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SMR 1216 - 19

Joint INFM - the Abdus Salam ICTP School on "Magnetic Properties of Condensed Matter Investigated by Neutron Scattering and Synchrotron Radiation Techniques"

1 - 11 February 2000

PHOTOEMISSION FROM MAGNETIC SYSTEMS

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These are preliminary lecture notes, intended only for distribution to participants.

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Forschungszentrum Jülich

Photoemission from Magnetic Systems

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Forschungszentrum Jülich

I. Photoemission and Bandstructure

Basic Aspects of the Method

Bandstructure of Magnetic Materials

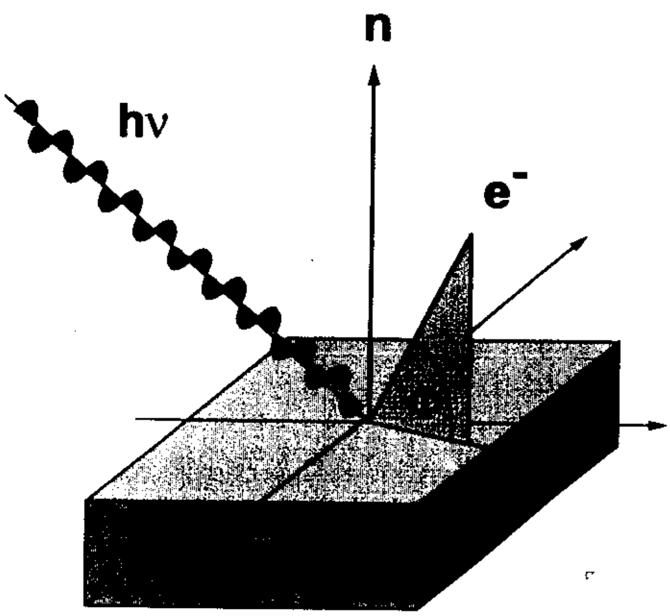
II. Electronic Structure and Magnetism

Finite temperature effects

Finite size effects in low-dimensional structures

Trieste, 11-2-2000

Photoemission



photon in ====> electron out

Photoemission

Einstein (1905) :
Theory of the photoelectric effect

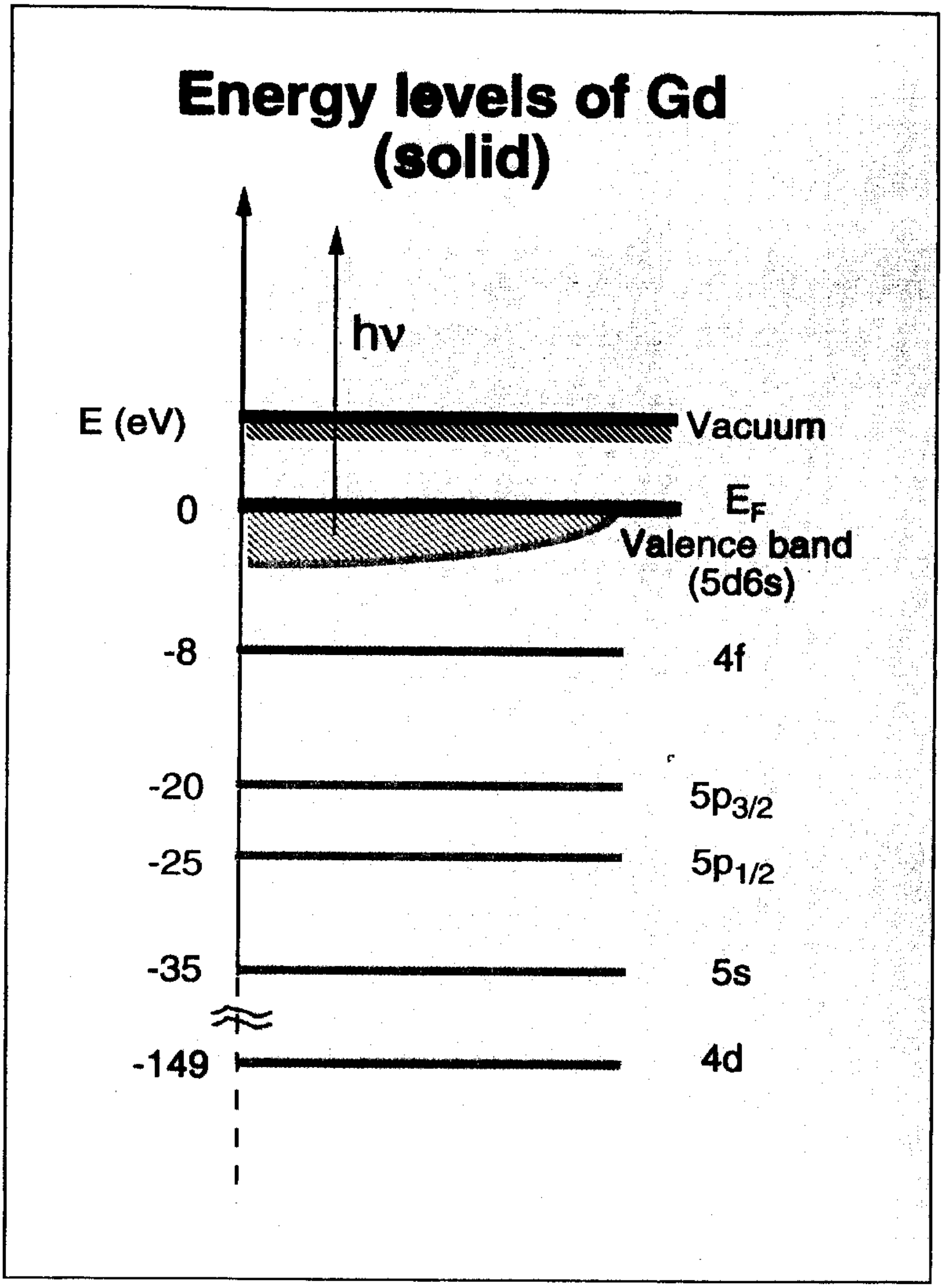
A photon is absorbed in the photoemission process. It transfers its *energy*, *momentum*, and *angular momentum* to an electron, which is excited

The energy of the excited (emitted) electron is proportional to the energy (wavelenght) of the photon

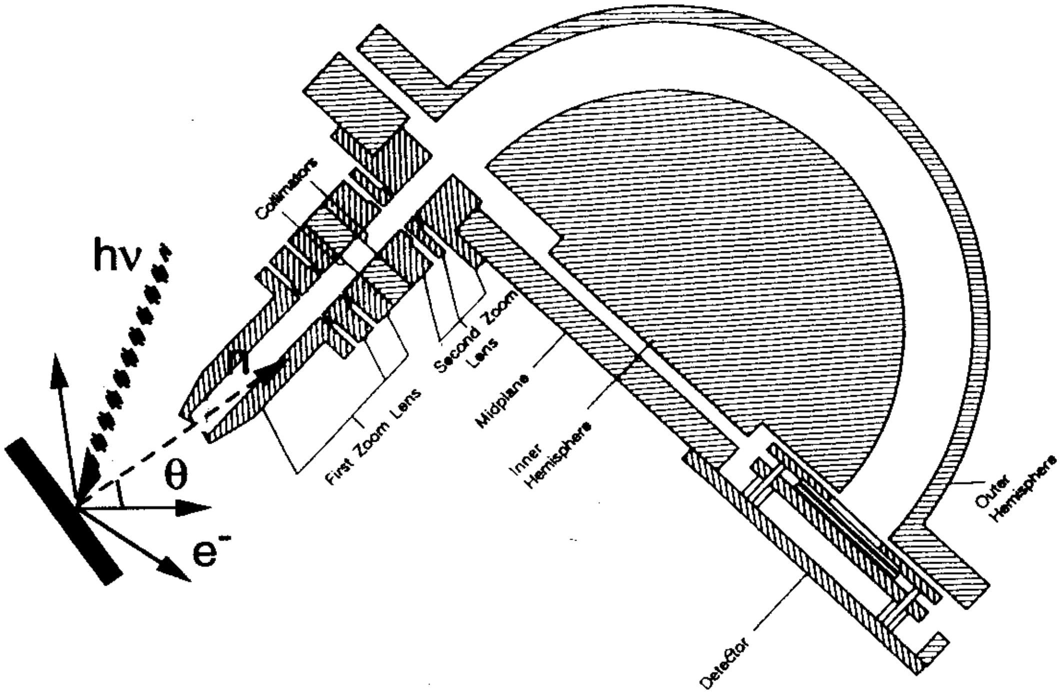
The number of the emitted electrons is proportional to the intensity of the incoming photons

Energy conservation :

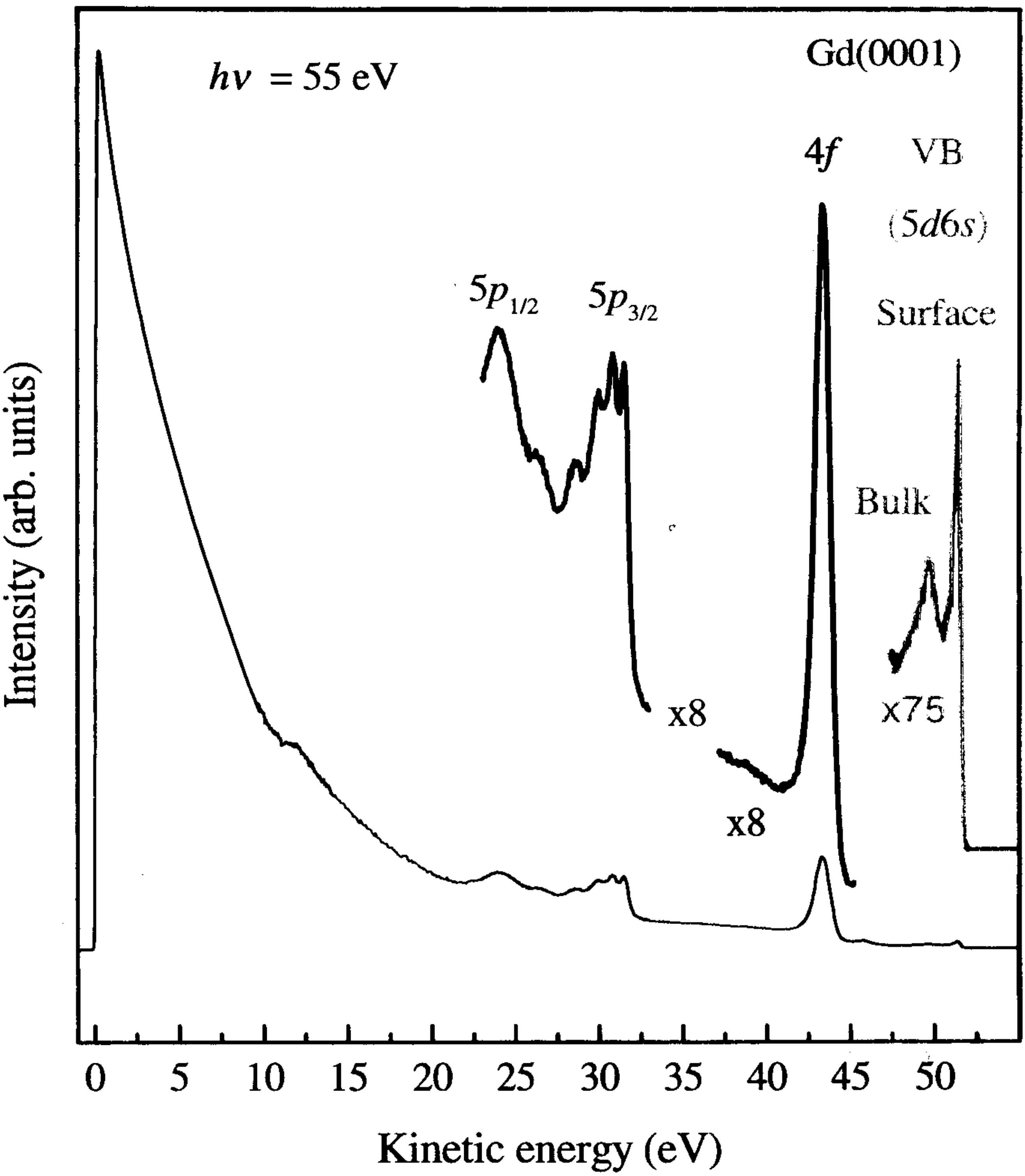
$$E_f = E_i + h\nu$$


Energy levels of Gd
(solid)
hν
E (eV)
Vacuum
0
E_F
Valence band
(5d6s)
-8
4f
-20
5p3/2
-25
5p1/2
-35
5s
-149
4d

Electron Energy Analyzer

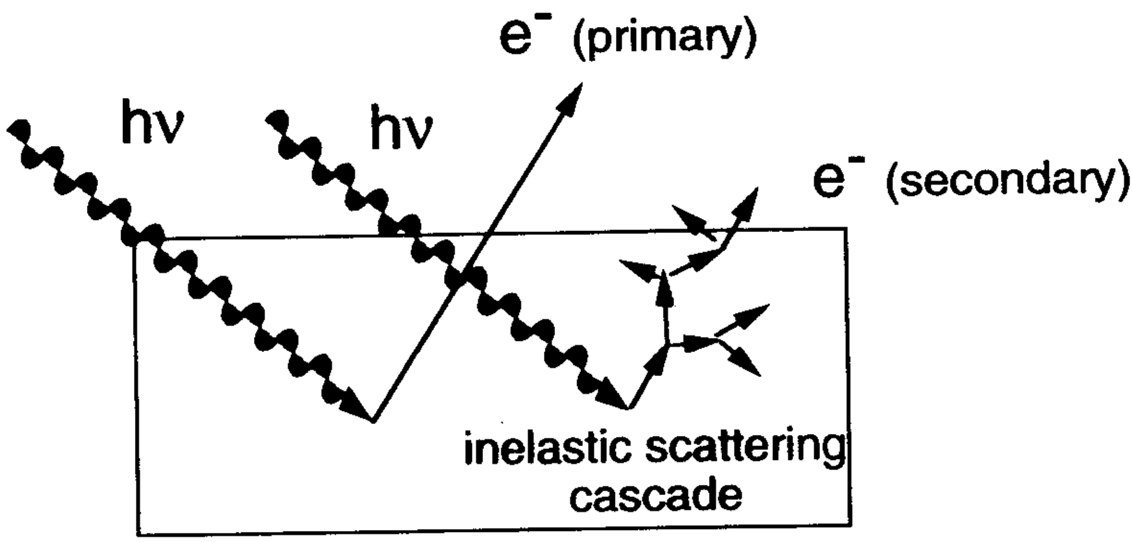


measure photoelectron E_{kin} and emission angle (θ)

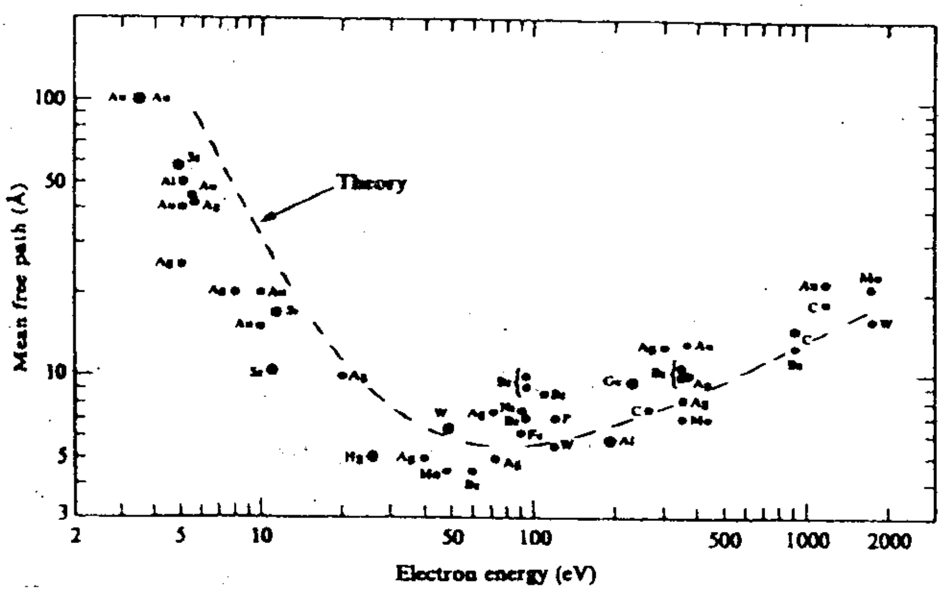


$h\nu$ = 55 eV
Gd(0001)
4f
VB
(5d6s)
5$p_{1/2}$
5$p_{3/2}$
Surface
Bulk
x8
x75
x8
Intensity (arb. units)
0 5 10 15 20 25 30 35 40 45 50
Kinetic energy (eV)

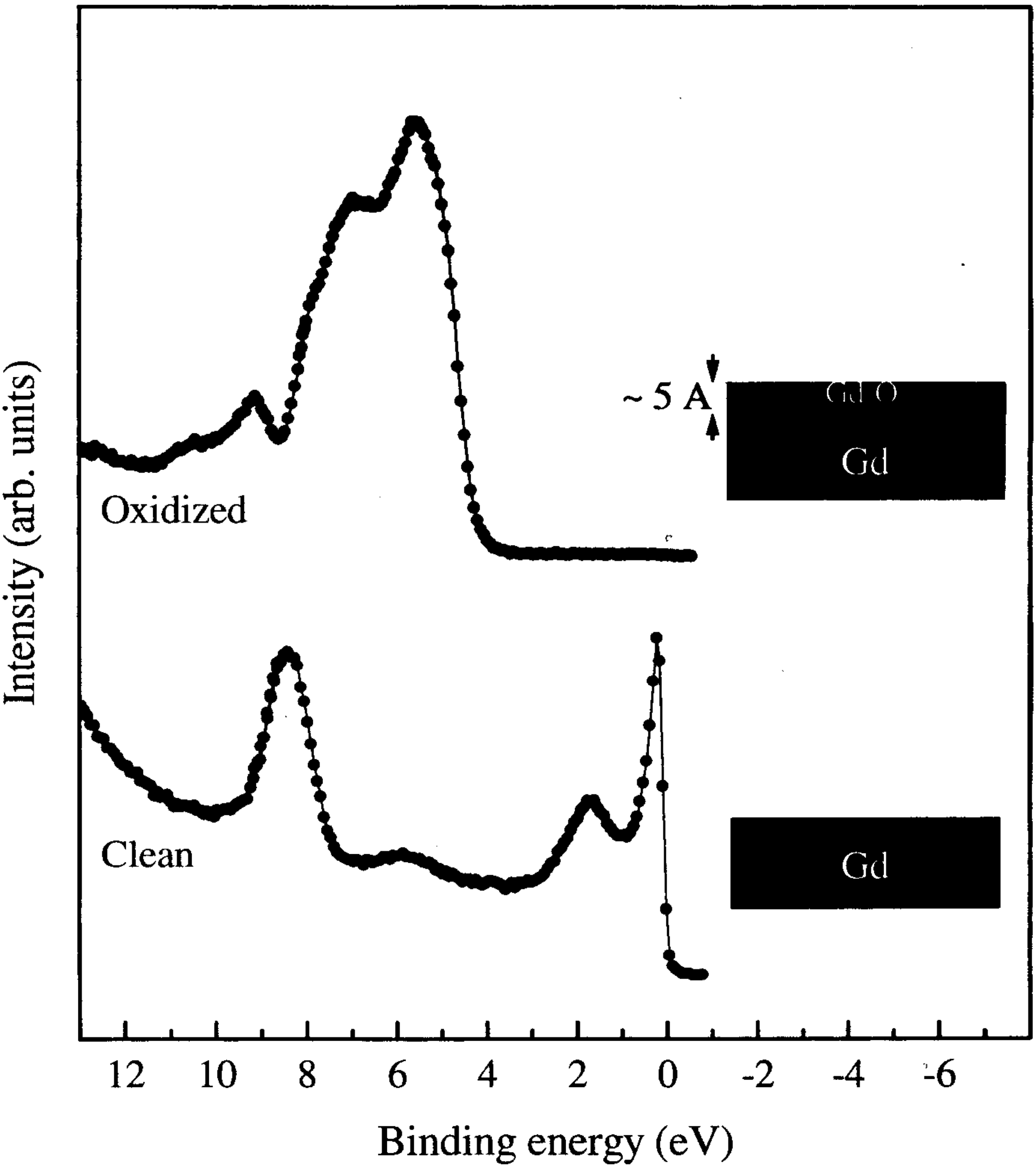
Inelastic scattering and electron mean free path



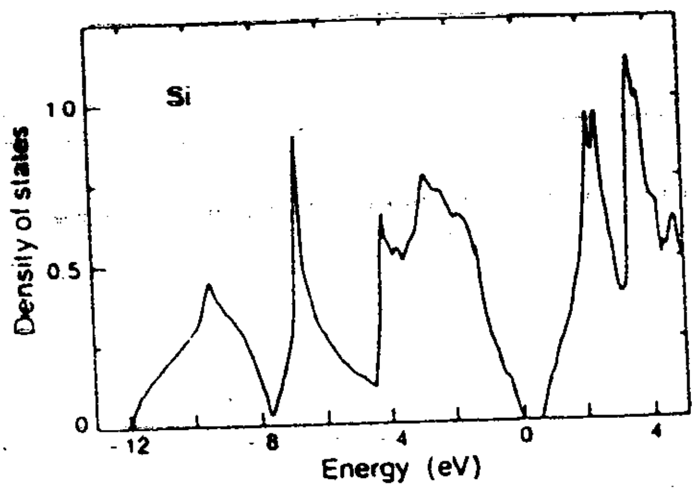
Electron mean free path



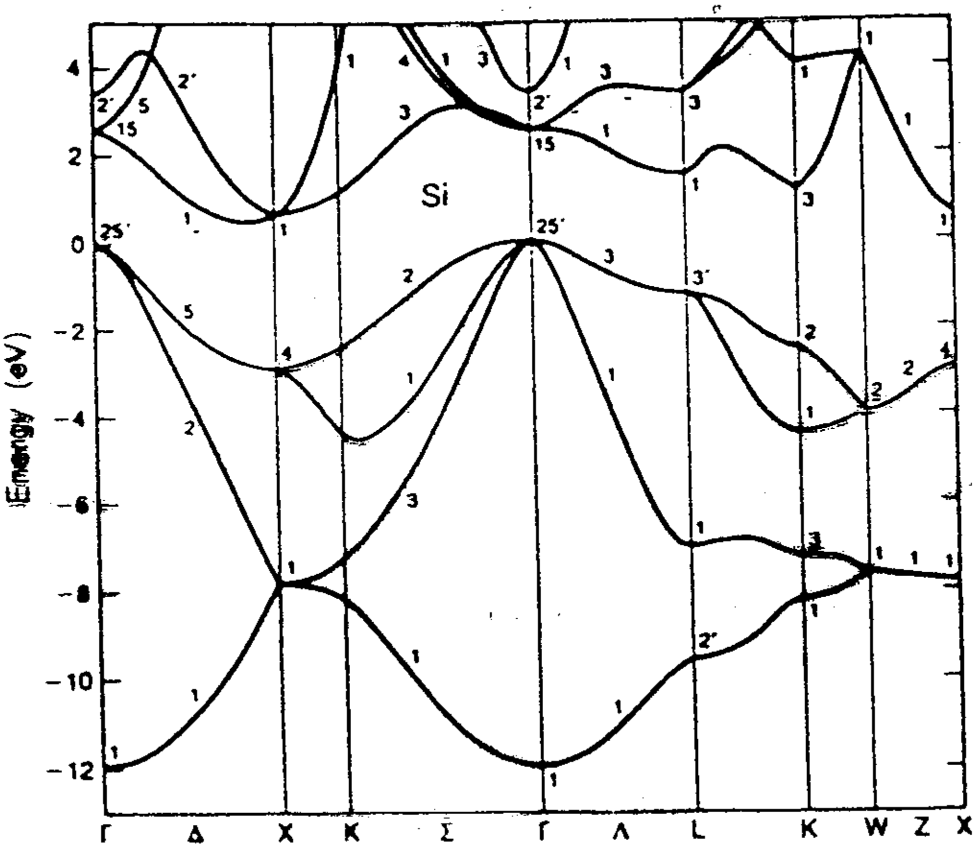
Surface sensitivity



Density of States



Bandstructure: E = E (**k**)



Transition rates, Matrix elements

"Fermi Golden Rule"

$$W \propto \langle f|H'|i\rangle^2 \ \delta\left(E_f - E_i - h\nu\right)$$

$$H' = \frac{e}{2mc}(\mathbf{A}\cdot\mathbf{P} + \mathbf{P}\cdot\mathbf{A}) + \frac{\mathrm{e}^2}{2\mathrm{mc}^2}|\mathbf{A}|^2 - e\Phi$$

$$[\mathbf{A},\mathbf{P}] = -i\hbar\nabla\mathbf{A}$$

$$W \propto \left|\langle f|2\mathbf{A}\cdot\mathbf{P} - i\hbar\overline{\nabla}\cdot\mathbf{A}|i\rangle\right|^2 \delta\left(E_f - E_i - h\nu\right)$$

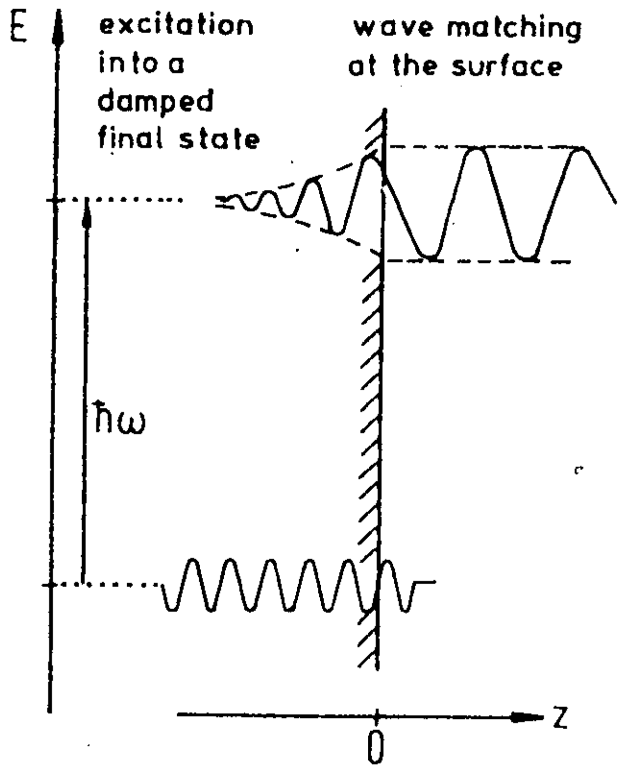
with $\overline{\nabla}\cdot\mathbf{A} = 0$

$$W \propto \left|\langle f|\mathbf{A}\cdot\mathbf{P}|i\rangle\right|^2 \delta(E_f - E_i - h\nu)$$

Dipole Matrix Element

$$\langle f|\mathbf{A}\cdot\mathbf{P}|i\rangle$$

One Step Model



/i> Bloch state in solid

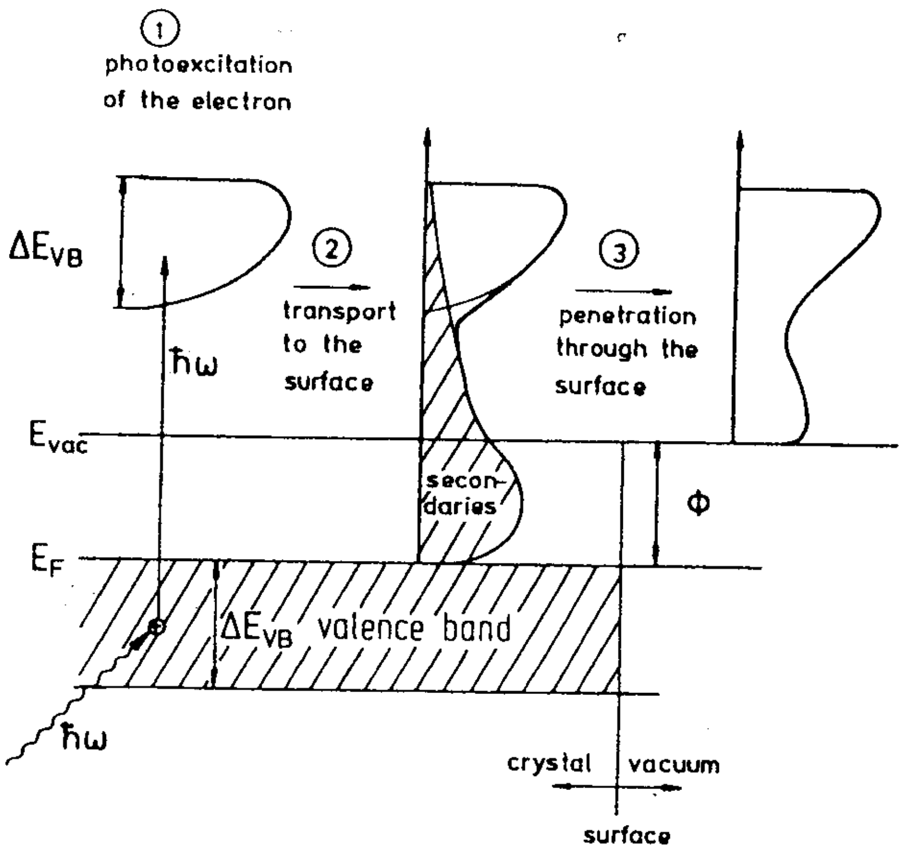
/f> freely propagating wave in vacuum

The Three Step Model

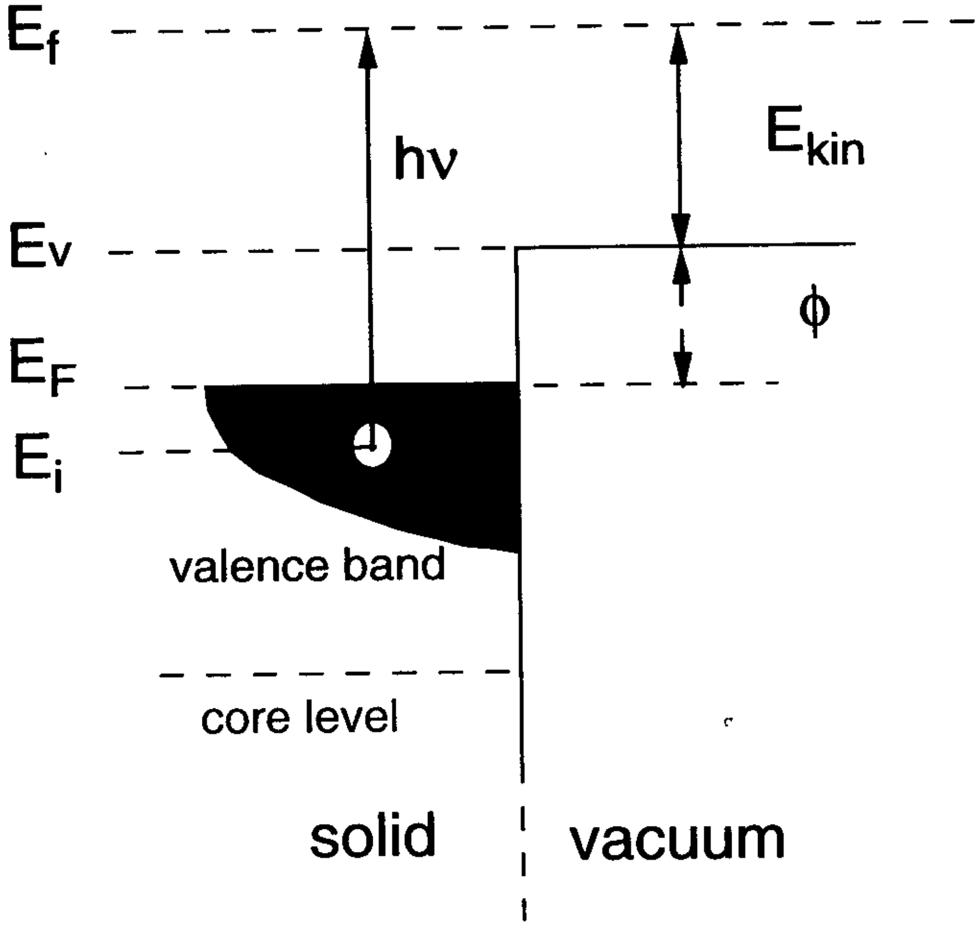
1) photoexcitation

2) transport to the surface

3) escape into vacuum



Energy Conservation

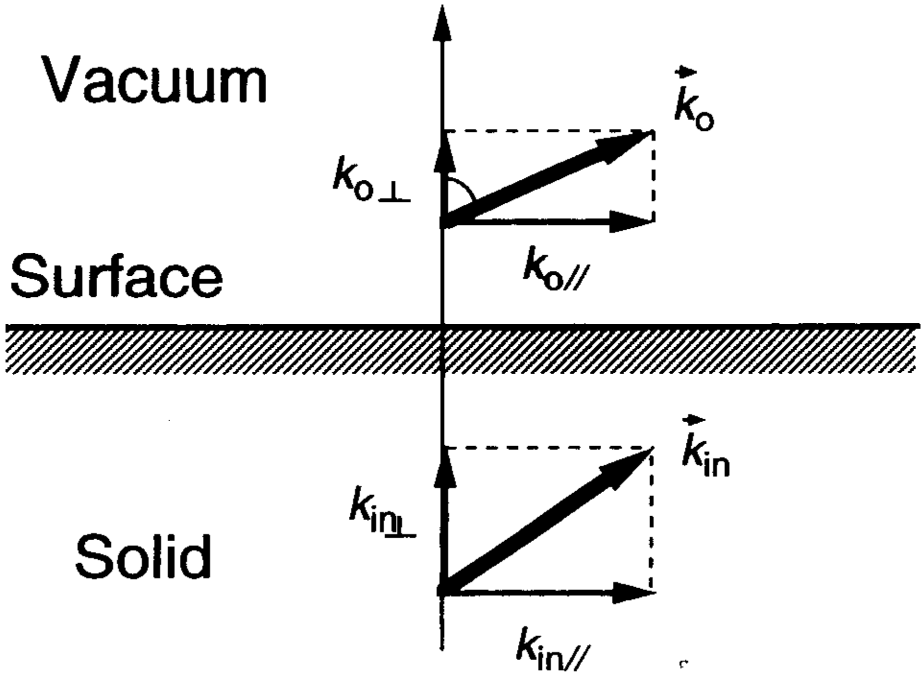


$$E_f = E_i + h\nu$$

$$E_{kin} = h\nu - E_B - \phi$$

$$E_B = E_F - E_i$$

Momentum Conservation

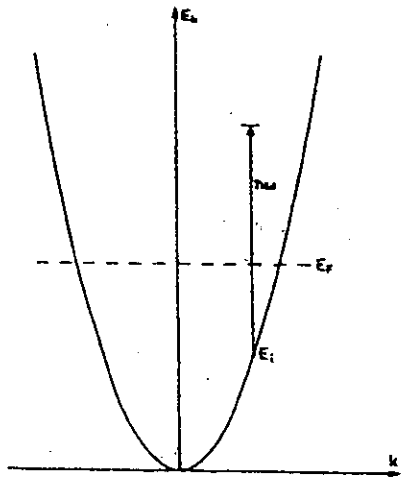


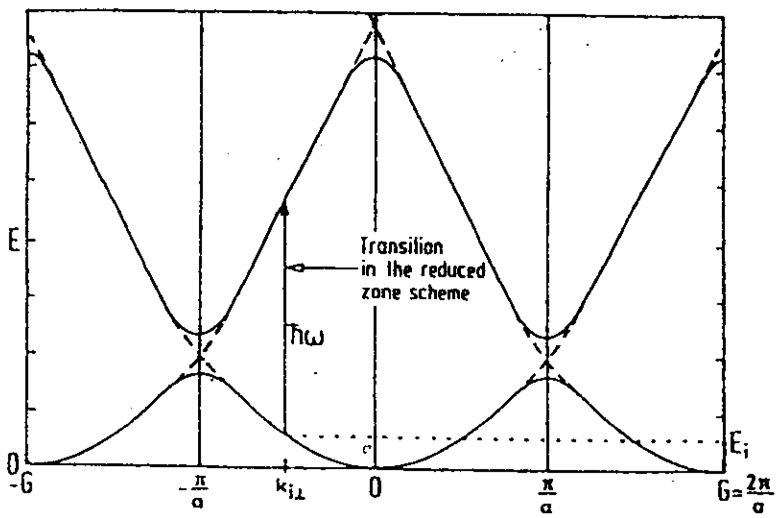
Periodic crystal structure :

