united nations educational, scientific and cultural organization

international atomic energy agency

the
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international centre for theoretical physics

SMR/1270-34

SCHOOL ON SYNCHROTRON RADIATION

6 November – 8 December 2000

Miramare - Trieste, Italy

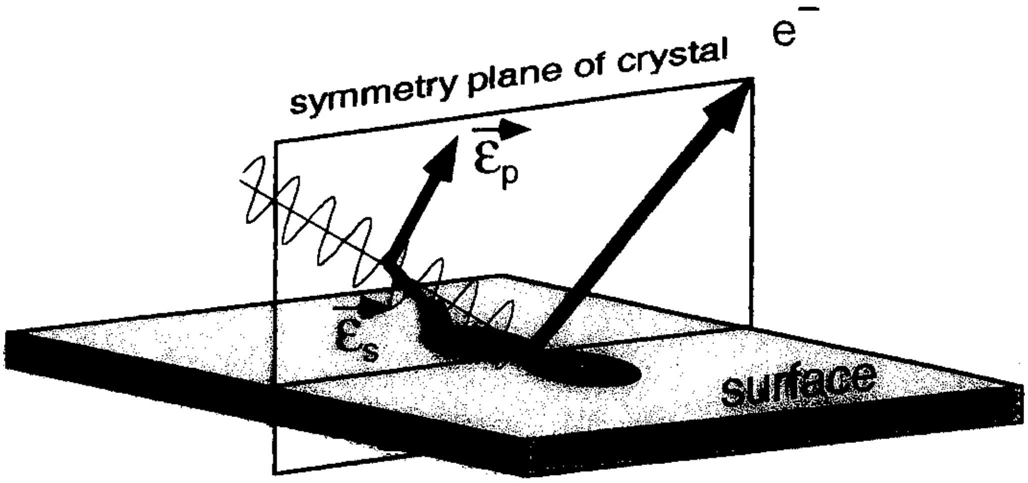
Supported in part by the Italian Ministry of Foreign Affairs in connection with the SESEME project

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

Photoemission Intensities and Line Widths

Juerg Osterwalder
Universitaet Zuerich-Irchel
Zurich, Switzerland

Exploitation of Photon Polarization for Symmetry Analysis of Valence States



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

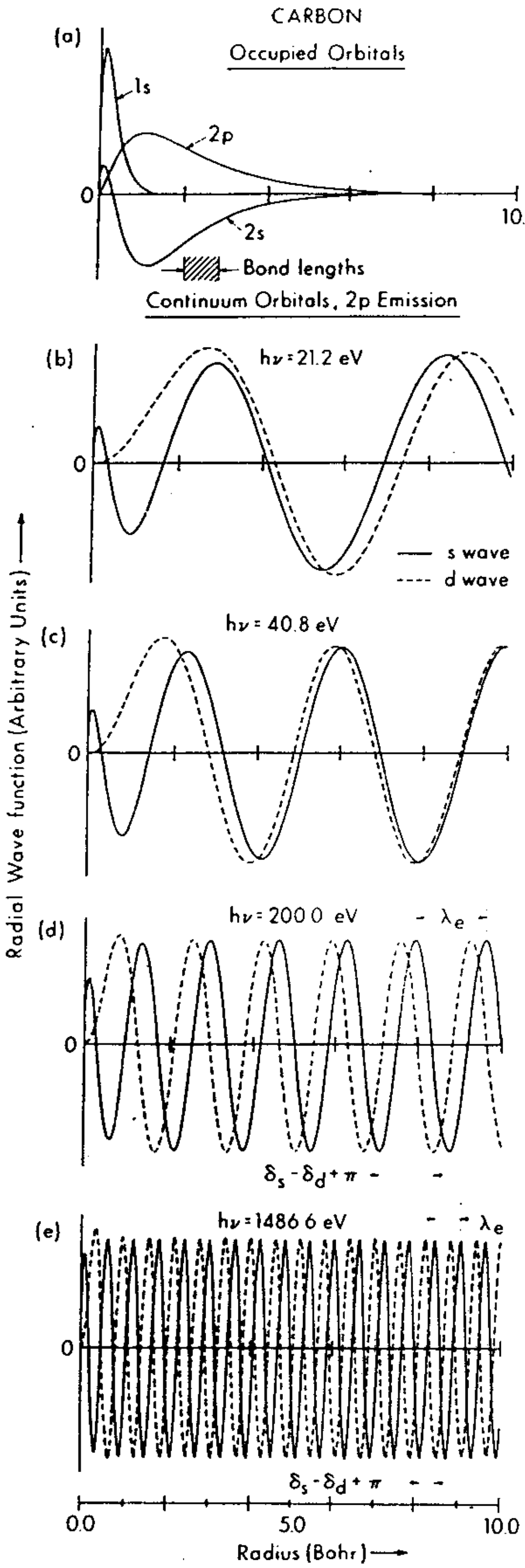
$\vec{\varepsilon}_s$ ... perpendicular ("senkrecht") to ... scattering plane

photoemission matrix element:

$\left| <$ [redacted] $| \vec{r}_k \cdot$ [redacted] [redacted] $> \right|^2 \longrightarrow$ Intensity

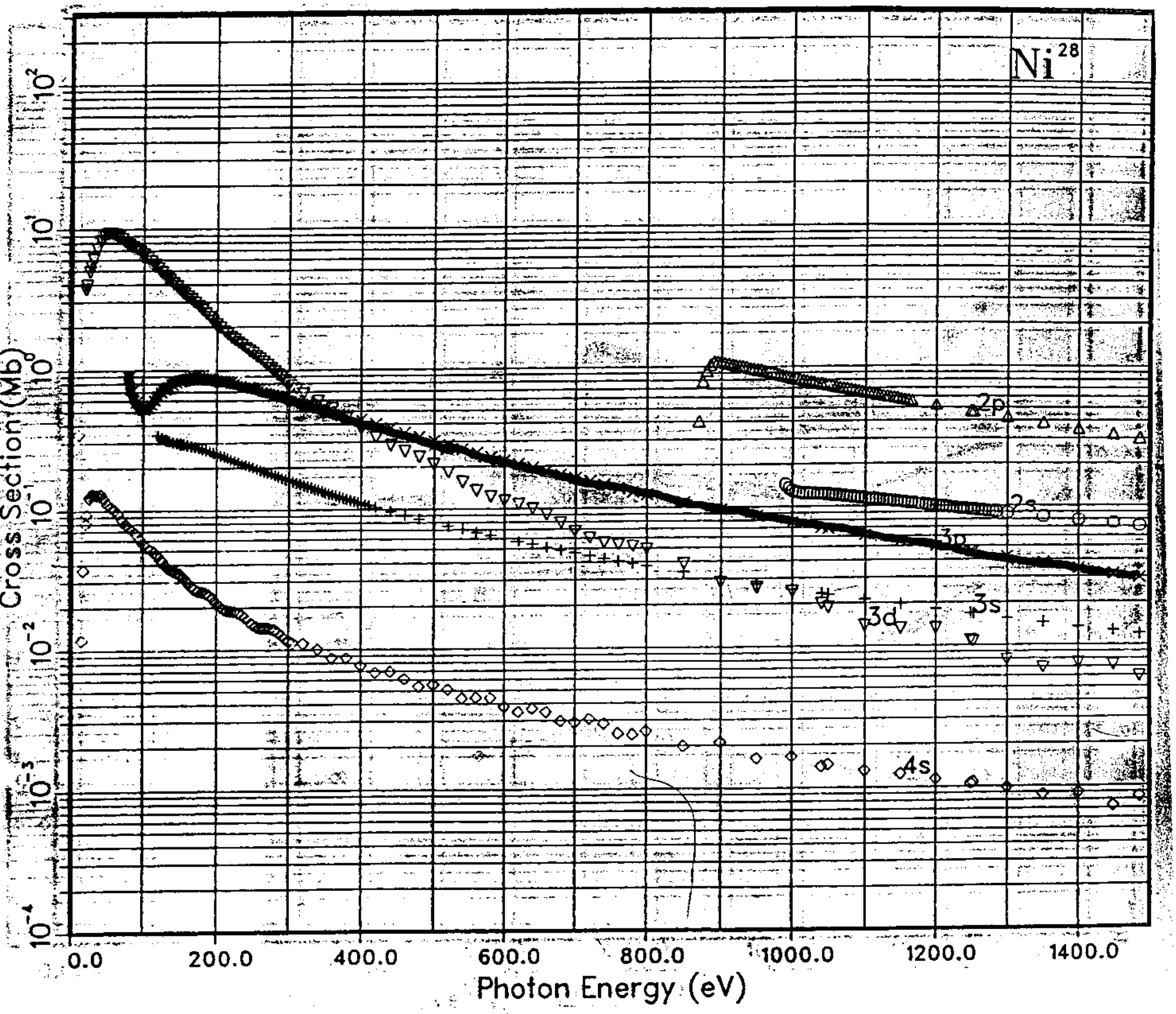
mirror reflection symmetries:

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


CARBON
Occupied Orbitals
(a)
1s
2p
2s
0
10.0
Bond lengths
Continuum Orbitals, 2p Emission
(b)
hν = 21.2 eV
0
s wave
d wave
(c)
hν = 40.8 eV
0
(d)
hν = 200.0 eV
λe
0
δs - δd + π
(e)
hν = 1486.6 eV
λe
0
δs - δd + π
0.0
5.0
10.0
Radius (Bohr)
Radial Wave function (Arbitrary Units)

GRAPH I. Atomic Subshell Photoionization Cross Sections for 0–1500 eV, $1 \leq Z \leq 103$

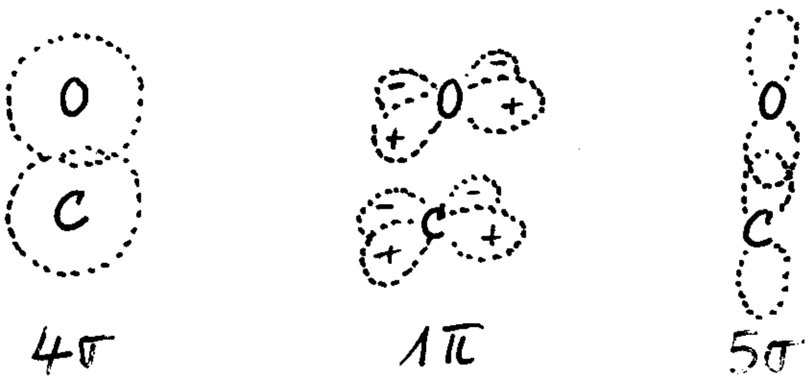
See page 6 for Explanation of Graphs

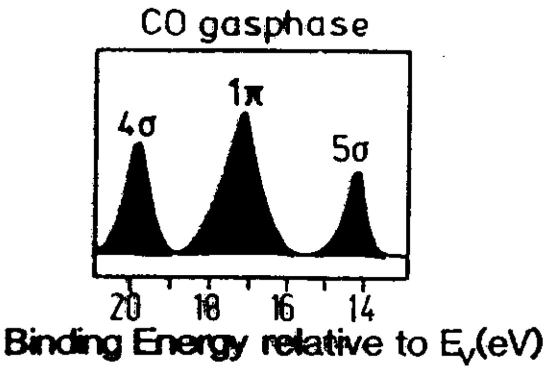


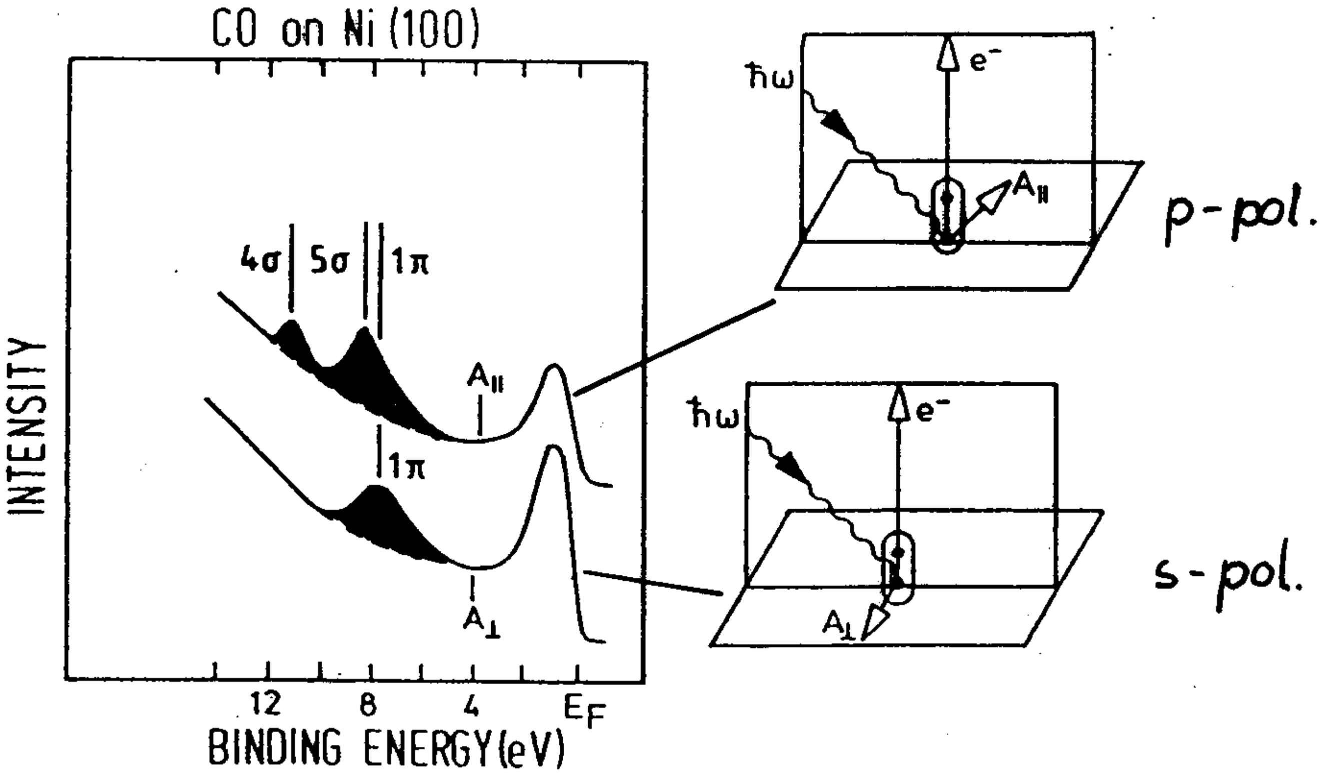
Ni binding energies(eV) are:

