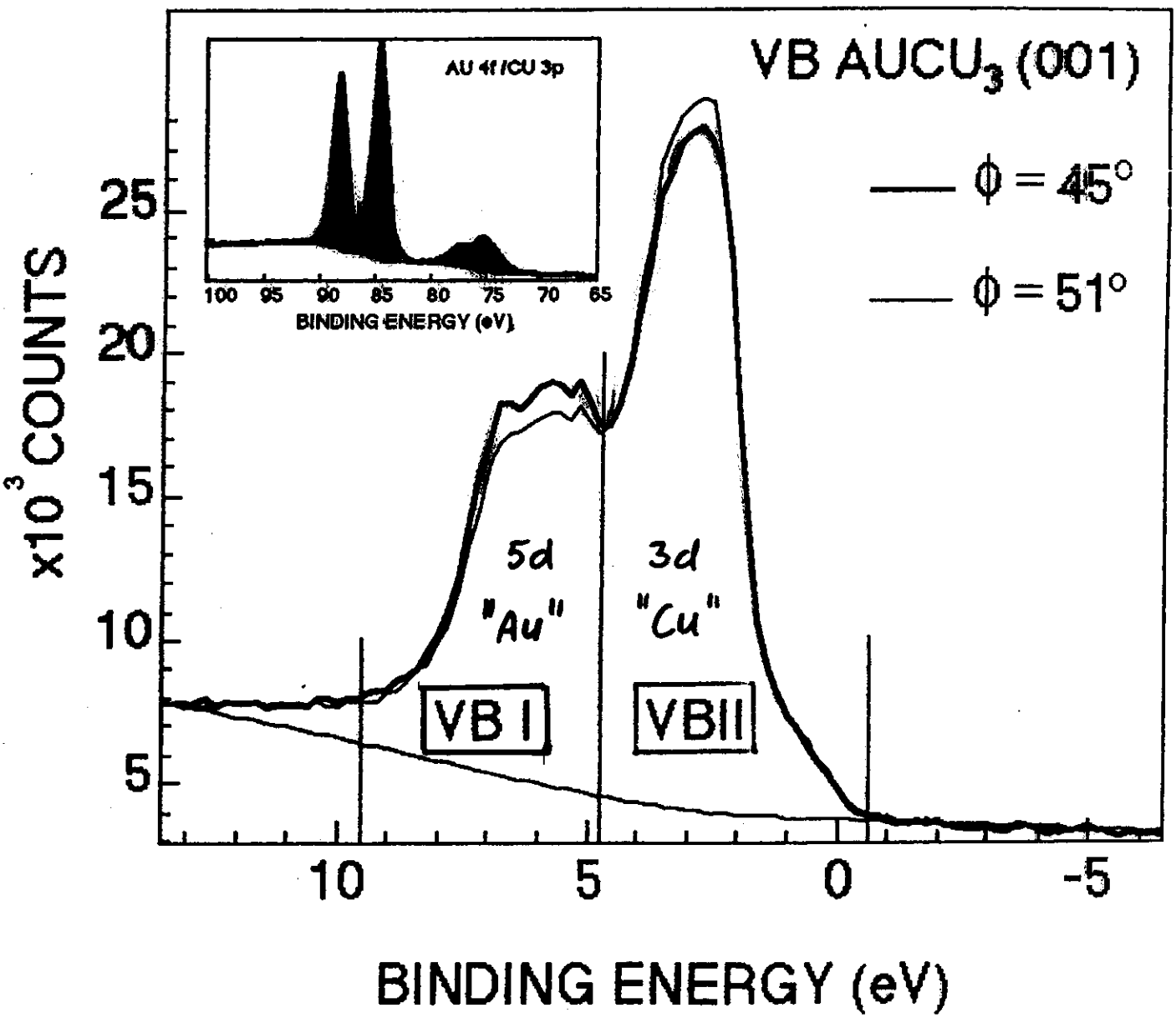
... can be considered a
incoherent superposition of the
spectral contributions of A & B.

→ partial densities of states (PDOS)