$$k_{in//} = k_{o//}$$

$$k_{o//} = \frac{1}{\hbar}\sqrt{2\,m\,E_{kin}}\,\sin\theta$$

Momentum Conservation : Direct Transitions



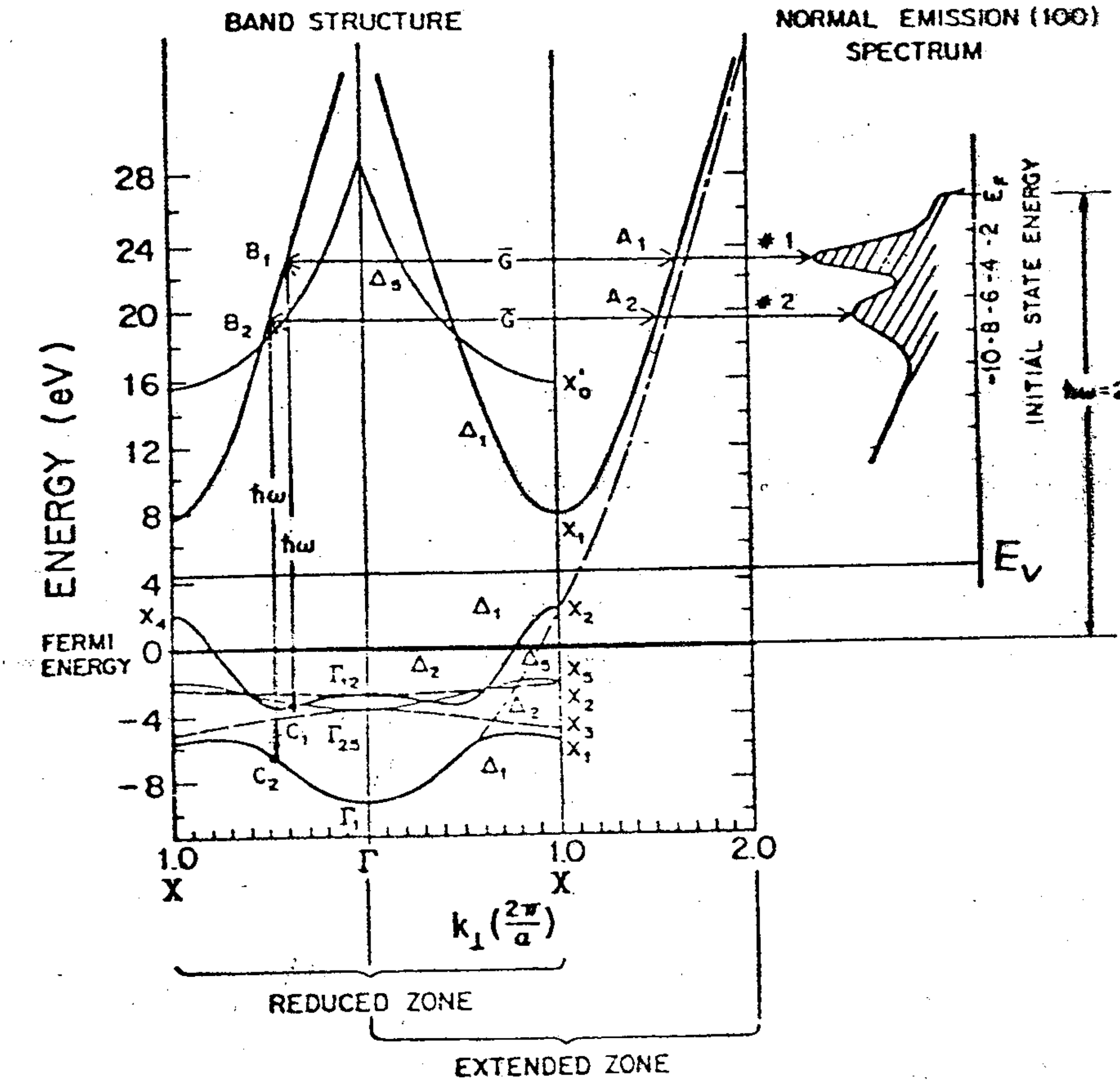


free electron

nearly free electron in a solid

$$k_f = k_i \pm \vec{G}$$

Direct Transitions in Solids



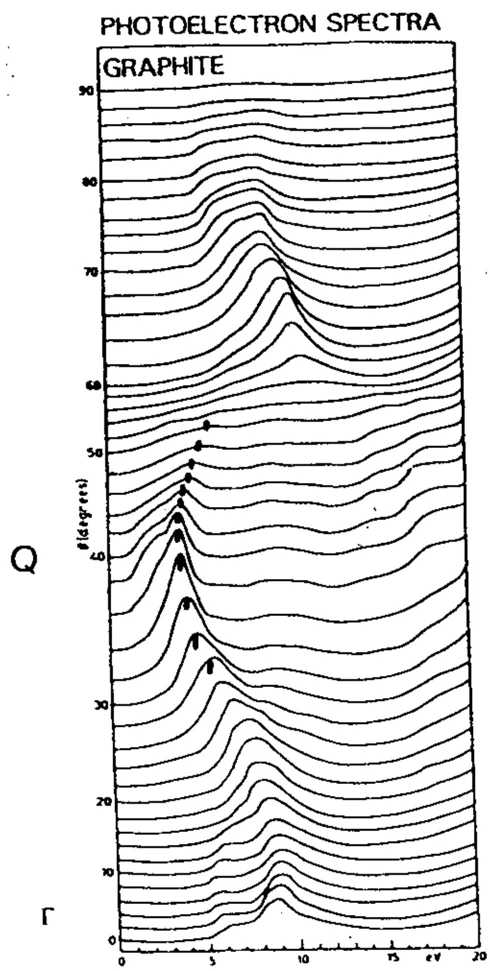
$$k_f = k_i \pm \vec{G}$$

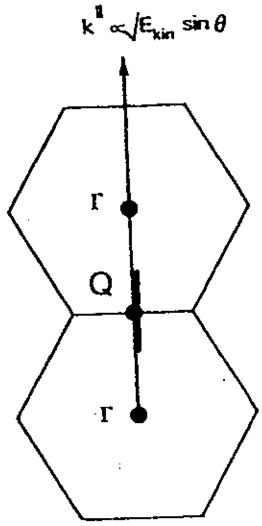
Two-dimensional states: $E = E(k_{//})$

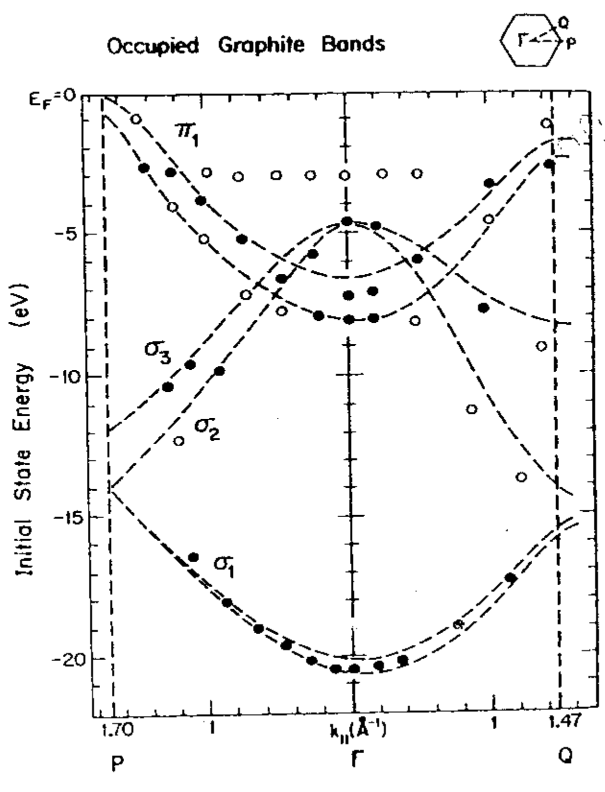
electrons confined in 2-D:

- layered materials
- surfaces
- surface adsorbates
- thin films

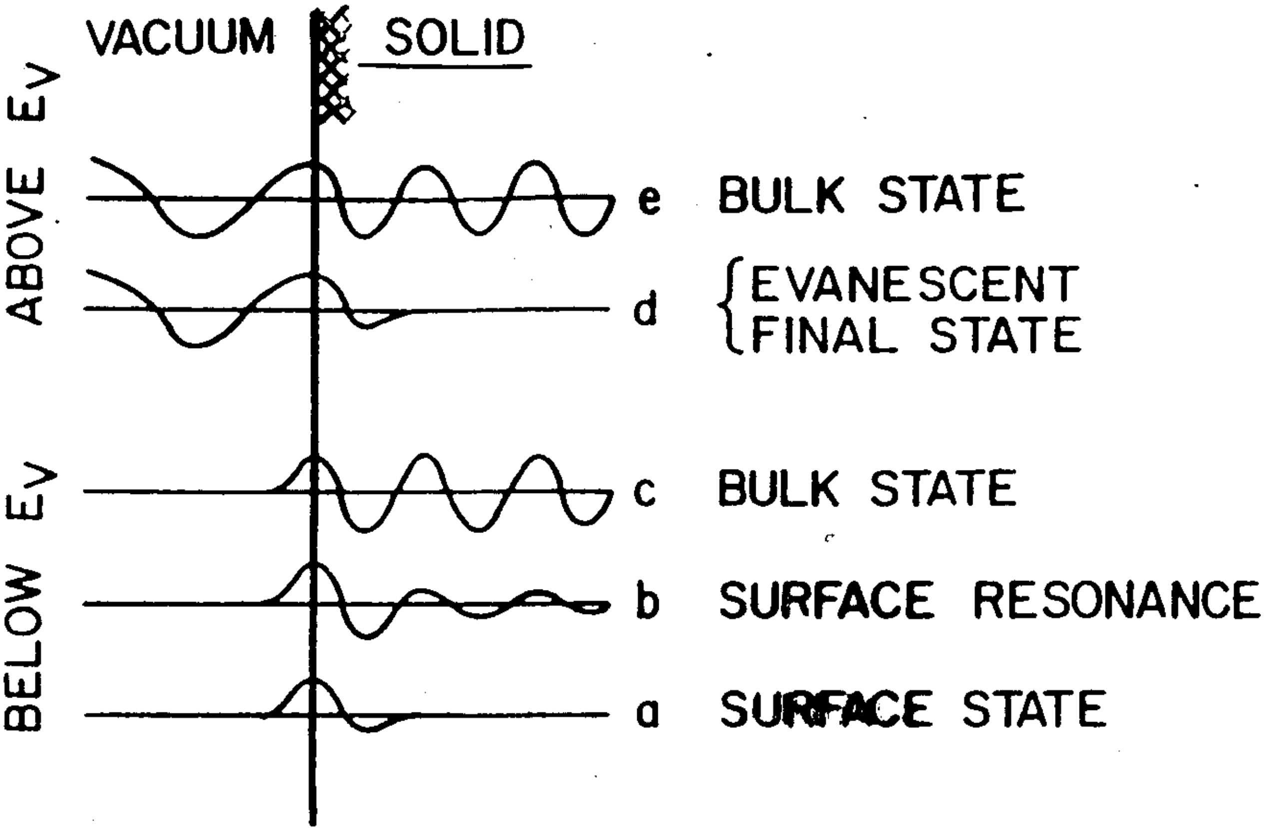
$$k_{in//} = k_{o//} = \frac{1}{\hbar}\sqrt{2\,m\,E_{kin}}\ \sin\theta$$



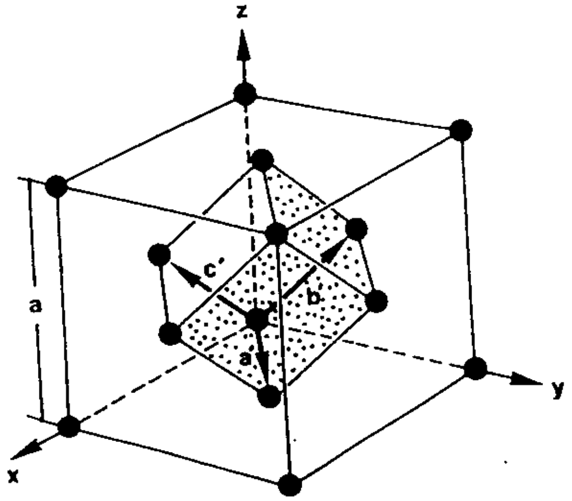




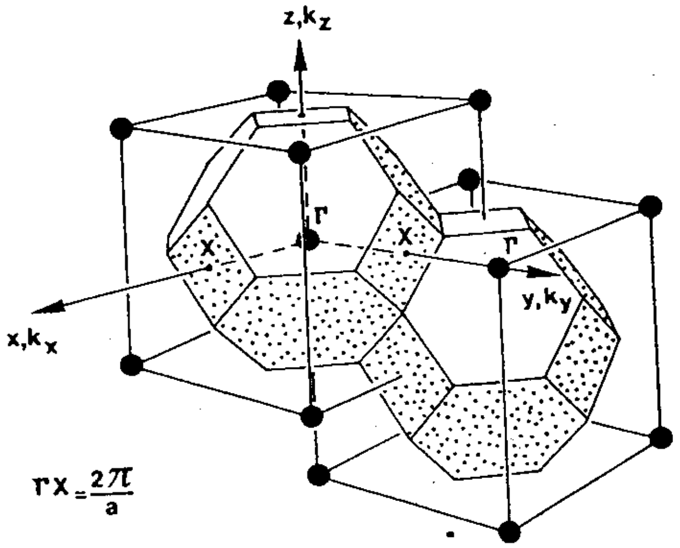
WAVE FUNCTIONS AT THE SURFACE



Face Centered Cubic Structure

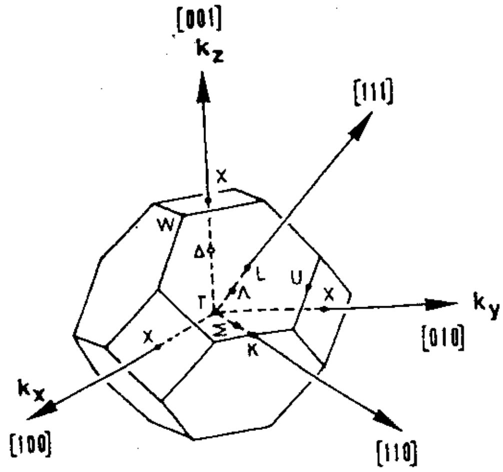


Real Space



Reciprocal Space

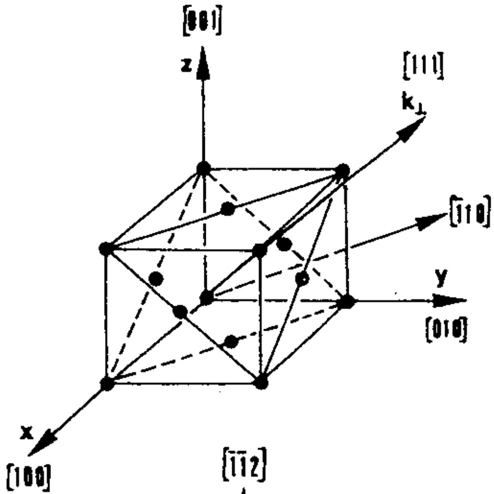
(and Brillouin Zone)



1st Brillouin Zone

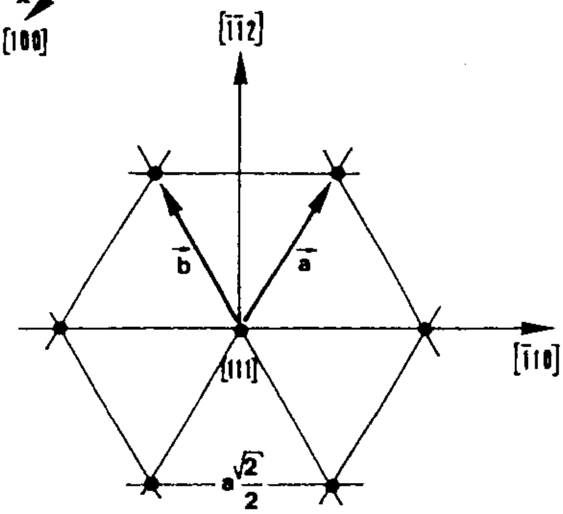
(and high symmetry directions

Face Centered Cubic Structure

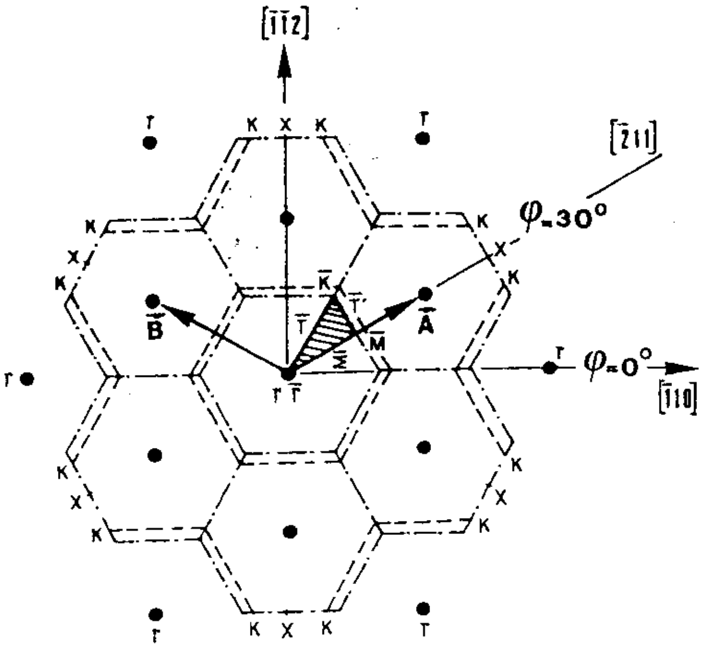


Real Space

(111) Face



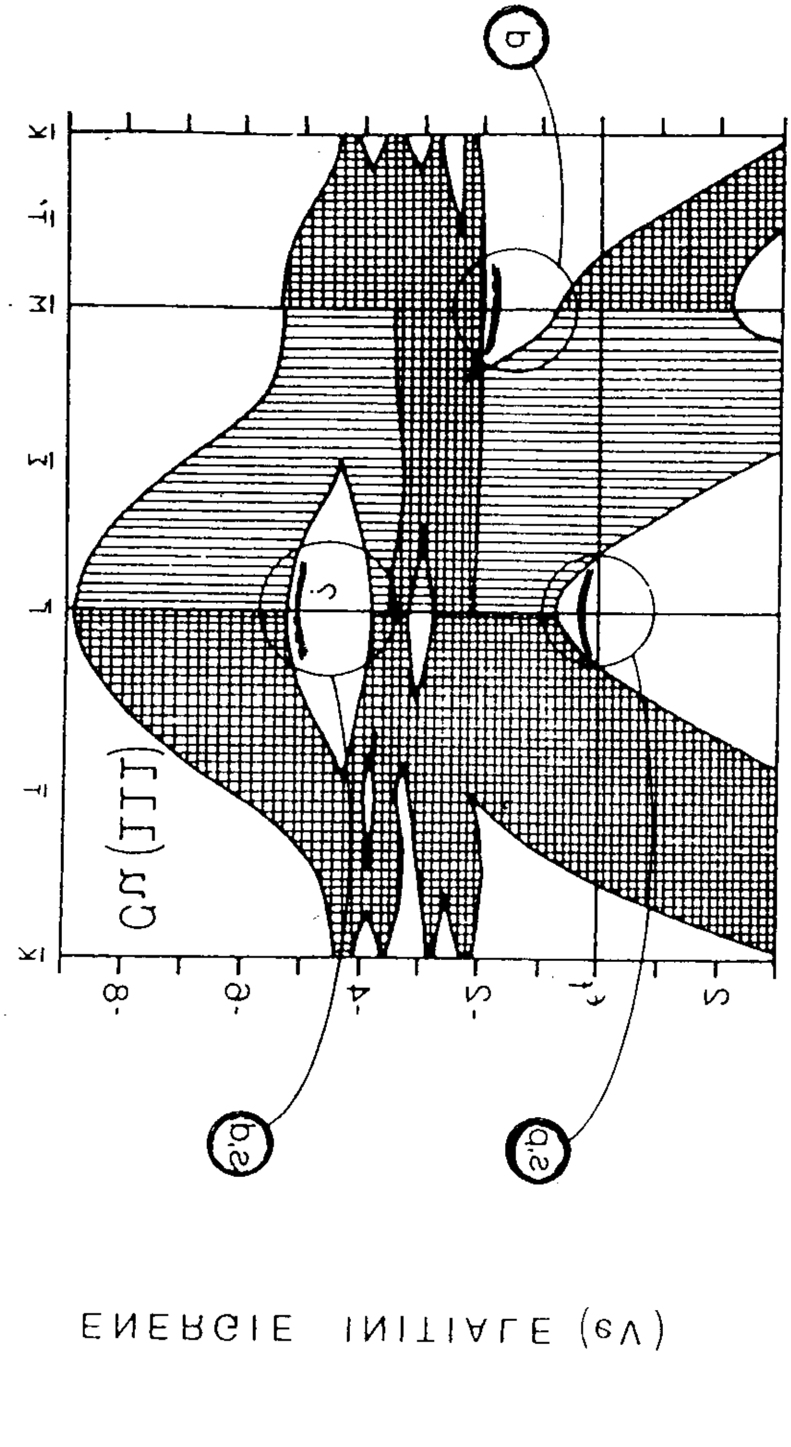
(111) Surface



Reciprocal

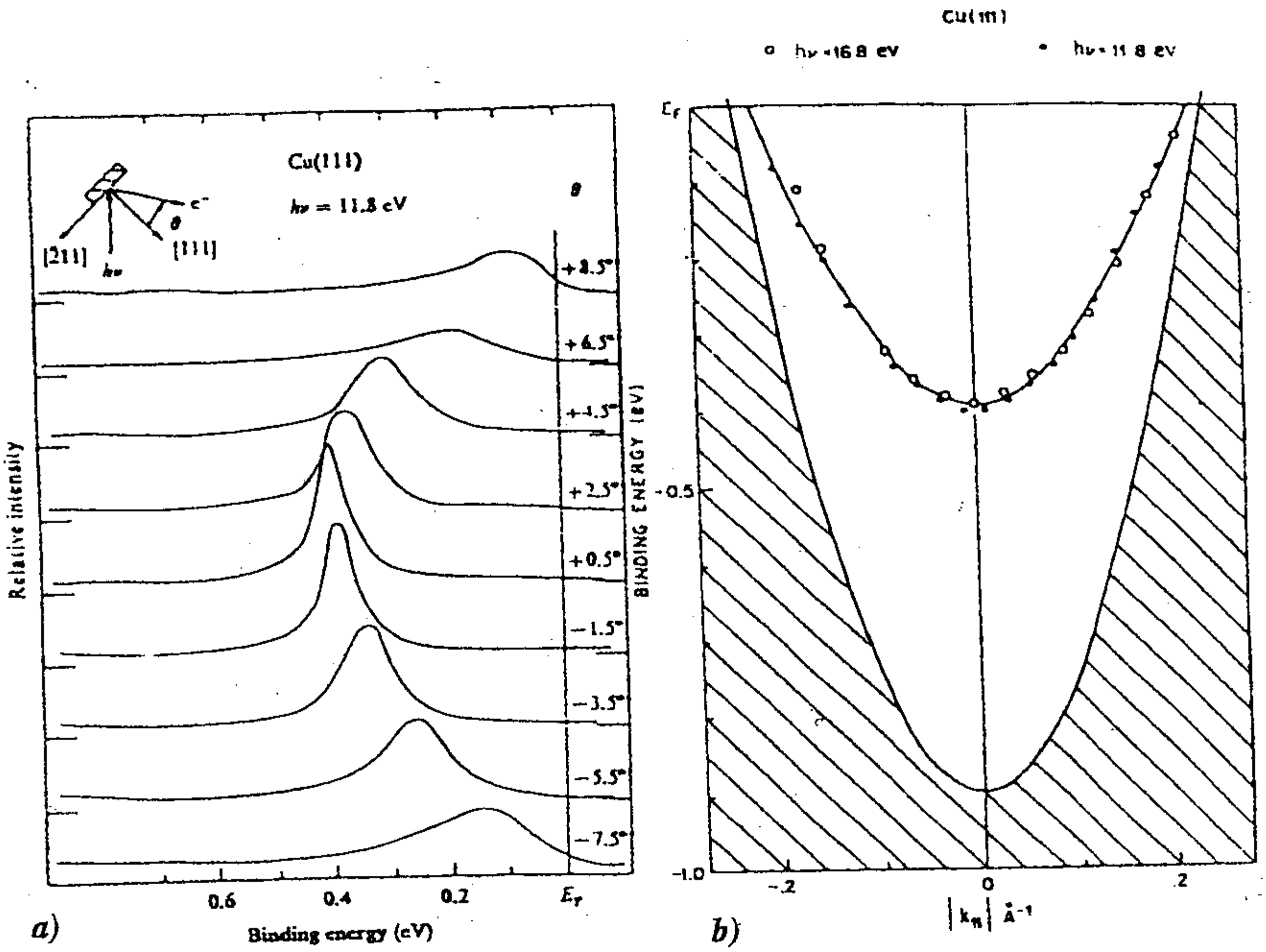
Surface Lattice

1st Surface Brilloinn Zone



Cu (111)
ENERGIE INITIALE (eV)
-8
-6
-4
-2
0
2

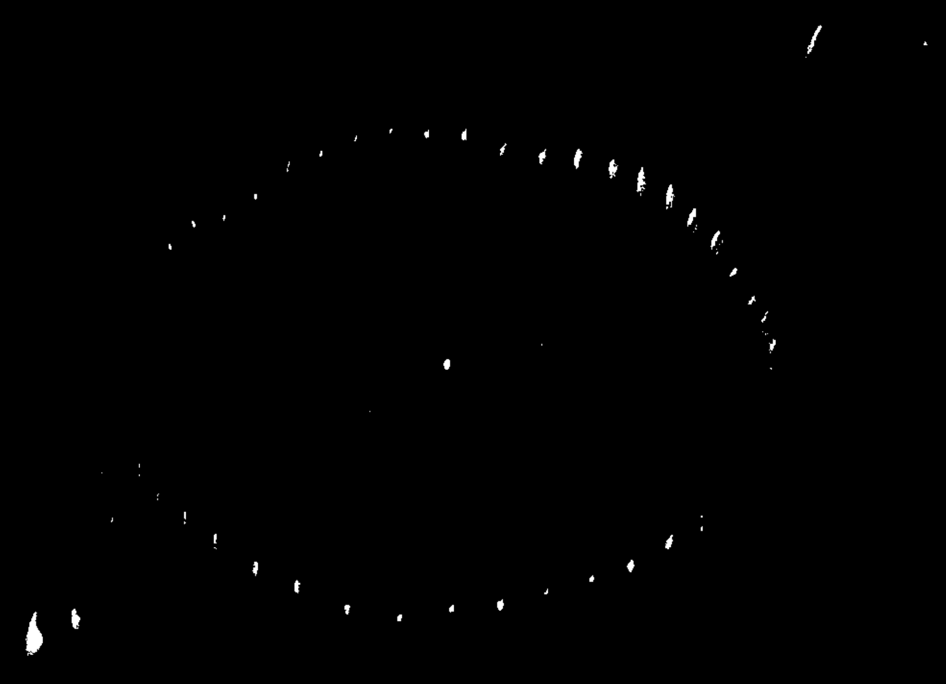
Cu(111): Surface State Band



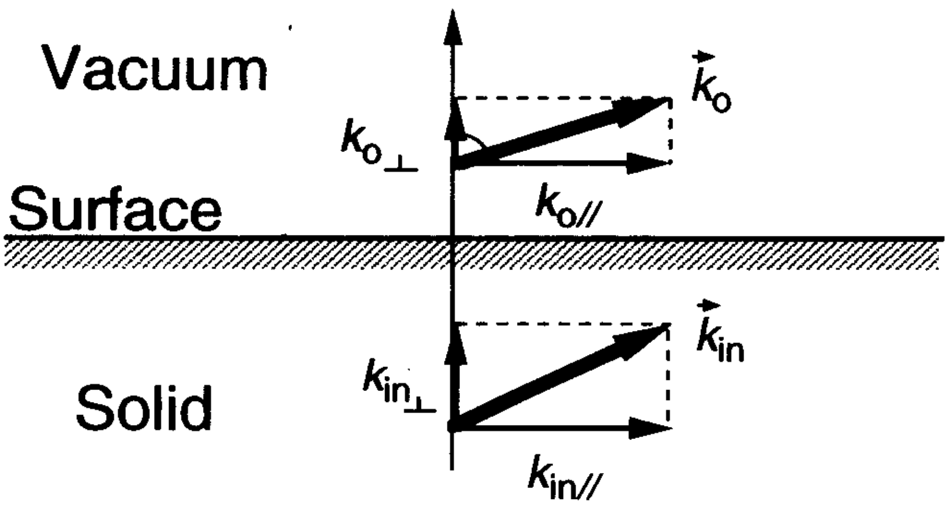
$$k_{in//} = k_{o//} = \frac{1}{\hbar}\sqrt{2\, m\, E_{kin}}\ \sin\theta$$

PHYSICS TODAY

NOVEMBER 1993



3-D System: $E = E(\vec{k})$

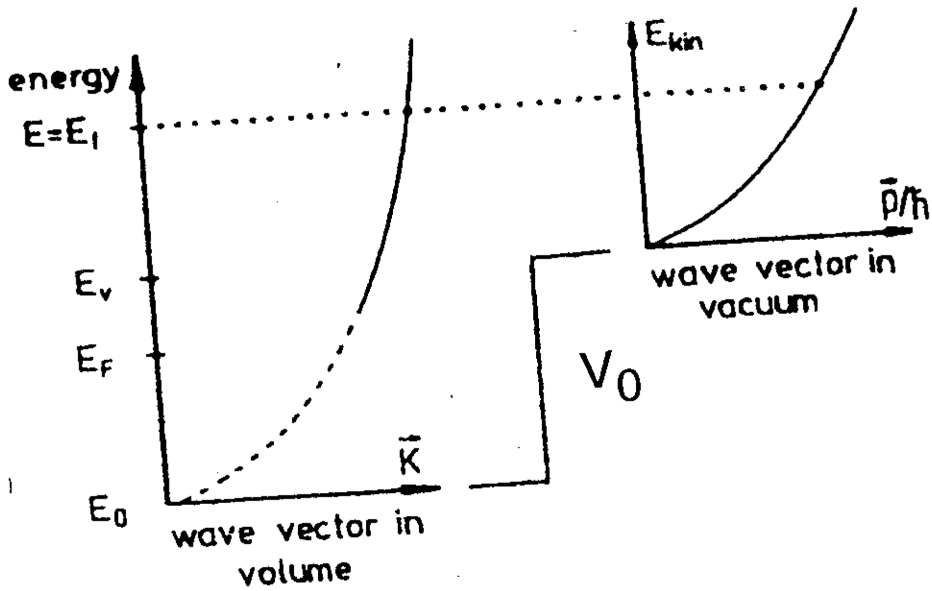


$$k_{in//} = k_{o//} = \frac{1}{\hbar}\sqrt{2\,m\,E_{kin}}\ \sin\theta$$

$$k_{in\perp} \neq k_{o\perp} = \frac{1}{\hbar}\sqrt{2\,m\,E_{kin}}\ \cos\theta$$

how to determine $k_{i\perp}$?