1s(2) 8213.02	2s(2) 987.301	2p(6) 868.772
3s(2) 115.630	3p(6) 78.2927	4s(2) 7.93172
3d(8) 15.1614		

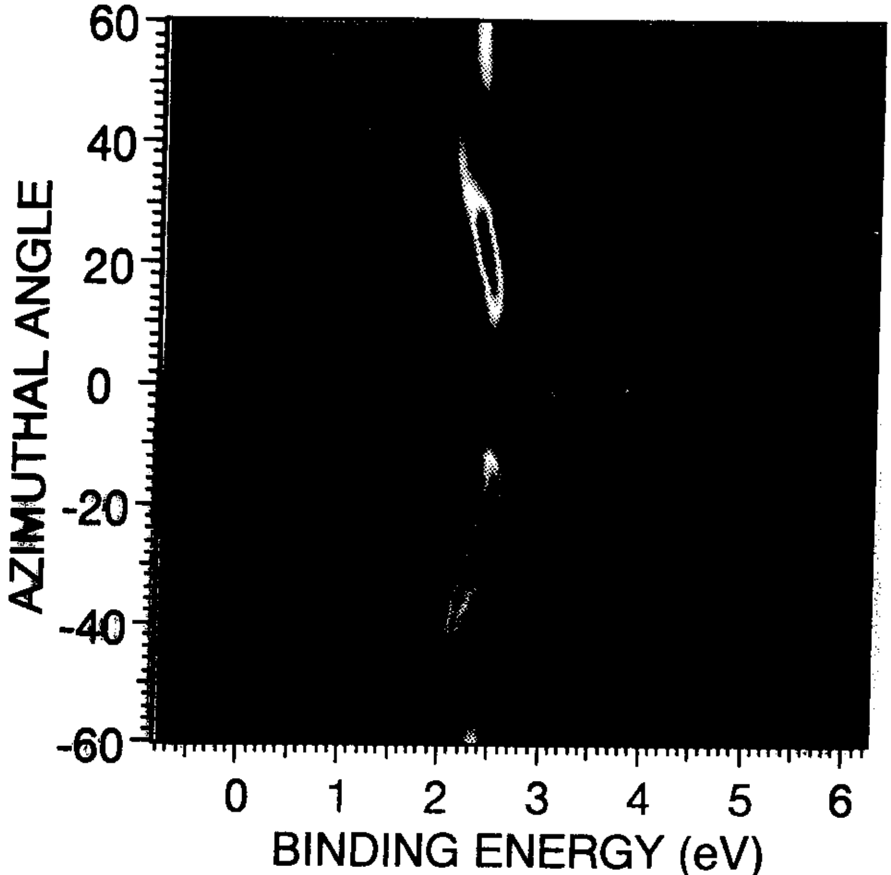
CO Molecular Orbitals







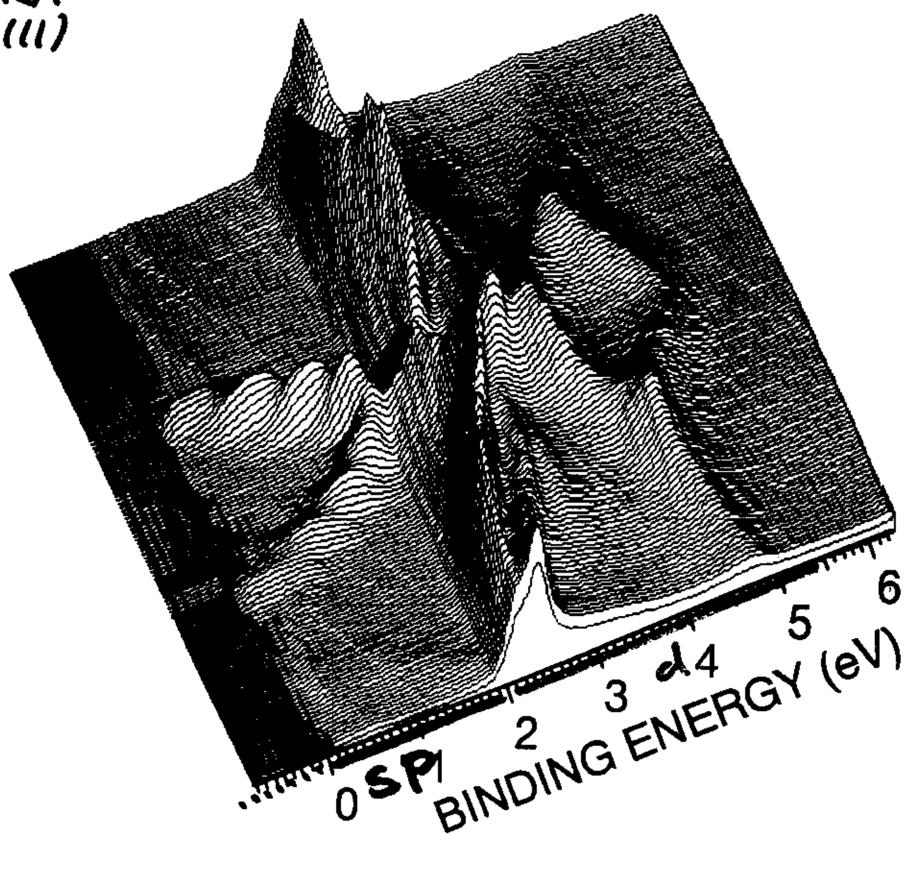
from Hüfner



UPS SPECTRA
FROM Cu(111)

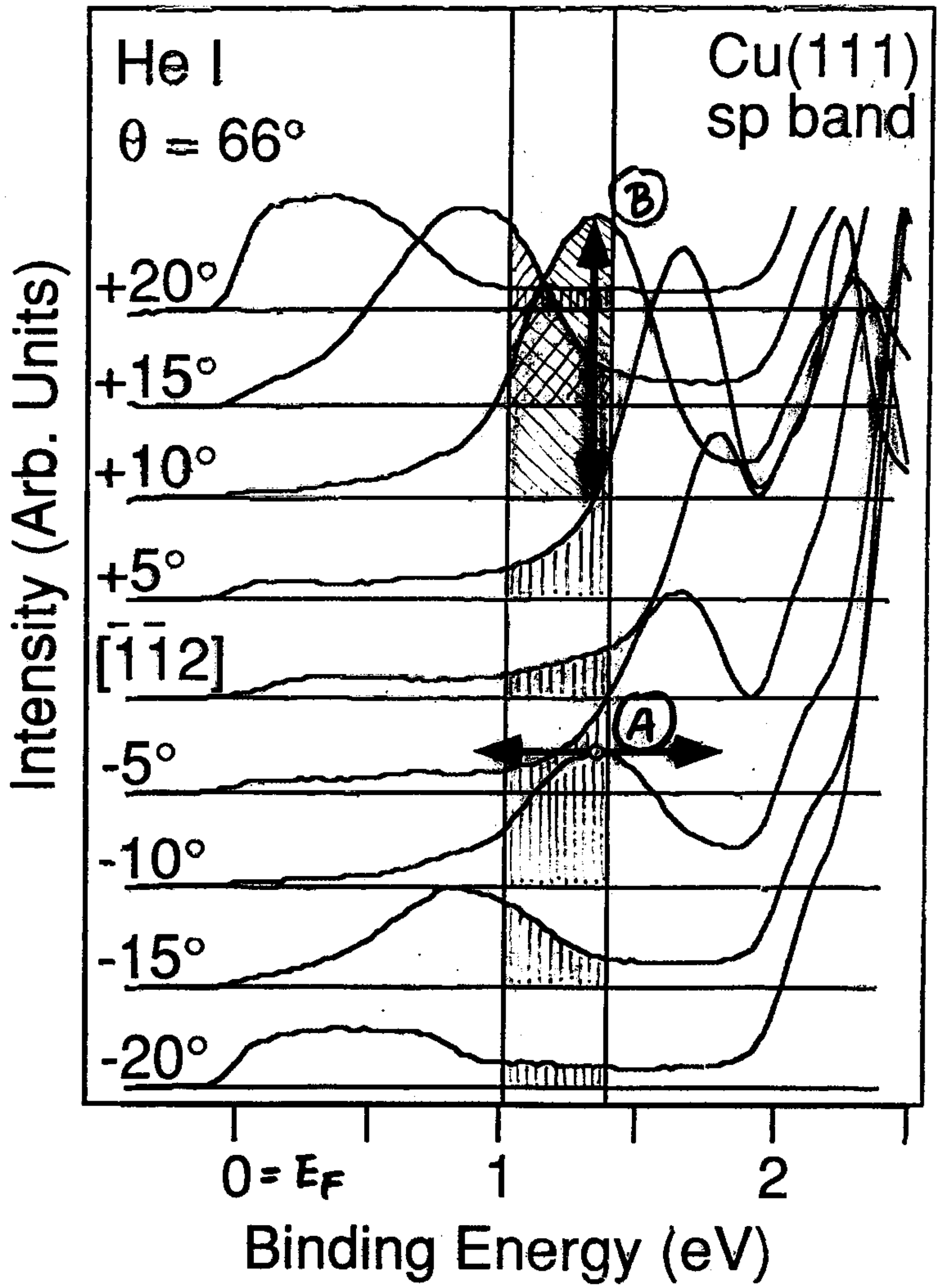
$h\nu = 21.2 eV$

$\theta = 66°$



UV EXCITATION

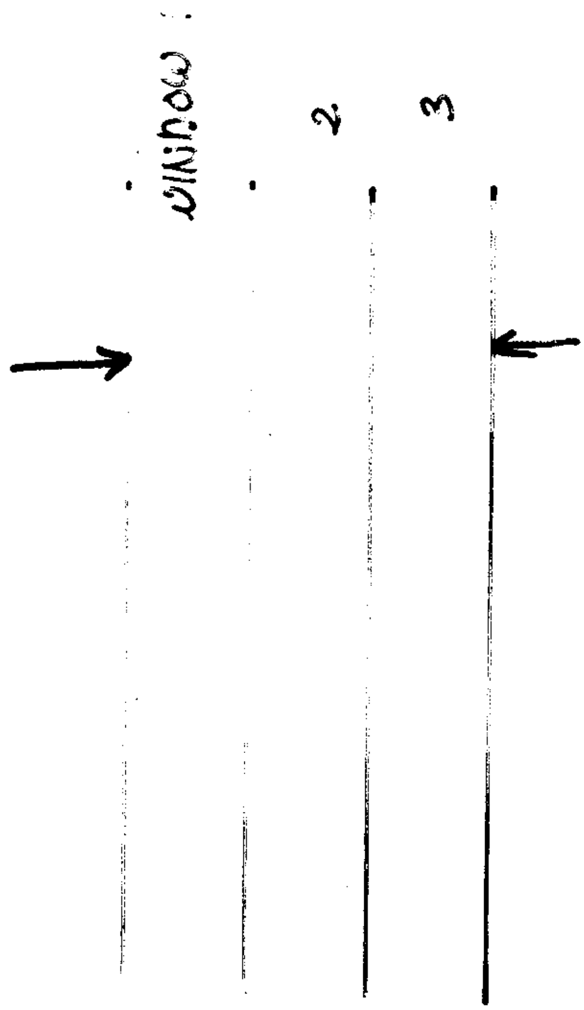
DISPERSION !