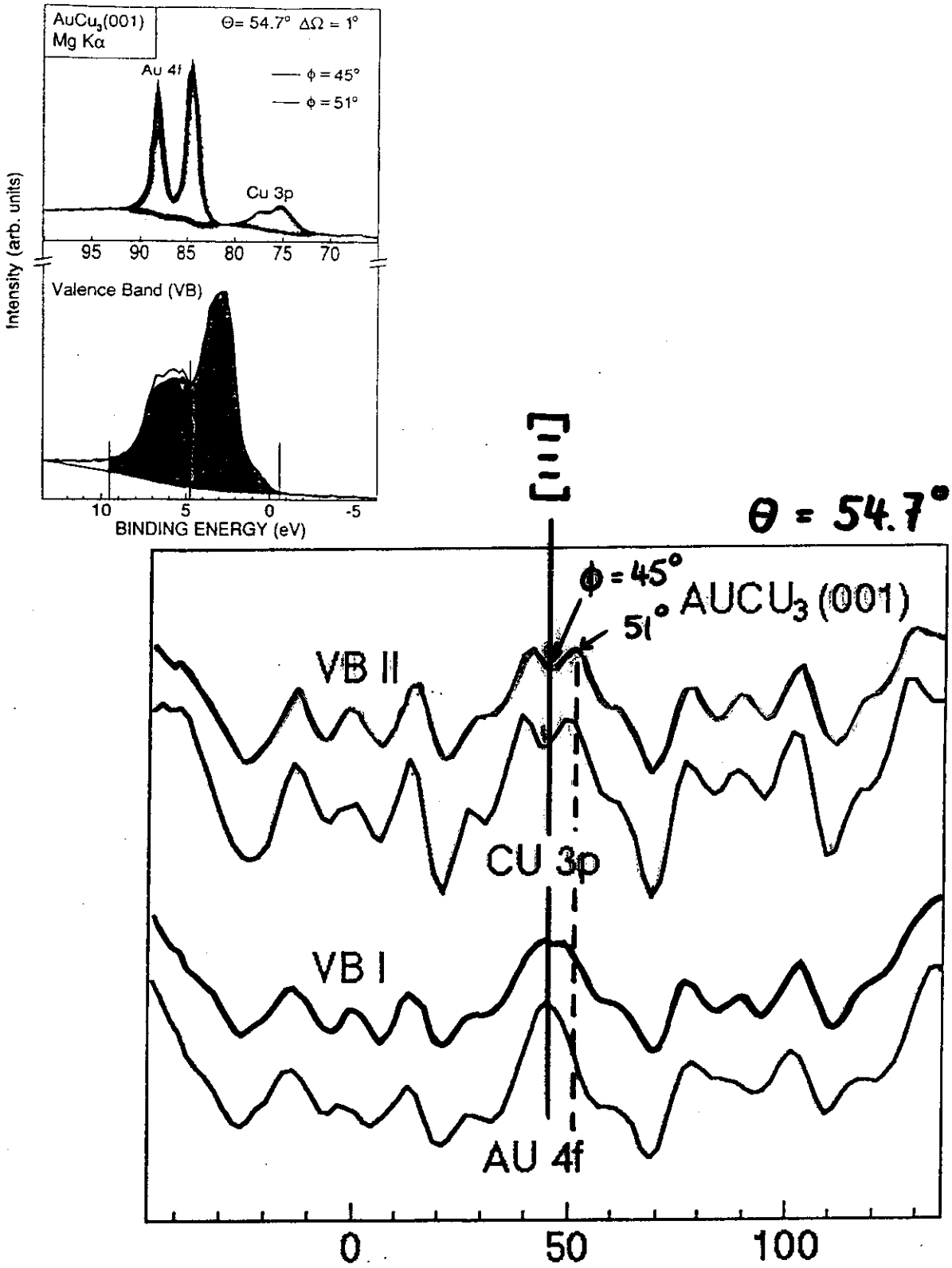
The $AuCu_3$ (001) Surface



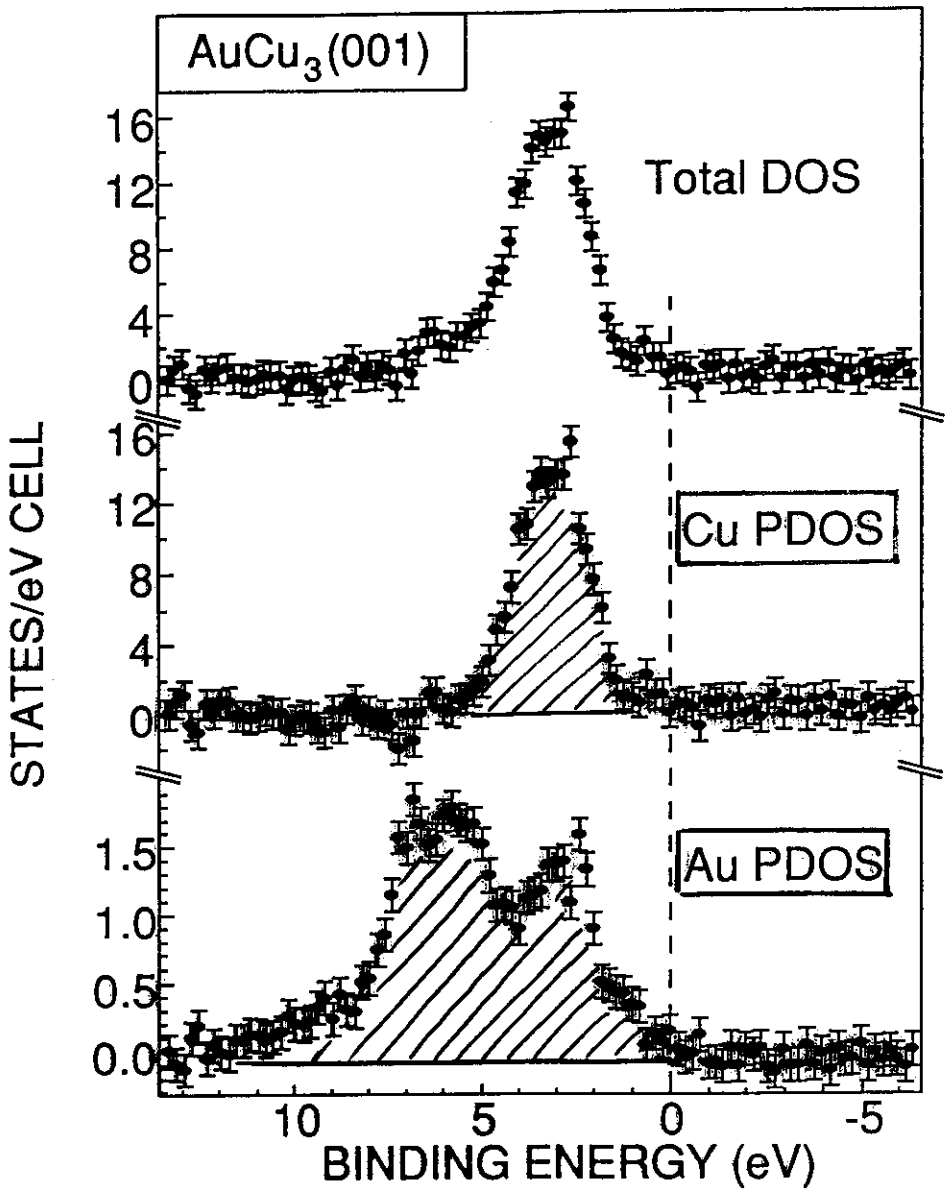
ISS, LEED: - surface well ordered
- at T = 300K :
compositional order up to top layer
→ no segregation



A. STUCK ET AL., P.R.L. 65, 3029 (1990)



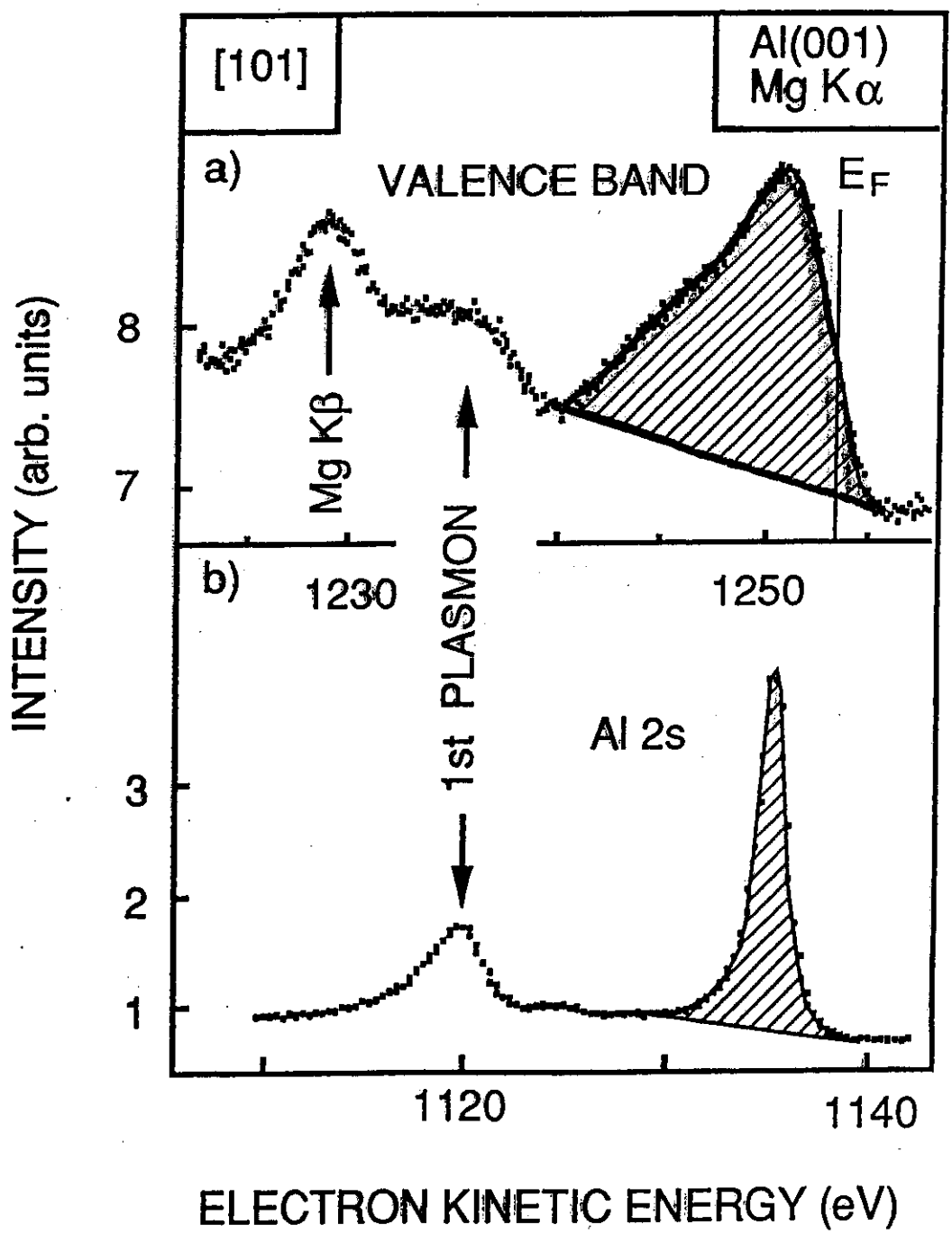
⇒ EQUIVALENCE CORE XPD - VB XPD !


AuCu3(001)
Total DOS
Cu PDOS
Au PDOS
STATES/eV CELL
BINDING ENERGY (eV)
16
12
8
4
0
1.5
1.0
0.5
0.0
10
5
0
-5

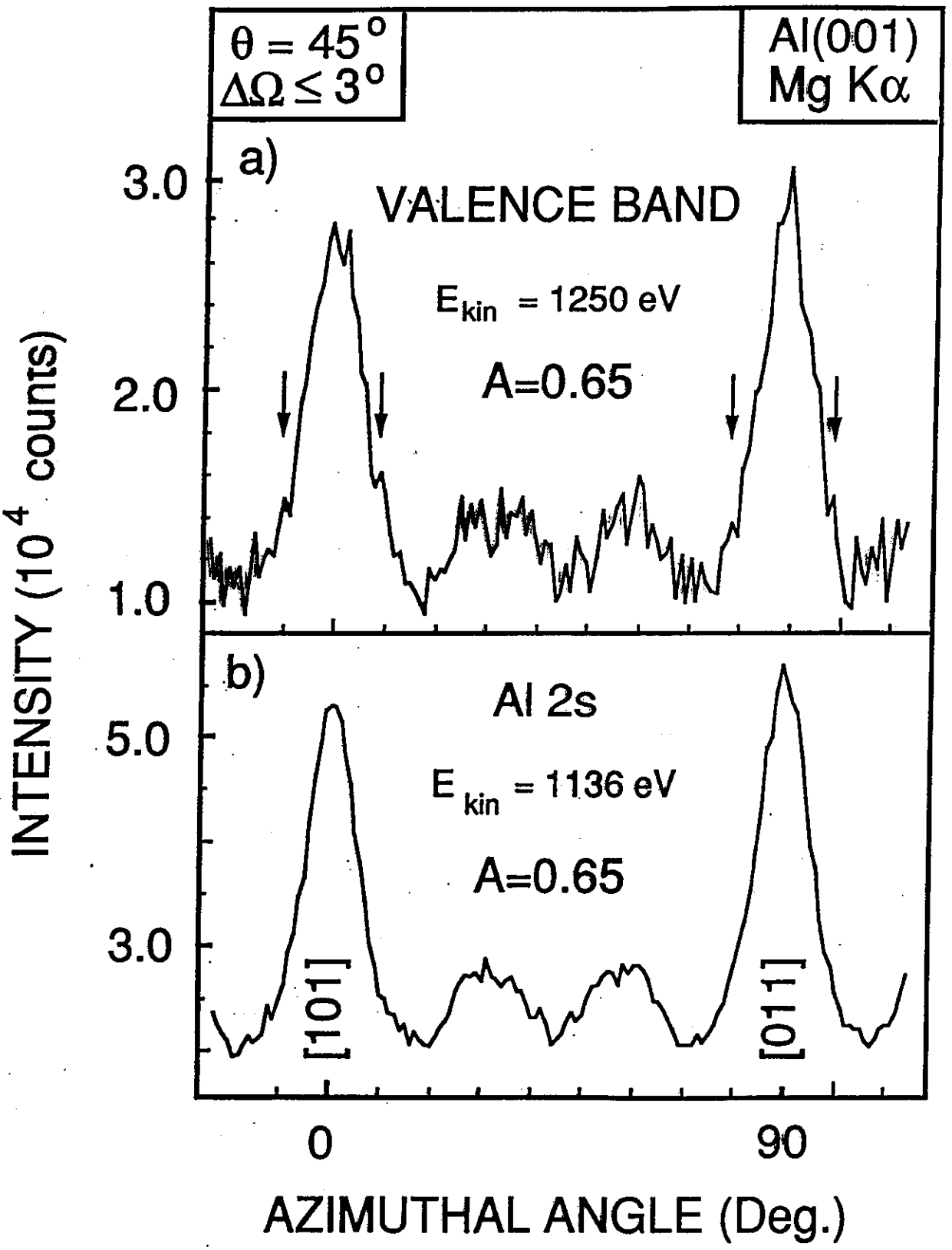
X-RAY EXCITATION

ANGLE RESOLVED VALENCE BAND SPECT.