Free electron final states



$$E_{kin} = \frac{\hbar^2}{2m} (k_{o//}^2 + k_{o\perp}^2) = \frac{\hbar^2}{2m} (k_{in//}^2 + k_{in\perp}^2) - V_0$$

substituting :

$$k_{o//} = k_{in//} \qquad k_{o\perp} = \frac{1}{\hbar}\sqrt{2\,m\,E_{kin}}\cos\theta$$

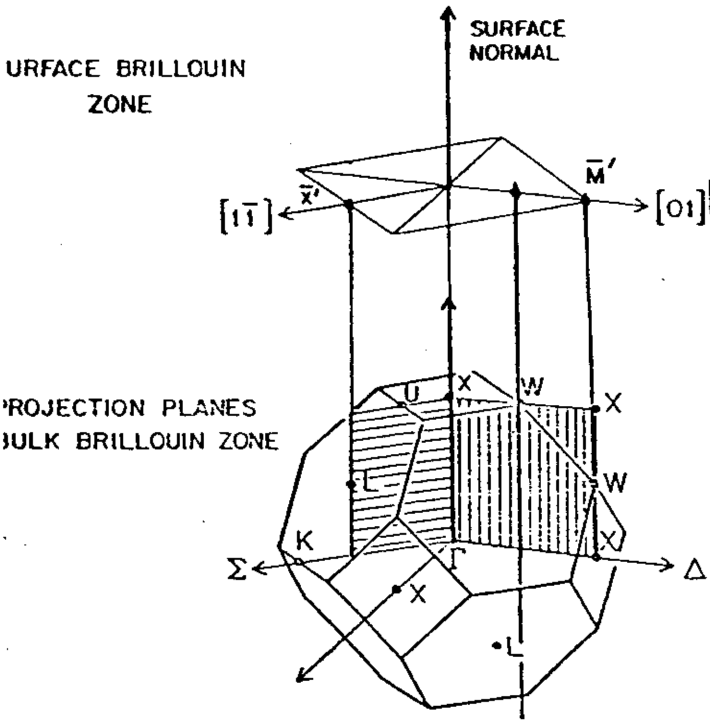
$$\longrightarrow$$

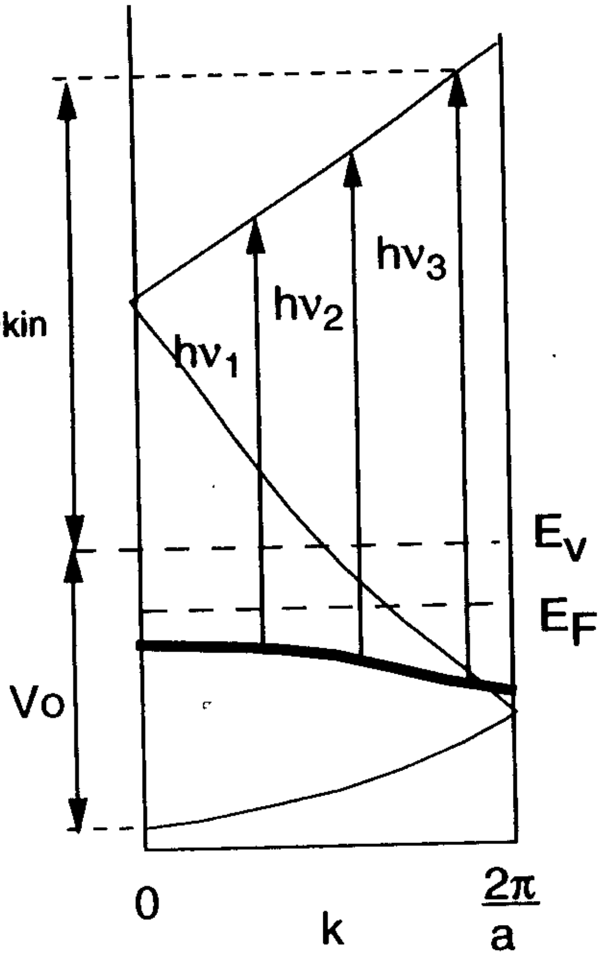
$$k_{in\perp} = \sqrt{k_{o\perp}^2 + \frac{2mV_o}{\hbar^2}}$$

$$= \frac{\sqrt{2m}}{\hbar^2}\sqrt{E_{kin}\cos^2\theta + V_0}$$

Band Mapping

Example : normal emission





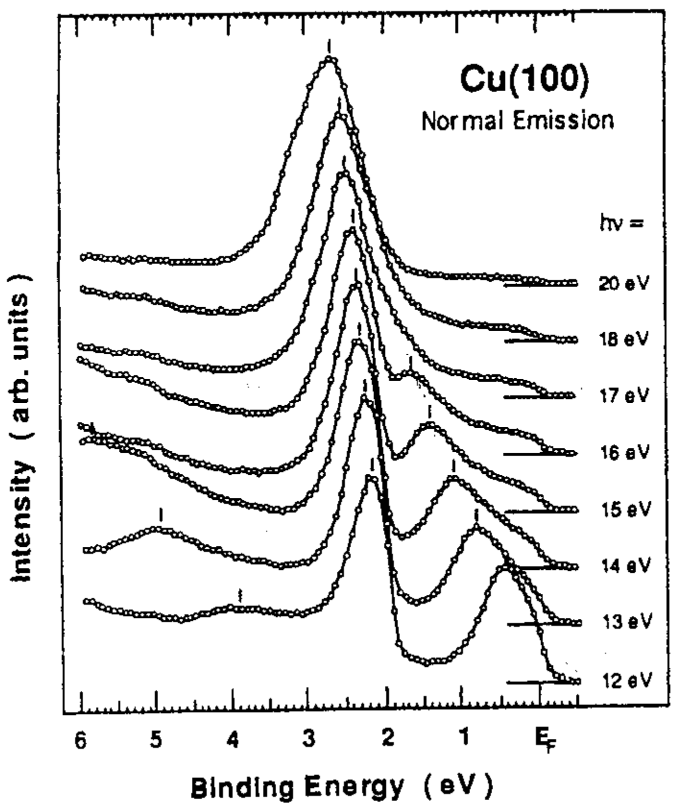
$$k_{o//} = k_{in//} = 0$$

$$k_{in\perp} = \frac{\sqrt{2m}}{\hbar^2} \sqrt{E_{kin} + V_0} \quad (\pm \vec{G})$$

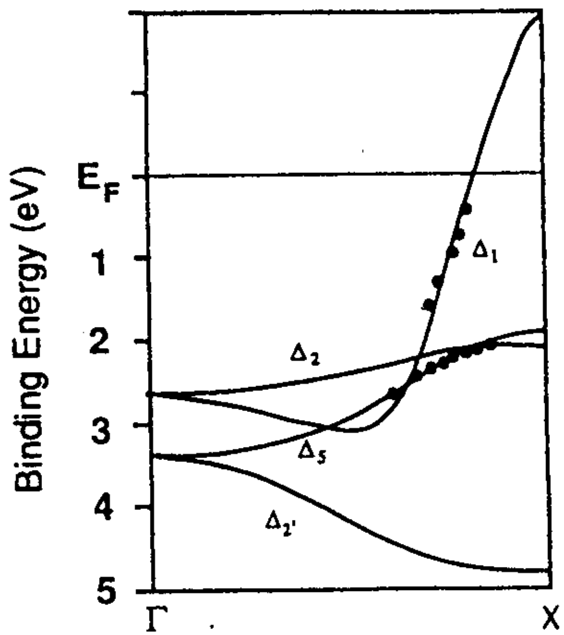
$$\frac{\sqrt{2m}}{\hbar^2} \sqrt{E_i + h\nu - \phi + V_0} \quad (\pm \vec{G})$$

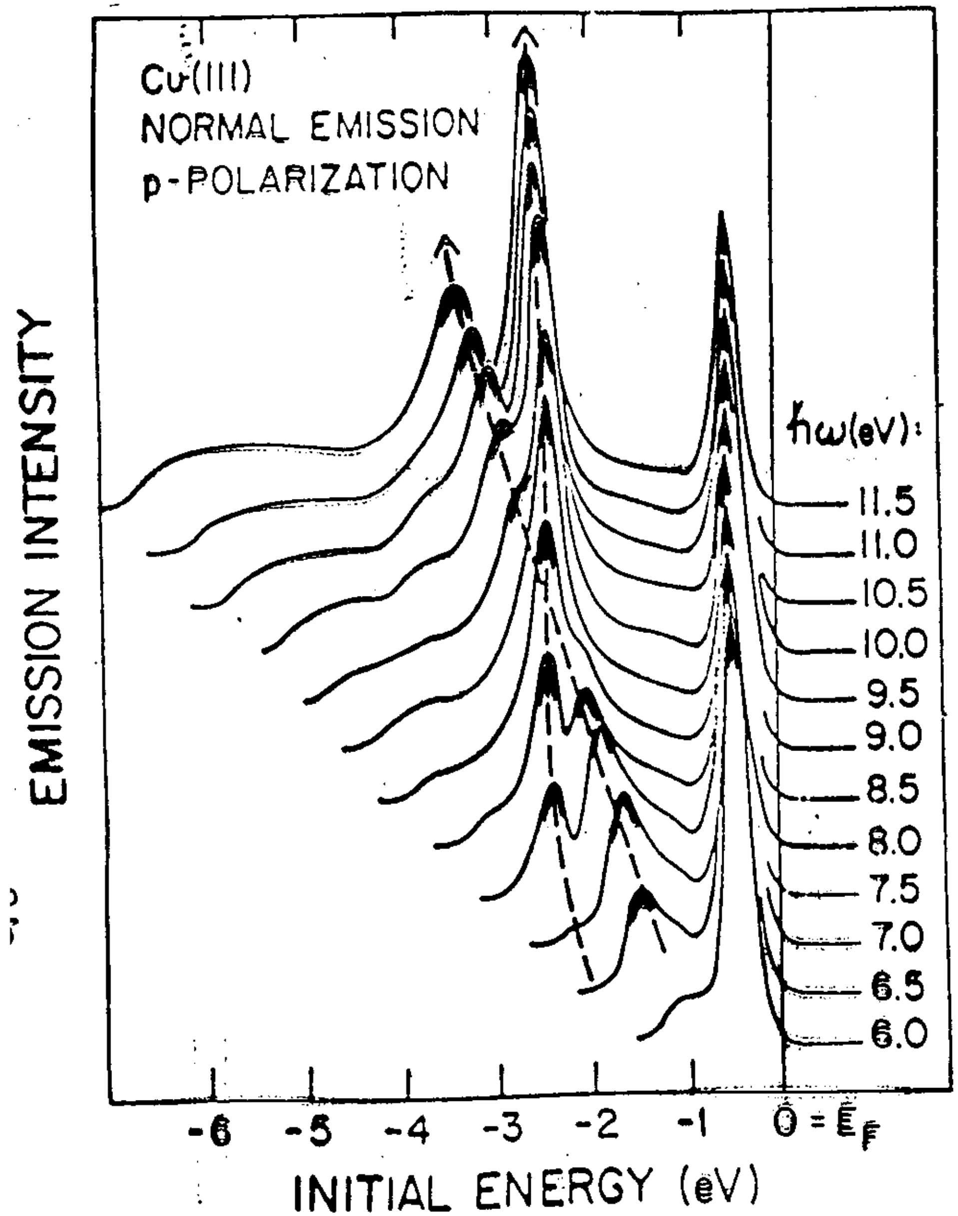
Photoemission from Cu (100)

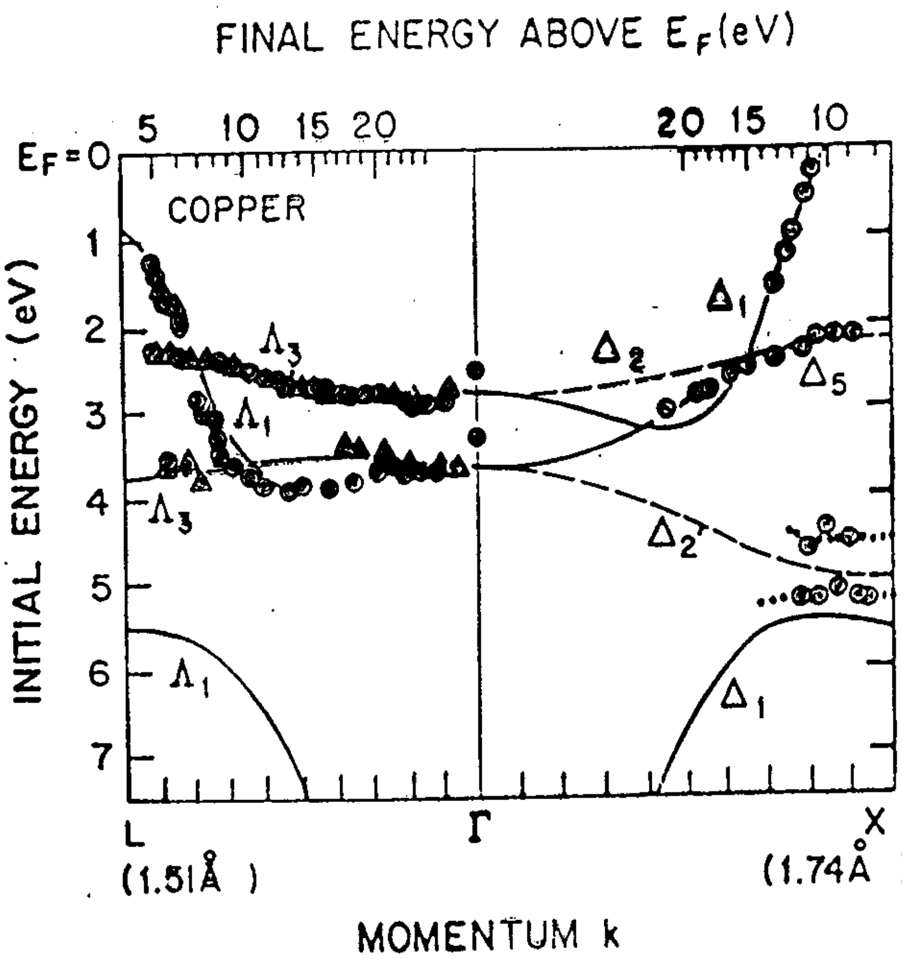
Spectra vs. Photon Energy



Band dispersion.







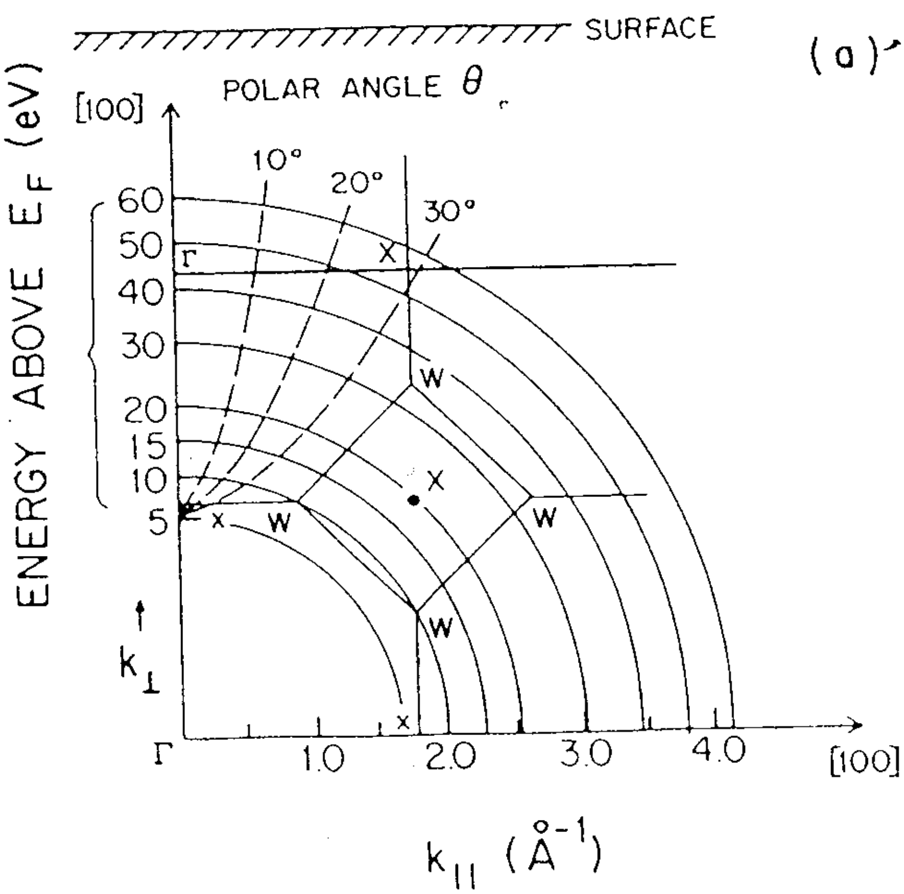
Knapp et al. PRB 19, 4952 (79)

Band Mapping

The general case : off-normal emission

$$k_{in//} = k_{o//} = \frac{\sqrt{2m}}{\hbar^2} \sqrt{E_{kin} \sin^2 \theta}$$

$$k_{in\perp} = \frac{\sqrt{2m}}{\hbar^2} \sqrt{E_{kin} \cos^2 \theta + V_0}$$



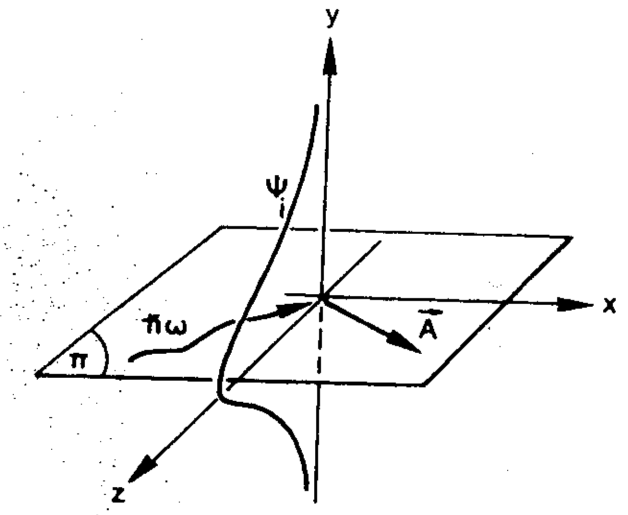
Free electron final state : circles $E = \frac{\hbar^2}{2m} (k_{in//}^2 + k_{in\perp}^2)$

Symmetry selection rules

$$\langle f | \mathbf{A} \cdot \mathbf{P} | i \rangle$$

Emission in a mirror plane : $\langle f | \equiv g$

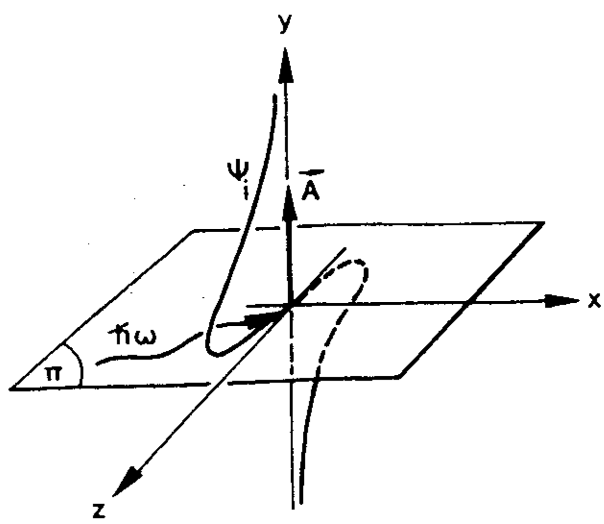
(detector in mirror plane) $| \quad | \rangle \equiv g$



$\mathbf{A} \parallel \pi$

$\mathbf{A} \cdot \mathbf{P} \equiv g$

$| i \rangle \equiv g$

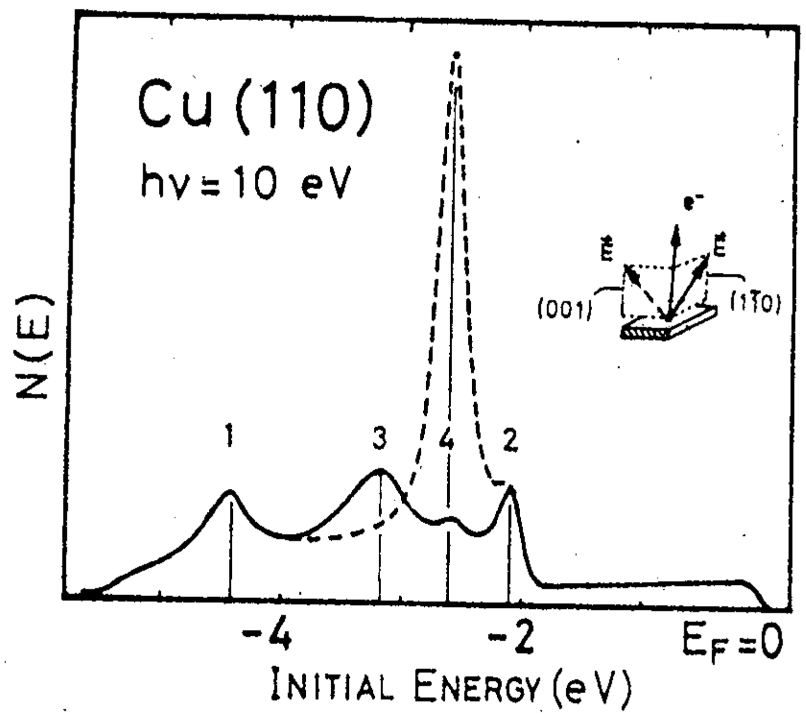


$\mathbf{A} \perp \pi$

$\mathbf{A} \cdot \mathbf{P} \equiv u$

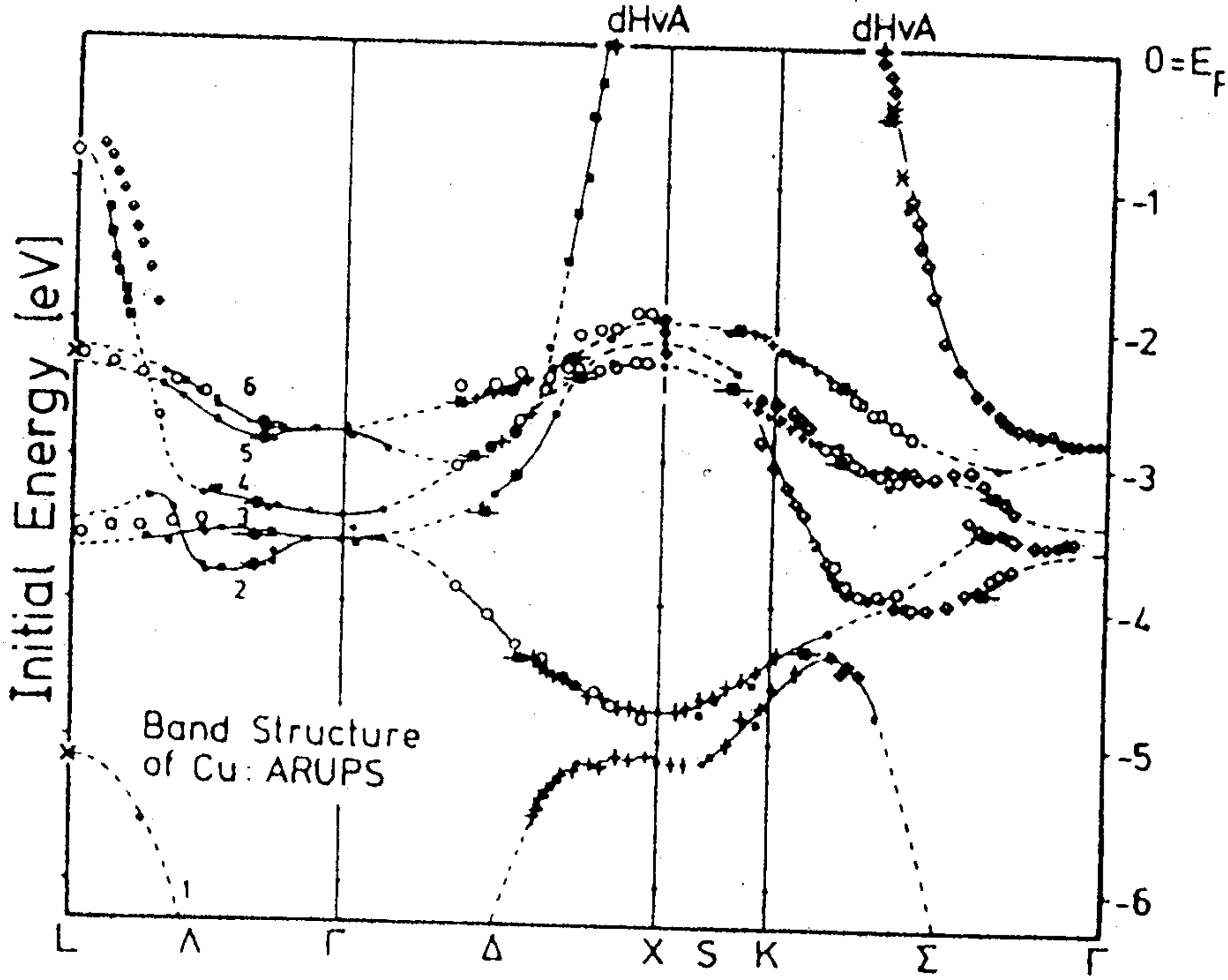
$| i \rangle \equiv u$

POLARIZATION SELECTION RULES



Kristall-fläche	Koordinaten Achsen x	y	z	Irreduzierbare Darstellungen	Symmetrie des Anfangszustandes A‖x	A‖y	A‖z
(001)	$\langle 100\rangle$	$\langle 010\rangle$	$\langle 001\rangle$	$\Delta_1\ \Delta_1'\ \Delta_2\ \Delta_2'\ \Delta_5$	Δ_5	Δ_5	Δ_1
(110)	$\langle 001\rangle$	$\langle 1\bar{1}0\rangle$	$\langle 110\rangle$	$\Sigma_1\ \Sigma_2\ \Sigma_3\ \Sigma_4$	Σ_3	Σ_4	Σ_1
(111)	$\langle \bar{1}10\rangle$	$\langle \bar{1}\bar{1}2\rangle$	$\langle 111\rangle$	$\Lambda_1\ \Lambda_2\ \Lambda_3$	Λ_3	Λ_3	Λ_1

Cu Bandstructure

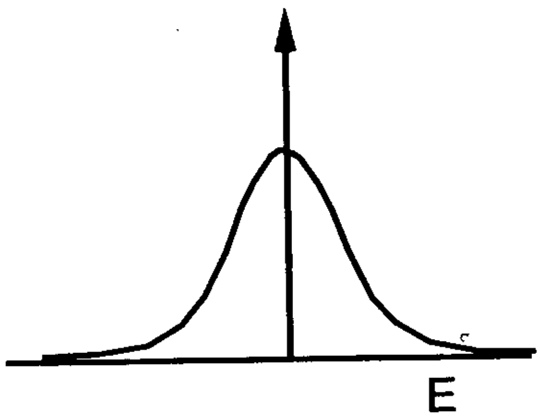


Beyond the single particle picture

electron and hole lifetime

e.g. Lifetimebroadening of the „initial state“ :

$$\delta\left(E_f - E_i - h\nu\right) \text{ -------> } \frac{1}{\pi}\frac{\Gamma_i}{(E_f - E_i - h\nu)^2 + \Gamma_i^2}$$



+ hole screening (Coulomb interaction)

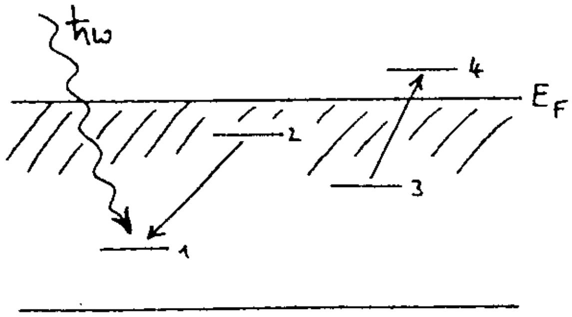
In general : Spectral distribution of the hole state $A_i(E_f - h\nu)$

$$A_i(E) = \frac{1}{\pi}\frac{\operatorname{Im}\Sigma_i(E)}{(E - E_i - \operatorname{Re}\Sigma_i(E))^2 + (\operatorname{Im}\Sigma_i(E))^2}$$

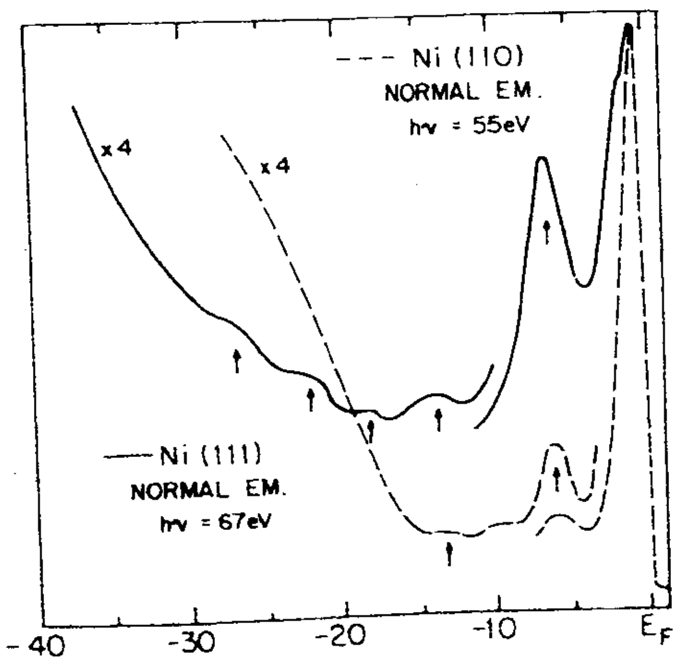
with complex self energy $\Sigma_i(E)$

Photoemission measures the excitation spectrum !