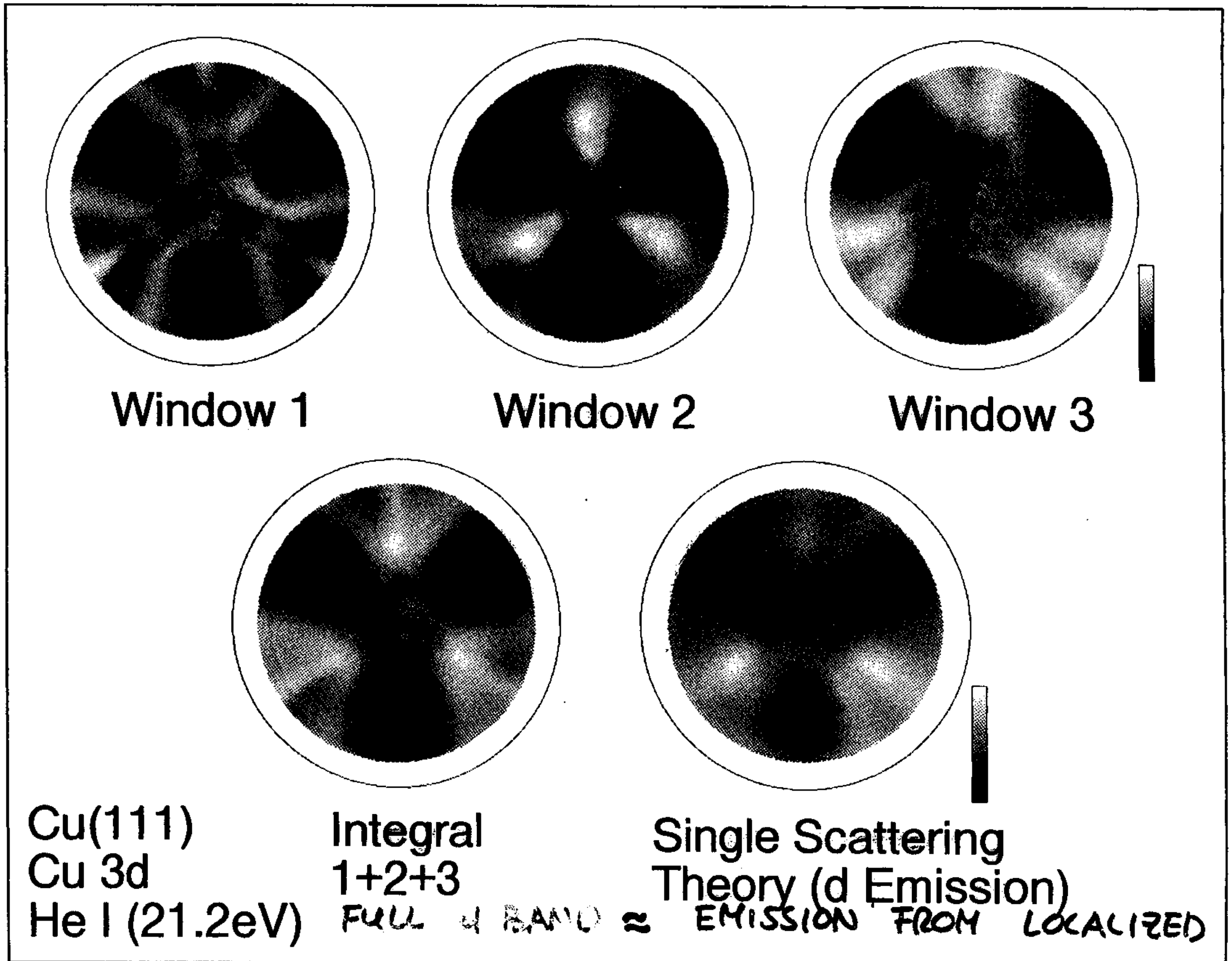
INTENSITY VARIATION DUE TO

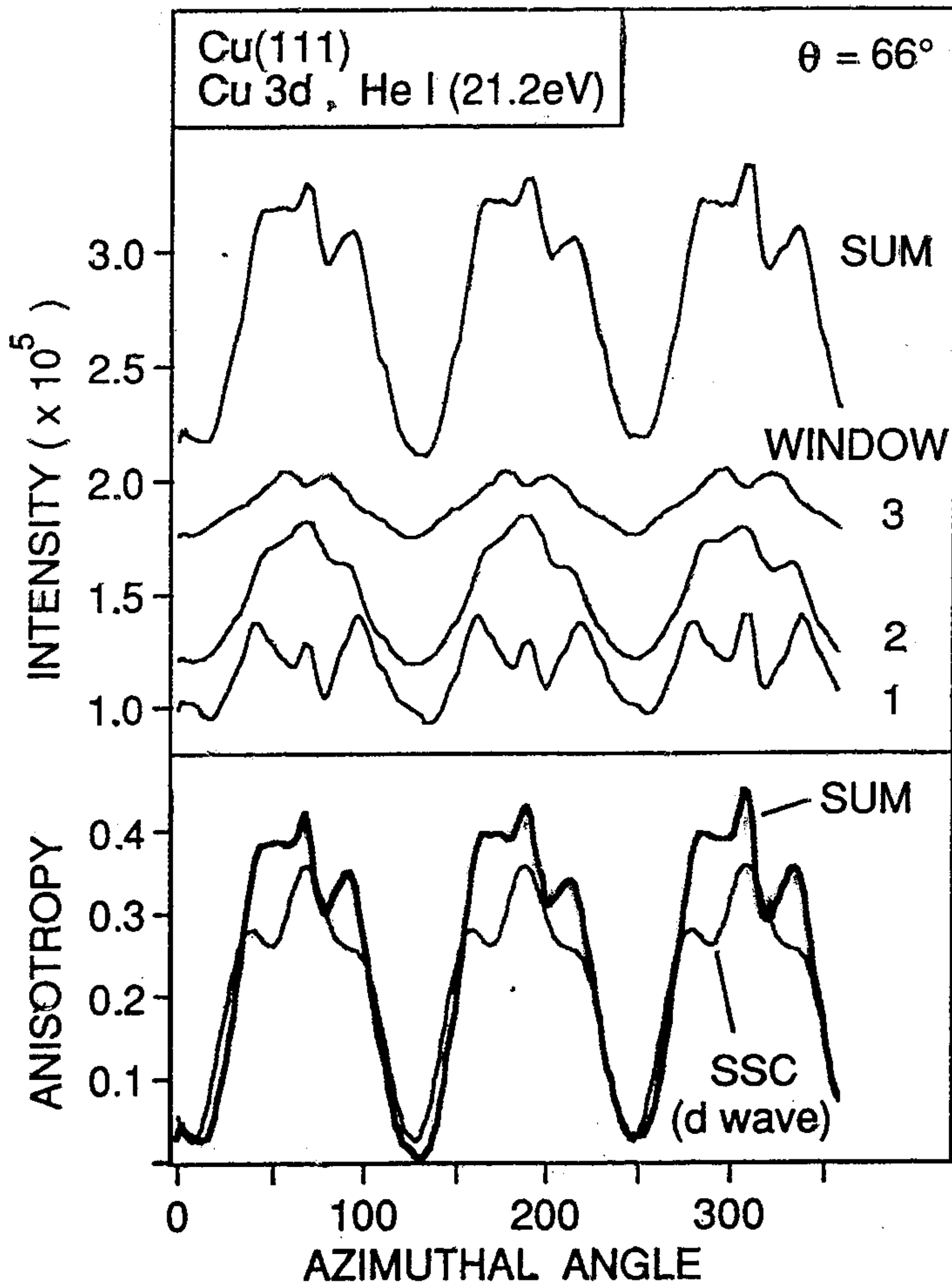
(A) DISPERSION IN/OUT OF WINDOW

(B) INTENSITY CHANGES OF DT PEAK



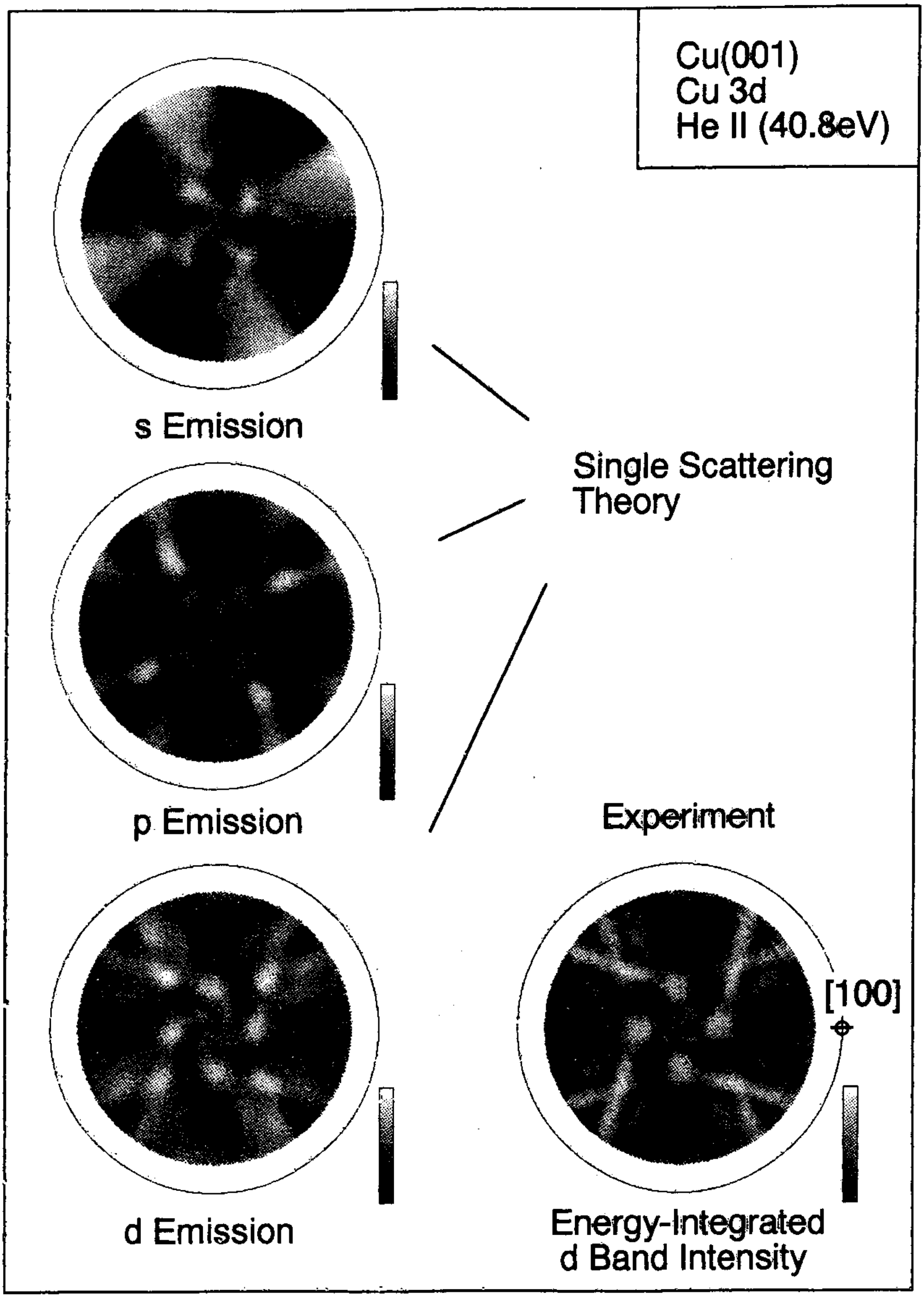
INTEGRATION
OVER FULL
d BAND


Window 1
Window 2
Window 3
Cu(111)
Cu 3d
He I (21.2eV)
Integral
1+2+3
Single Scattering
Theory (d Emission)
FULL d BAND ≈ EMISSION FROM LOCALIZED d ORBITAL (XPD THEORY!)

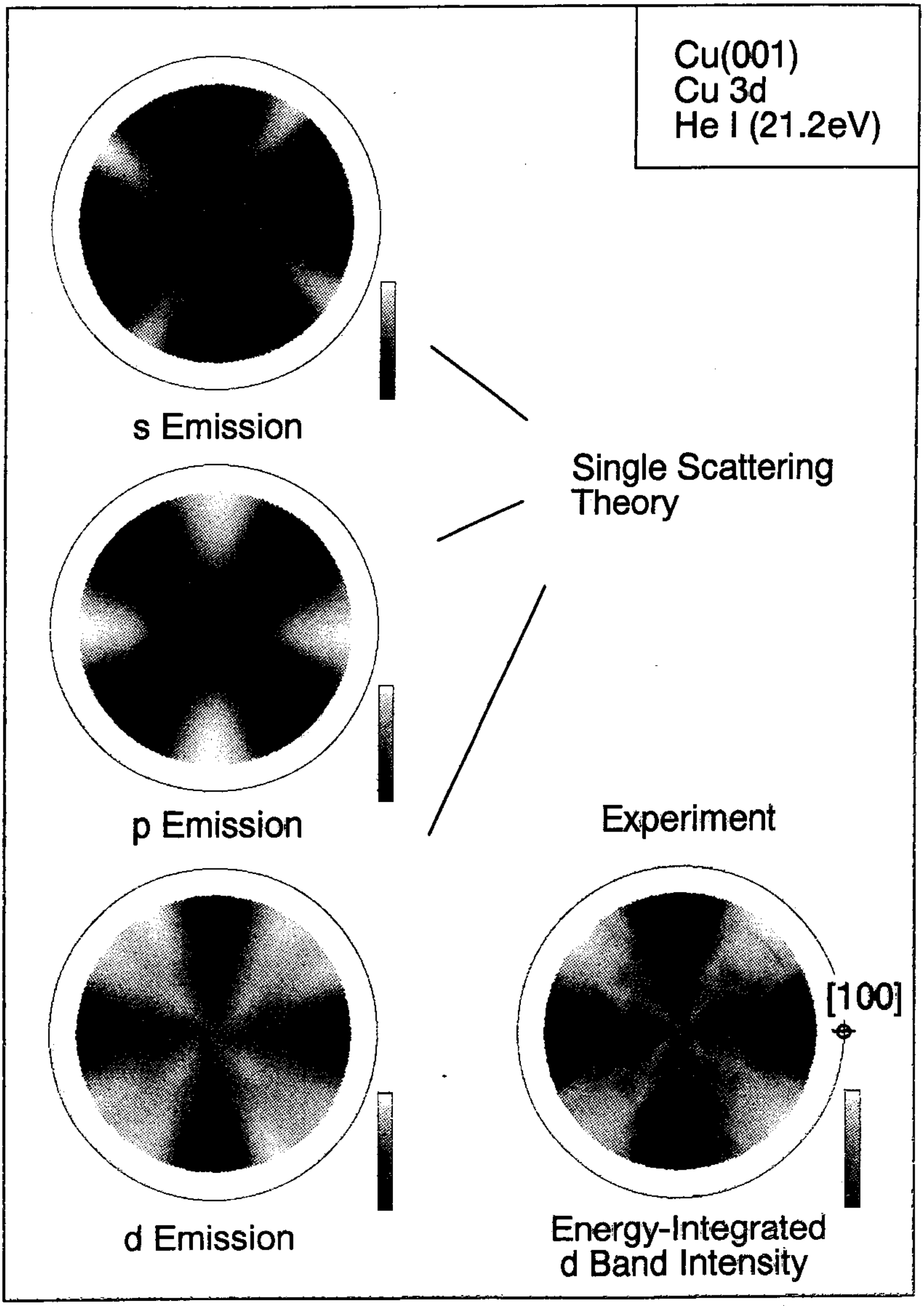


Cu(111)
Cu 3d , He I (21.2eV)
θ = 66°
SUM
WINDOW
3
2
1
INTENSITY (x 10^5)
3.0
2.5
2.0
1.5
1.0
SUM
SSC
(d wave)
ANISOTROPY
0.4
0.3
0.2
0.1
0
100
200
300
AZIMUTHAL ANGLE