$\Rightarrow$ DOES NOT CHANGE SHAPE WITH ANGLE



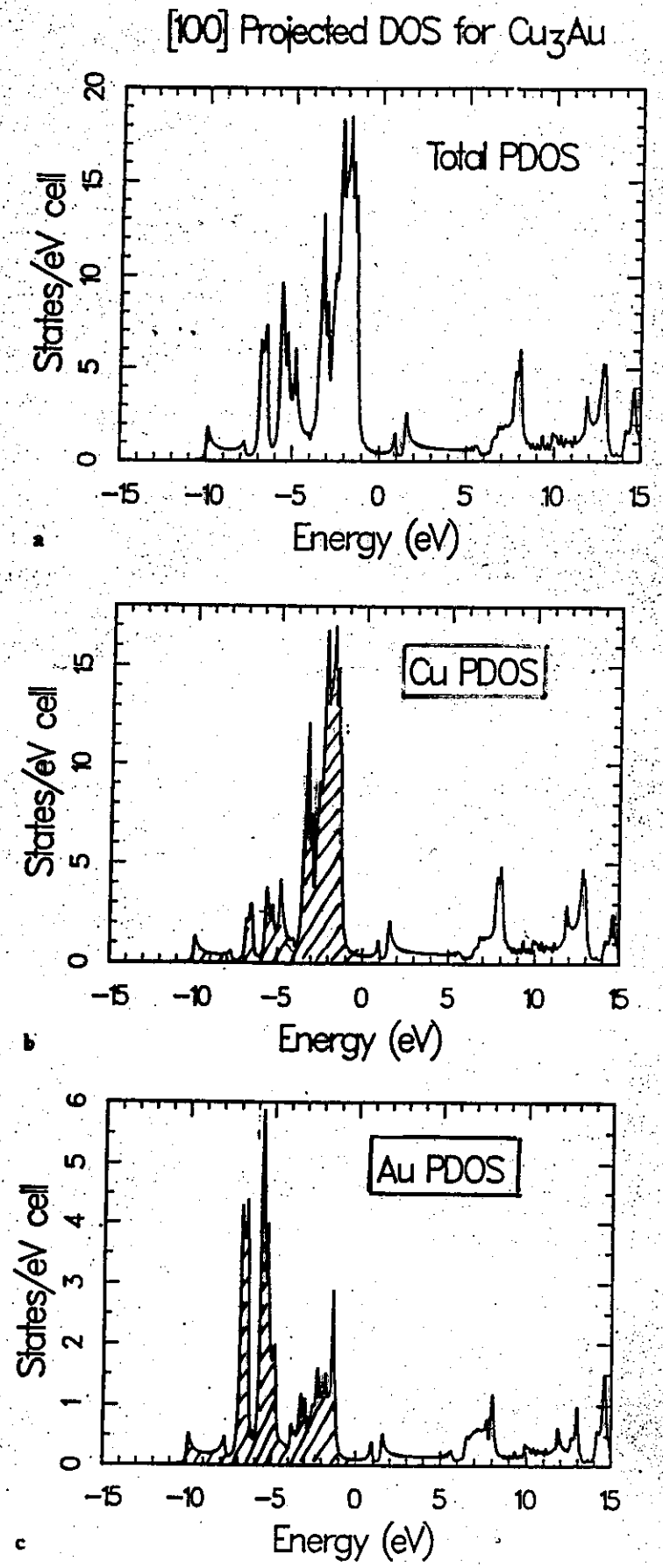
... BUT CHANGES INTENSITY !



LIKE CORE LEVEL XPD !

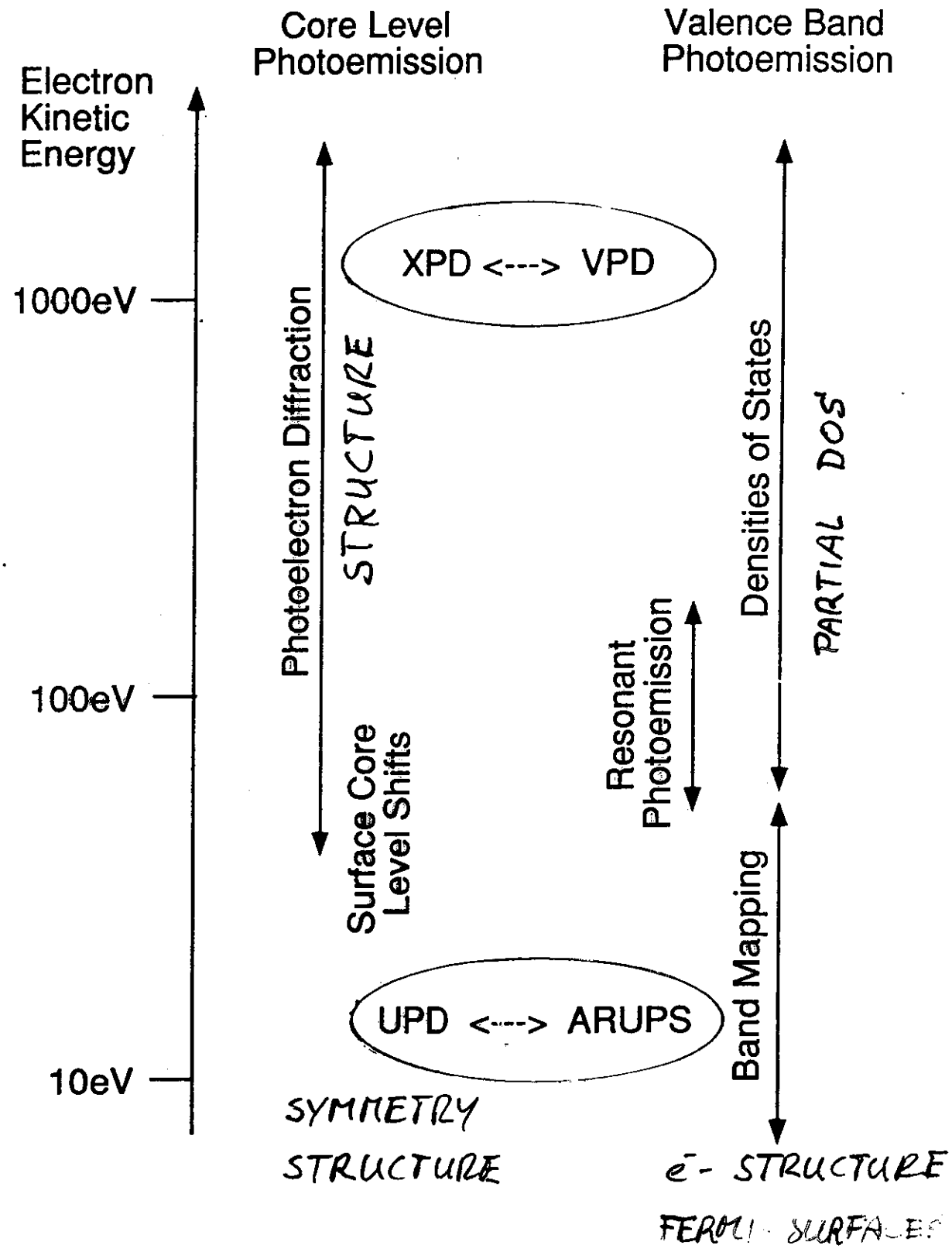
$\Delta\lambda \approx 5\%$

From Bandstructure Calculation:

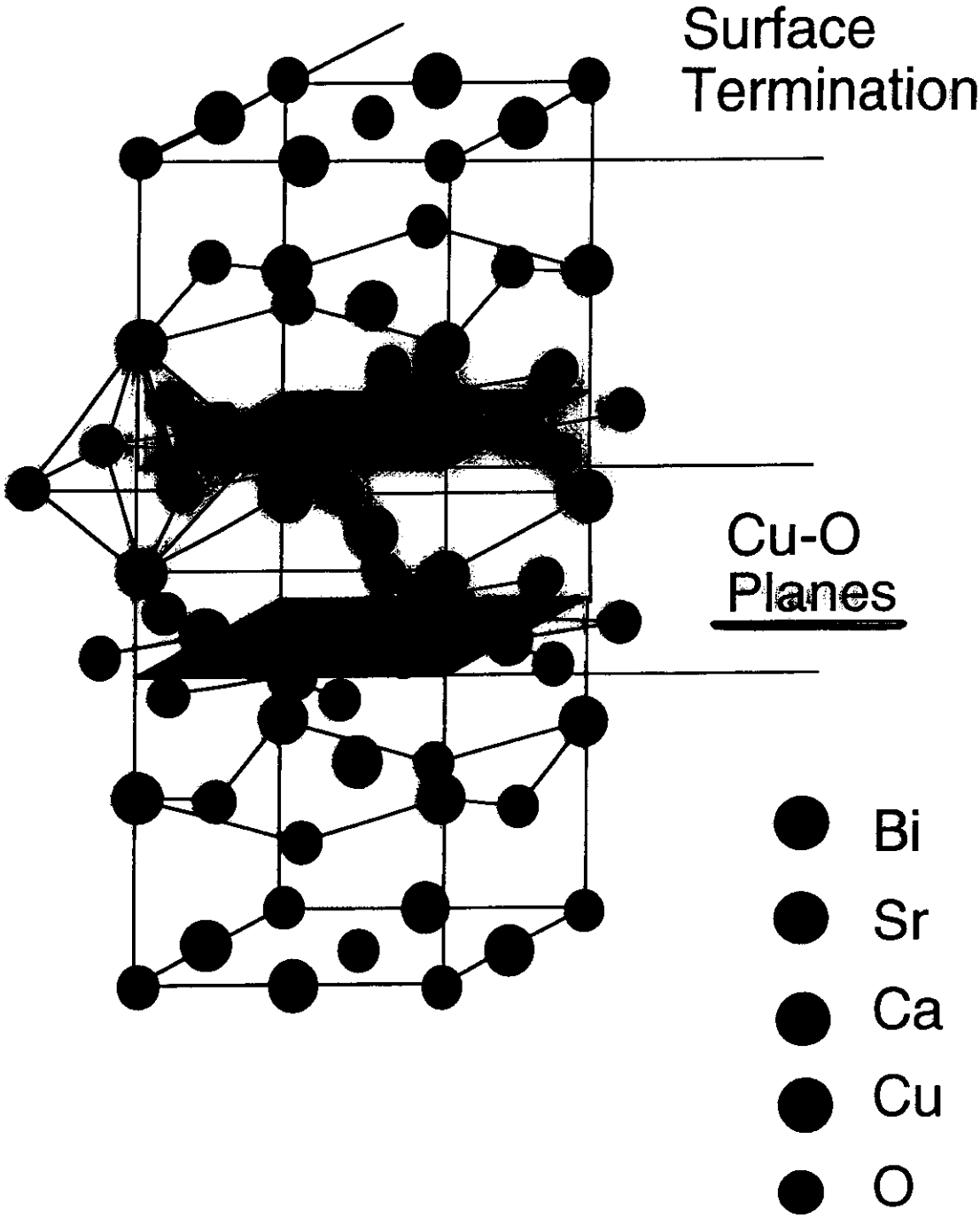


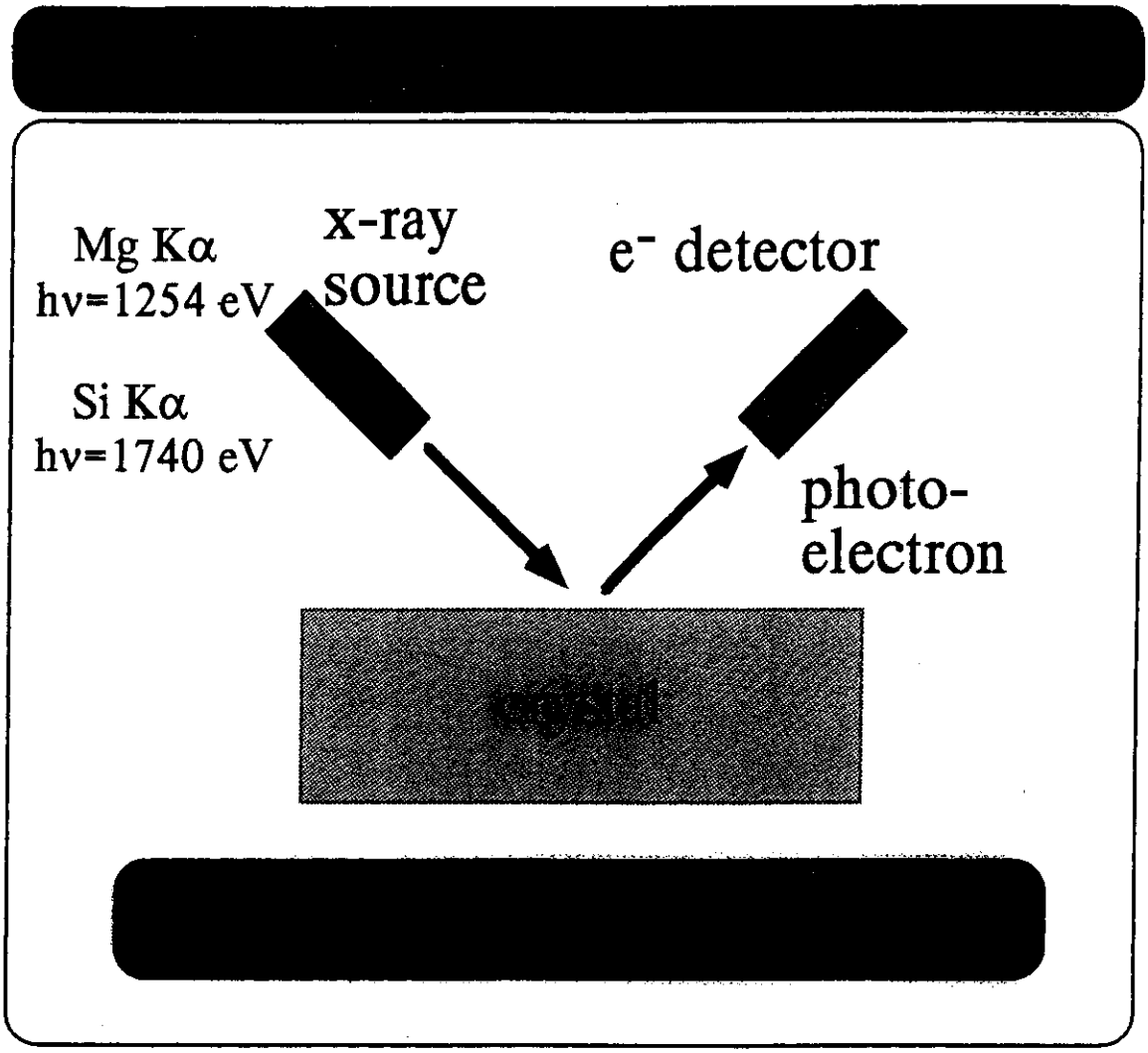
A. Fahal et al., Z. Phys. B 78, 295 (1990)