Many-body excitations

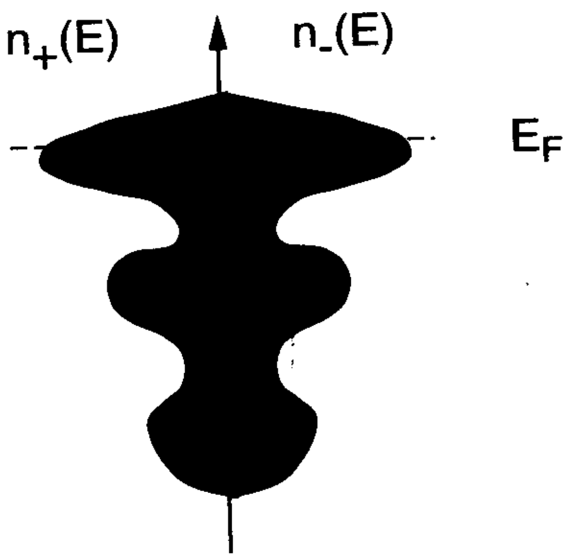


"Satellites" in Ni photoemission spectra



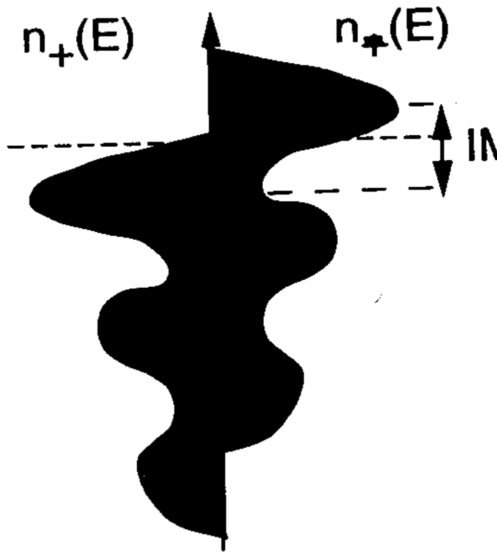
Stoner Model - Ferromagnetic Electronic Structure

PARAMAGNETIC DOS



$n_+(E) = n_-(E) = 0.5\, n_o(E)$

FERROMAGNETIC DOS



$n_\pm(E) = n_o(E \pm 0.5\, IM)$

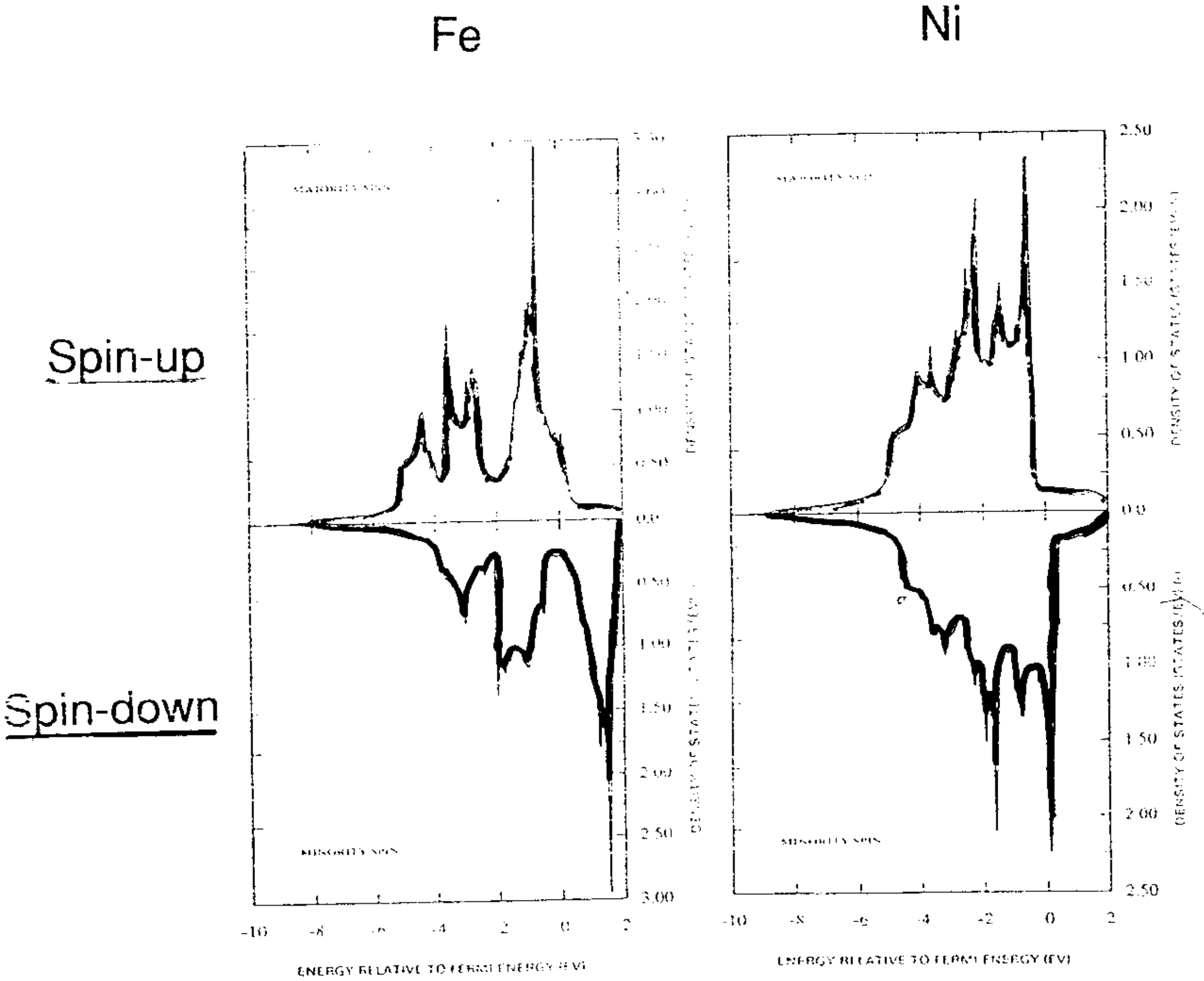
I exchange integral

M local moment

$$M = \int^{E_F} \{ n_+(E) - n_-(E) \}\, dE$$

FERROMAGNETIC METALS

SPIN DEPENDENT DENSITY OF STATES

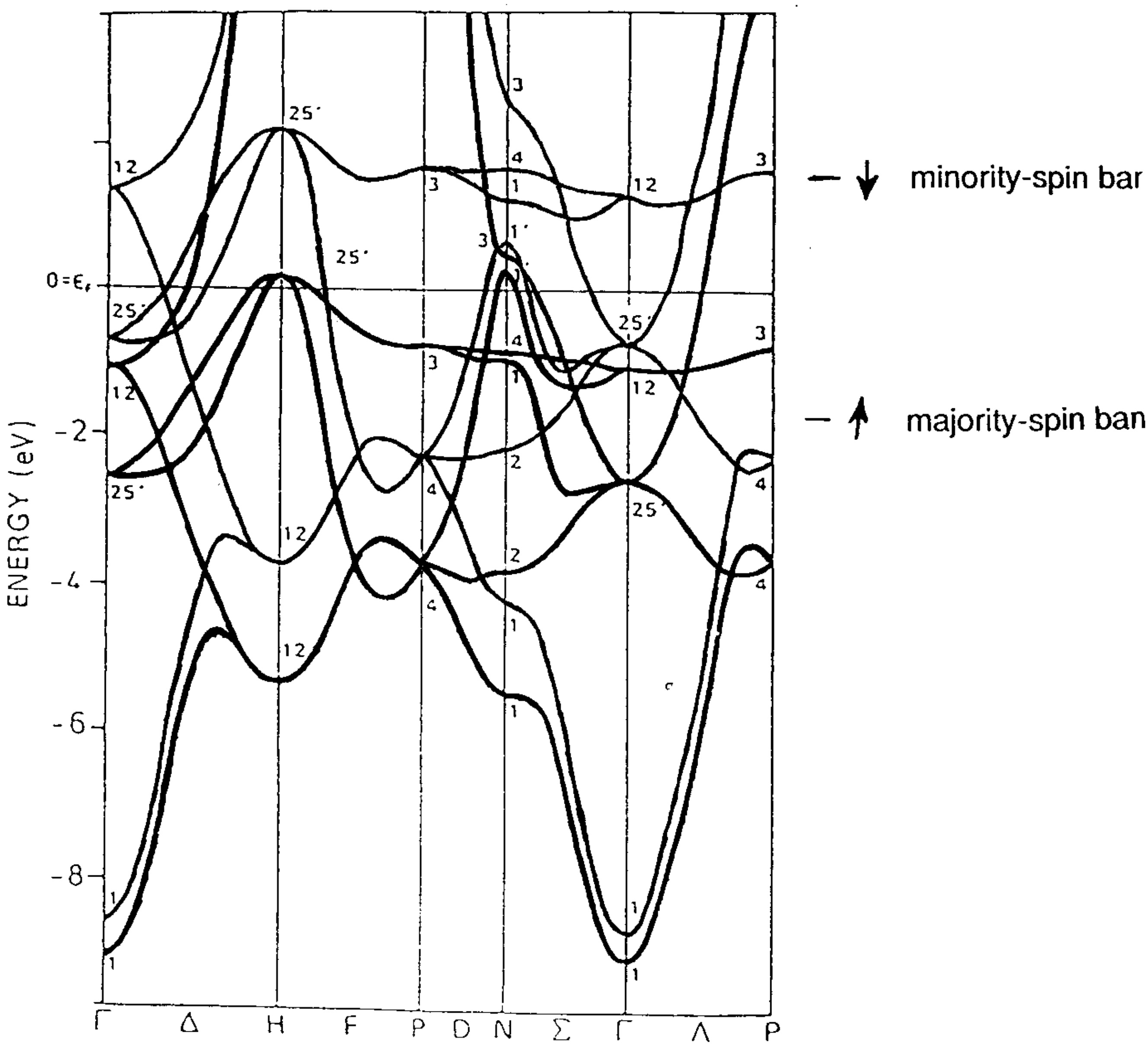


Magnetic Moments [μ_B / atom]

	Fe	Co	Ni	
Theory	2.15	1.56	0.59	(spin)
Exp.	2.12	1.57	0.55	(spin)
" (spin+orb.)	2.22	1.71	0.61	(tot.)

V.L. Moruzzi et al., "Calculated Properties of Metals" (1978)

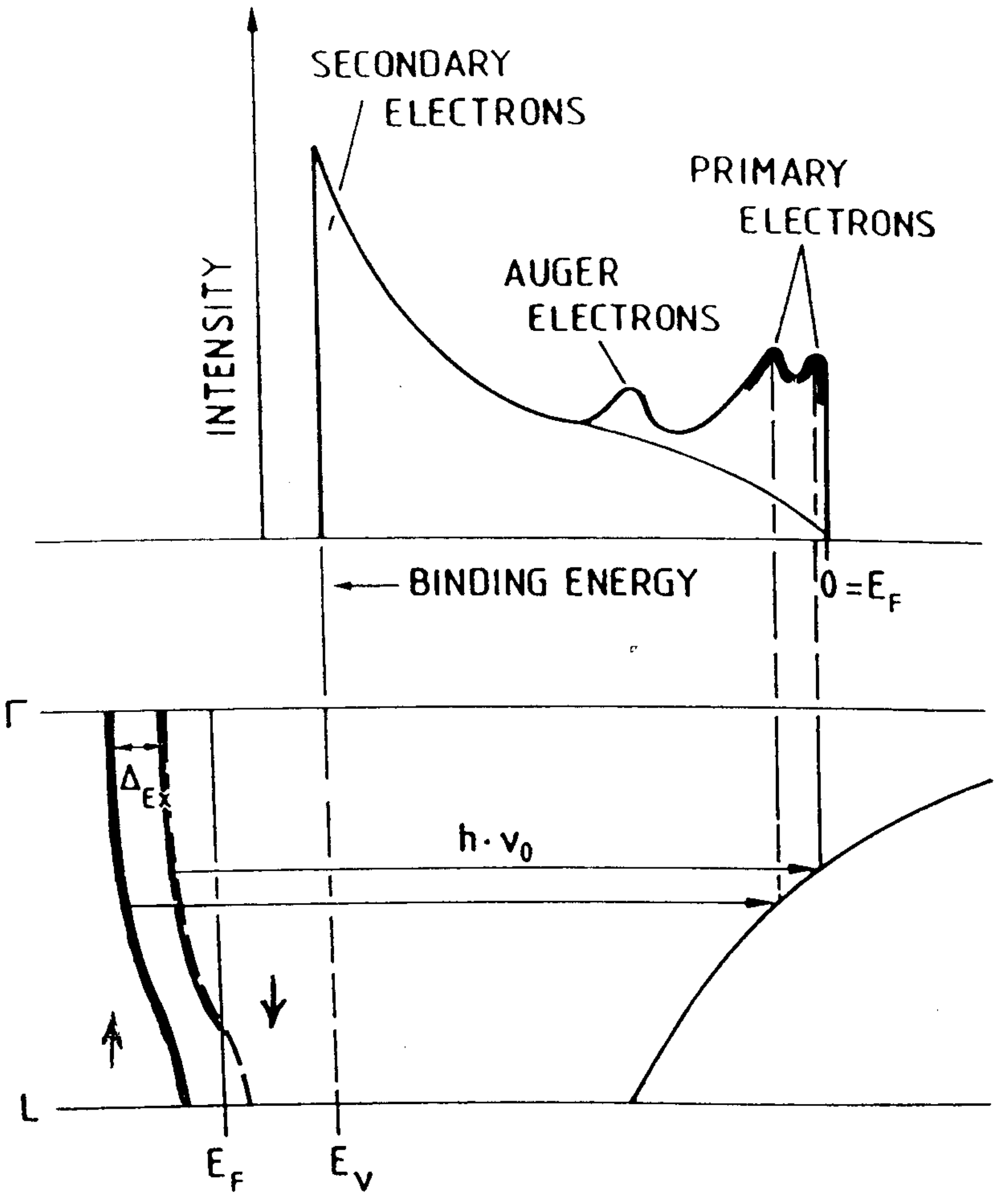
Fe Band Structure



Calculated bandstructure along high symmetry directions. Hathaway et al PRB 31, 7601 (1985)

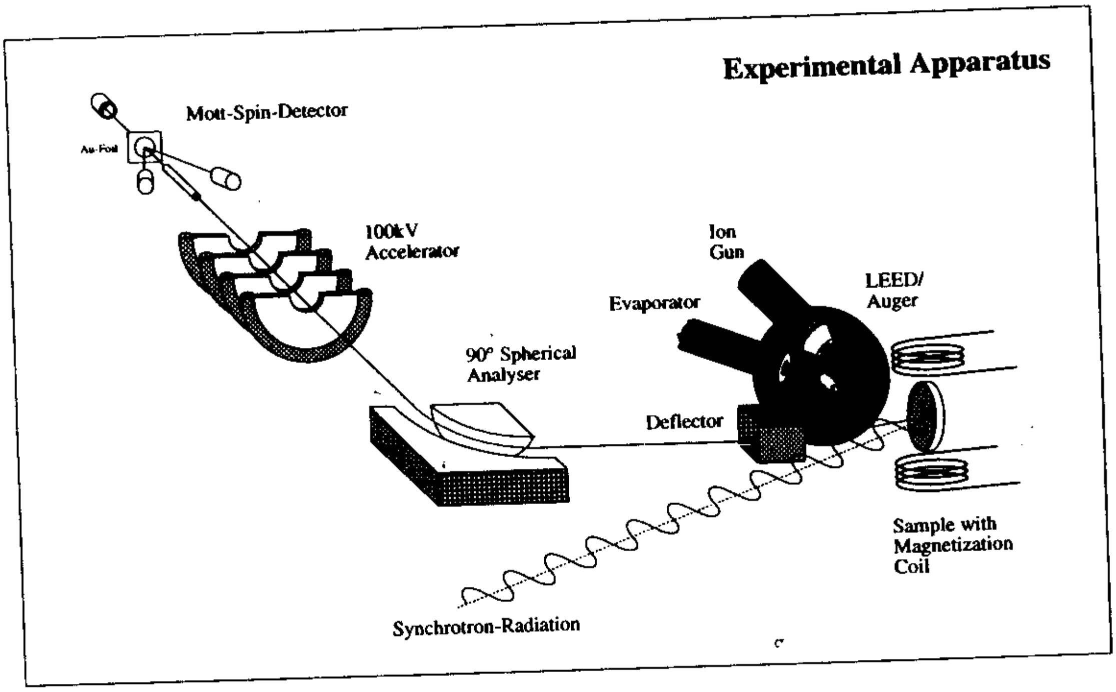
$$E = E(\bar{k}, \bar{\sigma})$$

Photoelectron Spectroscopy: Principles



{ kinetic energy ---> binding energy
{ emission angle ---> k vector
polarization ---> spin

Spin- and Angle-Resolved Photoemission



<u>MEASURE</u> :

E_k (kinetic energy)

$\vec{p}$ (momentum)

$\vec{P}$ (polarization)

outside

<u>TO OBTAIN</u> :

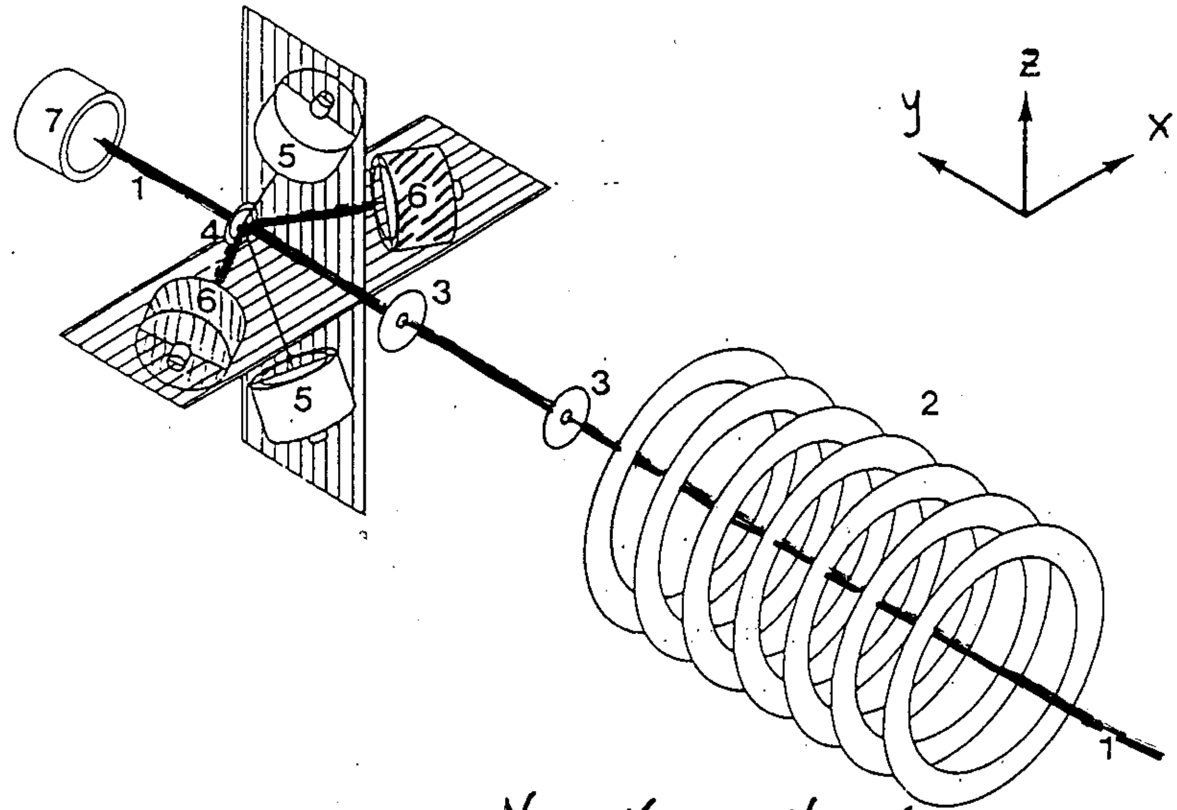
E_B (binding energy)

$\vec{k}_{\parallel}$ (wave vector)

$\vec{\sigma}$ (spin)

inside

MOTT DETECTOR



1) INCOMING ELECTRON BEAM

2) ACCELERATOR (30- 100 KeV)

3) COLLIMATOR

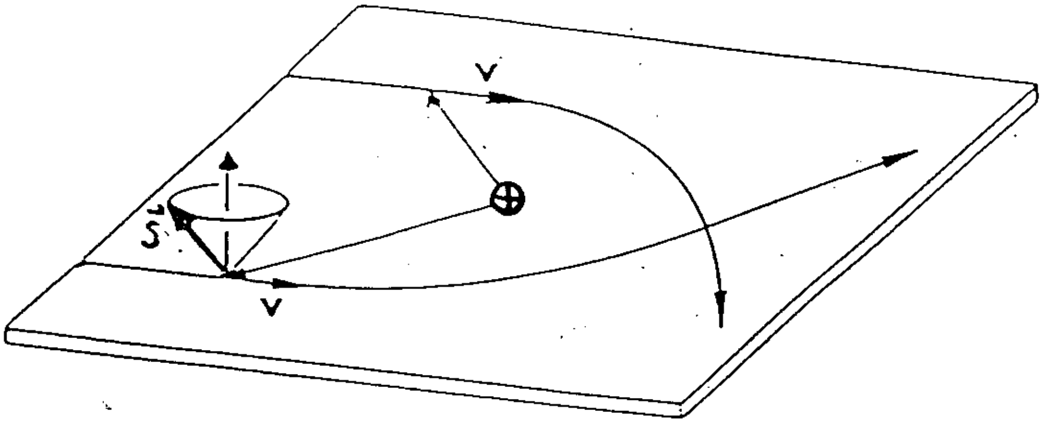
4) Au TARGET

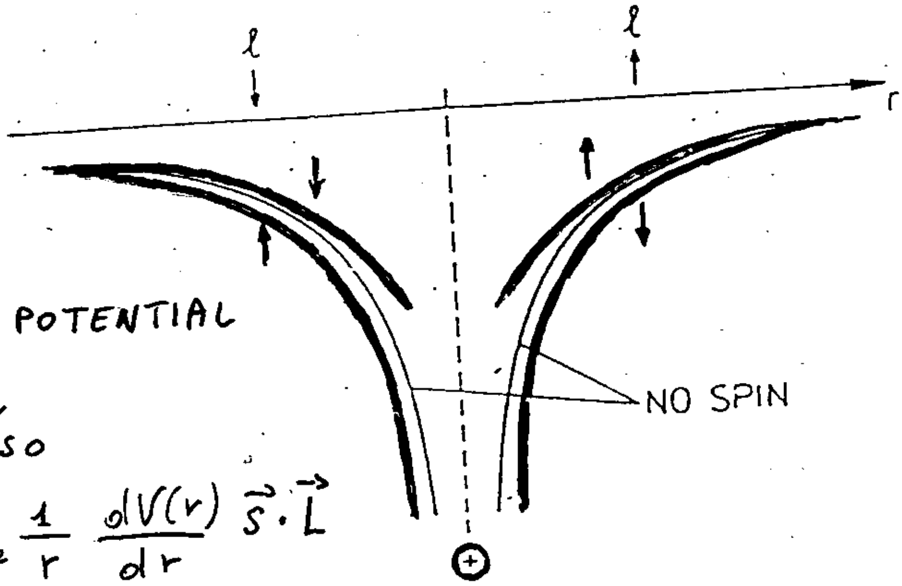
5-6) BACKSCATTERED ELECTRON DETECTORS

7) TRANSMITTED ELECTRON DETECTOR

$$P_z = \frac{1}{S} \frac{N_l - N_r}{N_l + N_r} = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}$$

$$FM = S^2 \left(\underline{N_l + N_r} \right) \simeq 10^{-4}$$

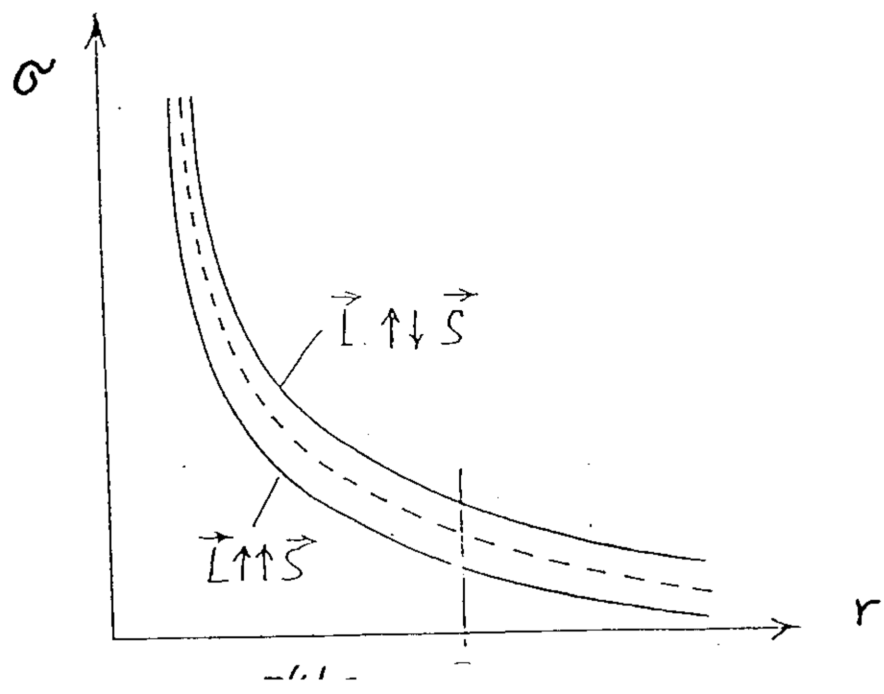


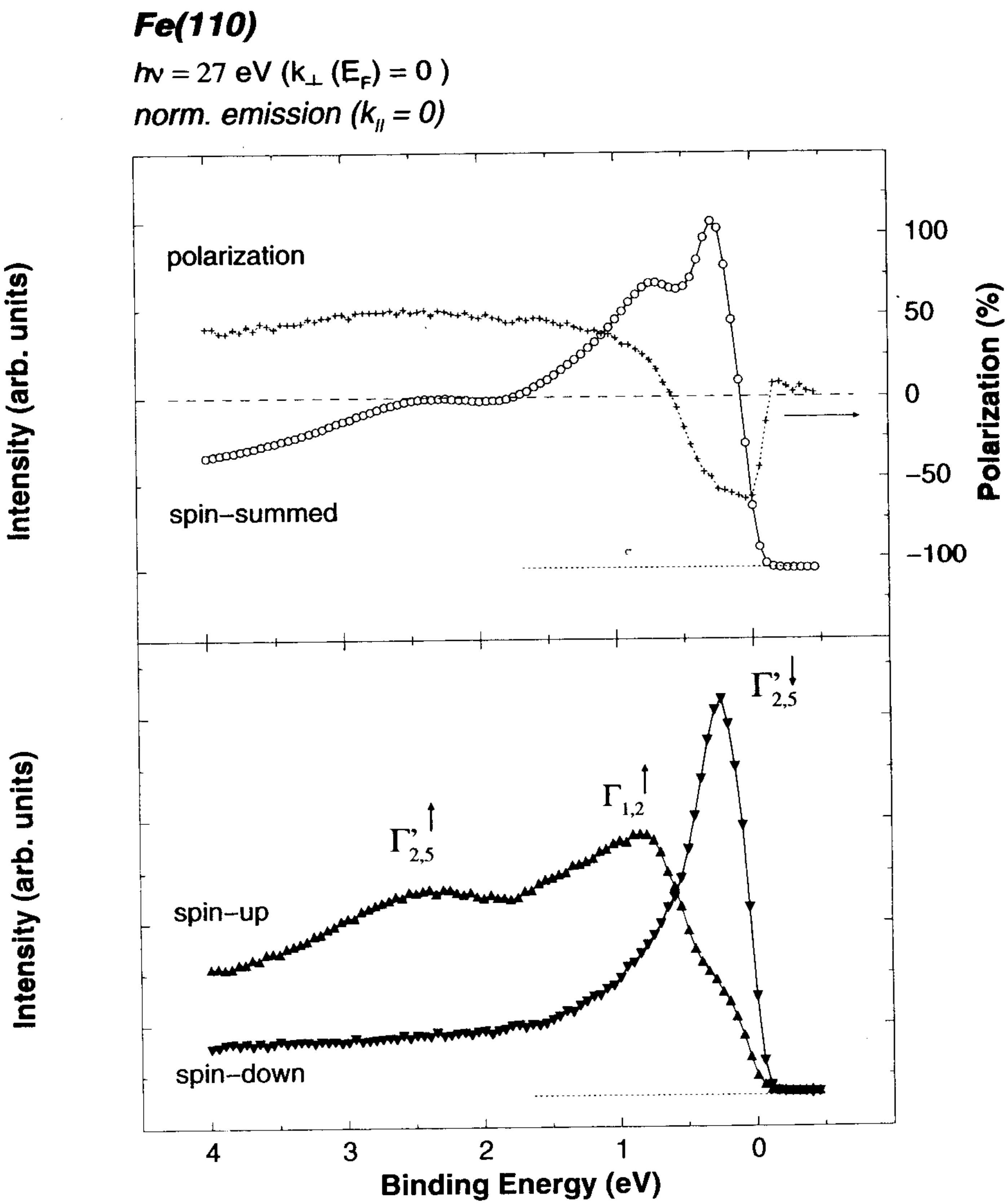


SCATTERING POTENTIAL

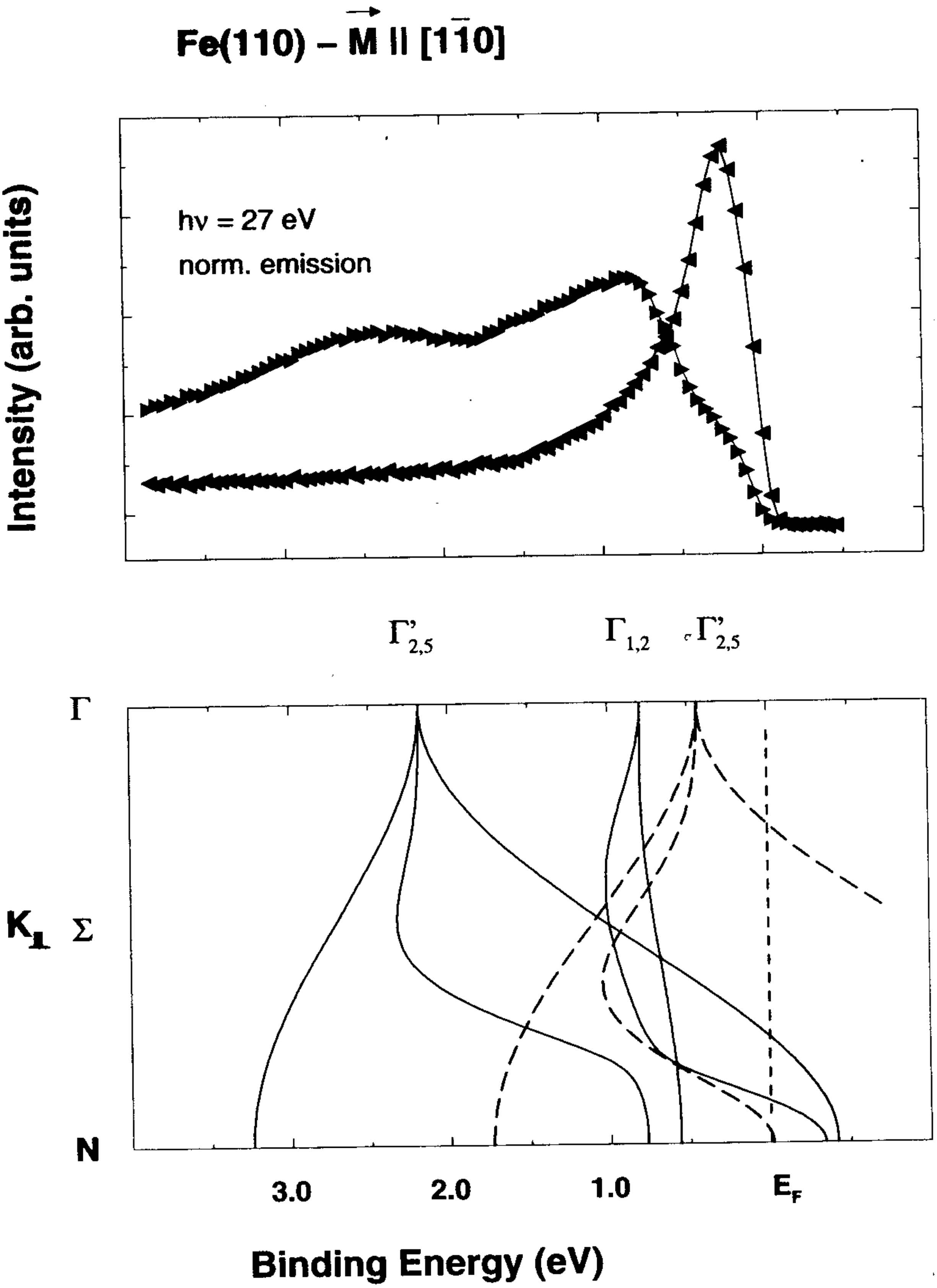
$$V = V_0 + V_{SO}$$

$$V_{SO} = \frac{1}{2m^2c^2}\,\frac{1}{r}\,\frac{dV(r)}{dr}\,\vec{S}\cdot\vec{L}$$