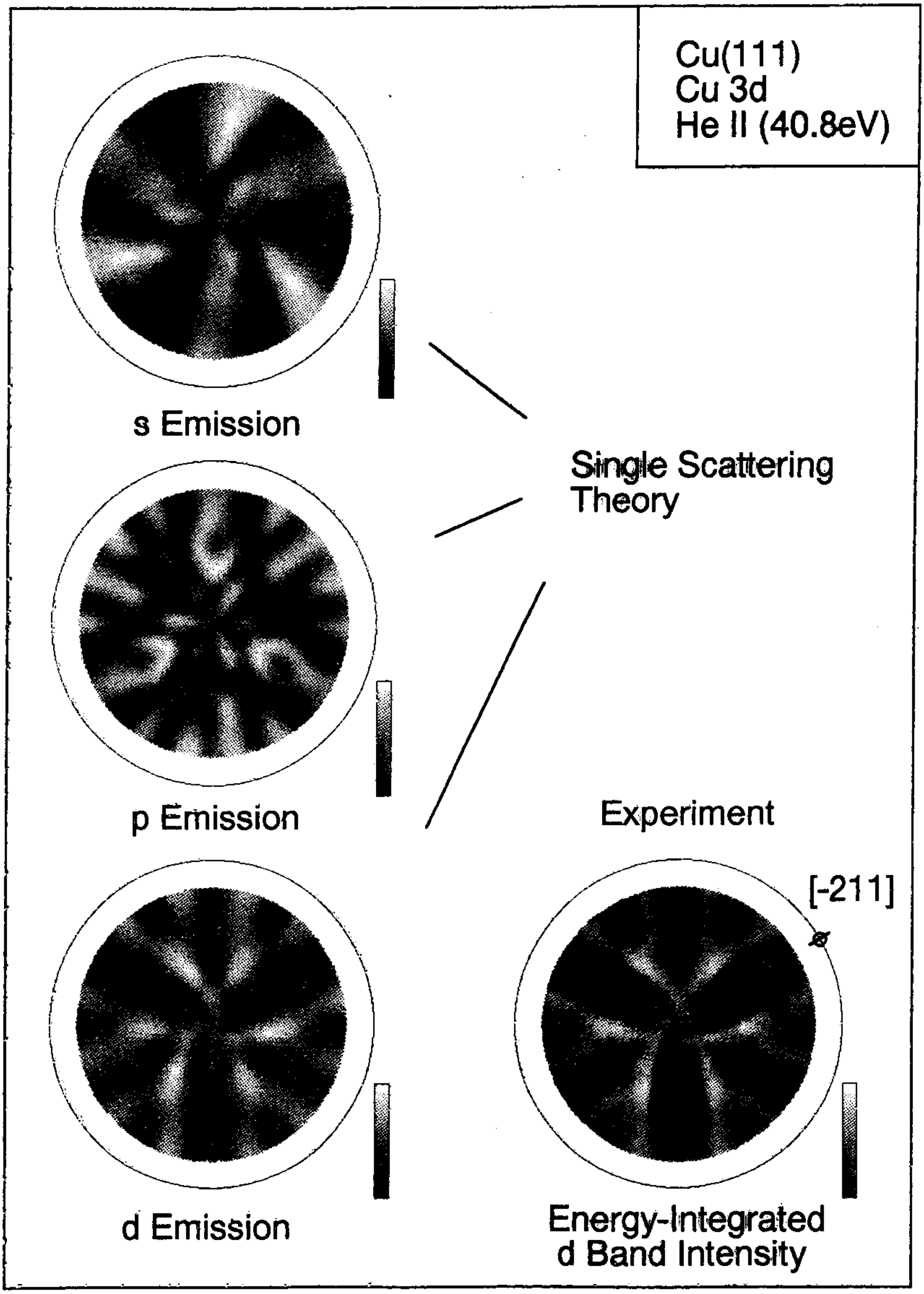
J. Osterwalder et al.
PRB 53, 10209 ('96)



... AND AGAIN !

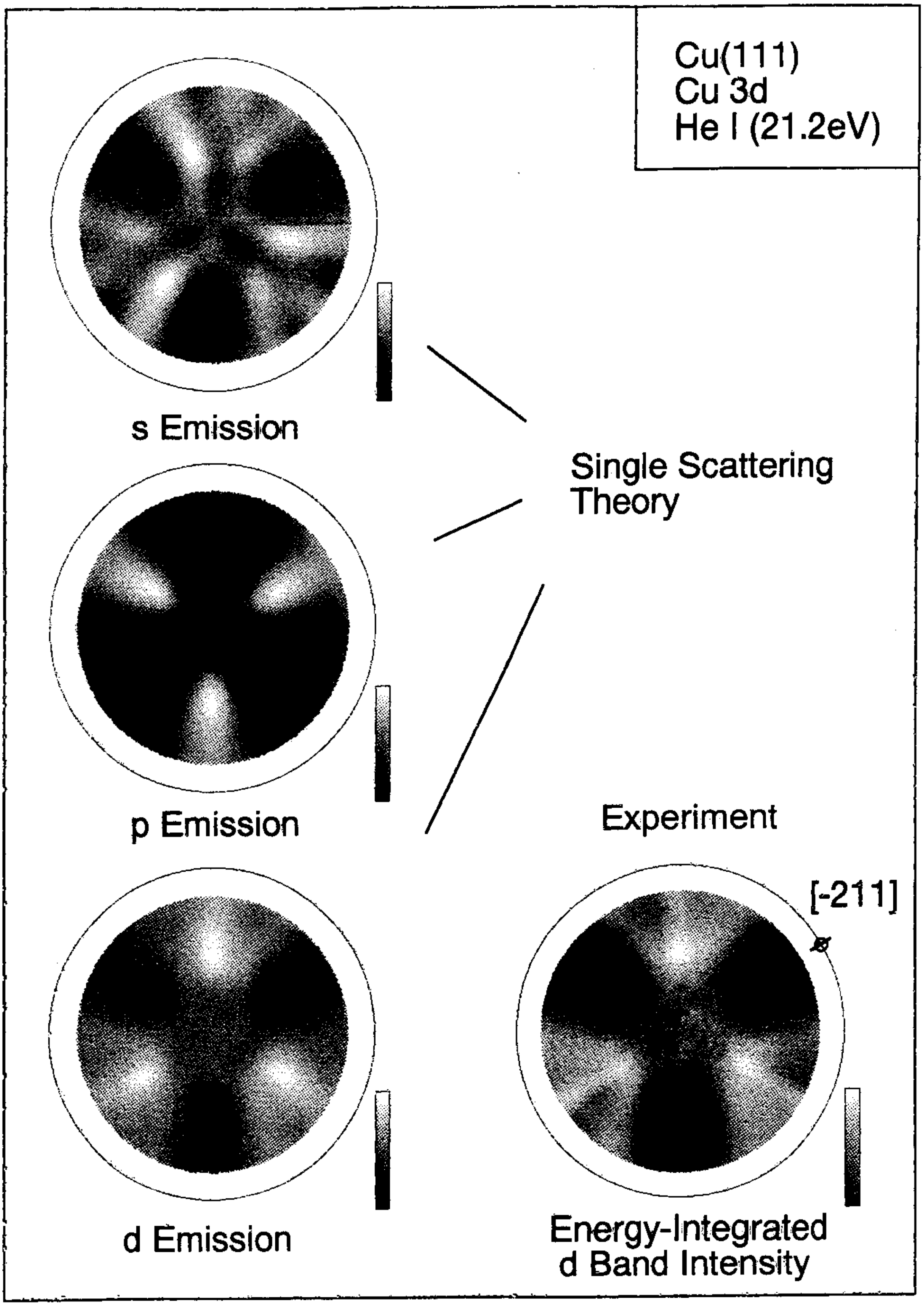

Cu(001)
Cu 3d
He I (21.2eV)
s Emission
Single Scattering
Theory
p Emission
Experiment
[100]
d Emission
Energy-Integrated
d Band Intensity

... AND AGAIN !


Cu(111)
Cu 3d
He II (40.8eV)
s Emission
Single Scattering Theory
p Emission
Experiment
[-211]
d Emission
Energy-Integrated d Band Intensity

... AGAIN !

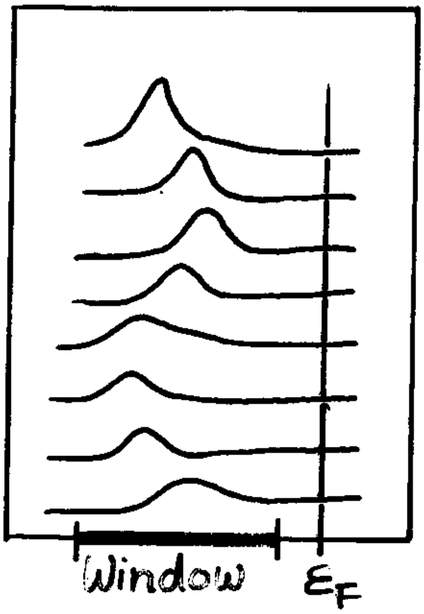
J. Osterwalder et al. Phys. Rev. B 53 (1996), 10 209



d ORBITAL WELL DISCRIMINATED!

UPD and Photoemission Intensities

filled shells:



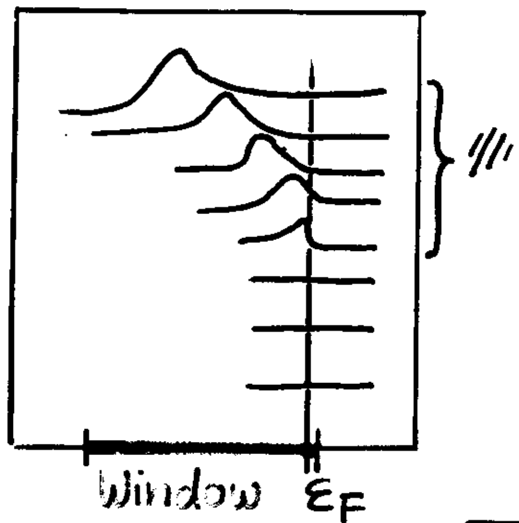
direct transition never disperses out of measurement window (e.g. Cu 3d).

⇓

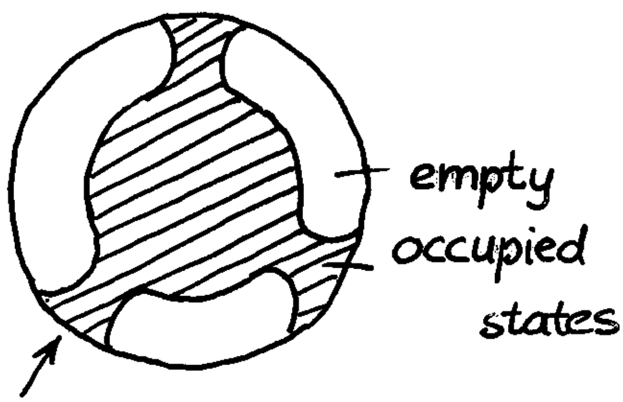
UPD describes overall band intensities !

(sum rule over several subbands)

unfilled shells: ?



direct transition is lost at Fermi surface.



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

But: Must know angular momentum compos. of occupied crystal field states !