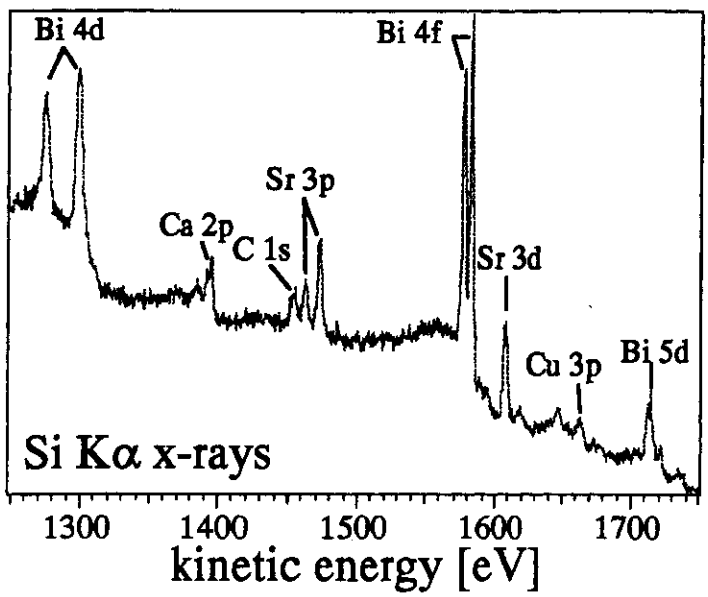
CONCLUSIONS



$Bi_2Sr_2Ca_1Cu_2O_{8+x}$: Crystal Structure



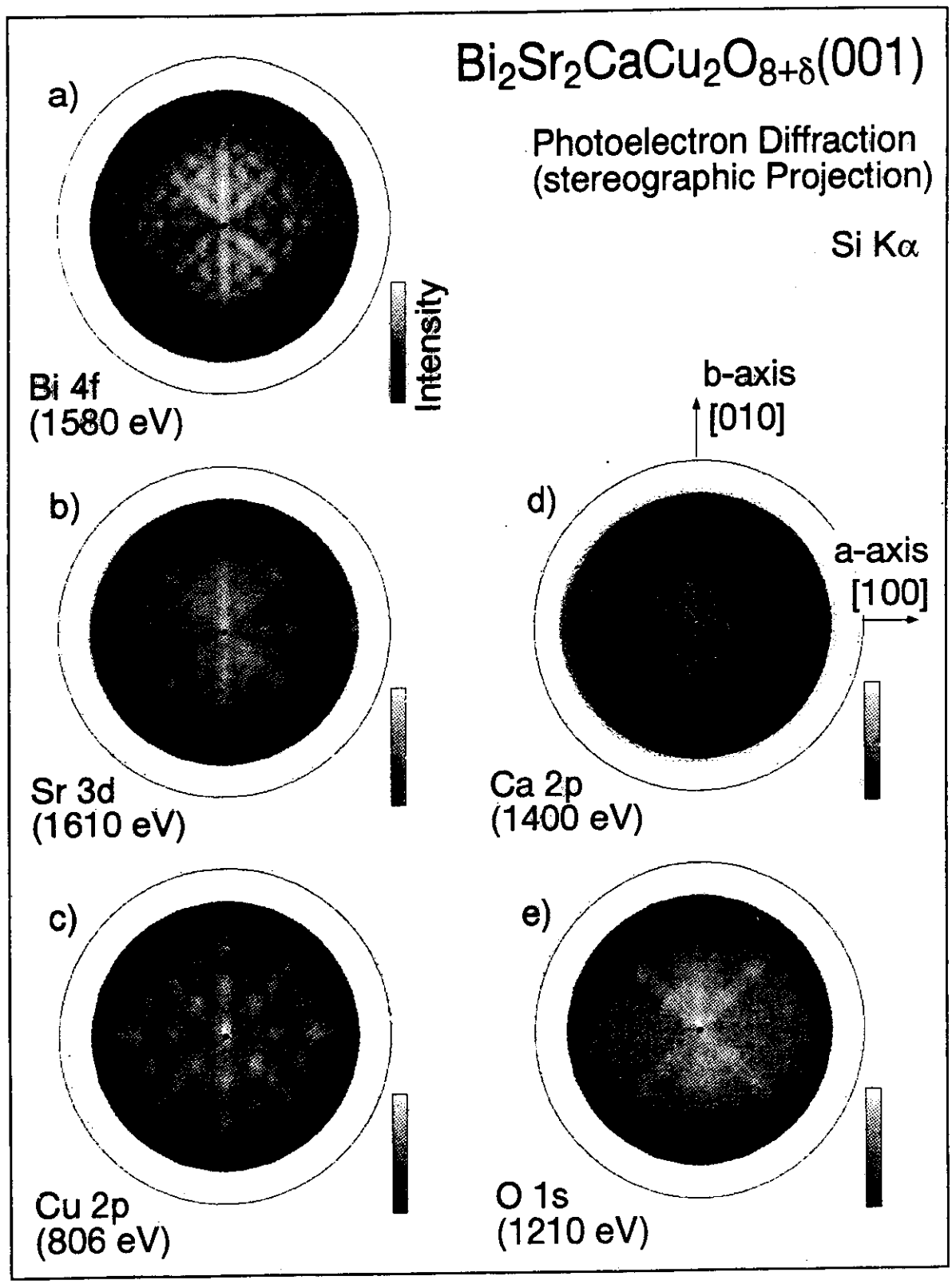




XPS spectrum from
a Bi-2212 single crystal

XPS gives chemical information of a material (type of components)

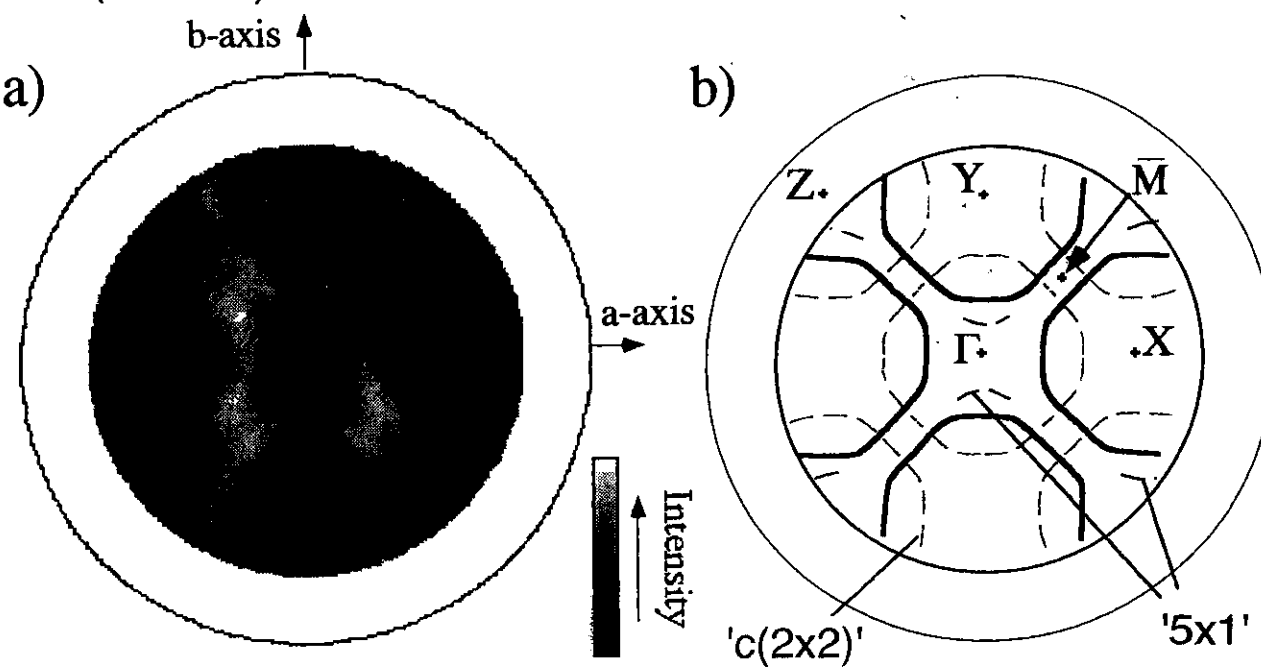
Sr-O
Cu-O
Ca
Cu-C
Sr-O

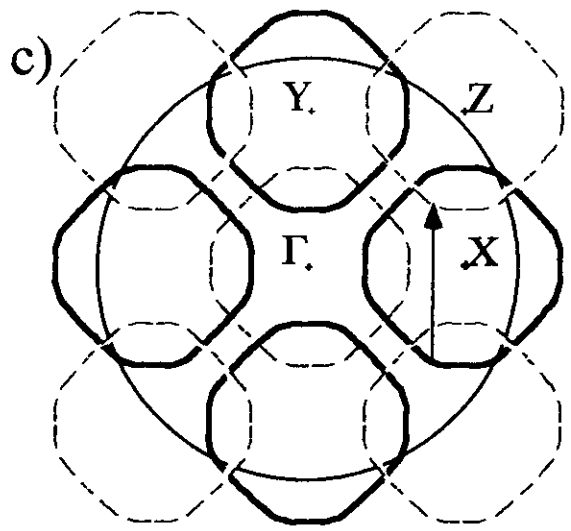


Fermi Surface Mapping from $Bi_2Sr_2CaCu_2O_{8+\delta}(001)$

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

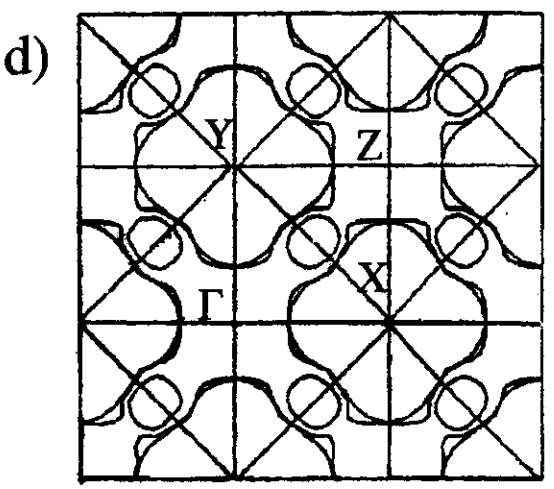
HeI (21.2 eV)





Shadow bands

Large Fermi surface



Band Theory (FLAPW)
(Massidda, Yu, Freeman
Physica 158C, 251 (1988))

Note: $X, Y \triangleq (\pi, \pi)$!