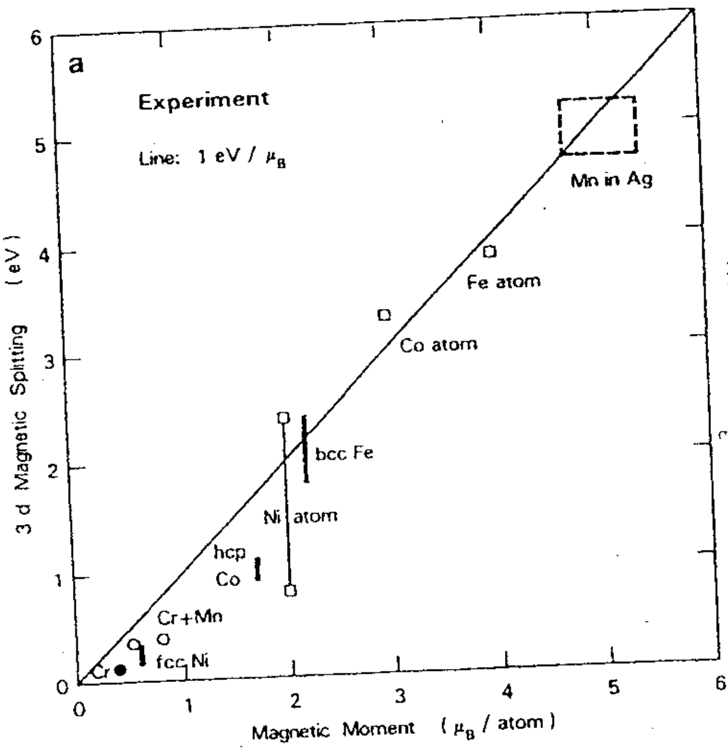


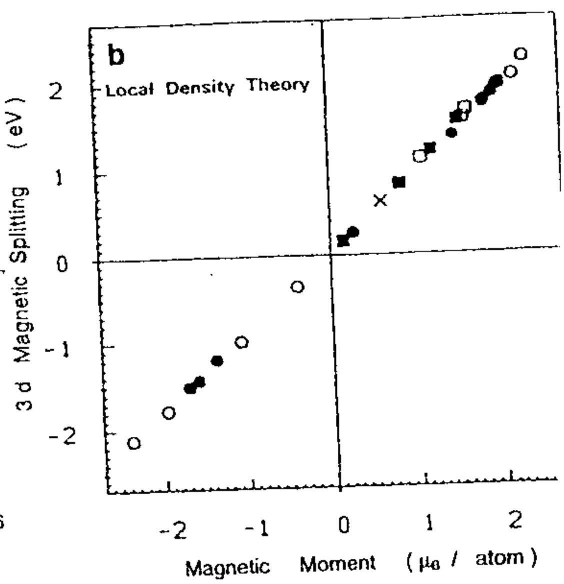
Fe(110)
hν = 27 eV (k⊥ (E_F) = 0)
norm. emission (k_// = 0)
polarization
spin–summed
Intensity (arb. units)
Polarization (%)
100
50
0
−50
−100
Γ'2,5↓
Γ1,2↑
Γ'2,5↑
spin–up
spin–down
Intensity (arb. units)
4
3
2
1
0
Binding Energy (eV)



Fe(110) – $\vec{M}$ II [1$\bar{1}$0]
Intensity (arb. units)
hν = 27 eV
norm. emission
Γ'2,5
Γ1,2
Γ'2,5
Γ
K⊥ Σ
N
3.0
2.0
1.0
EF
Binding Energy (eV)

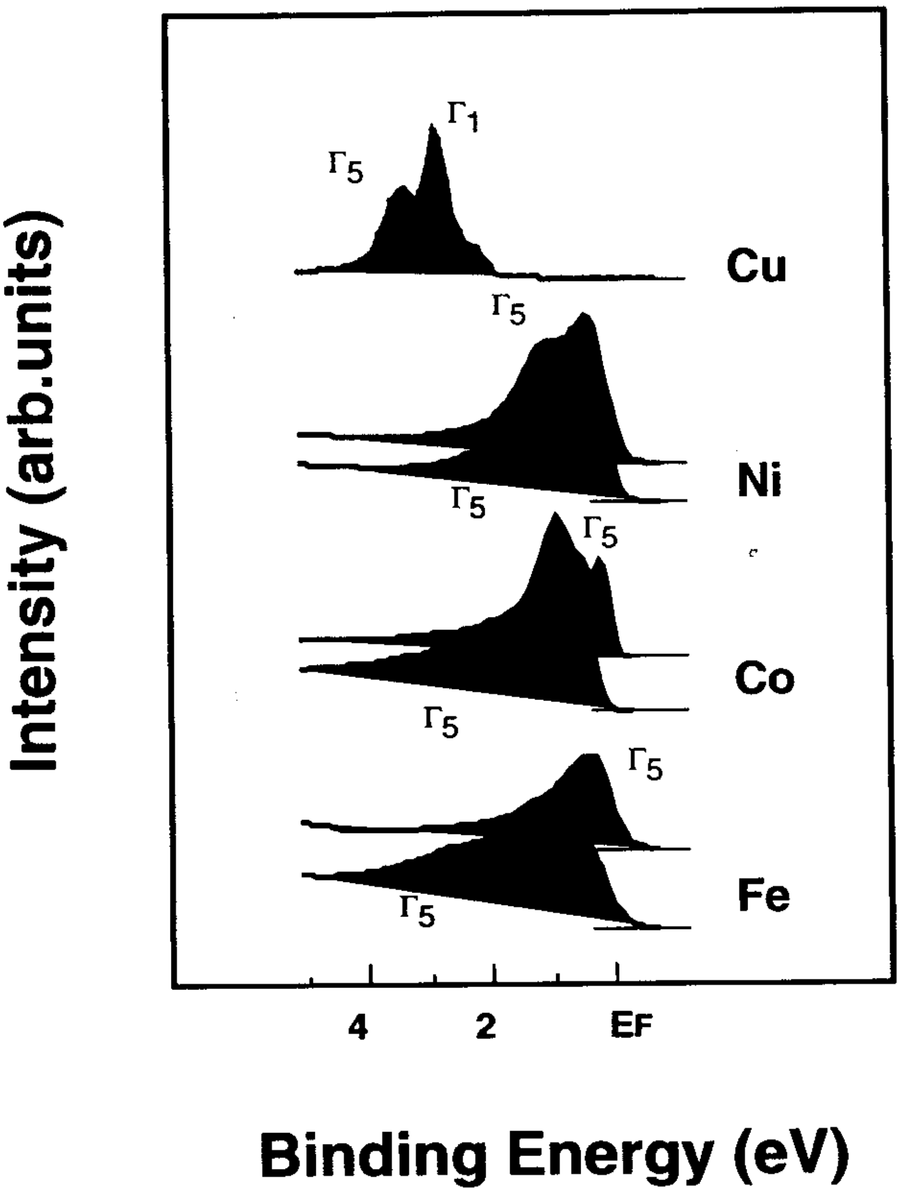
Magnetic Exchange Splitting δE_{ex} versus Magnetic Moment





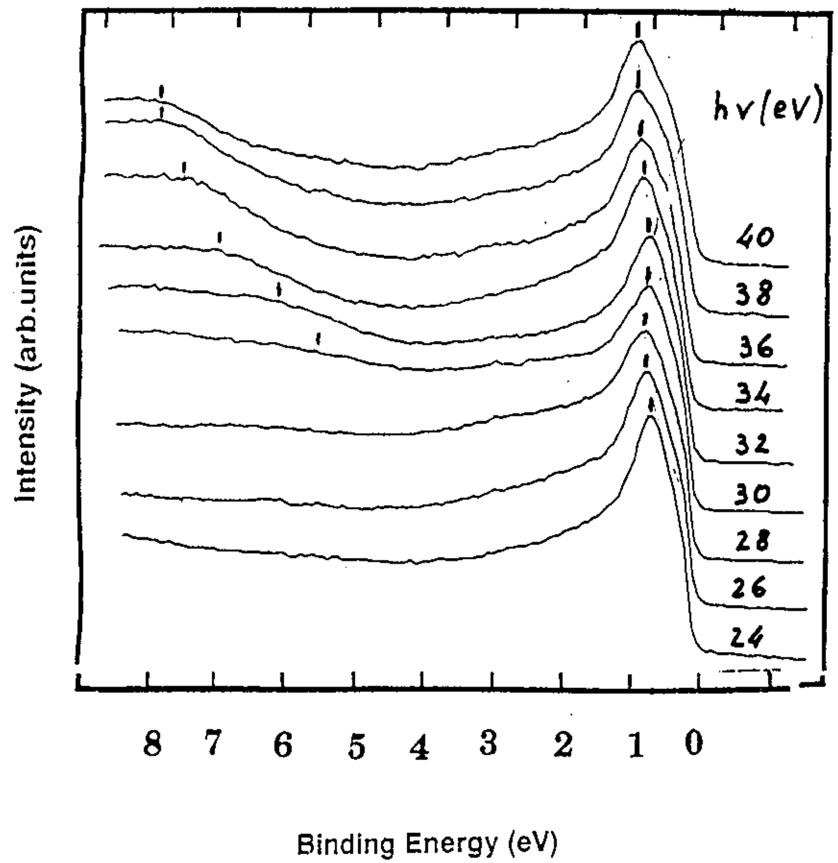
Epitaxial fcc Films

Spin-Resolved Photoemission

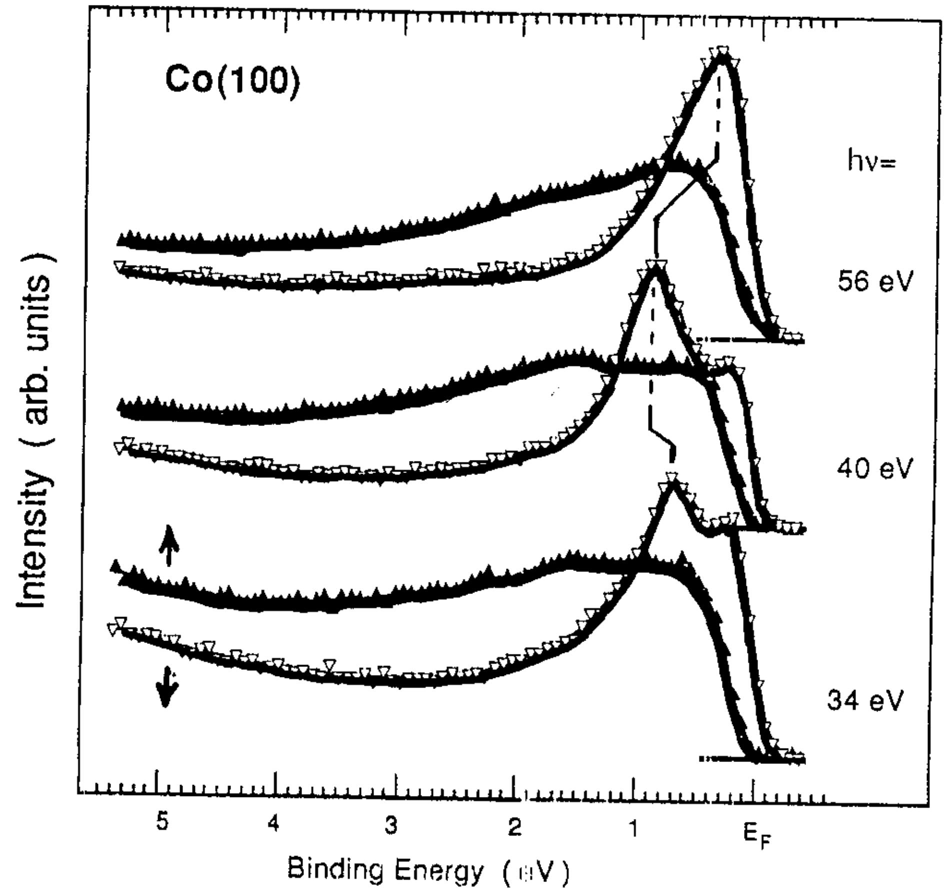


Band Mapping of Magnetic States **Fcc Co (100)**

Spin Integrated

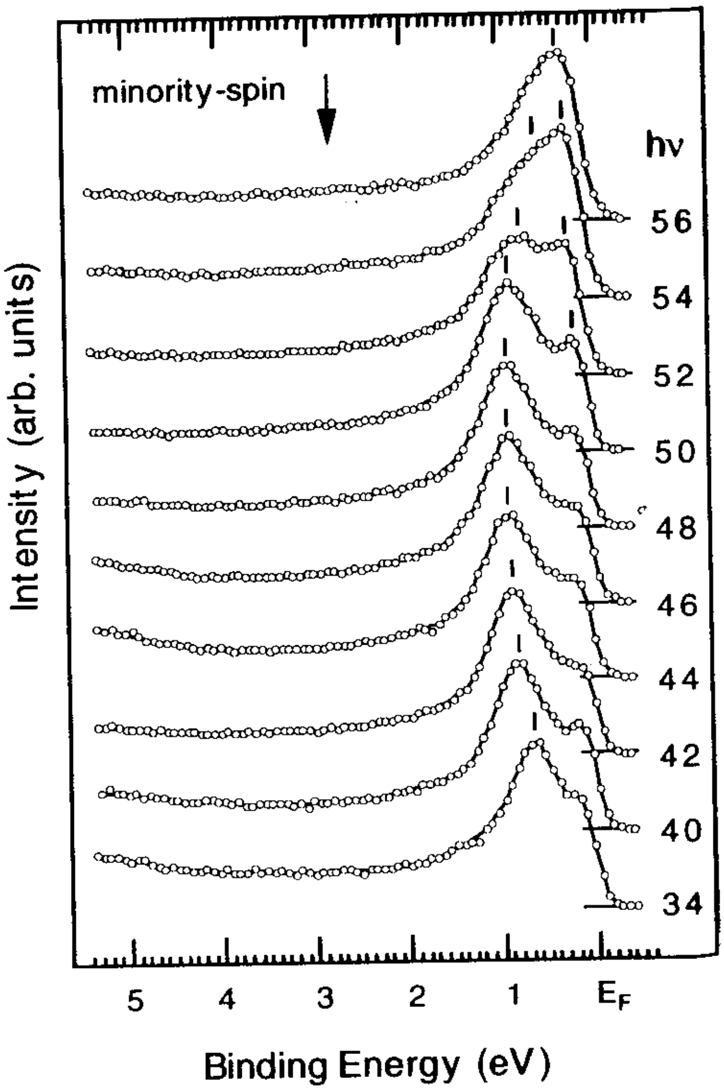


Spin Resolved



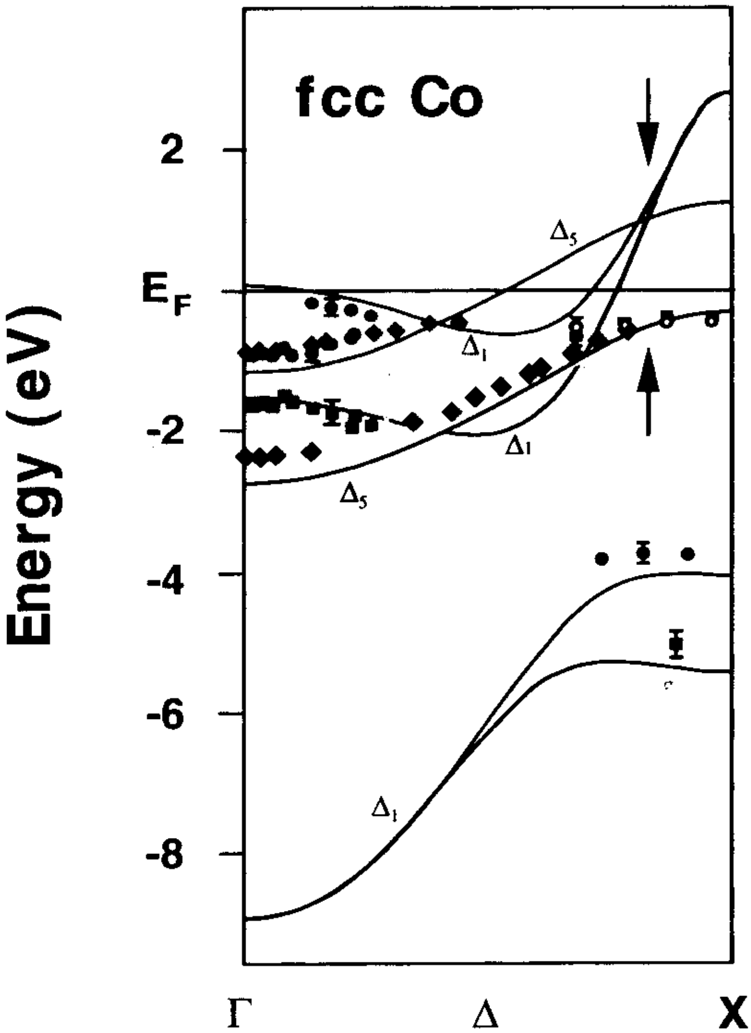
fcc-Co: bandstructure

Minority-Spin Emission Only



$E = E(k_{\perp}, \sigma_{\downarrow})$ $k_{\perp}$ along Γ-X

Fcc Co -Bandstructure



20 ML Co on Cu (100)

Experiment (symbols) vs.theory (lines)

Band disperion $E=E(k,\sigma)$

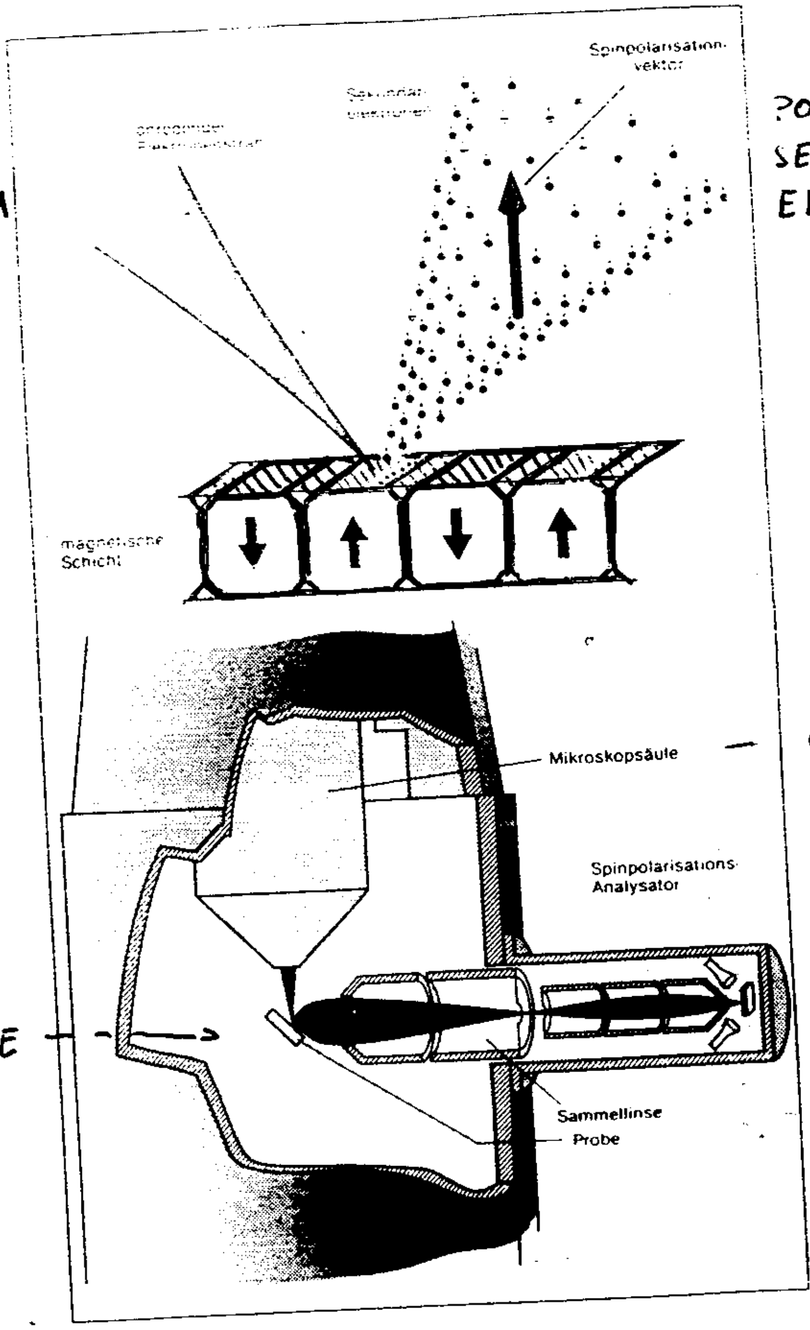
Exp.: R.Kläsges, PhD thesis, Köln (98)

Th: P.Bruno, Europhys. Lett. 23, 615 (93)

SCANNING ELECTRON MICROSCOPY OF POLARIZED ELECTRONS

UNPOLARIZED PRIMARY e^--BEAM

POLARIZED SECONDARY ELECTRONS



COLLIMATED SOURCE ($\simeq$ 20 nm)

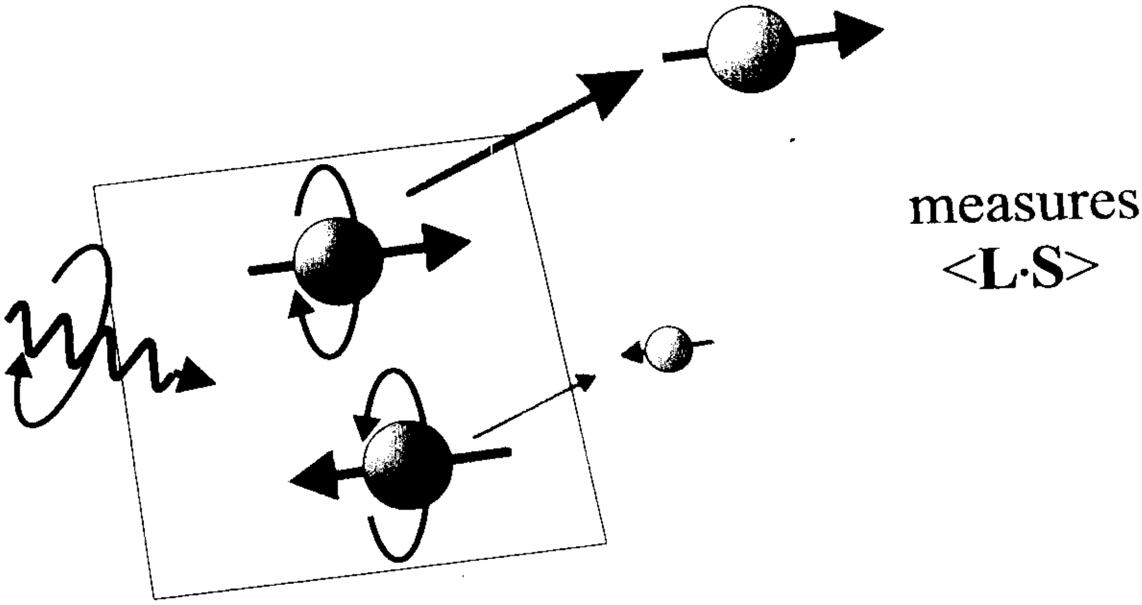
SPIN ANALYZER

SAMPLE

$$P \simeq \frac{n_B}{n_V}$$

n_B Bohr magnetons (per atom)

n_V valence electron (per atom)



spin-polarized PEEM

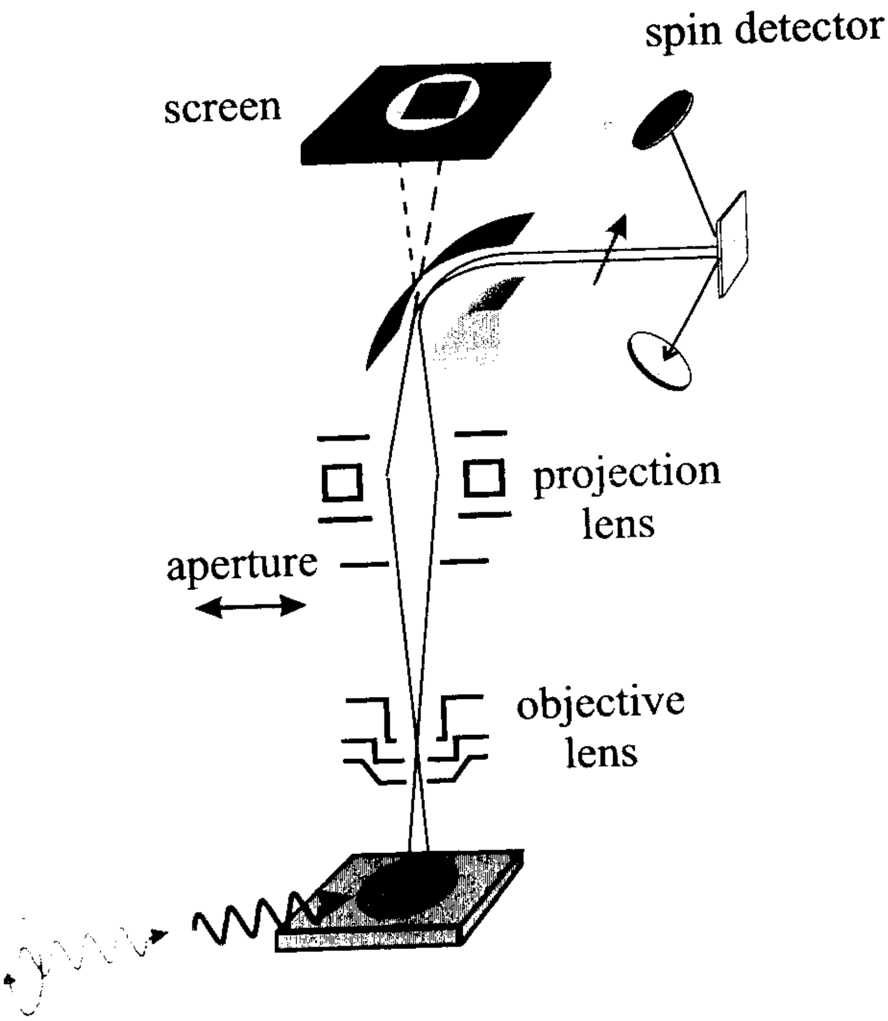
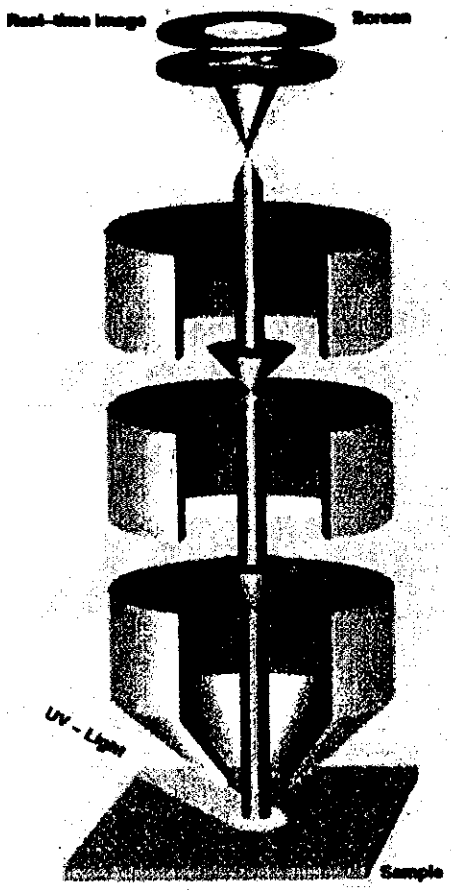
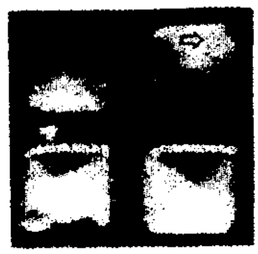


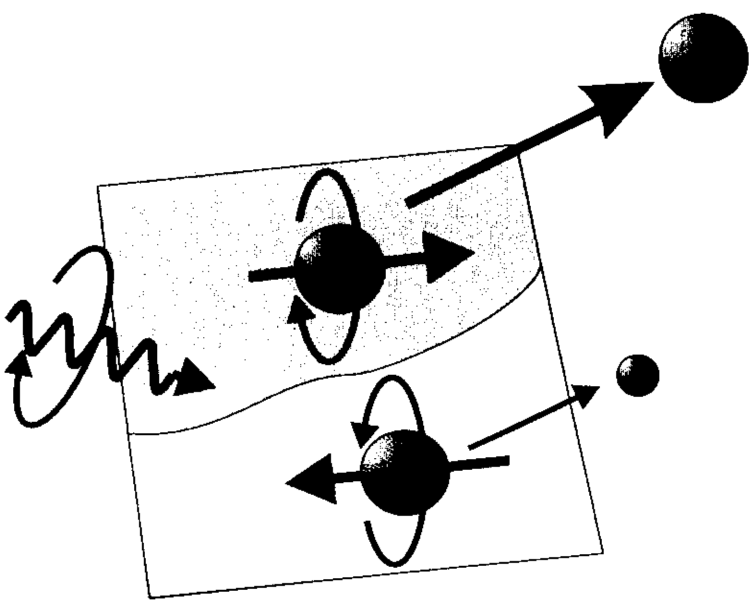
Photo Emission Electron Microscopy



Fe squares on Si

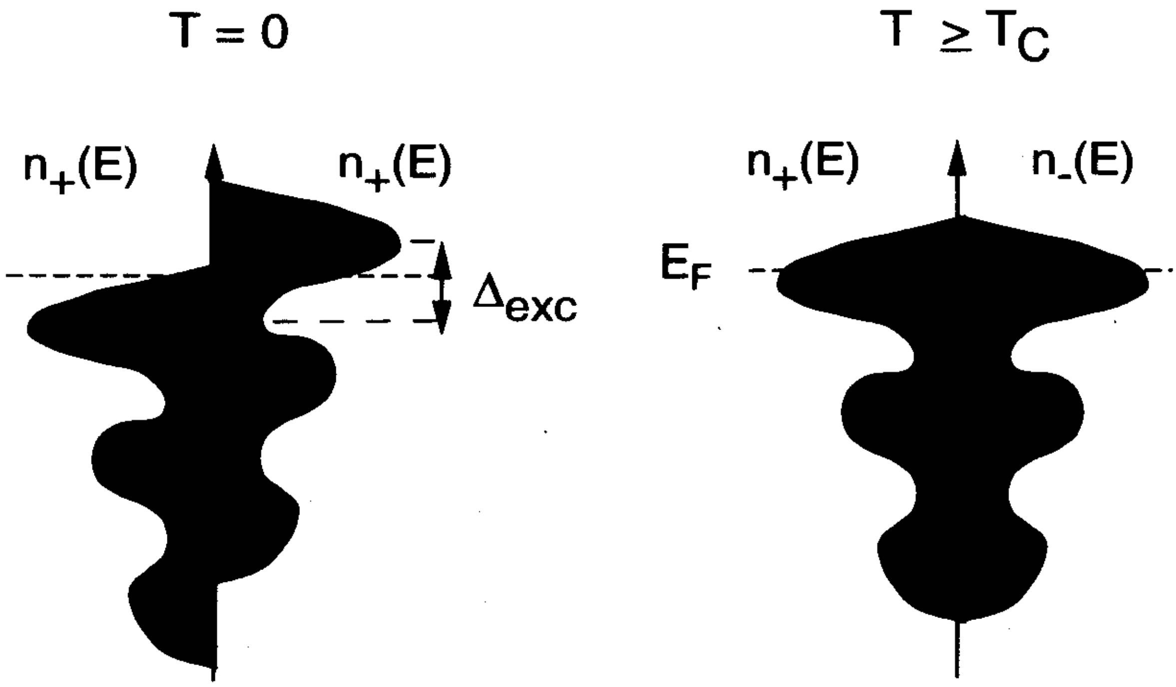
20μm



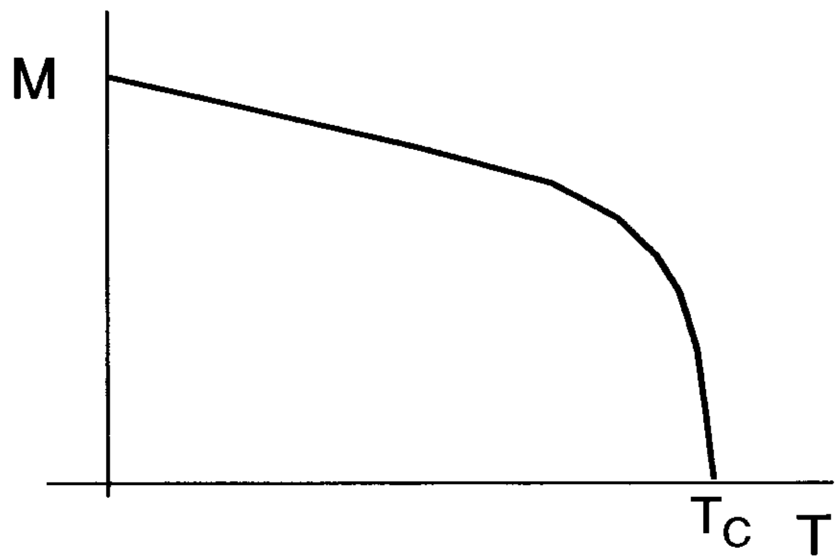


measures
<L> and <S>

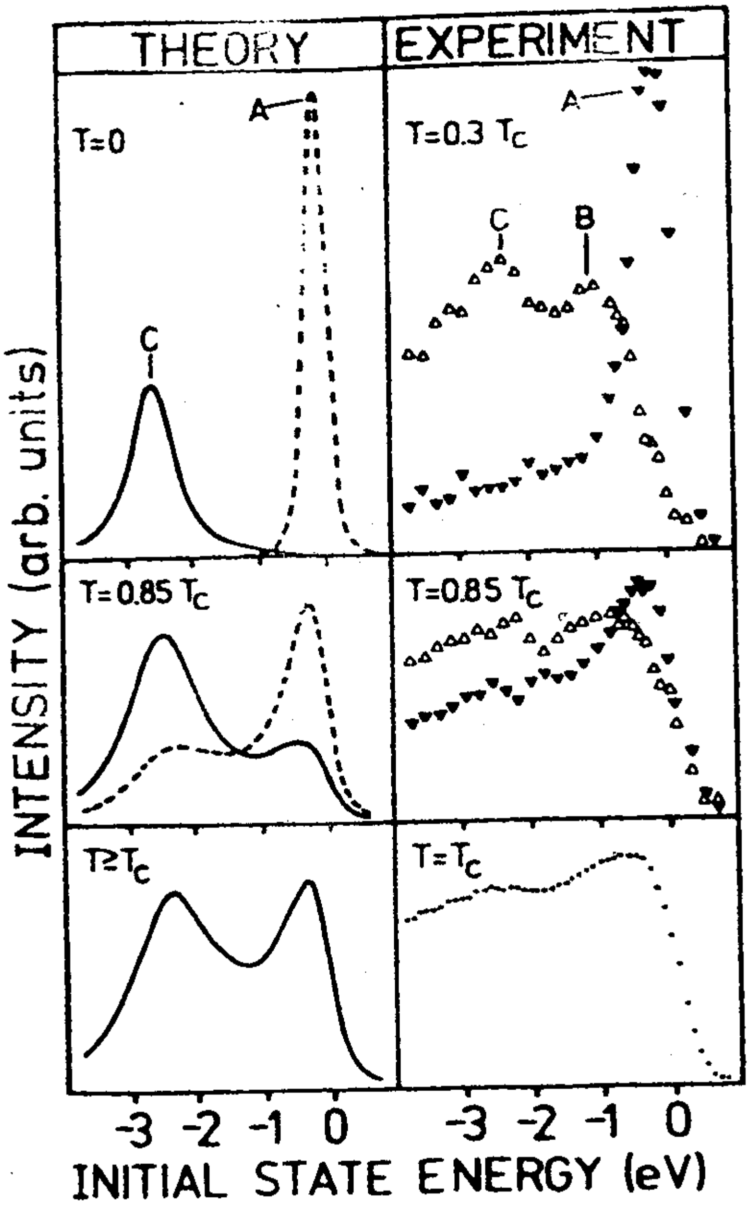
Stoner Model - Ferromagnetic Electronic Structure



$\Delta_{exc} \propto M$



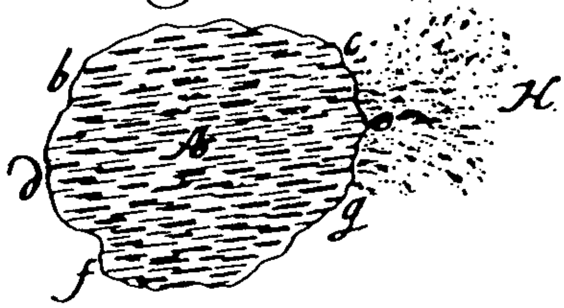
Fe: Temperature dependence



The exchange-splitting does not vanish approaching T_C

Order - Disorder

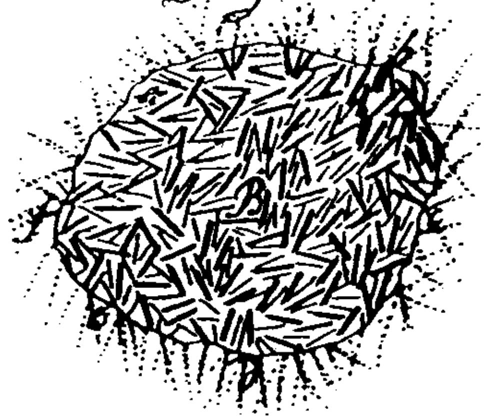
Fig. 1.