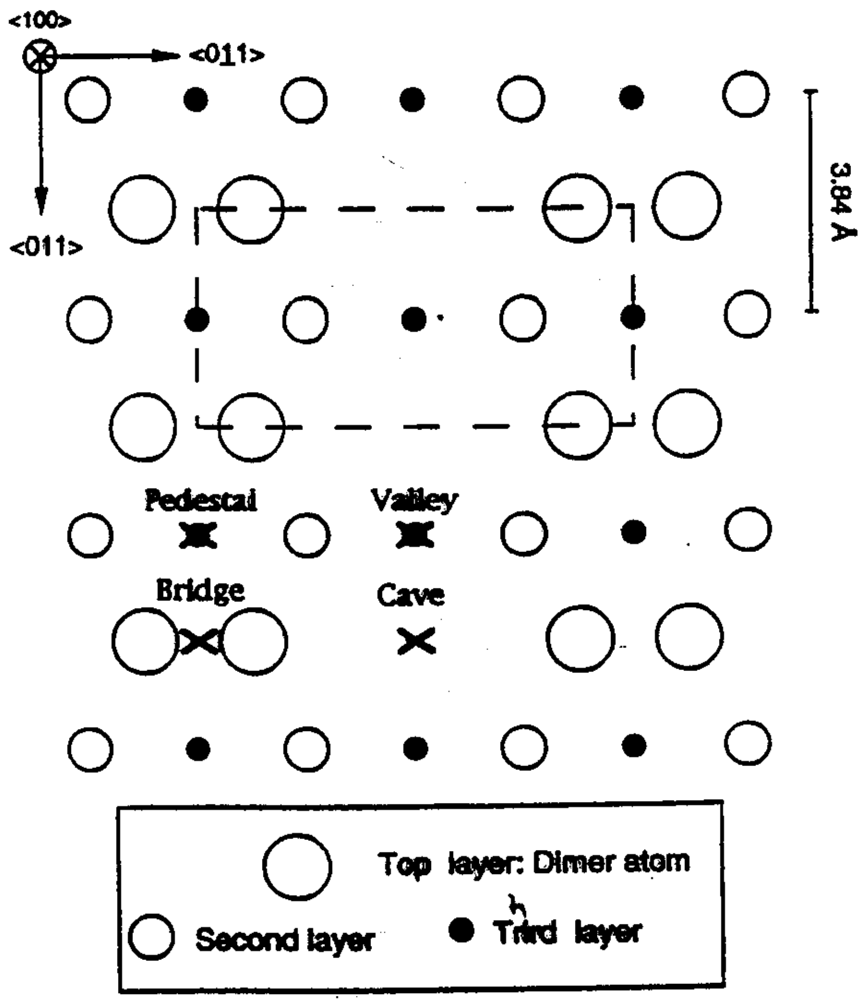
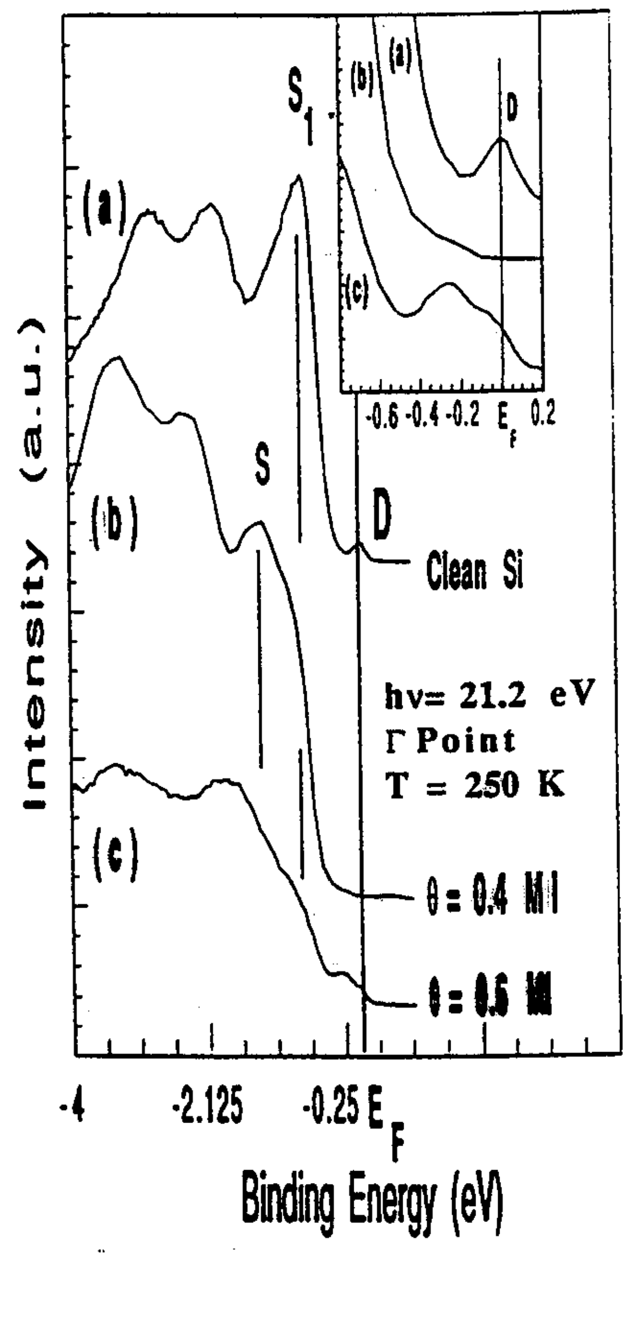
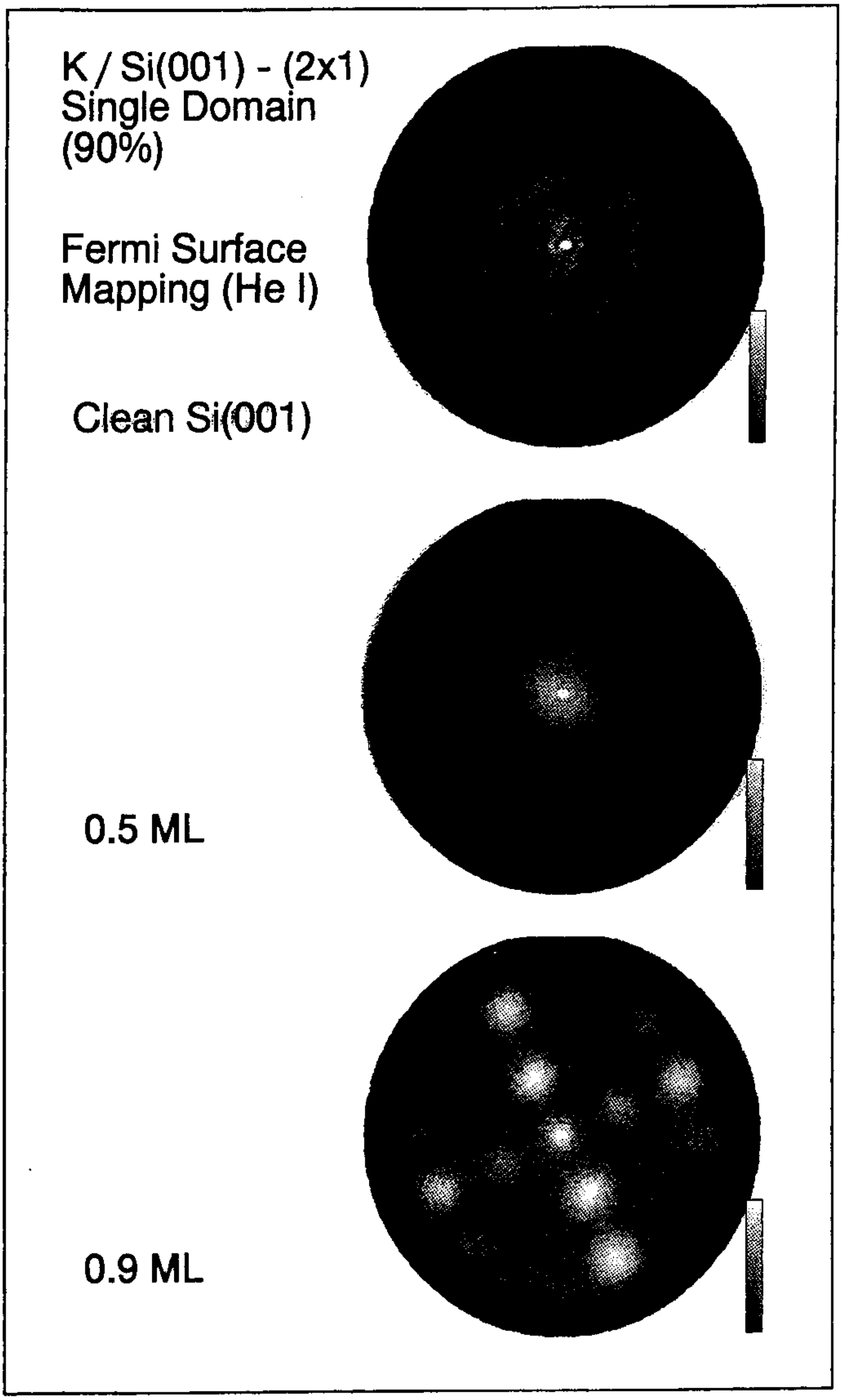

<100>
<011>
<011>
3.84 Å
Pedestal
Valley
Bridge
Cave
Top layer: Dimer atom
Second layer
Third layer

Fig. 1

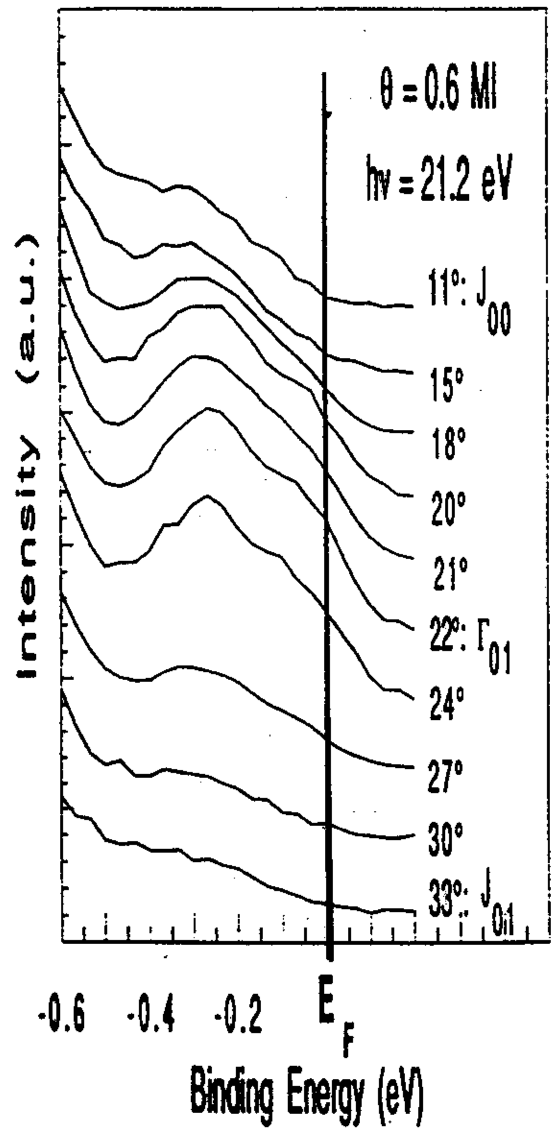


Intensity (a.u.)
(a)
(b)
(c)
S_1
S
D
Clean Si
hv= 21.2 eV
Γ Point
T = 250 K
θ = 0.4 Ml
θ = 0.6 Ml
-0.6 -0.4 -0.2 E_F 0.2
-4
-2.125
-0.25
E_F
Binding Energy (eV)

Fig. 2

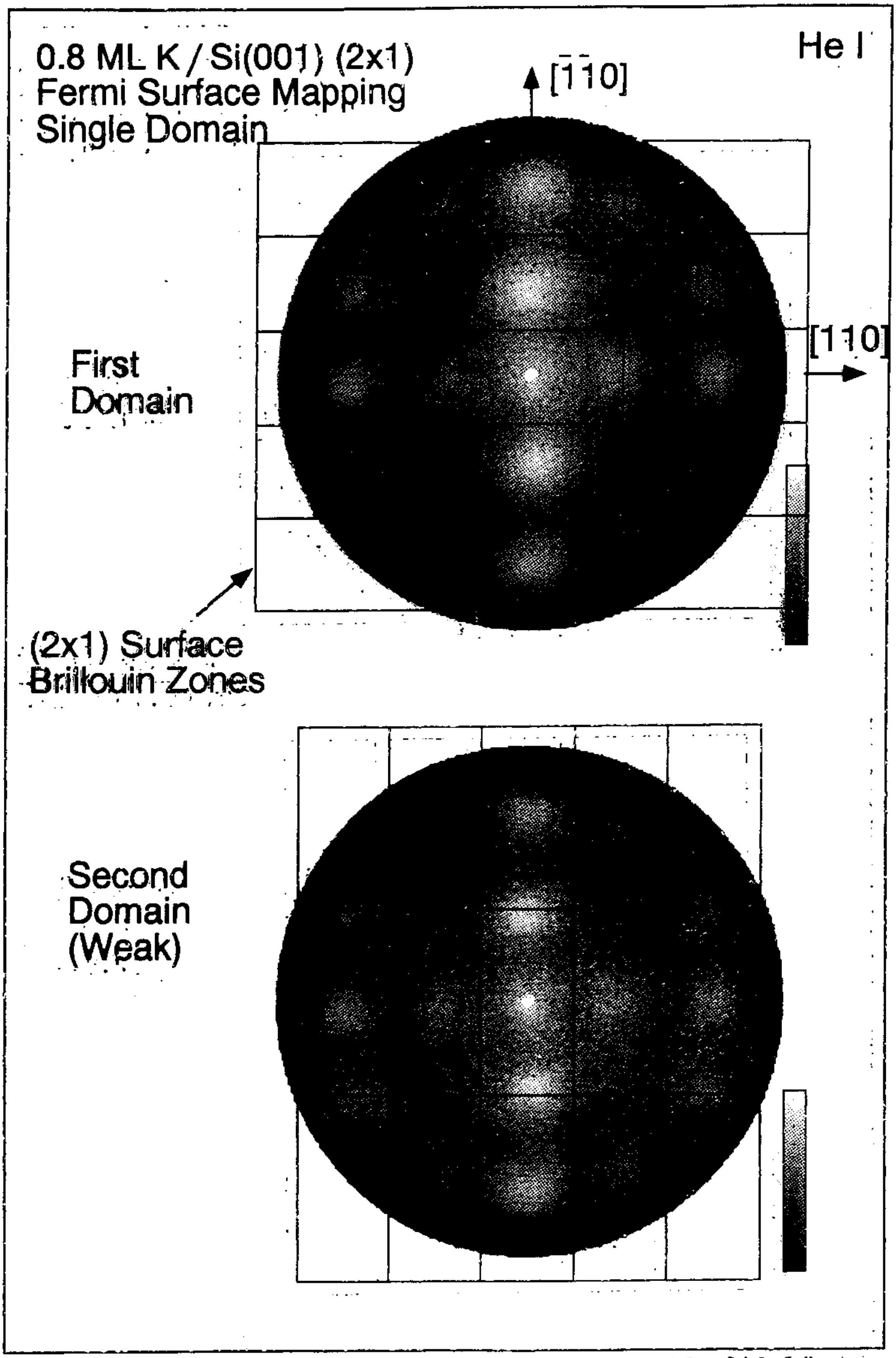

K / Si(001) - (2x1)
Single Domain
(90%)
Fermi Surface
Mapping (He I)
Clean Si(001)
0.5 ML
0.9 ML

J. A. MART[illegible]N - GA[illegible]



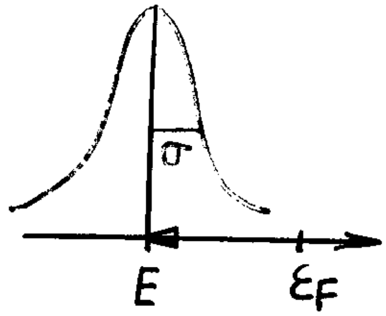
$I(\varepsilon_F)$ → dispersion
or
→ intensity modulation ?

⇒ check for periodicity in $\vec{k}$ - space !