Observation of a BCS Spectral Function in a Conventional Superconductor by Photoelectron Spectroscopy

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Universität des Saarlandes, Fachrichtung 7.2–Experimentalphysik, D-66041 Saarbrücken, Germany

U. Probst and E. Bucher
Universität Konstanz, Fakultät für Physik, D-78434 Konstanz, Germany
(Received 27 April 2000)

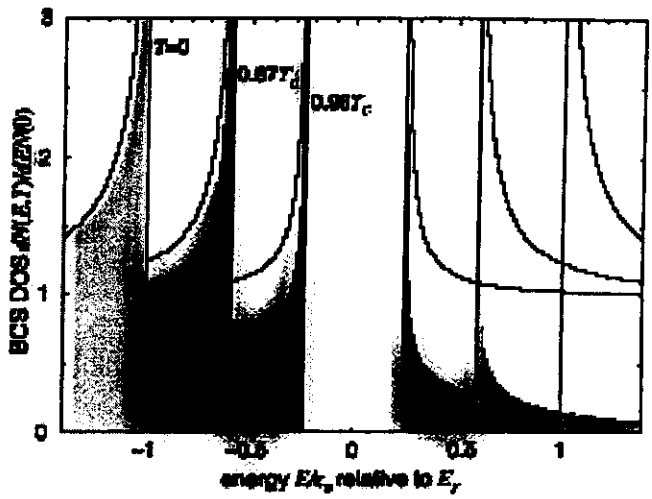
Conventional Superconductor

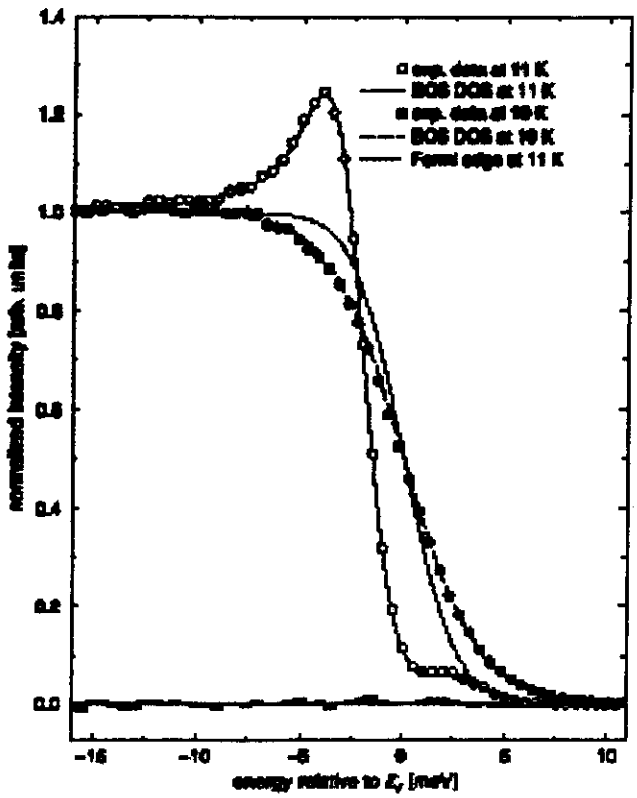
V_3Si

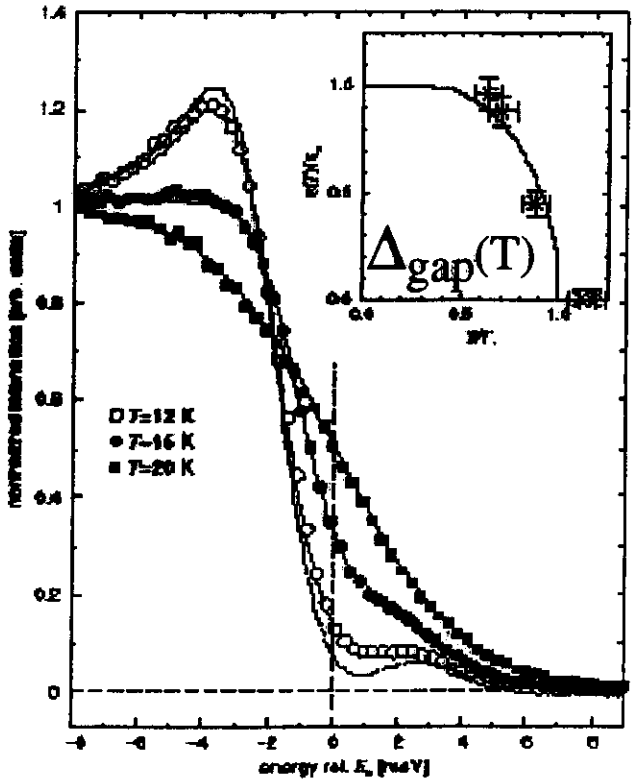
$T_c = 17$ K

$\Delta_{gap} = 5$ meV

Instr. Resolution 2.9 meV !

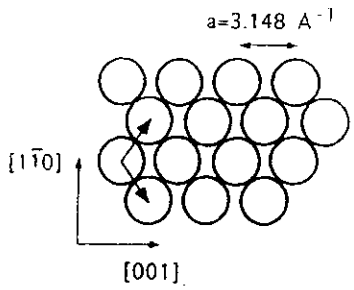




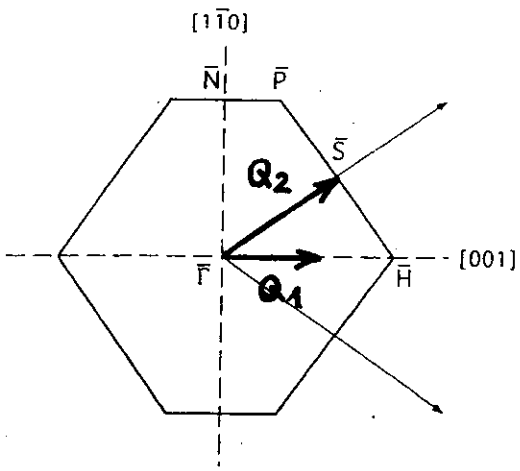


Surface Phonon Modes for H/Mo(110)

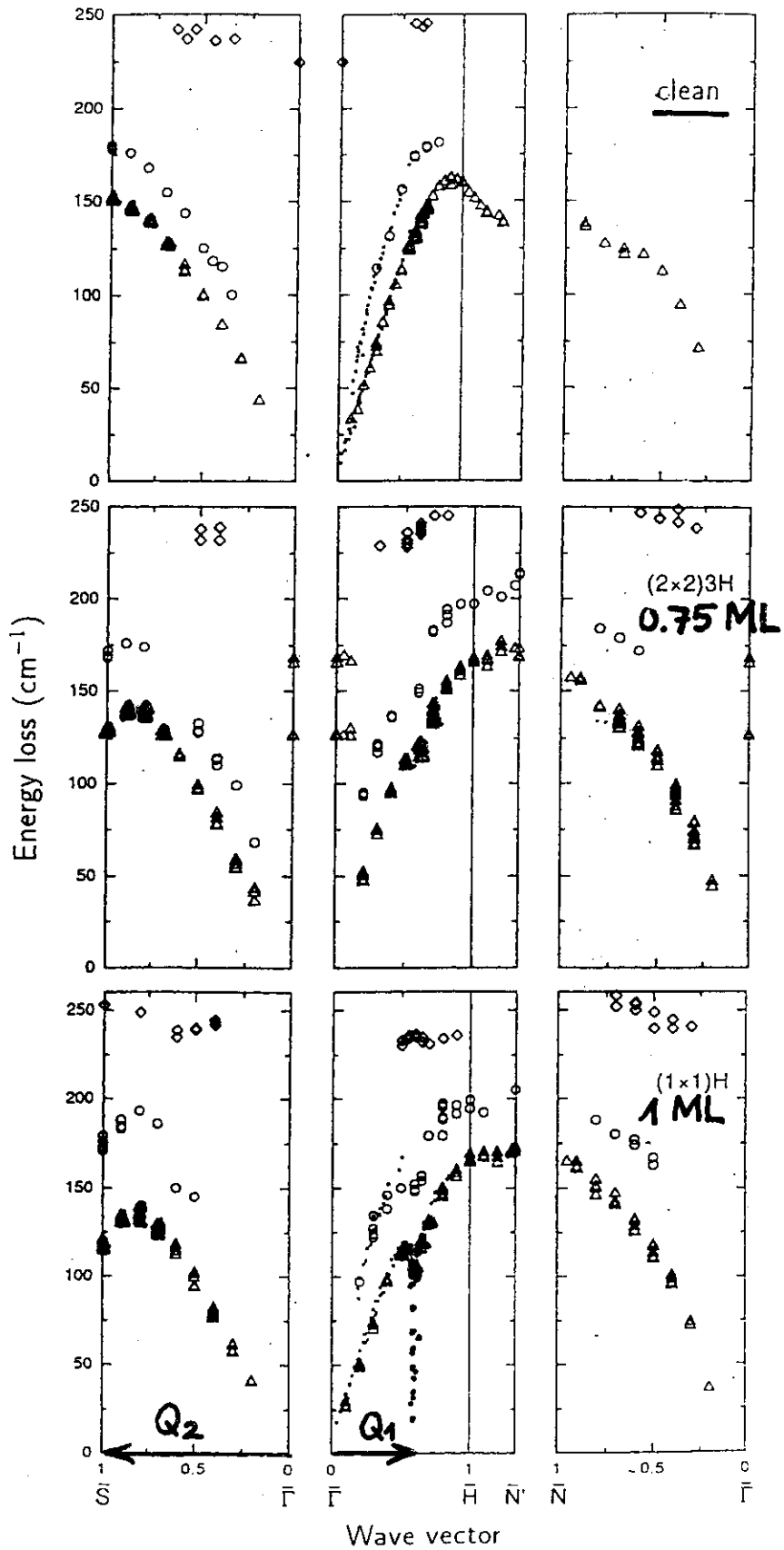
Giant Kohn Anomaly ?