Magnetized Fe

(e.g. $T < T_C$)

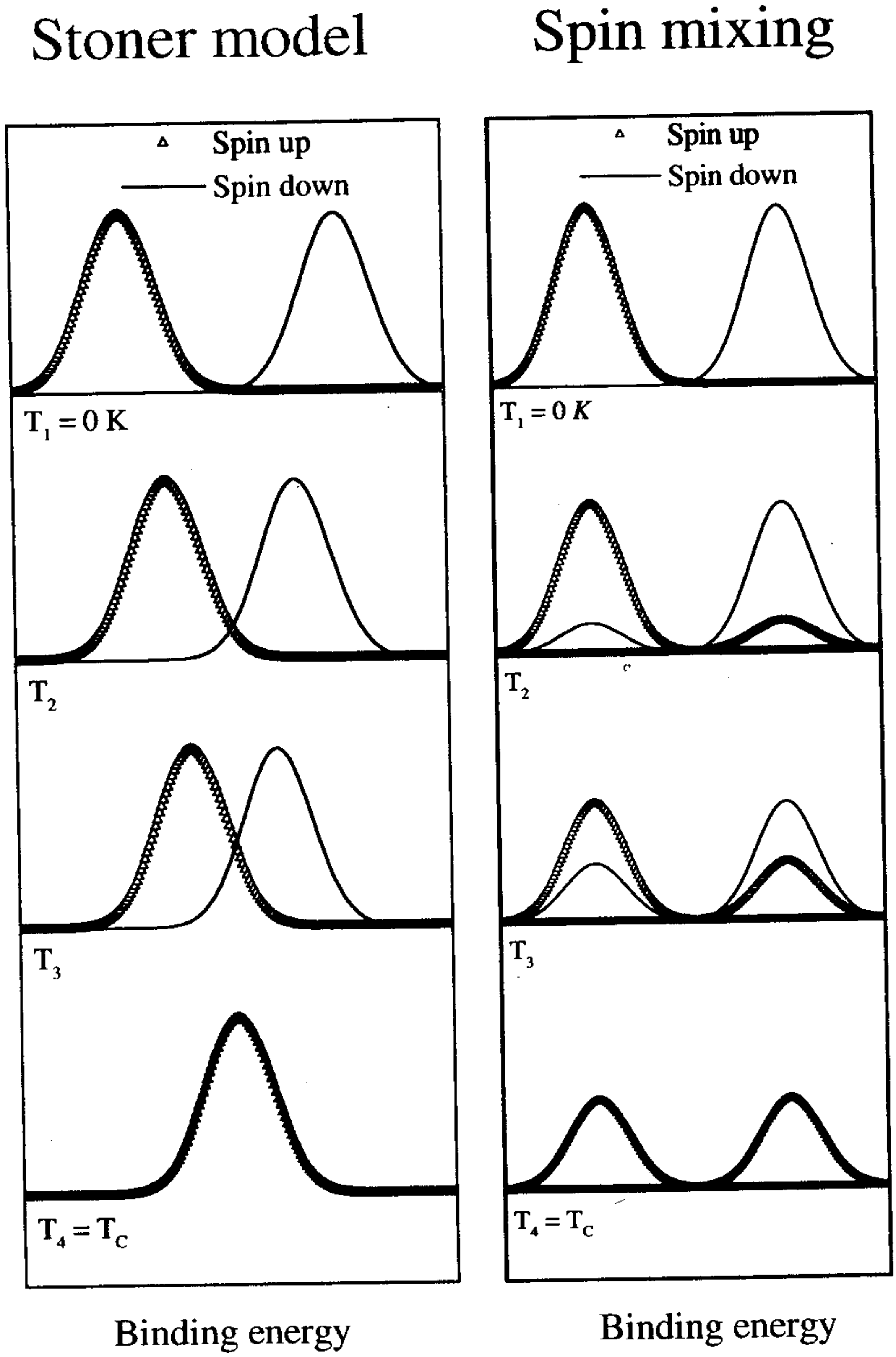
Fig. 2.

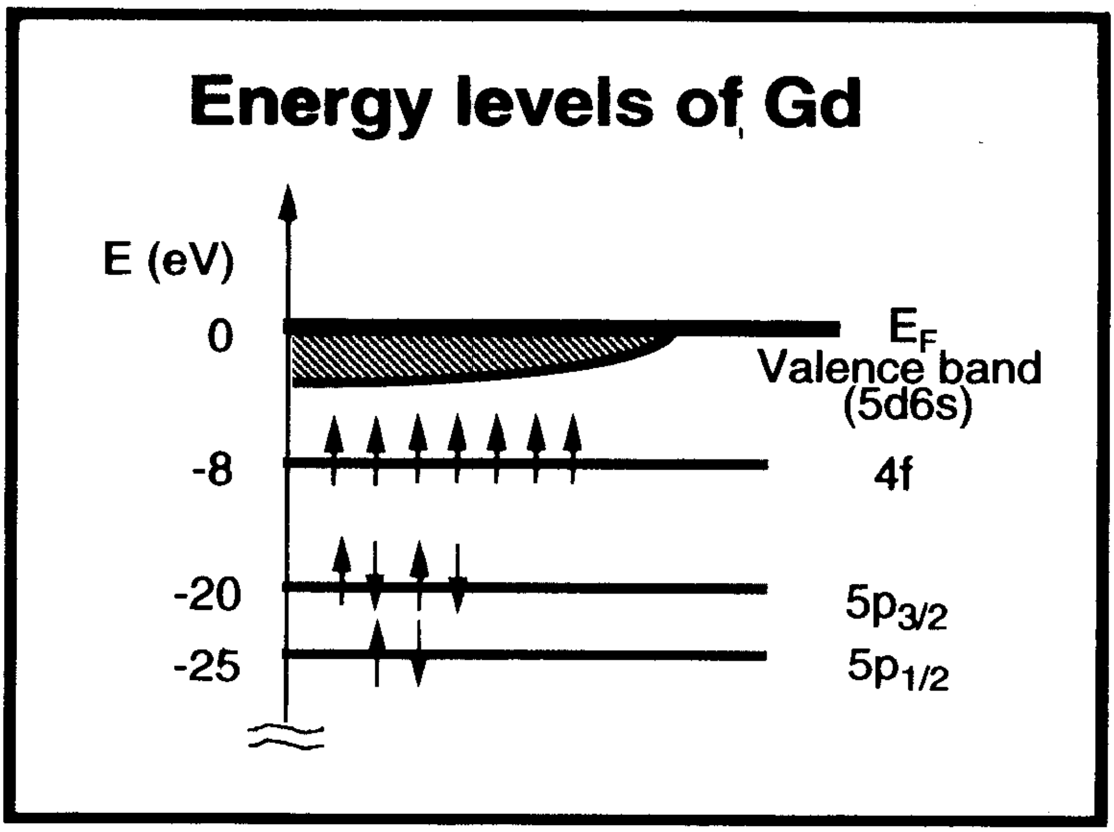


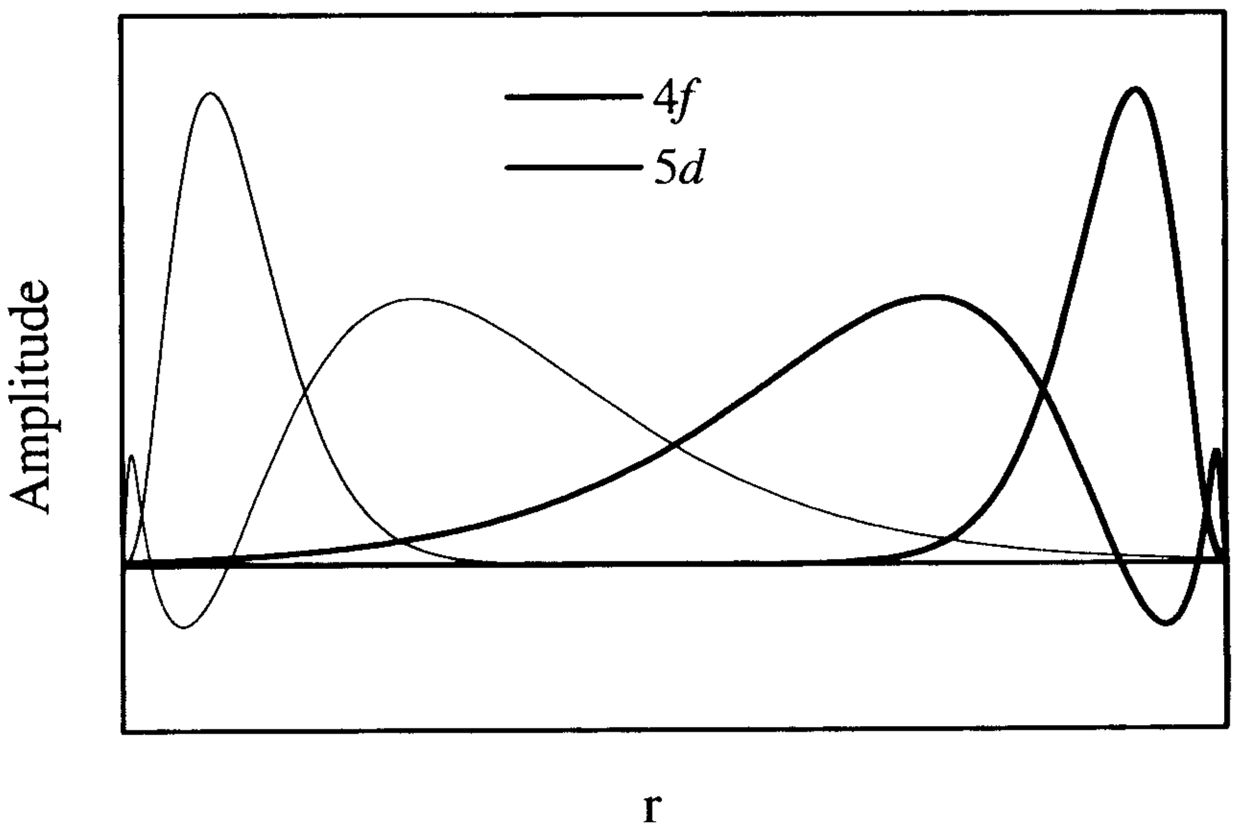
Non-Magnetized Fe

(e.g. $T \geq T_C$)

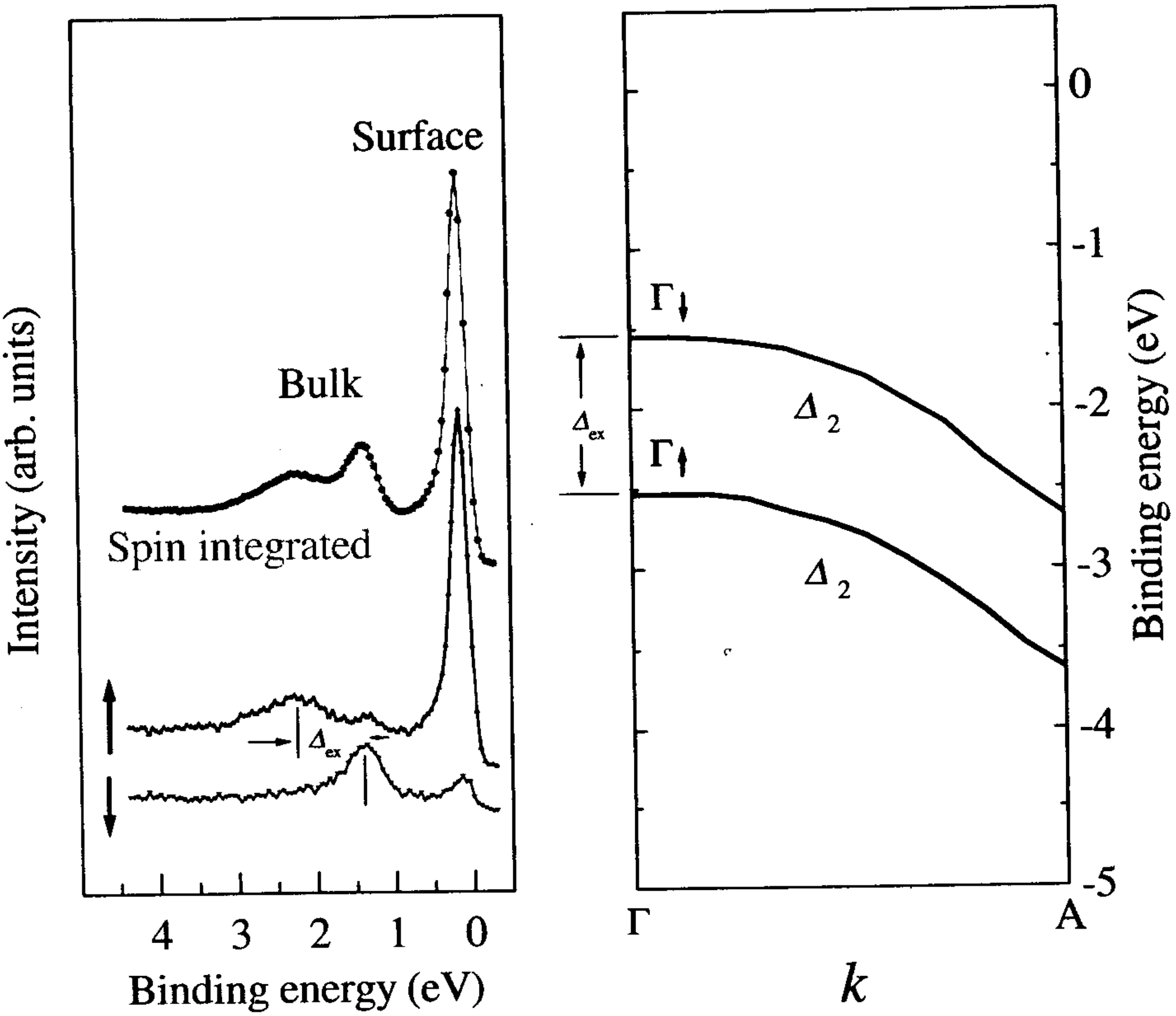
E.Swedenborg, Principia rerum naturalium (1734)

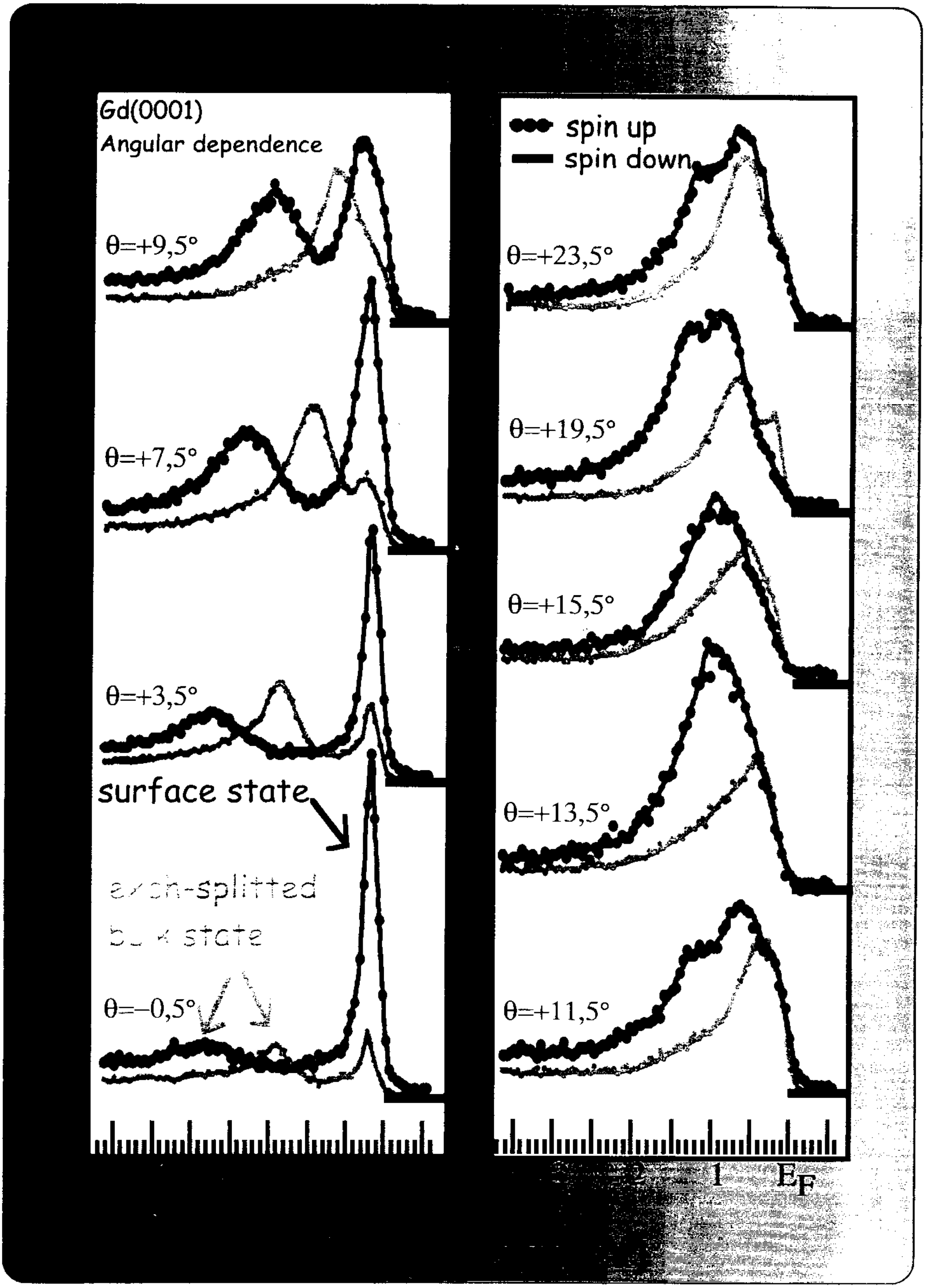

Stoner model
Spin mixing
Spin up
Spin down
Spin up
Spin down
T1 = 0 K
T2
T3
T4 = TC
T1 = 0 K
T2
T3
T4 = TC
Binding energy
Binding energy


Energy levels of Gd
E (eV)
0
-8
-20
-25
E_F
Valence band
(5d6s)
4f
$5p_{3/2}$
$5p_{1/2}$

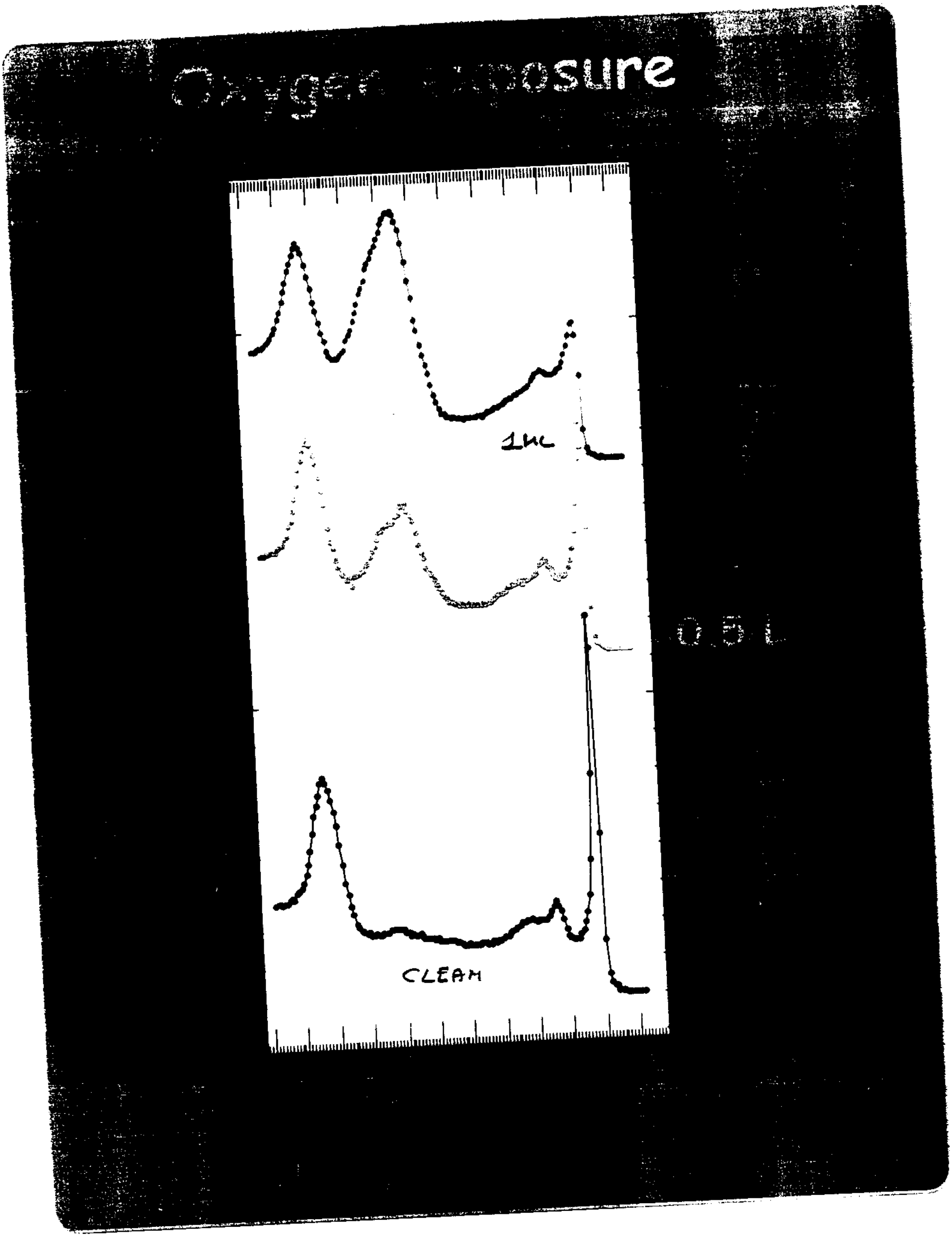

4f
5d
Amplitude
r

Gd : Valence band

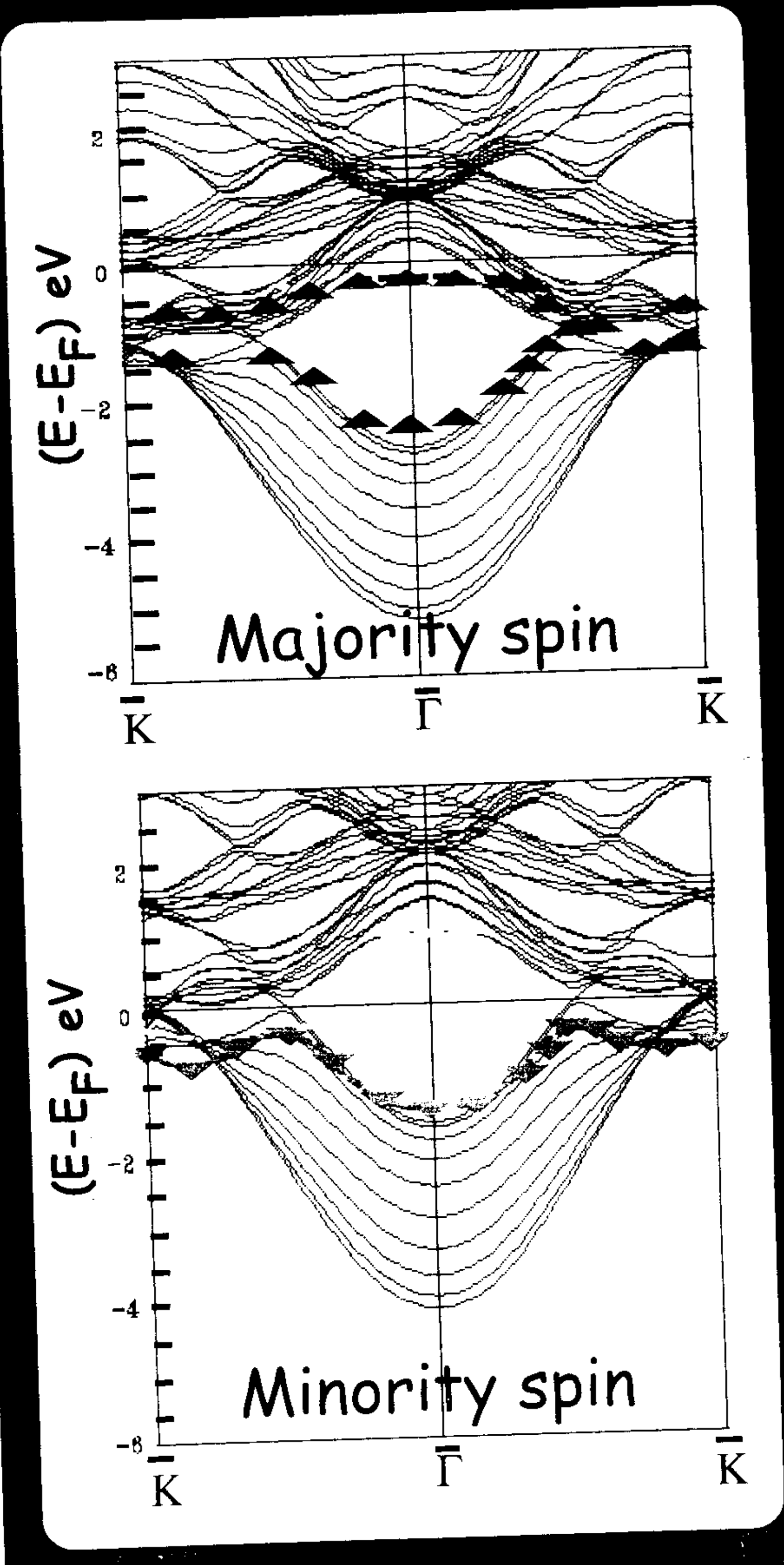




Gd(0001)
Angular dependence
θ=+9,5°
θ=+7,5°
θ=+3,5°
surface state
exch-splitted
bulk state
θ=−0,5°
spin up
spin down
θ=+23,5°
θ=+19,5°
θ=+15,5°
θ=+13,5°
θ=+11,5°
2
1
E_F



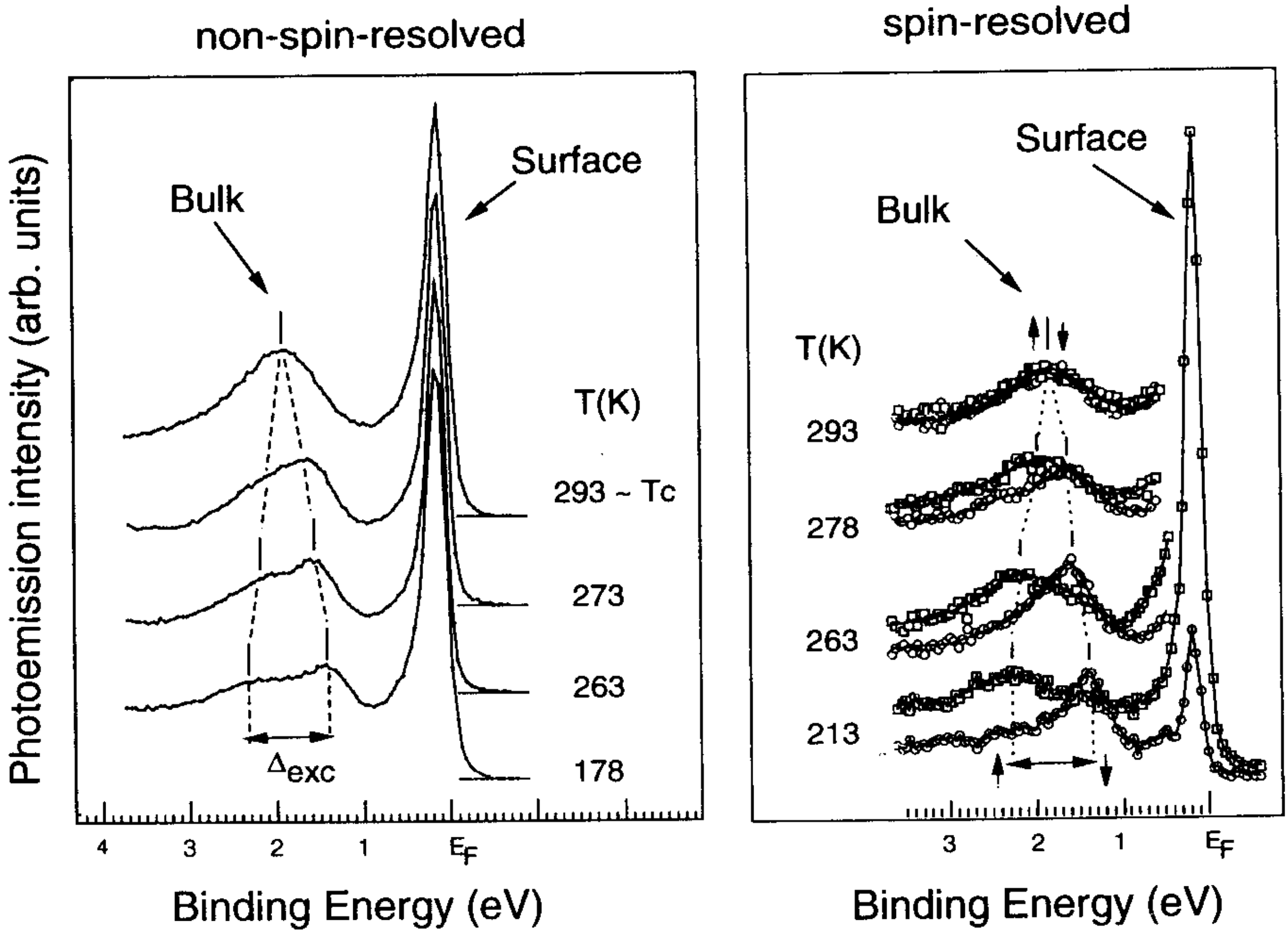
Oxygen exposure
1ML
0.5 L
CLEAN

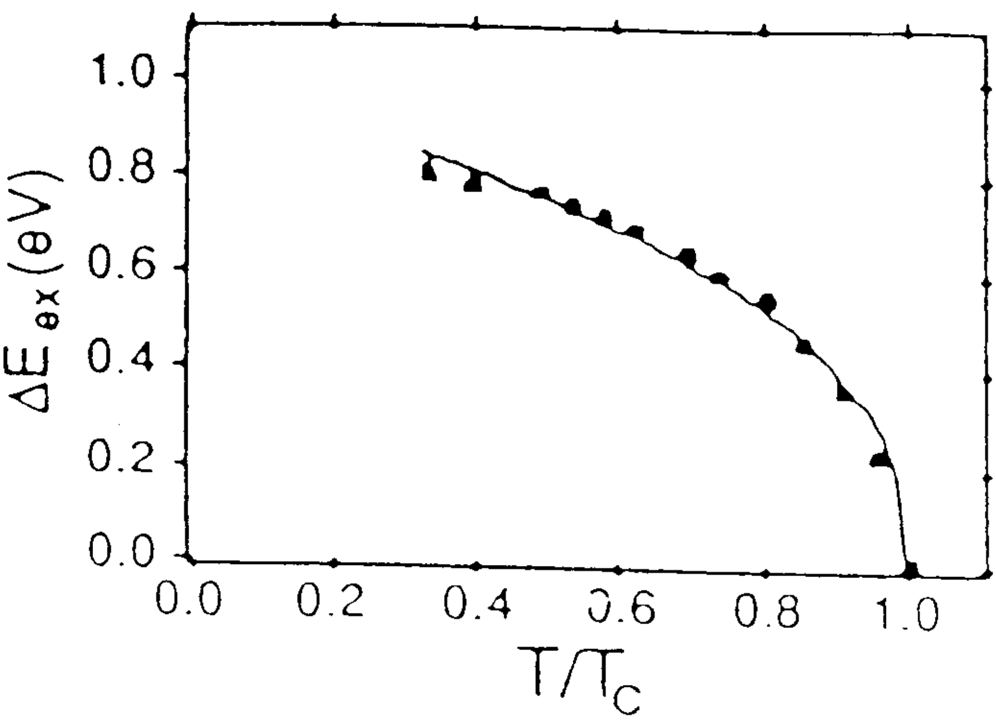


The measured variation of the binding energy as a function of the K value is compared with new LSDA calculations (coloured triangles represent experimental data).