M.C. ASENSIO J.A. MA

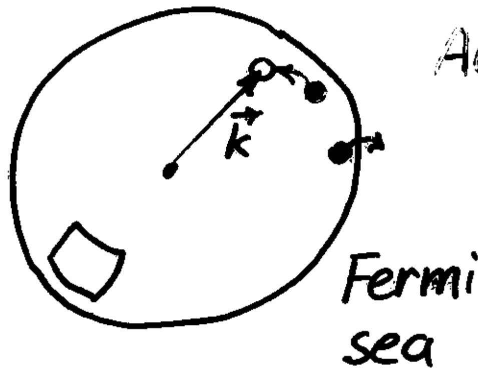
Interpretation of Line Widths



$$\sigma = \mathrm{Im}\,\Sigma(\vec{k},E) \sim \frac{\hbar}{\Delta t}$$

Q.P. life time

dominant hole decay processes:



Auger decay

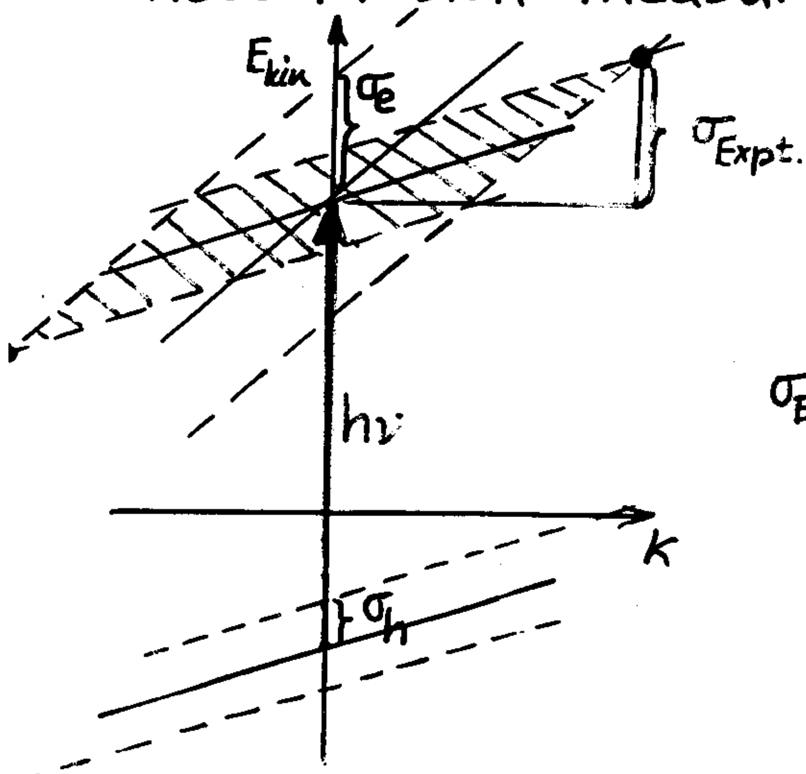
Fermi liquid theory

$$\Rightarrow \quad \Delta t \sim \frac{1}{E^2}$$

$$\Rightarrow \quad \boxed{\sigma \sim E^2}$$

Caution!

Photoemission measures
- hole lifetime $\frac{1}{\sigma_h}$
- and photoelectron lifetime $\frac{1}{\sigma_e}$



normal emission:

$$\sigma_{Expt.} = \frac{v_e^{\perp}/v_h^{\perp}}{v_e^{\perp} - v_h^{\perp}} \cdot \left(\frac{\sigma_h}{v_h^{\perp}} + \frac{\sigma_e}{v_e^{\perp}} \right)$$

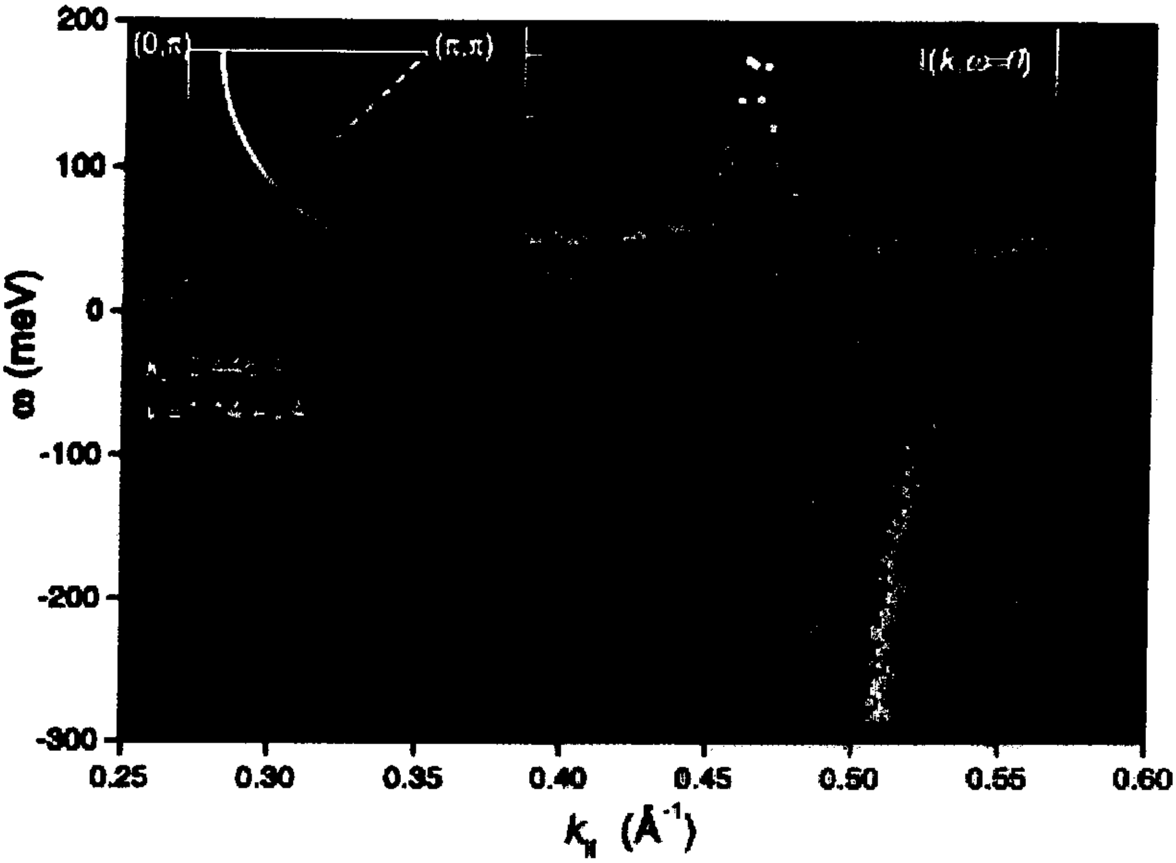
group velocities $\frac{\partial \varepsilon}{\partial k_{\perp}}$

(P. Thiry, 1981)

Energy Distribution Curves (EDCs) and Momentum Distribution Curves (MDCs)

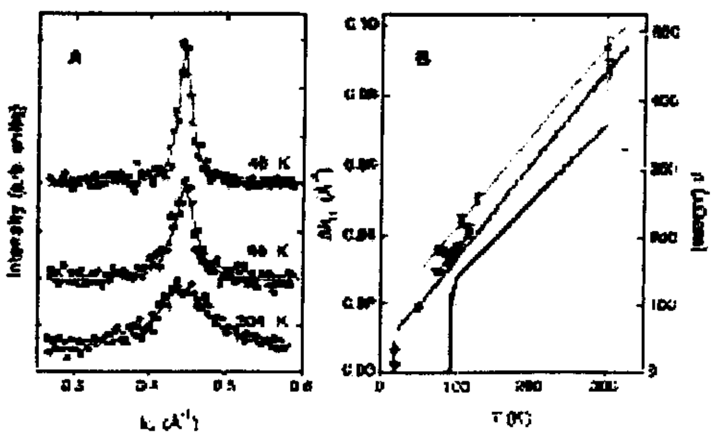
Example:
Dispersion Plot from BSCCO High Temperature Superconductor

T. Valla, A. V. Fedorov, P. D. Johnson et al., Science 285, 2110 (1999).



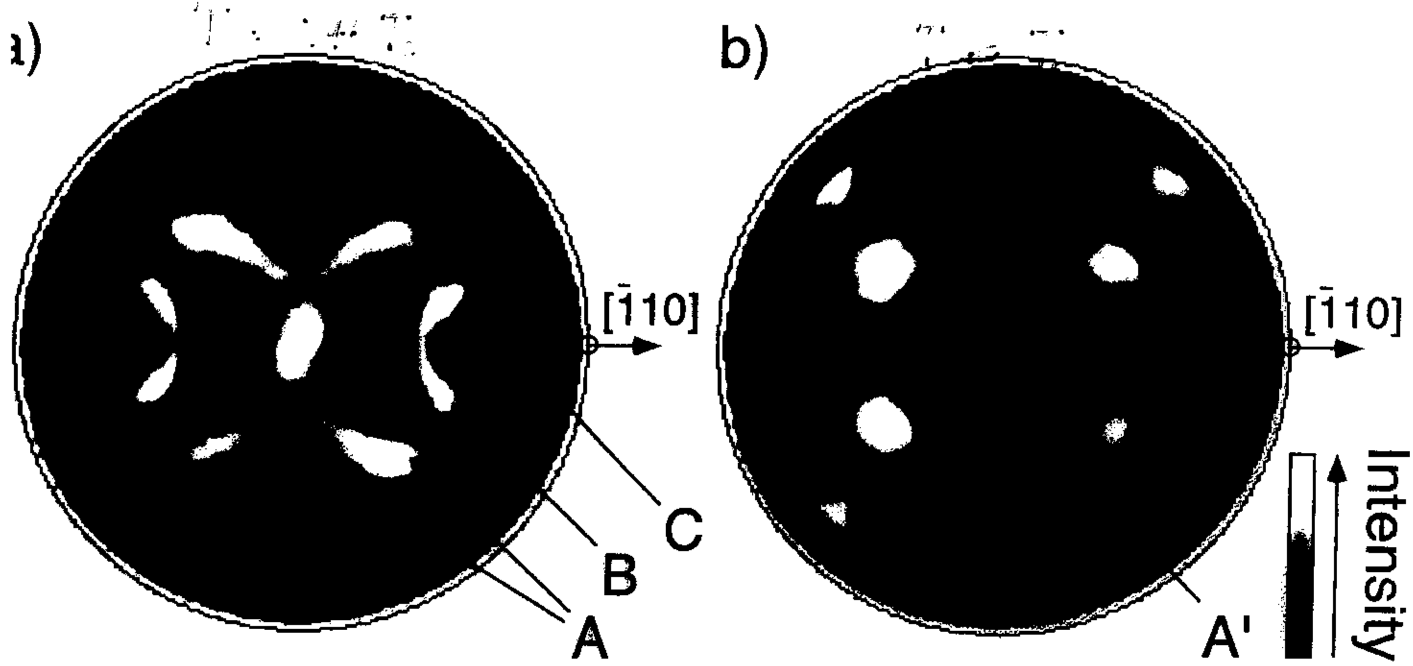
Line width Δk in MDCs : $$\hbar v_k \Delta k = \frac{\hbar v_k}{\Lambda} \approx \left|2\,\mathrm{Im}\,\Sigma(\vec{k},\omega)\right|$$

Λ : Mean free path of the electrons near the Fermi level

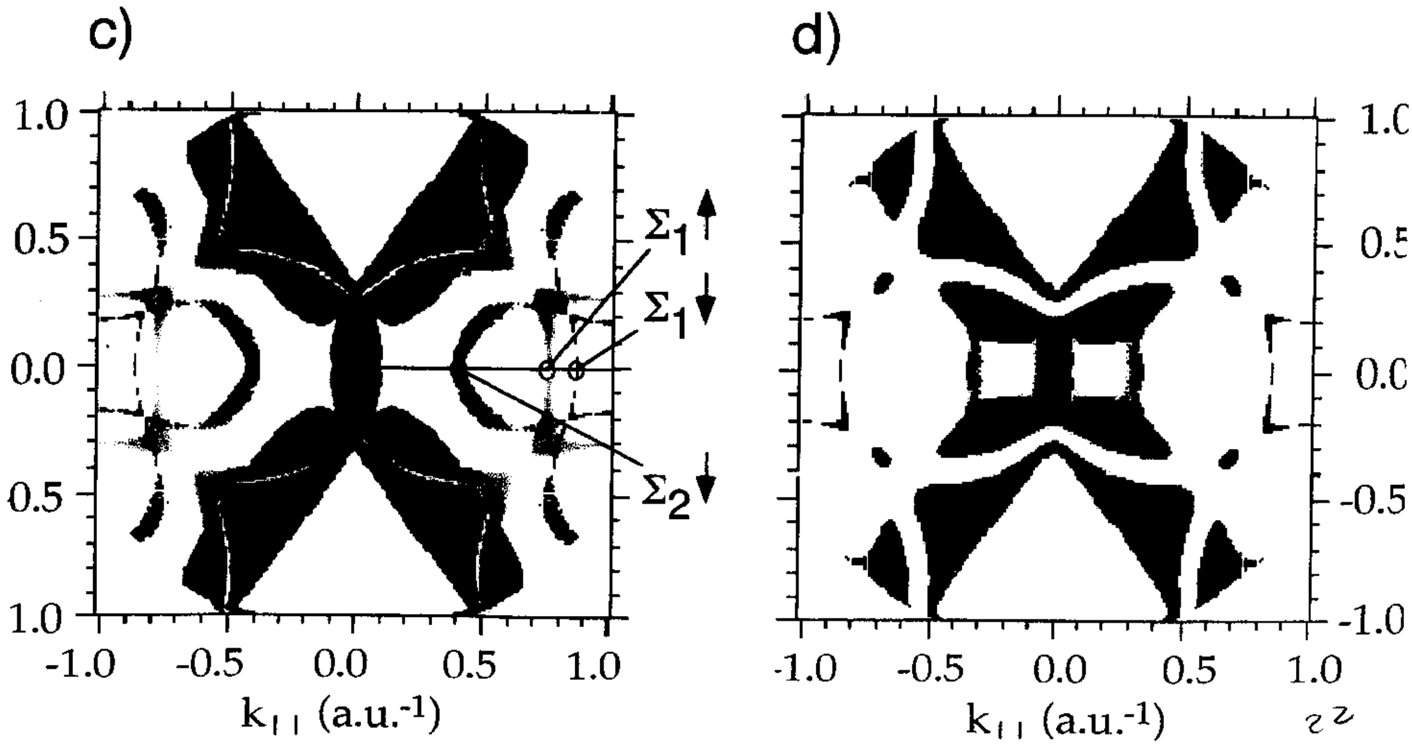


Connection between photoemission data and sample resistivity:

line widths of MDCs at the Fermi level

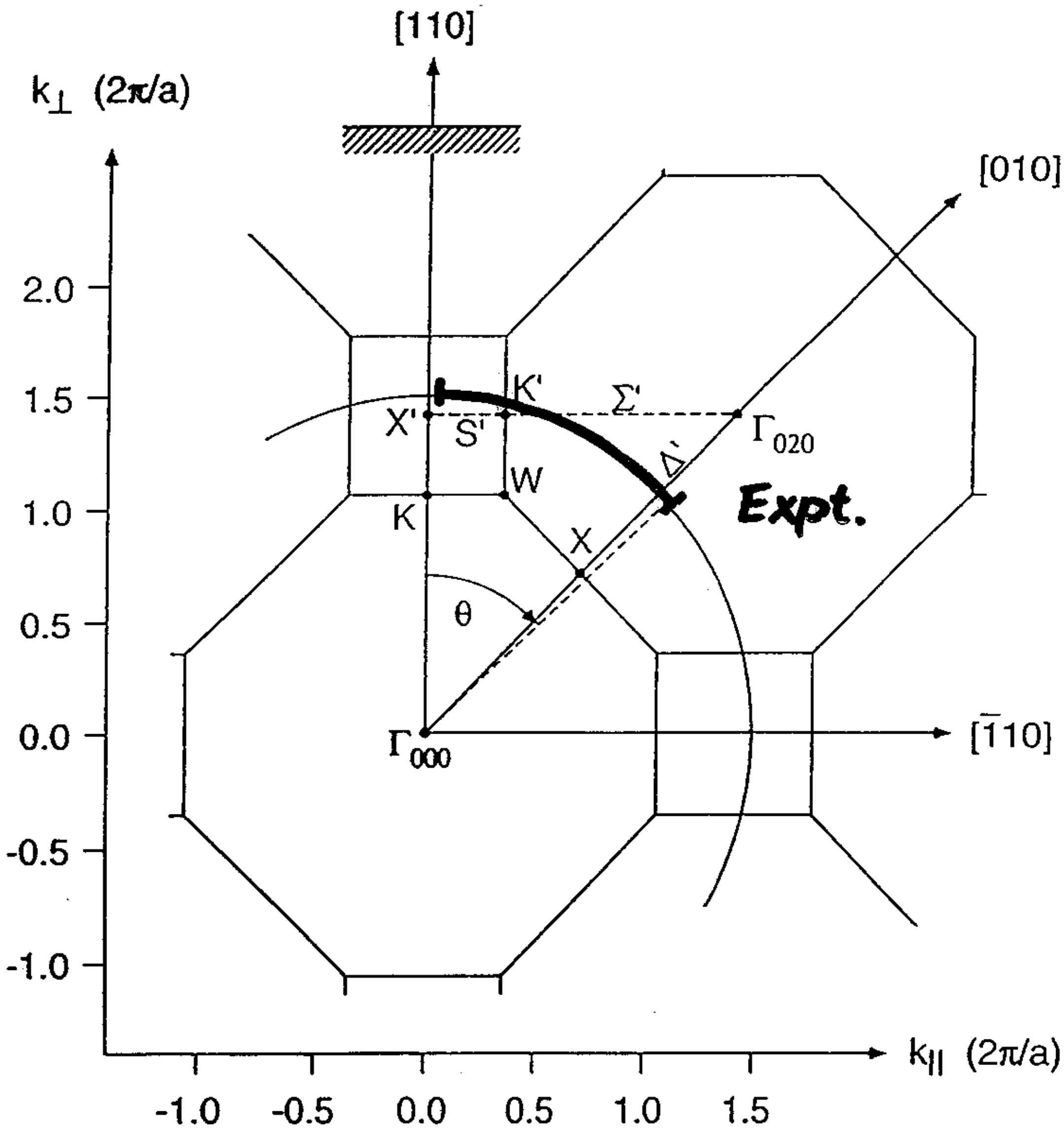


P. Aebi et. al.
PRL 76, 1150 ('96)



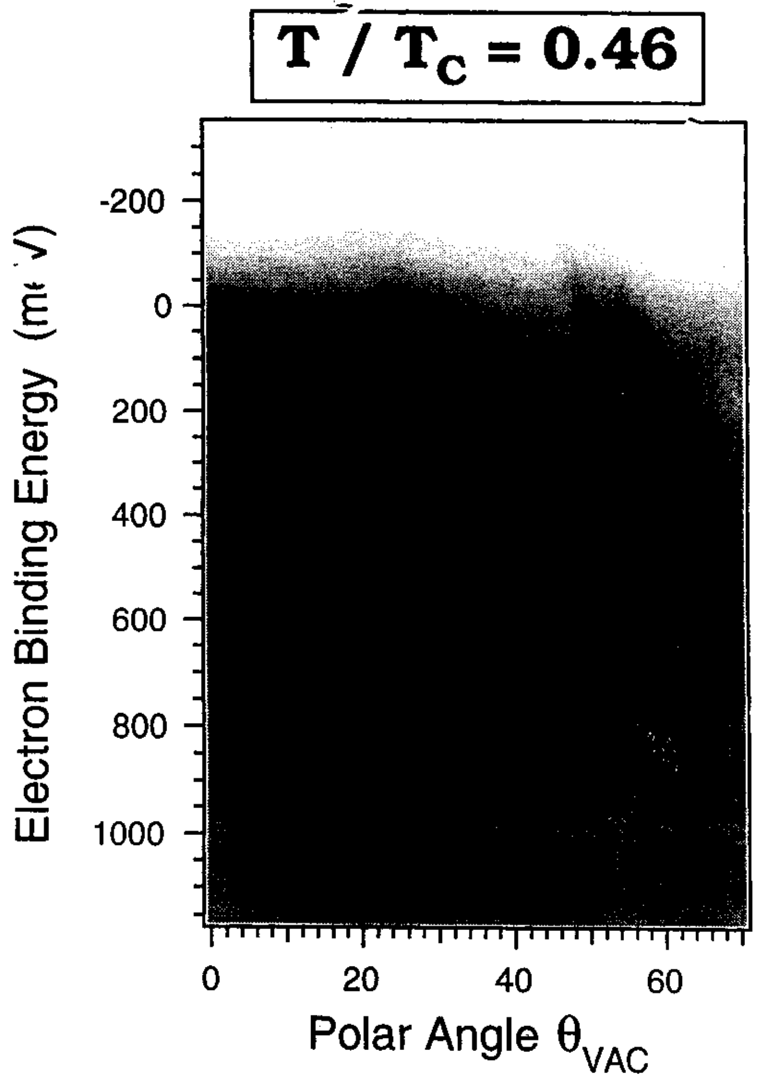
(001) Plane

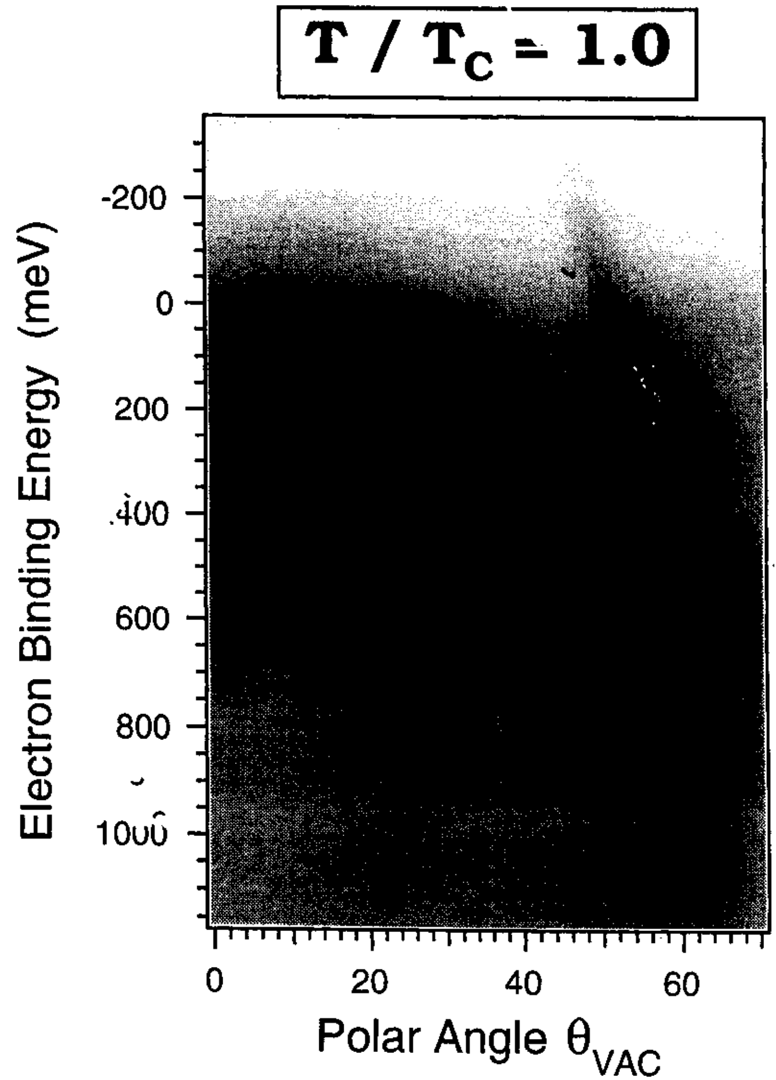
($\vec{k}$ space)



POLAR-ANGLE SCANNED ENERGY DISTRIBUTION CURVES FROM Ni(110)

Excitation: HeI (21.2 eV)

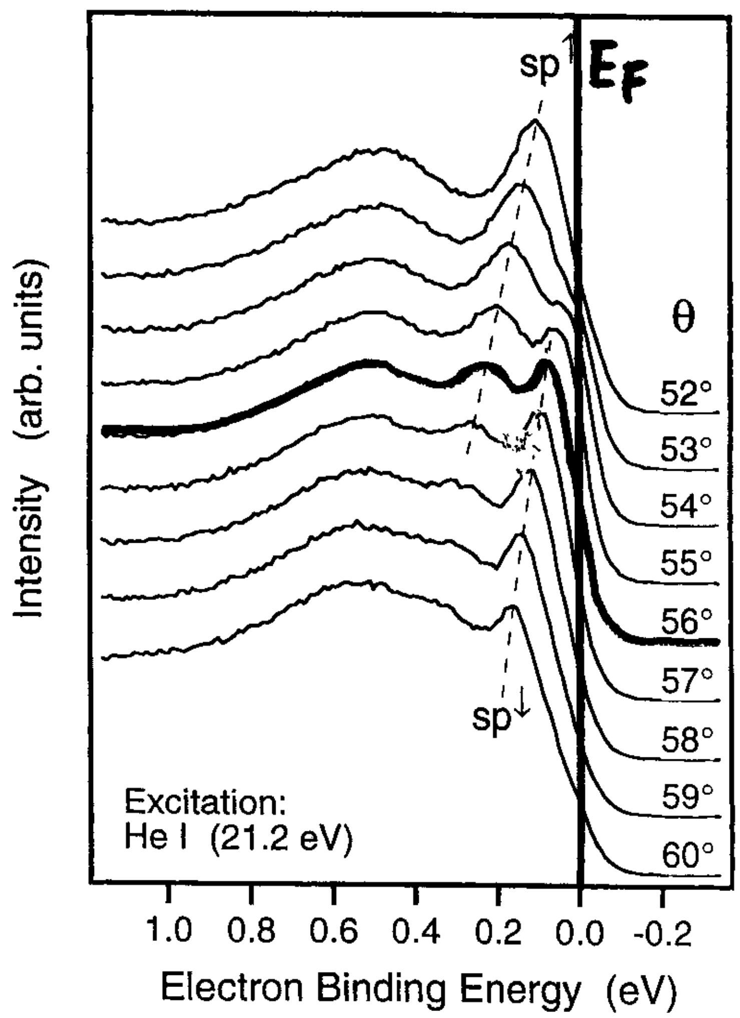




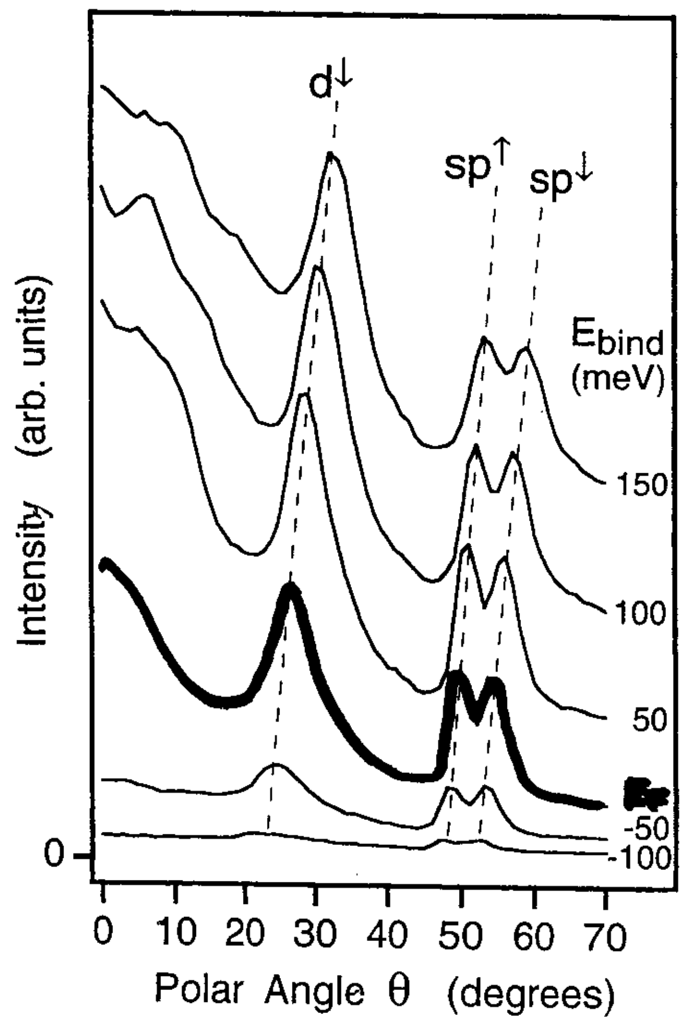
<??>From: T.J. Kreutz et al., Solid State Commun. **96**, 339 (1995)