Mo(110)-direct lattice

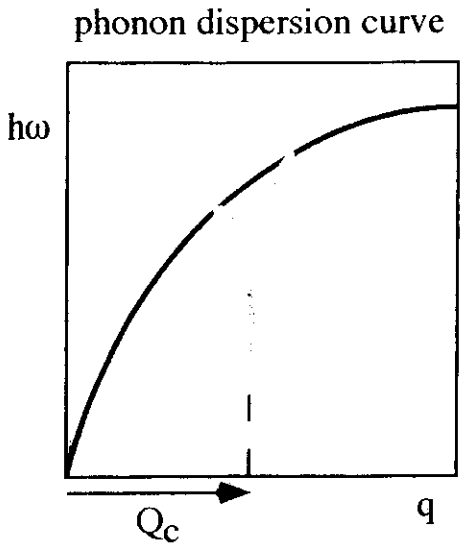


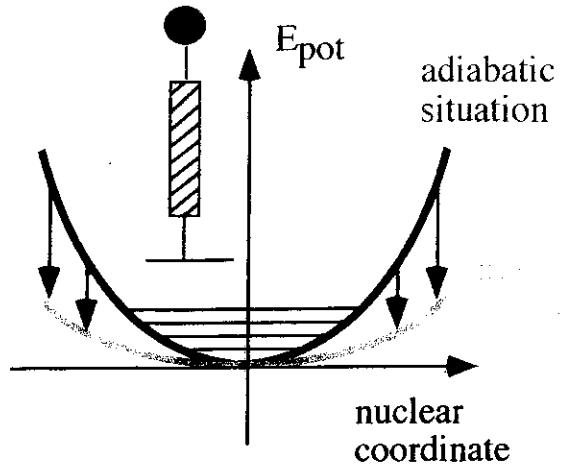
Mo(110)-reciprocal lattice



△ HREELS: J. Kröger et al., PRB 55 ('97) 10895.

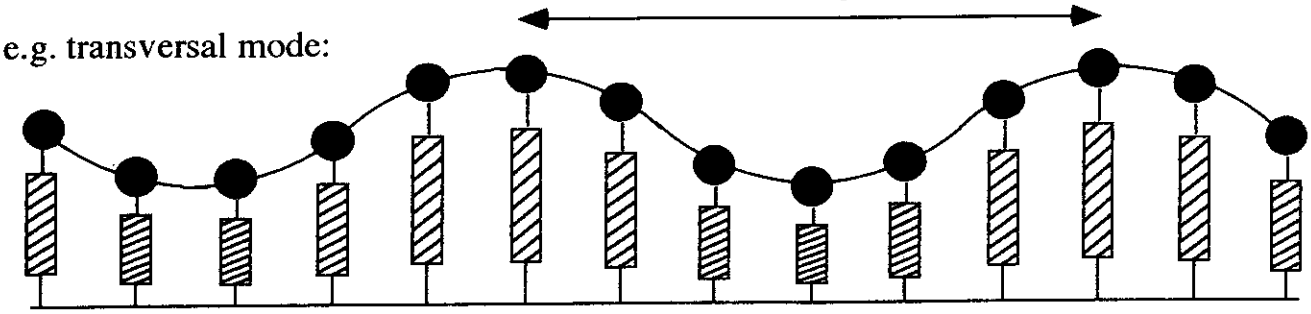
Giant Kohn Anomaly





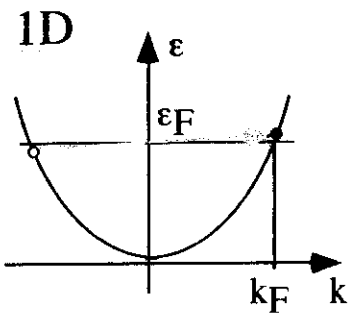
$$\Lambda = \frac{2\pi}{Q_c}$$

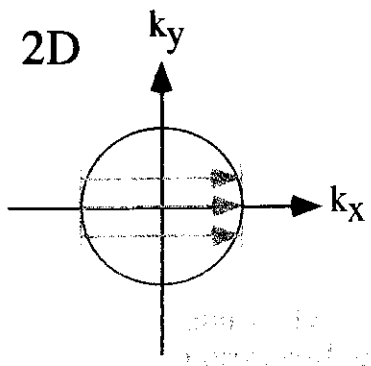
e.g. transversal mode:



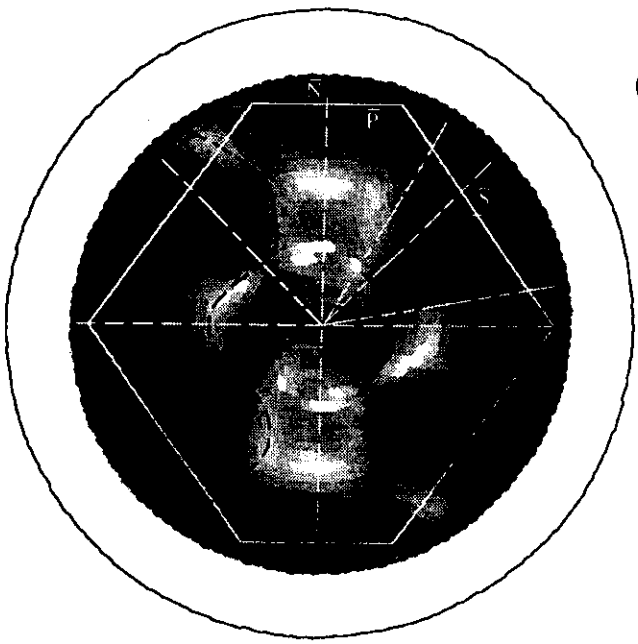
optimum screening:

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

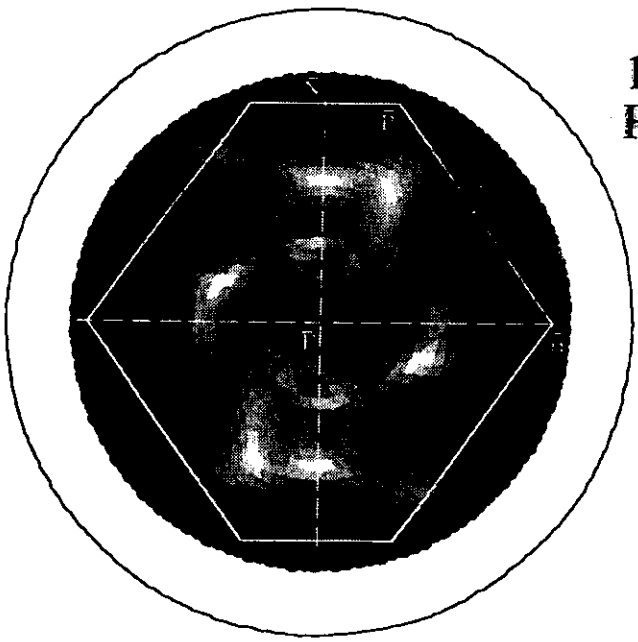




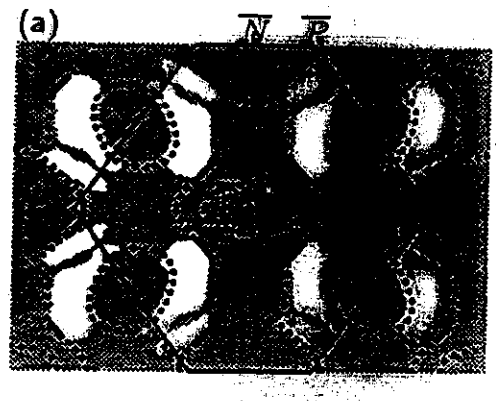
Fermi Surface Contours of Surface States on Mo(110)