Exchange splitting in Gd bands

Photoemission



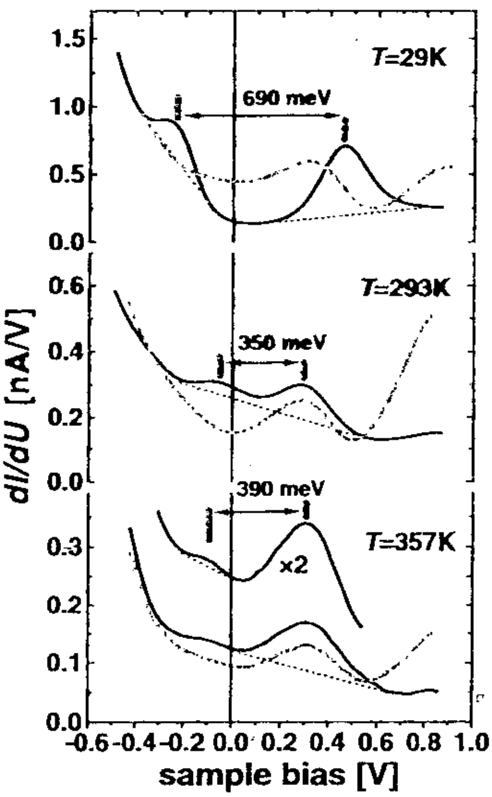


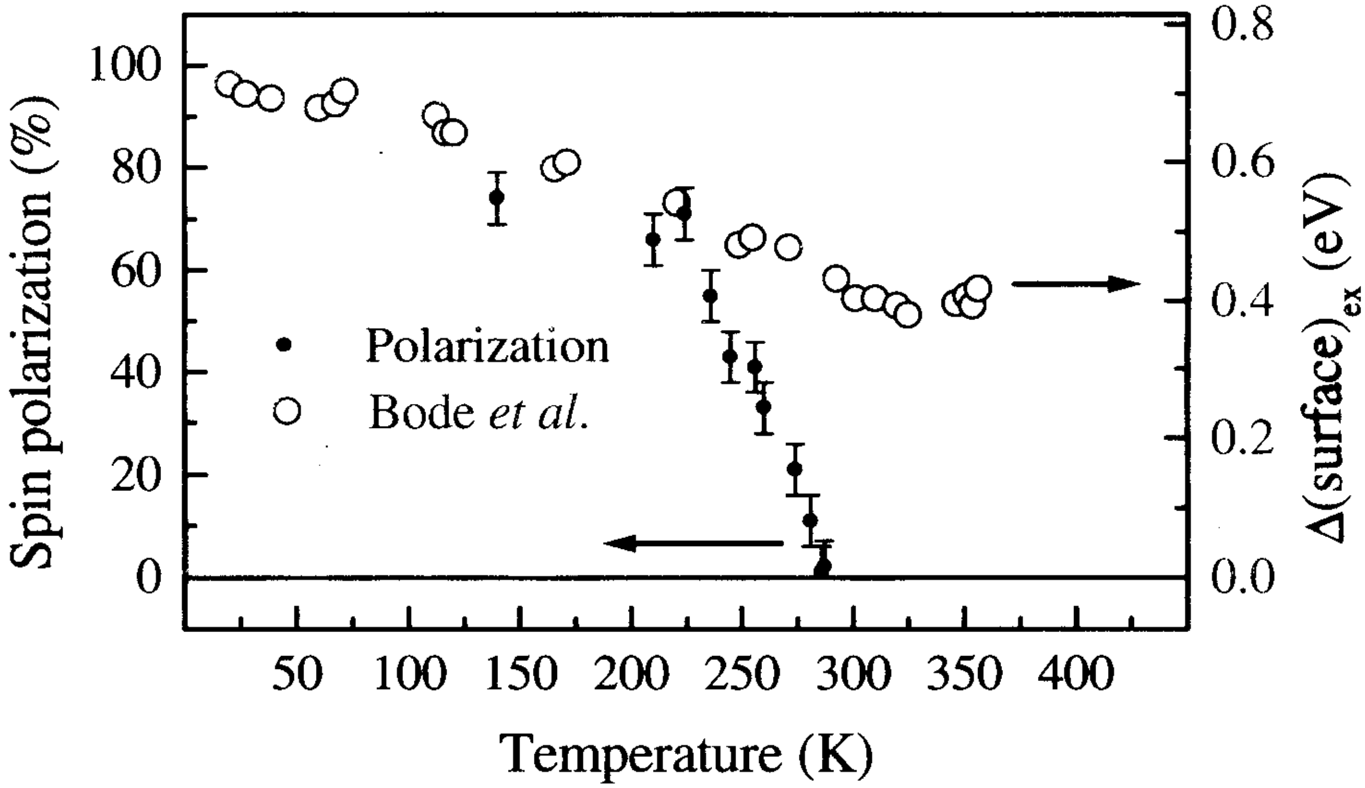
$$\Delta_{exc} = \left(1 - \frac{T}{T_c}\right)^{\beta}$$

$\beta \sim 0.35$

Kim et al. PRL 68, 1931 (92)

Tunneling spectra measured on Gd(0001) surface





Epitaxial thin film of $La_{0.7}Sr_{0.3}MnO_3$

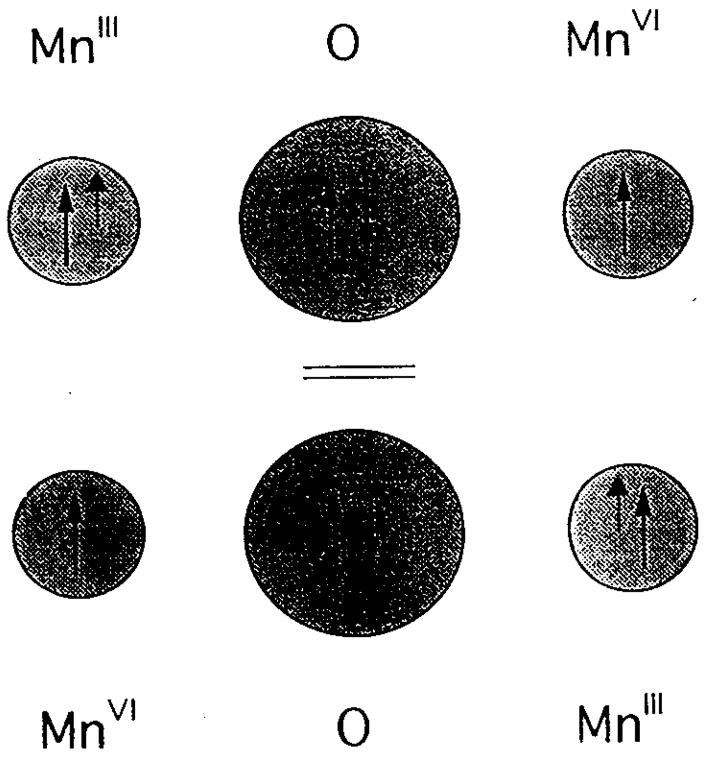
perovskite structure from the parent $LaMnO_3$

ferromagnetic/paramagnetic
metal/insulator } phase transitions

colossal magnetoresistence

Double Exchange mechanism

(Zener, Phys .Rev. <u>82</u>, 403 (9151))

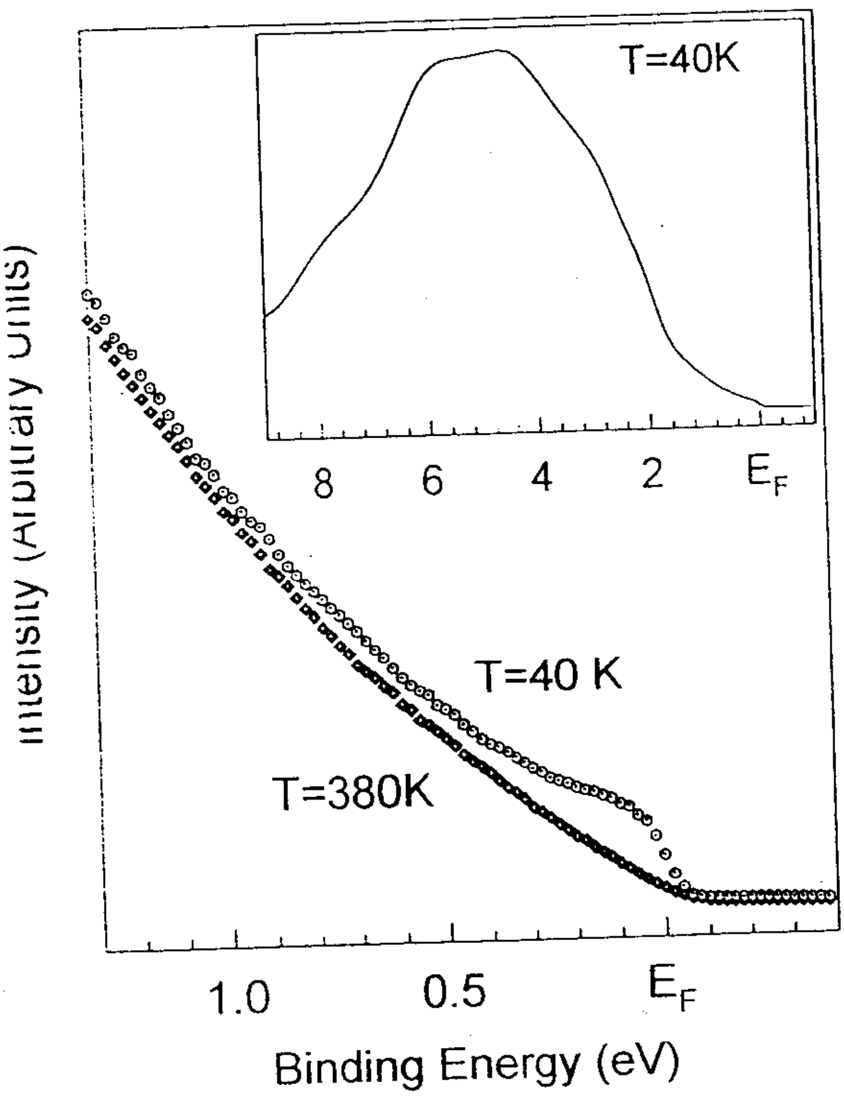


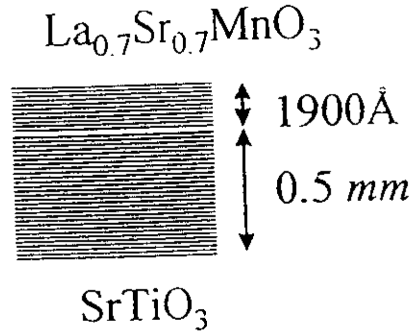
The linear combination lowers the total energy.
It implies the contemporary occurrence of:

a) metallicity
b) ferromagnetic order

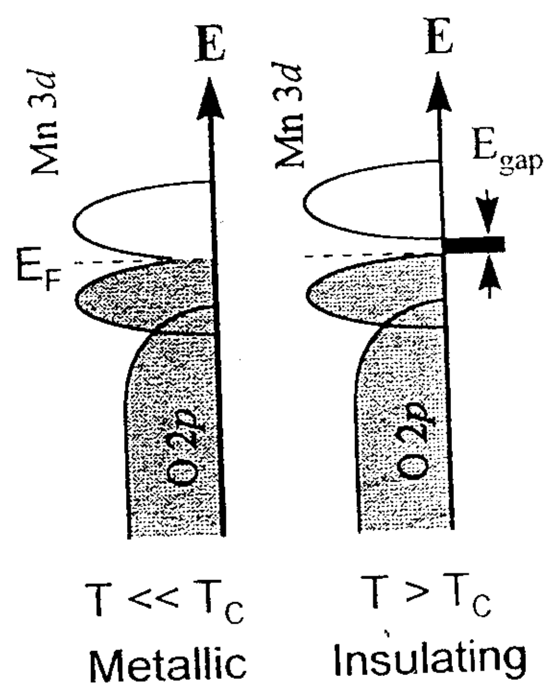
Photoemission Study of $La_{0.7}Sr_{0.3}MnO_3$ Thin Film

1900A $La_{0.7}Sr_{0.3}MnO_3$ on $SrTiO_3$



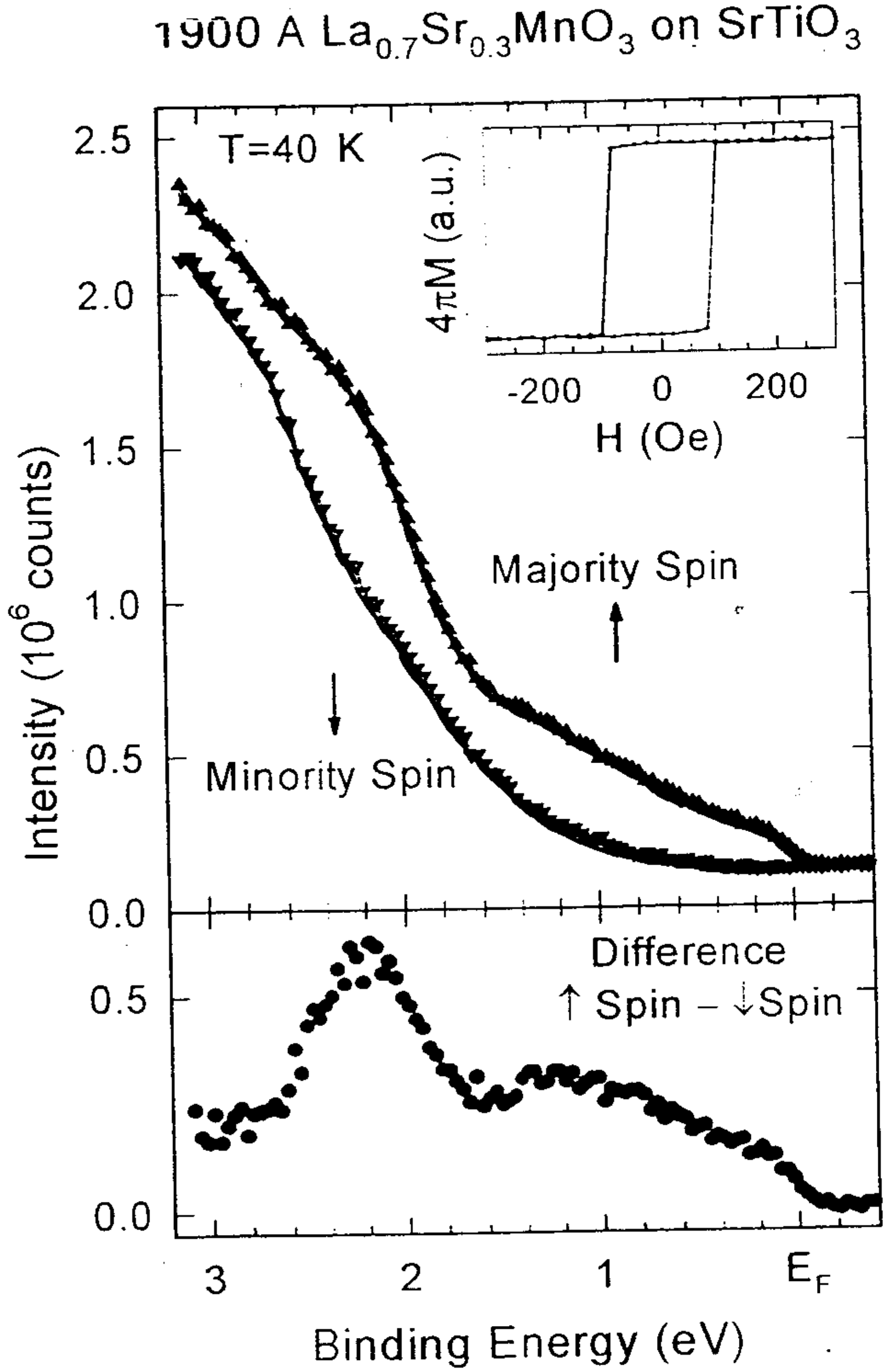


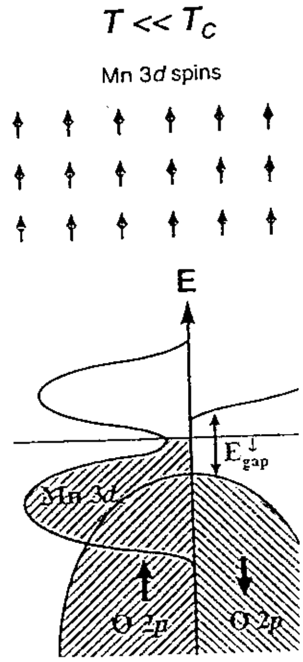
T_C = 350K
$h\nu$ = 40 eV
ΔE = 0.12 eV



Metal-Insulator Transition !!

Spin resolved photoemission spectra

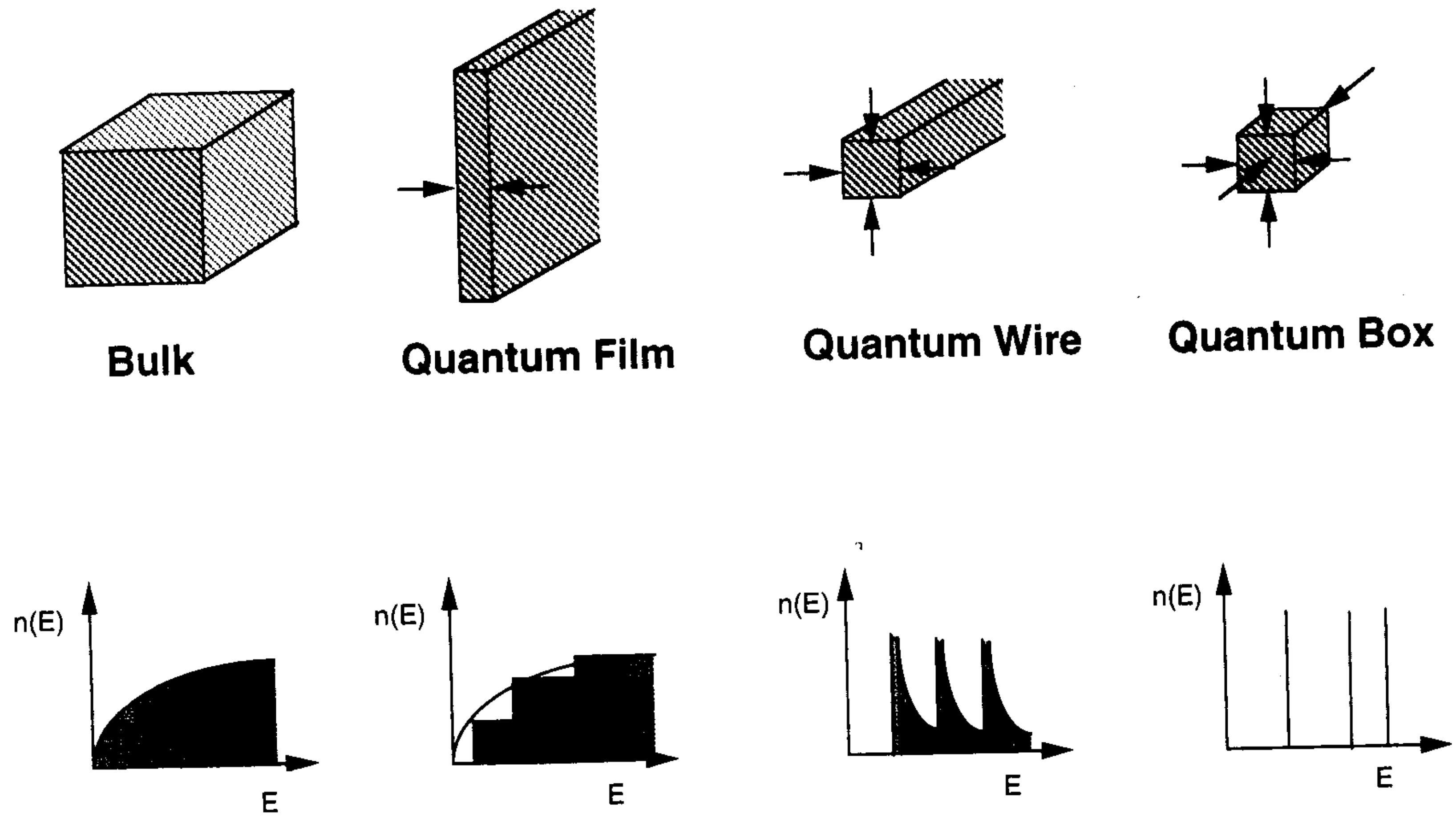




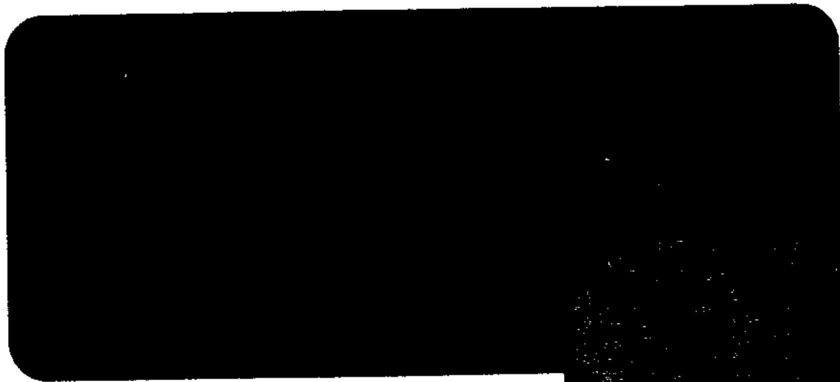
Half metal

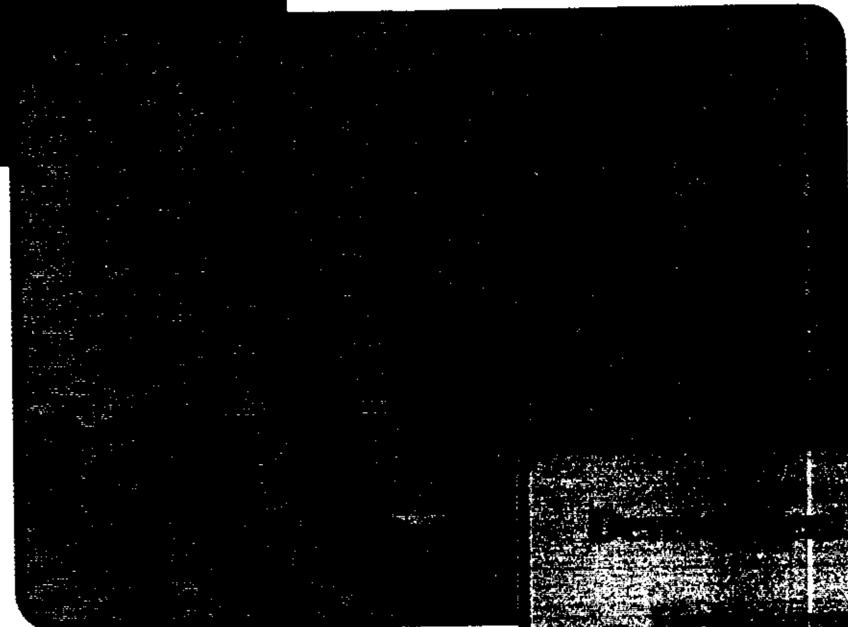
J.H. Park, E. Vescovo et al., Nature

Electron confinement and density of states



MAGNETIC NANOSTRUCTURES





[illegible] application

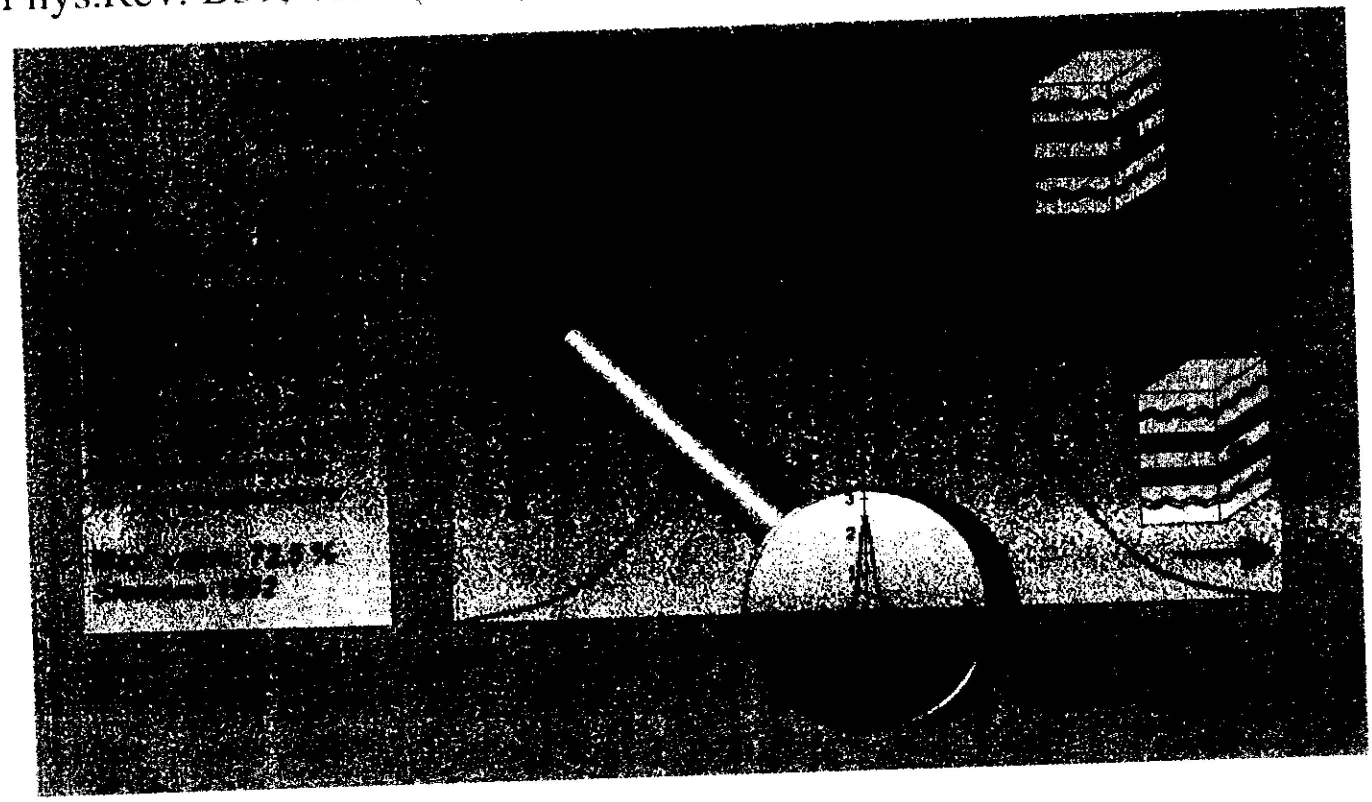
- [illegible]
- [illegible]c devices
- M[illegible] media for information storage

Giant Magnetoresistance Effect

Publications

M.N. Baibich, J.M. Broto, A. Fert, F. NguyenVanDan, F. Petroff, P. Etienne, G. Creuzet, A. Friederich, J. Chazelas
Phys. Rev. Lett. 61, 2472 (1988)

G. Binasch, P. Grünberg, F. Saurenbach, W. Zinn
Phys.Rev. B39, 4828 (1989)



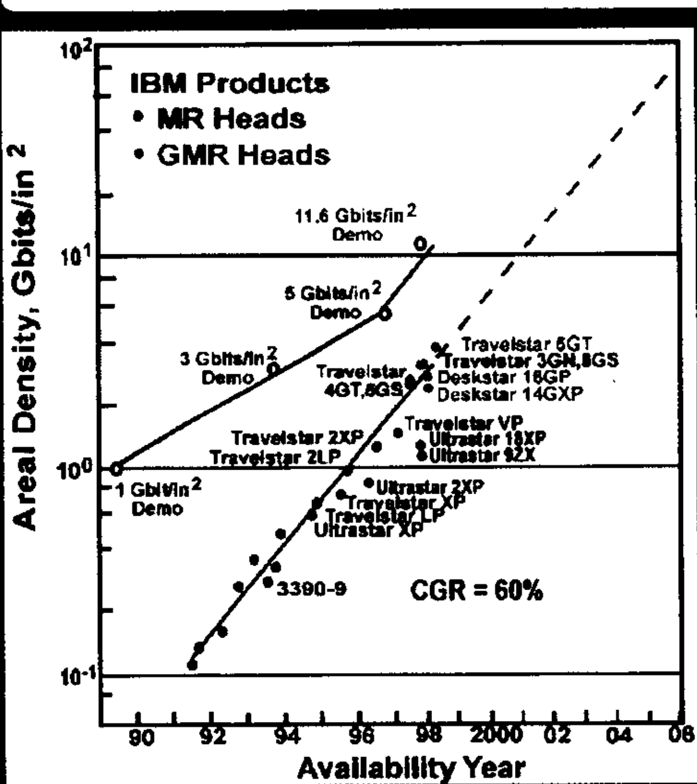
Patent (U.S. No. 4949039)

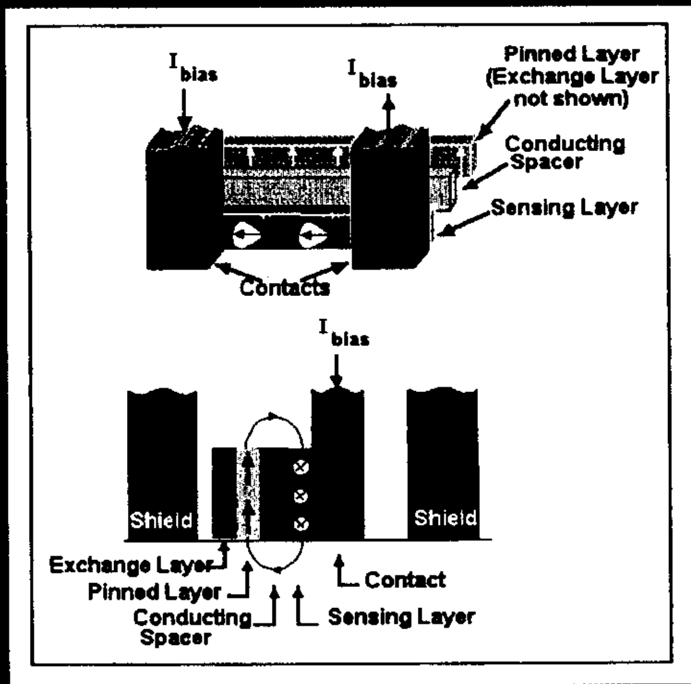
P. Grünberg IFF, Forschungszentrum Jülich
Magnetic Field Sensor with Ferromagnetic thin layers having magnetically antiparallel polarized components