Angle-Resolved Photoemission from Ni(110)

Energy Distribution Curves

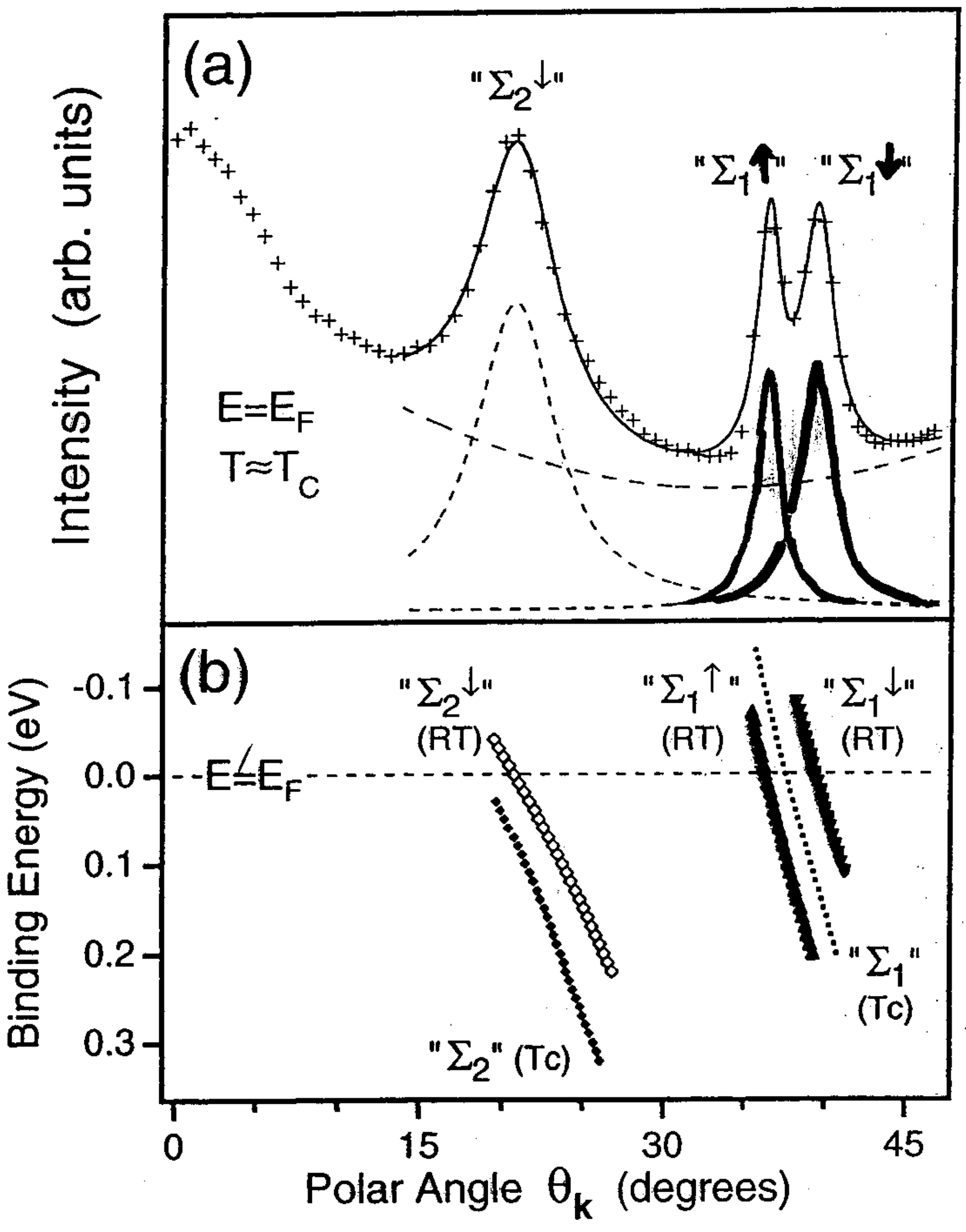


Polar Intensity Scans



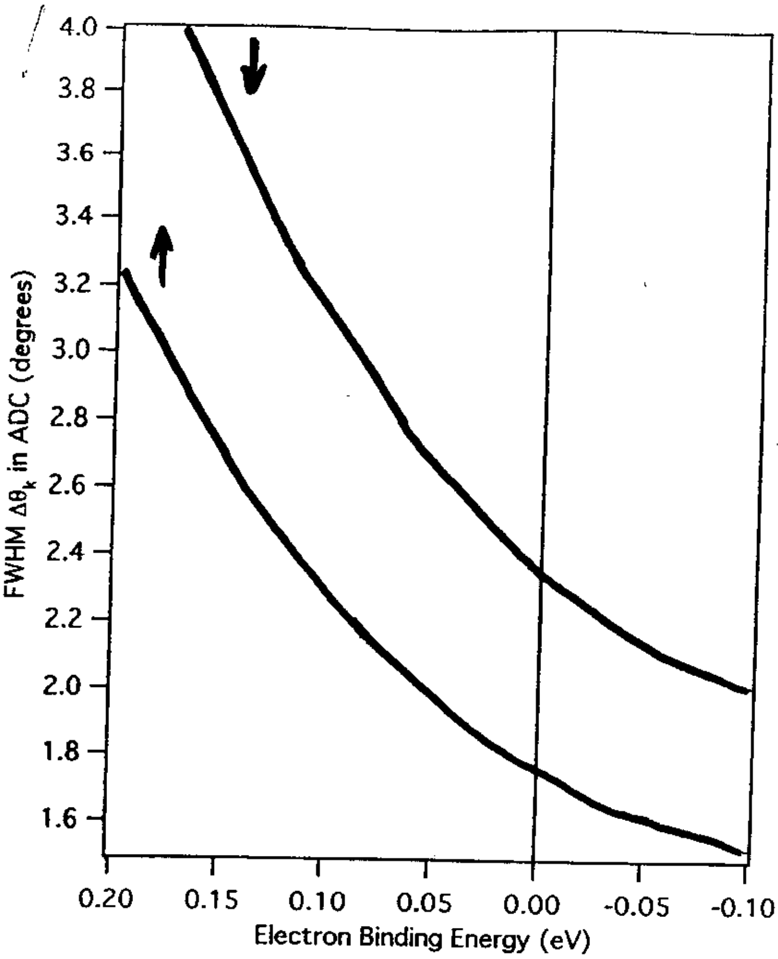
T =

⇒ dispersion



WIDTH:
$1.8°$
$2.4°$

$\Rightarrow \Delta E_{ex} = 2$[illegible]$4 \pm$ [illegible] meV

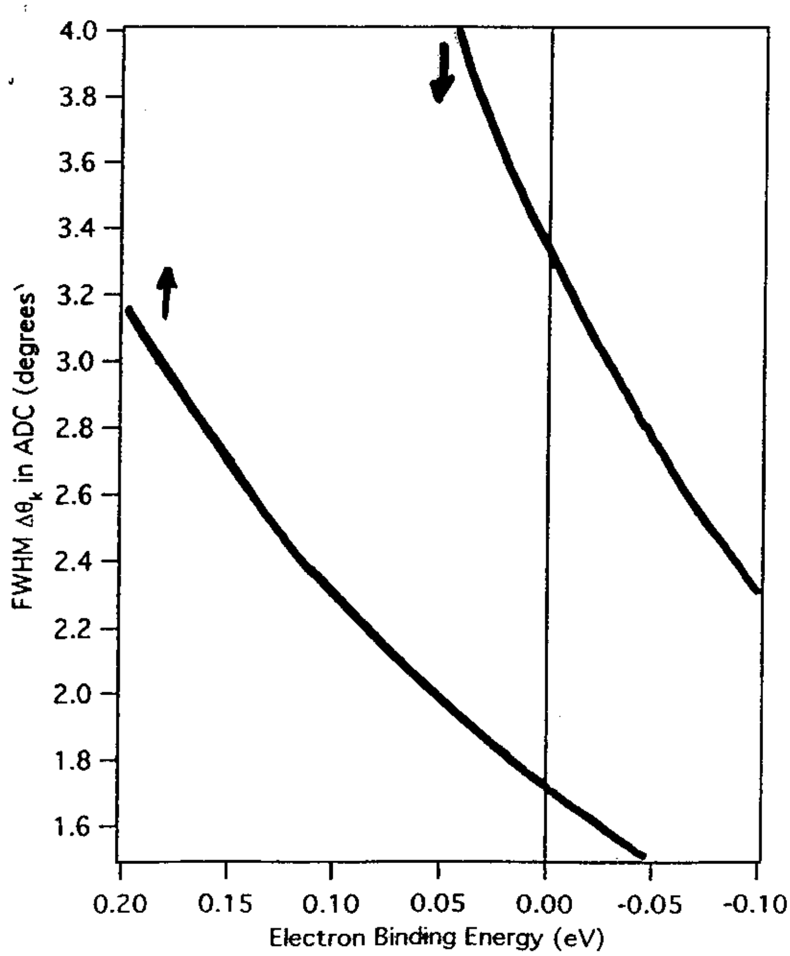


free-electron final + free-electron initial state

$\Gamma_f = 1.9$ eV

$\alpha = 2.0$ eV^{-1}

dispersion fitted

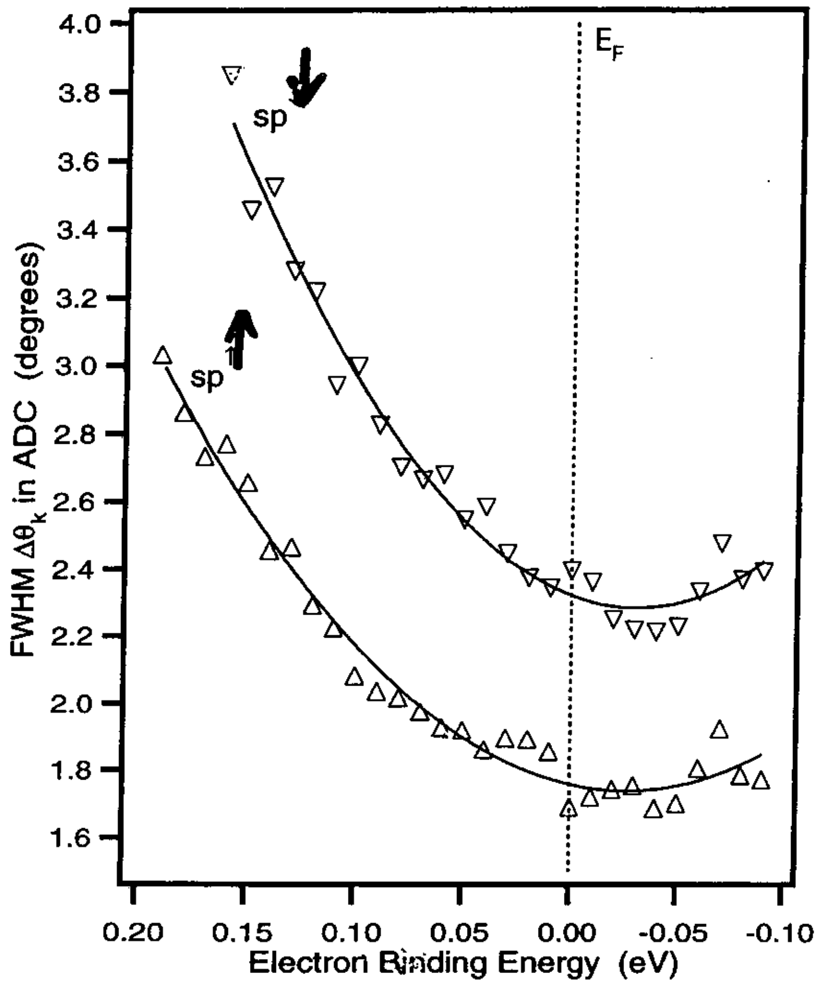


free-electron final + free-electron initial state

$\Gamma_f = 1.8$ eV

$\Gamma_i = 0.01$ eV = const

dispersion from experiment



Quasiparticle Lifetimes τ:

$$\frac{\hbar}{\tau} = \Gamma \propto (E - E_F)^2$$

(Fermi Liquid Theory)

The angular peak width is also influenced by the band structure (group velocities):

$$\Delta\theta = \frac{1}{\hbar k_{ext} cos\theta} \cdot \frac{\Gamma_i / |v_{i\perp}| + \Gamma_f / v_{f\perp}}{|v_{i\parallel}/v_{i\perp} - v_{f\parallel}/v_{f\perp}|}$$

(to be published)

. . . similar to peak widths in energy distribution curves:

$$\Delta E = \frac{\Gamma_i / |v_{i\perp}| + \Gamma_f / v_{f\perp}}{\left|(1 - \frac{msin^2\theta}{\hbar k_\parallel} v_{i\parallel})/v_{i\perp} - (1 - \frac{msin^2\theta}{\hbar k_\parallel} v_{f\parallel})/v_{f\perp}\right|}$$

(Thiry et al., 1981)