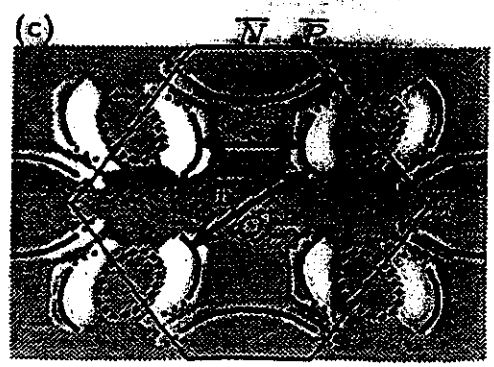


Clean Surface



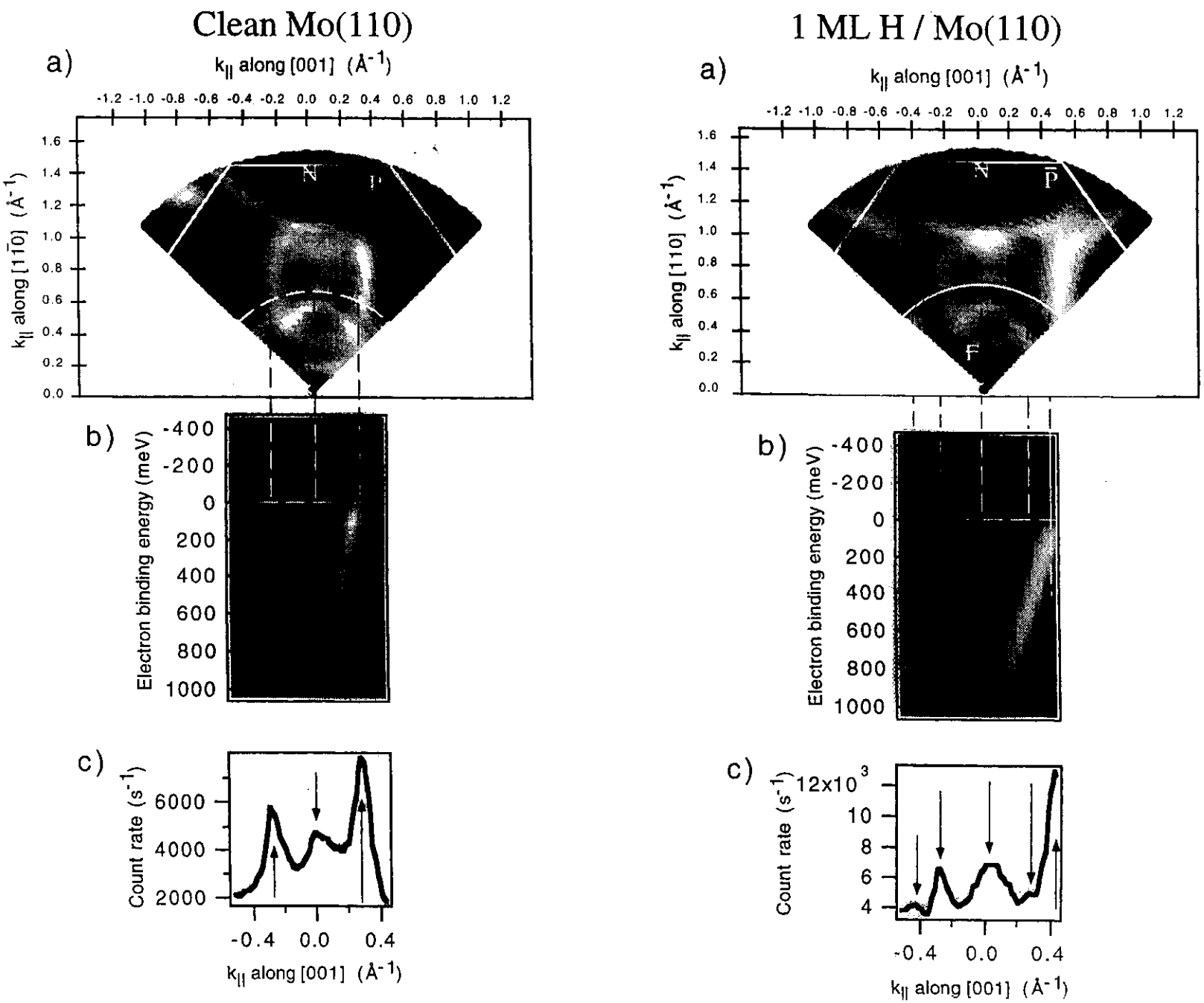
1 ML Hydrogen



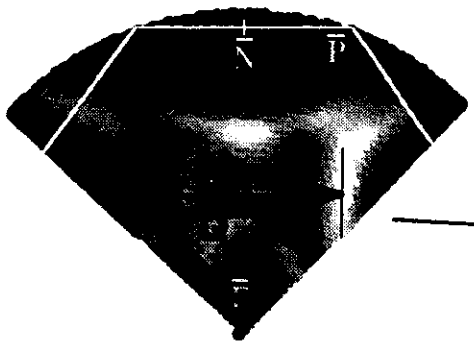


DFT: B. Kohler et al., PRL 74 (1995) 1387.

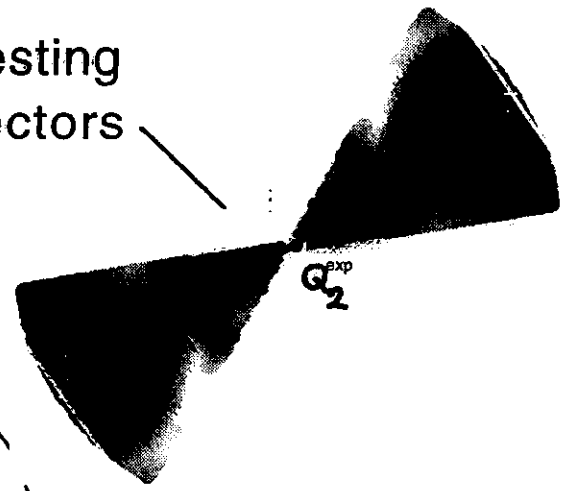
H-Induced Shift of Fermi Surface Contours on Mo(110)

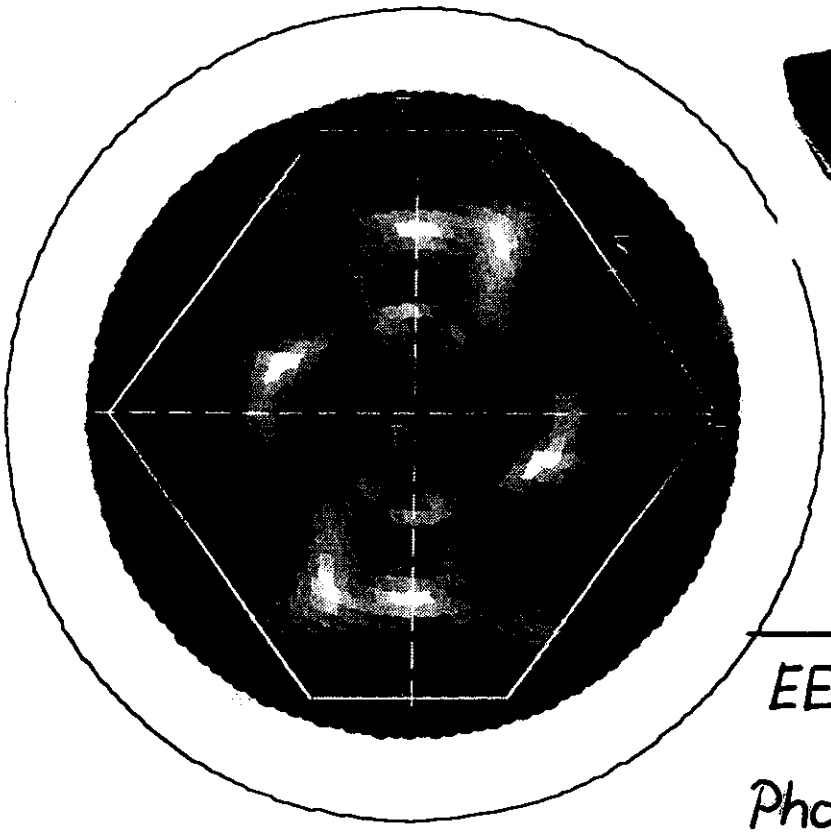


Fermi Surface Nesting
on 1 ML H/Mo(110)
Measured by Photoemission



nesting
vectors

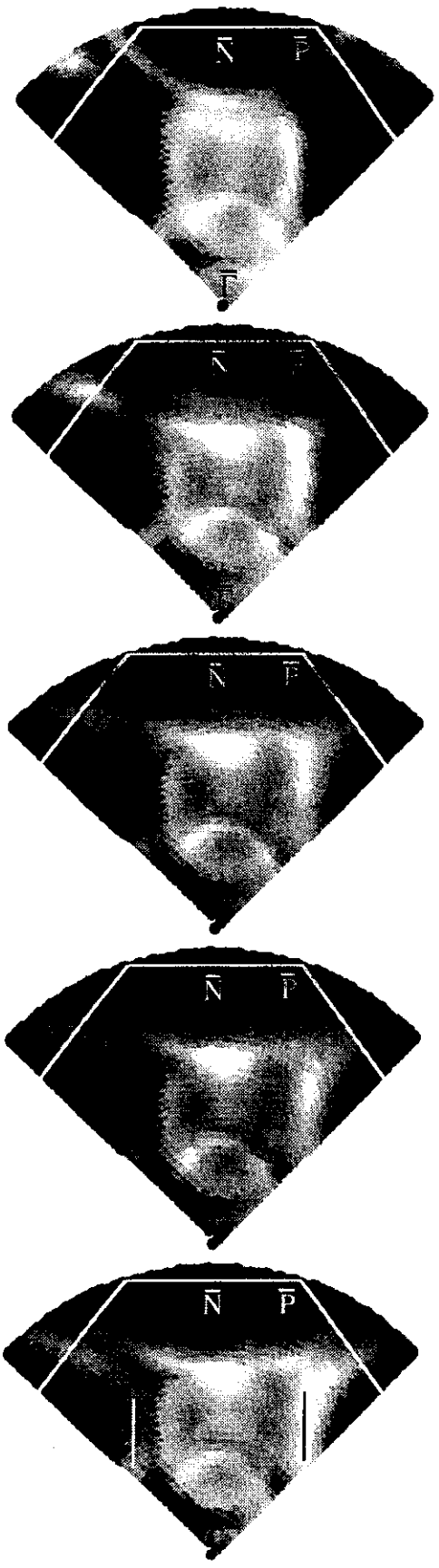




	Q_1	Q_2
EELS	0.90	1.22
Photo-emission	0.85	1.19
Theory (DFT)	0.86 $Å^{-1}$	1.23

Fermi Surface Contours of H/Mo(110):

Evolution with Coverage



clean

0.6 L H_2

1.5 L H_2

2.5 L H_2

80 L H_2

= 1 ML