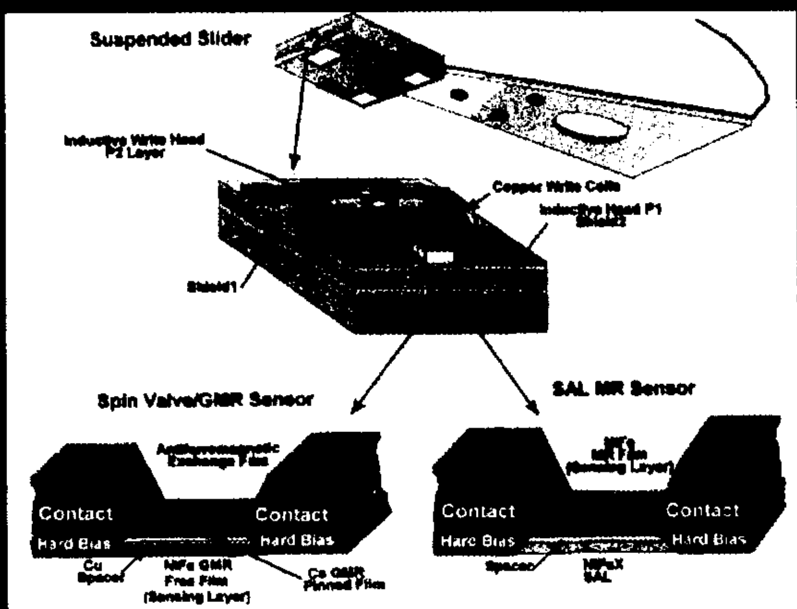
License agreements

IBM Corp	1995	Fujitsu	1997	Read Rite Corp 1998
Yamaha	1996	Hitachi	1997	
TDK Corp	1996	Siemens	1997	
Silmag	1996	Seagate	1997	
		Matsushita	1997	

GMR Readout Head Technology

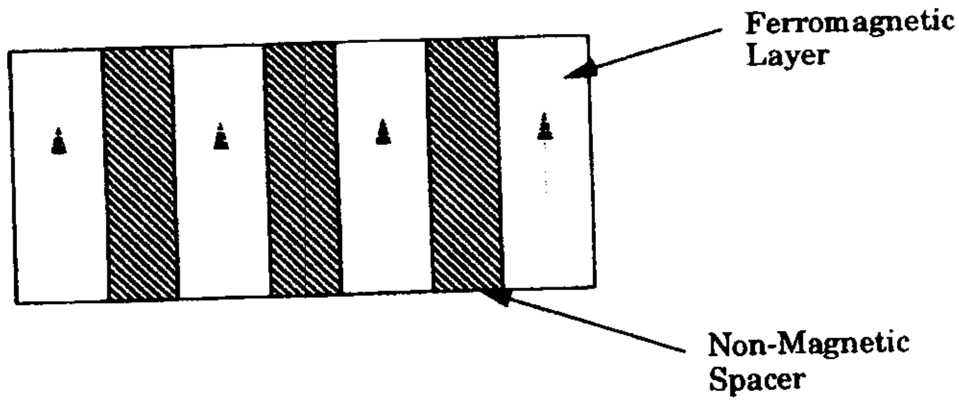




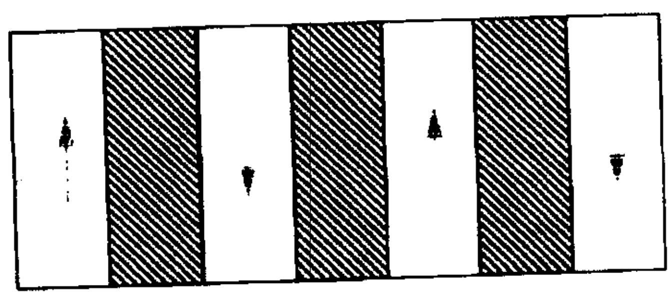


Exchange Coupling Through Non-Magnetic Layers

Ferromagnetic Coupling (FM)

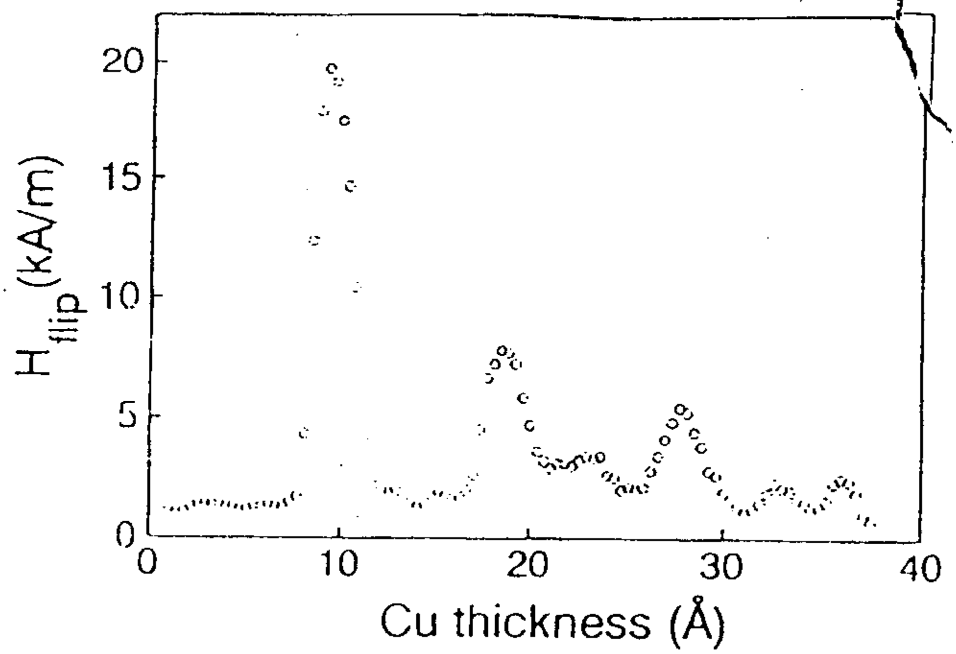


Antiferromagnetic Coupling (AF)



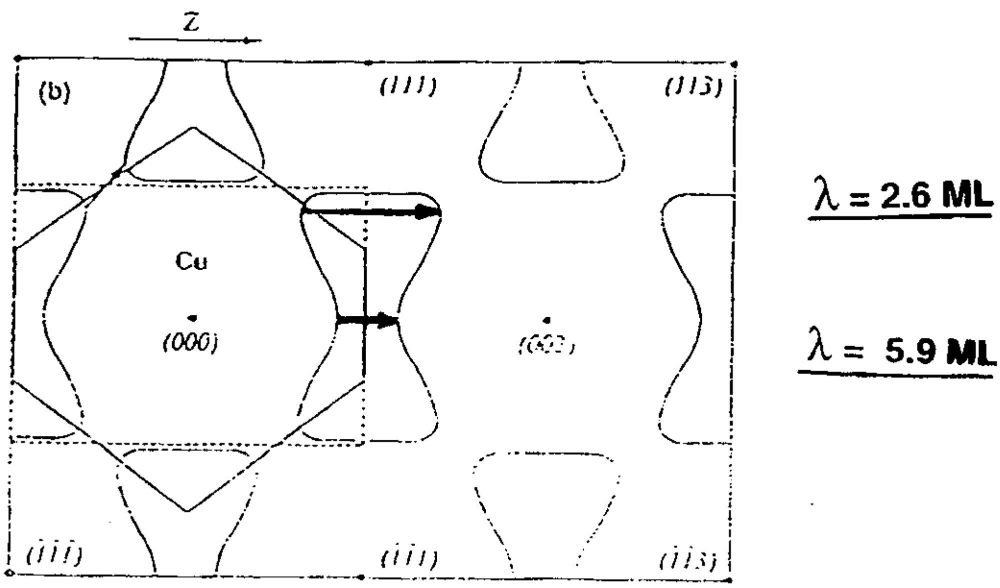
- The sign of the coupling depends on the thickness of the non-magnetic spacer
- It oscillates periodiically between AF and FM

Oscillatory Coupling of Co layers separated by Cu(100)



Bloemen et al., PRL 68, 2688 (1994)

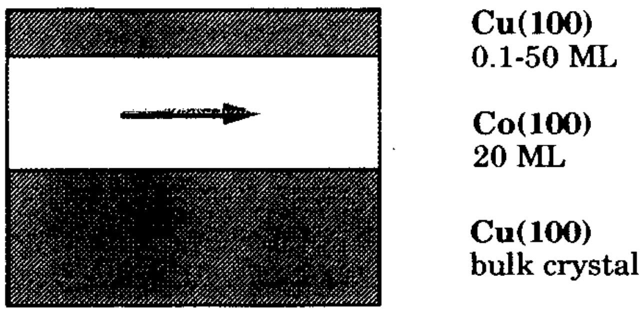
Cu Fermi Surface-RKKY coupling scheme

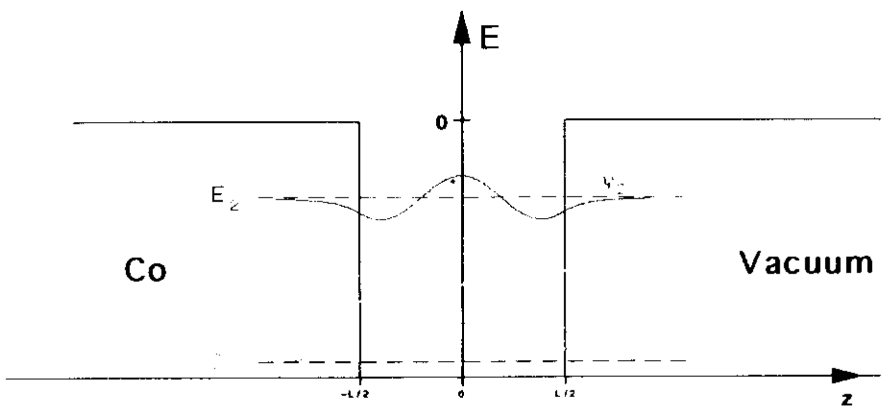


Bruno and Chappert, PRL 67, 1602 (1991); 67, 2592 (1991)

Quantum Well States in Cu on Co(100)

EPITAXIAL Cu LAYERS ON Co(100)



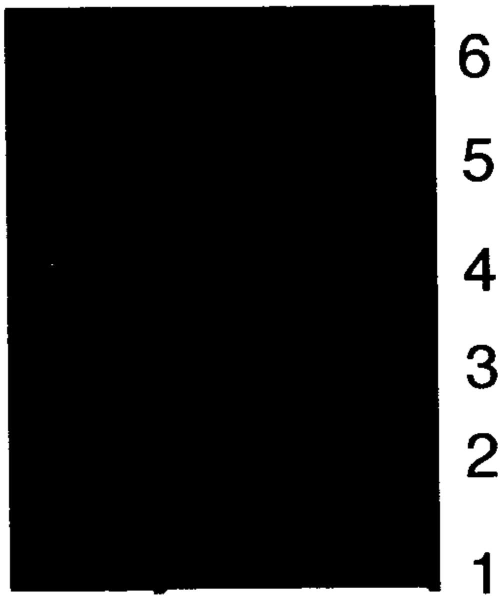


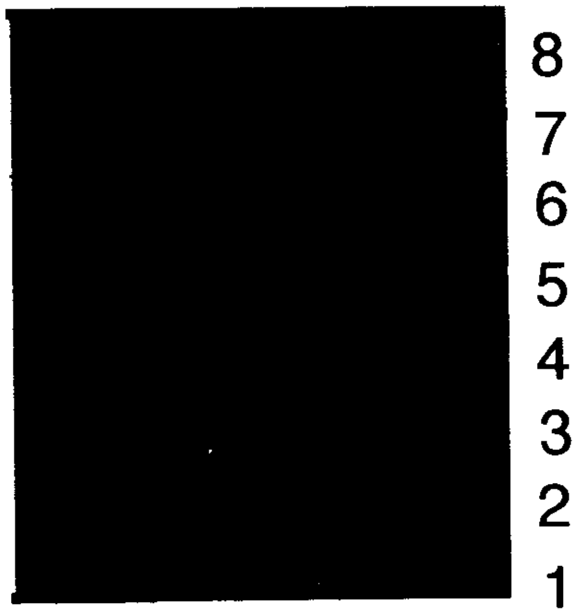
Discretization of $k_\perp$ in thin films ⟶ 2D-Quantum Well States

J. Ortega and F.J.Himpsel, PRL 69,844(92); Garrison et al, PRL71,2801(93), Carbone et al, PRL71,2805(93)

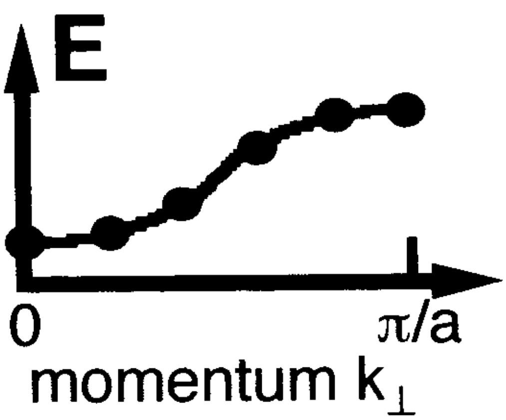
Quantum Well States

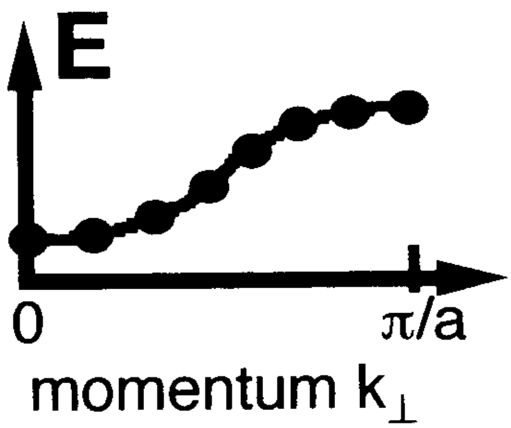
Real Space





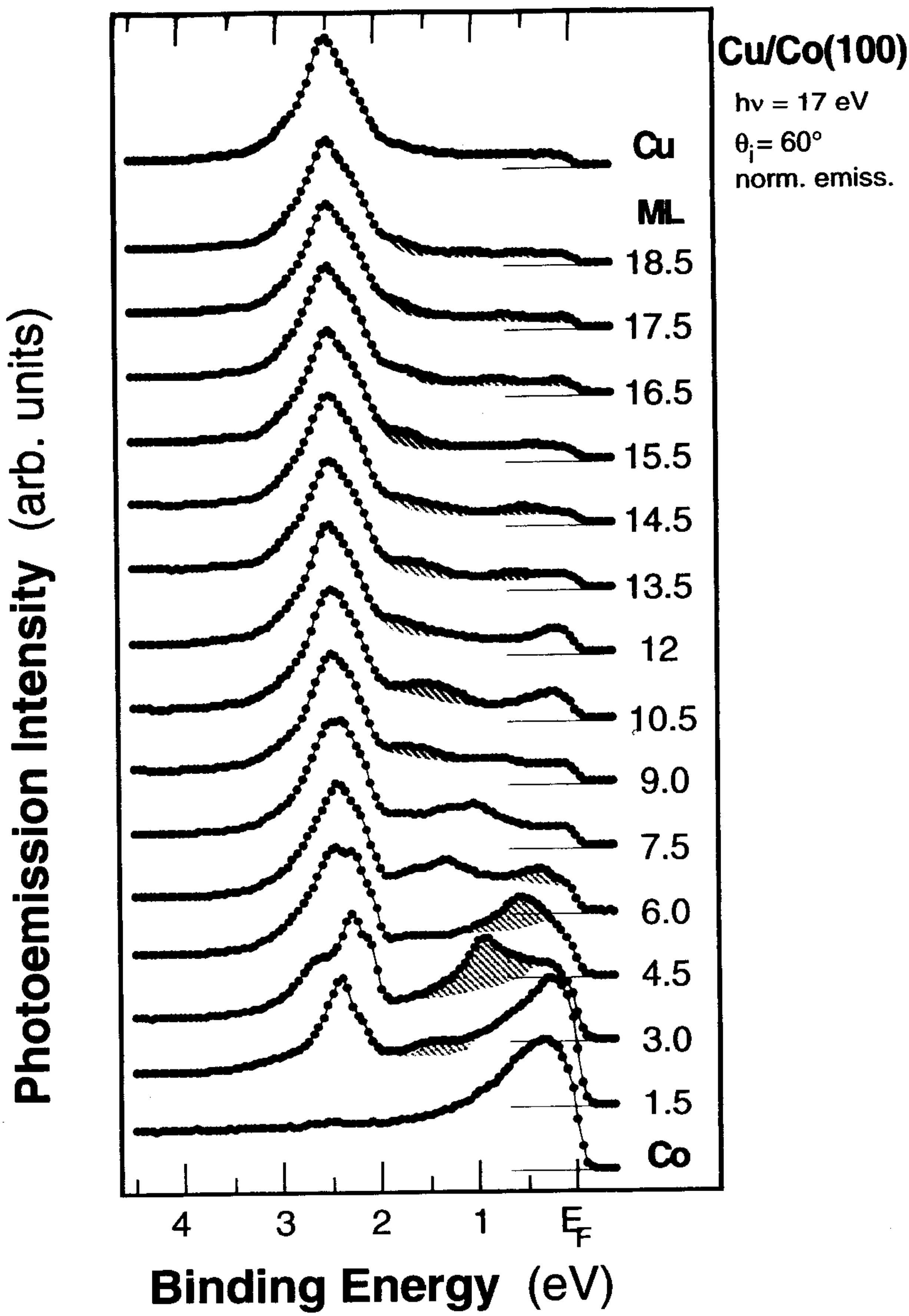
Reciprocal Space



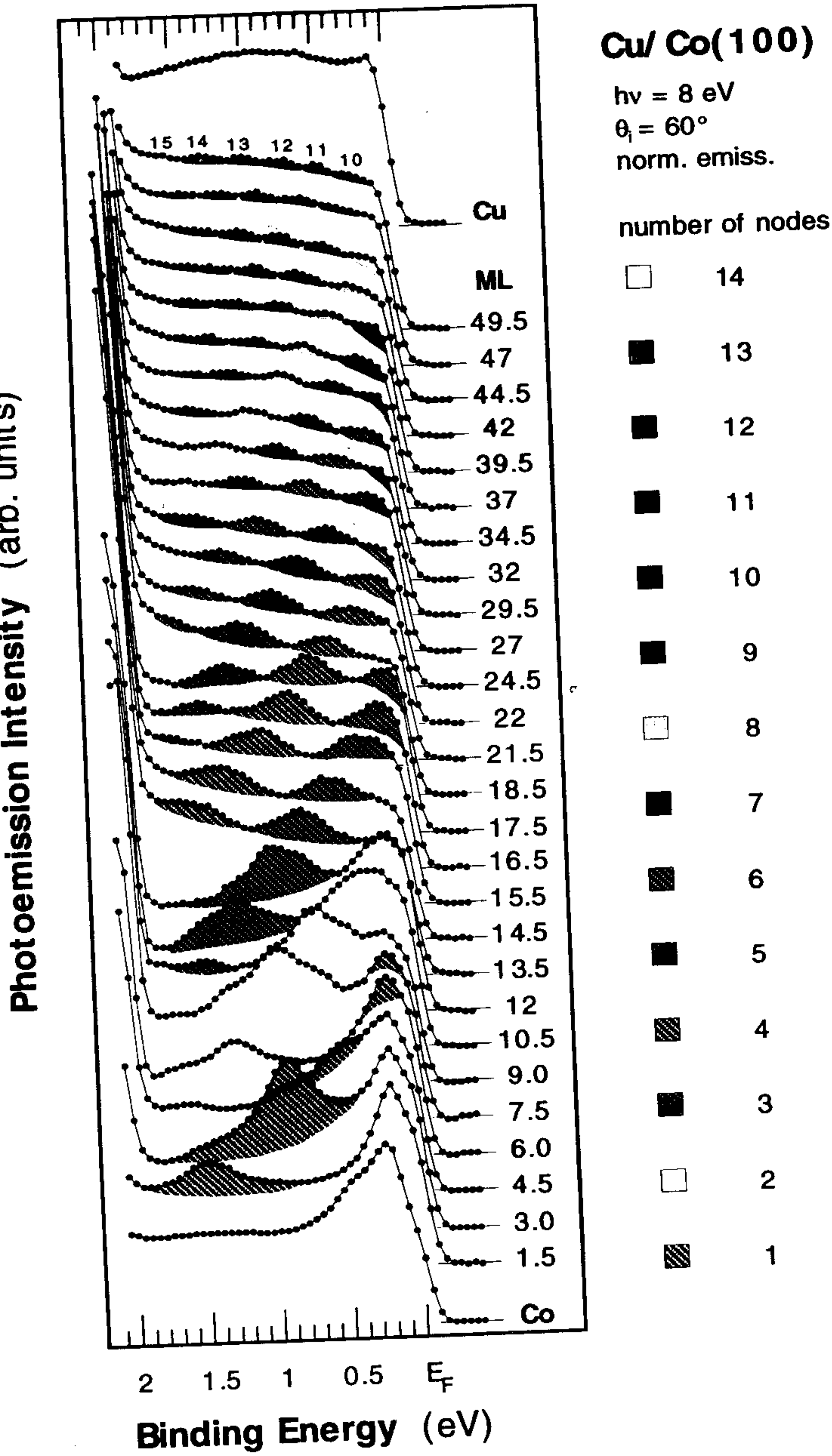


Reflectivity
Boundary Conditions

IFF-EE 94

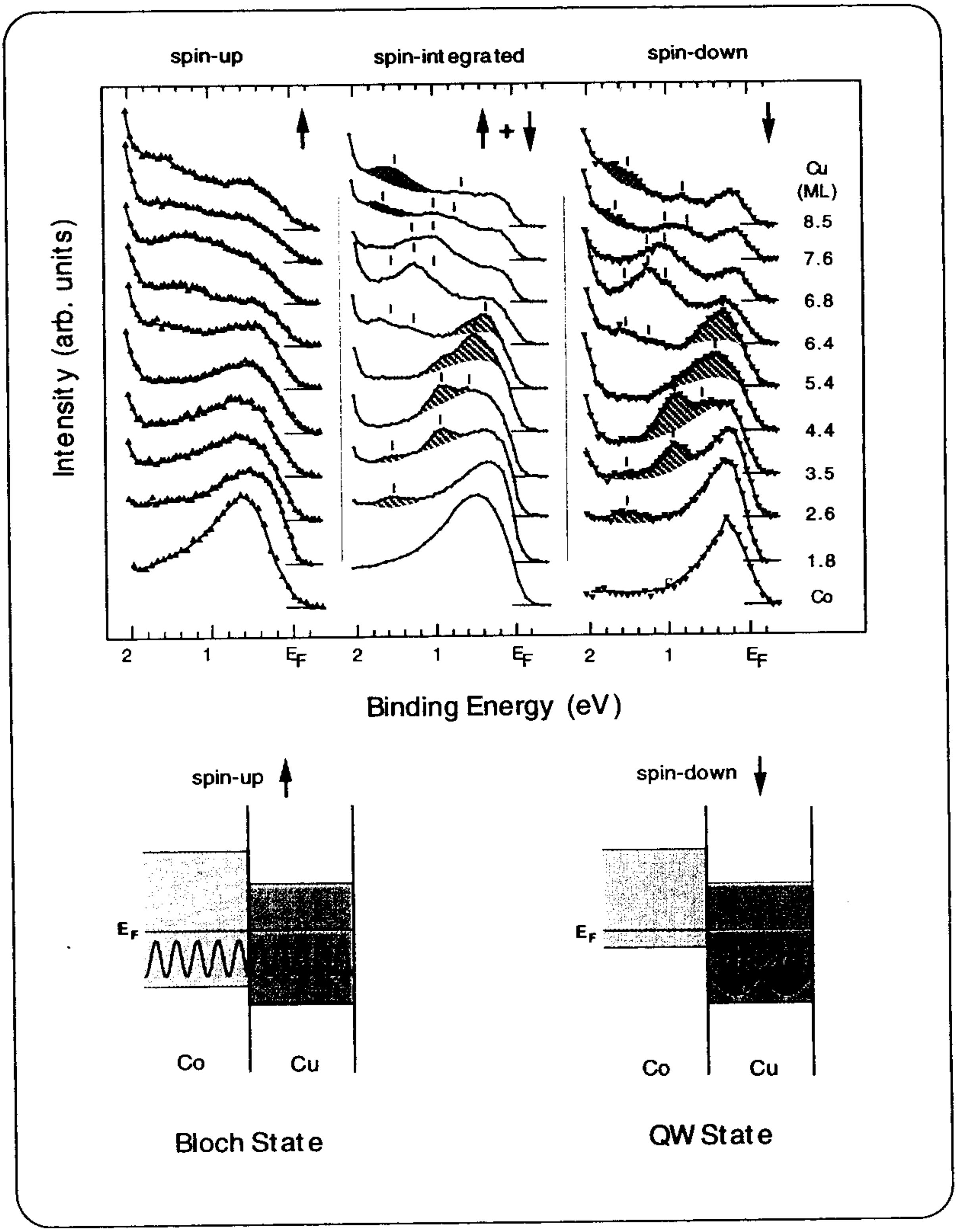


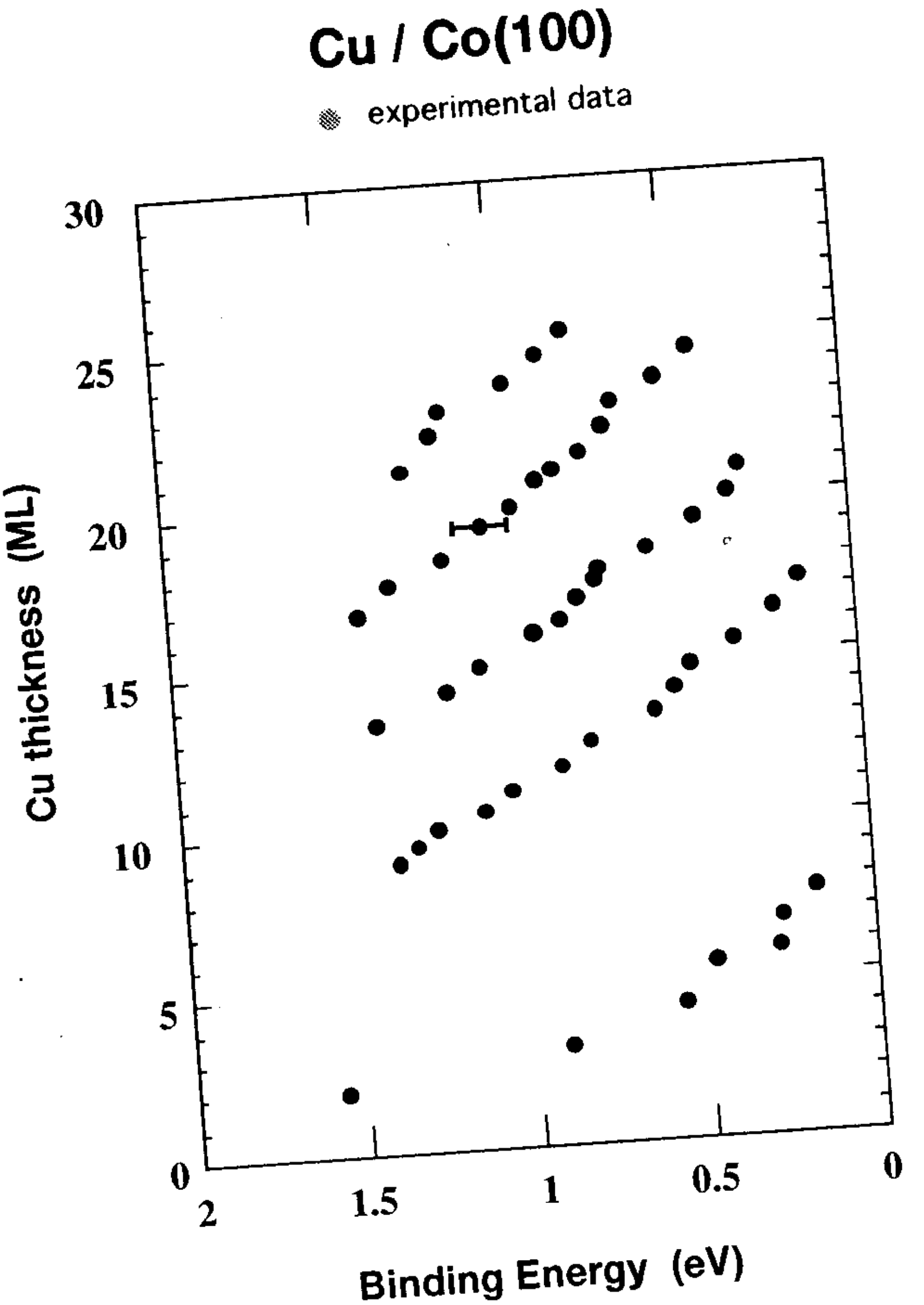
Cu/Co(100)
hν = 17 eV
θ_i = 60°
norm. emiss.
Cu
ML
18.5
17.5
16.5
15.5
14.5
13.5
12
10.5
9.0
7.5
6.0
4.5
3.0
1.5
Co
Photoemission Intensity (arb. units)
4
3
2
1
E_F
Binding Energy (eV)



Cu/ Co(100)
hv = 8 eV
θi = 60°
norm. emiss.
number of nodes
14
13
12
11
10
9
8
7
6
5
4
3
2
1
15 14 13 12 11 10
Cu
ML
49.5
47
44.5
42
39.5
37
34.5
32
29.5
27
24.5
22
21.5
18.5
17.5
16.5
15.5
14.5
13.5
12
10.5
9.0
7.5
6.0
4.5
3.0
1.5
Co
Photoemission Intensity (arb. units)
2 1.5 1 0.5 EF
Binding Energy (eV)

Spin polarisation of QW States in Cu/ Co(100)

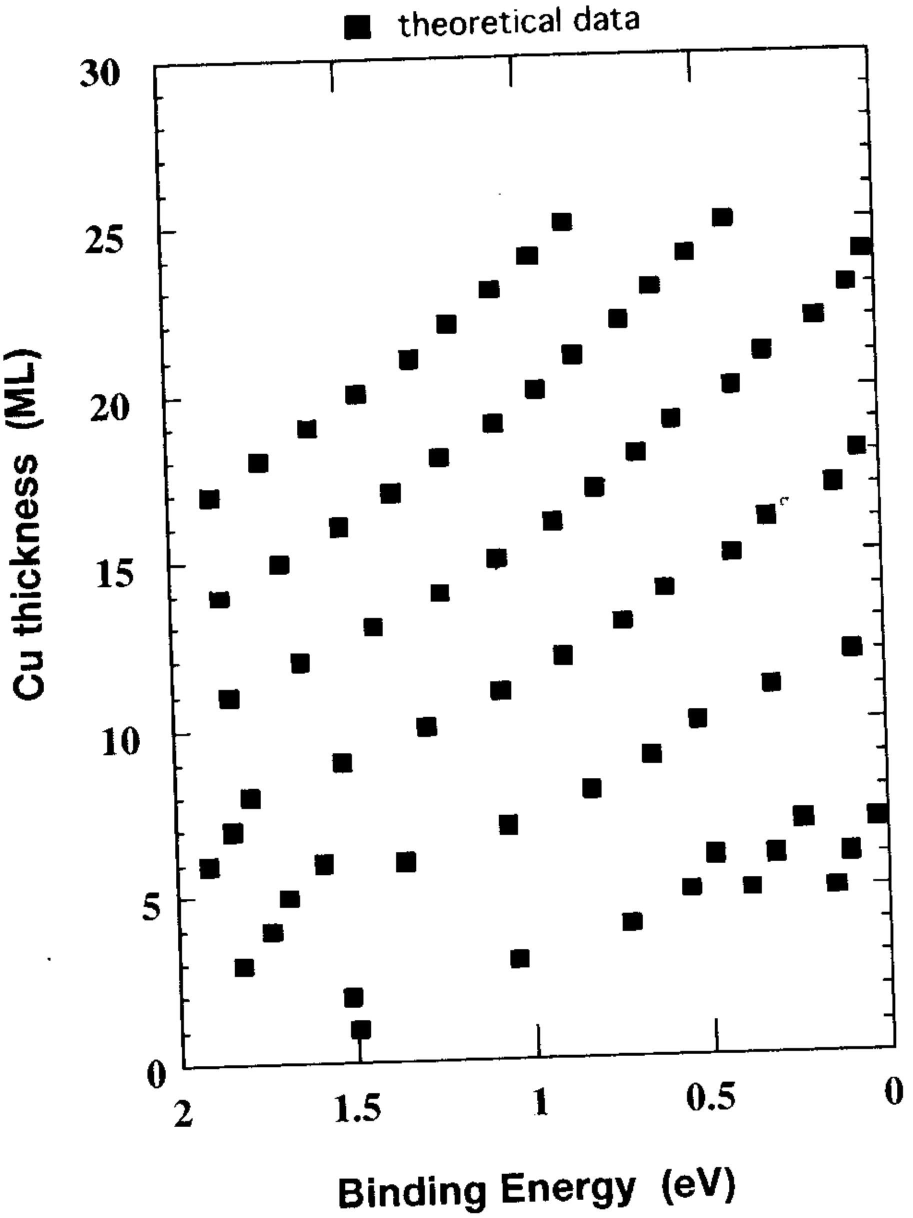




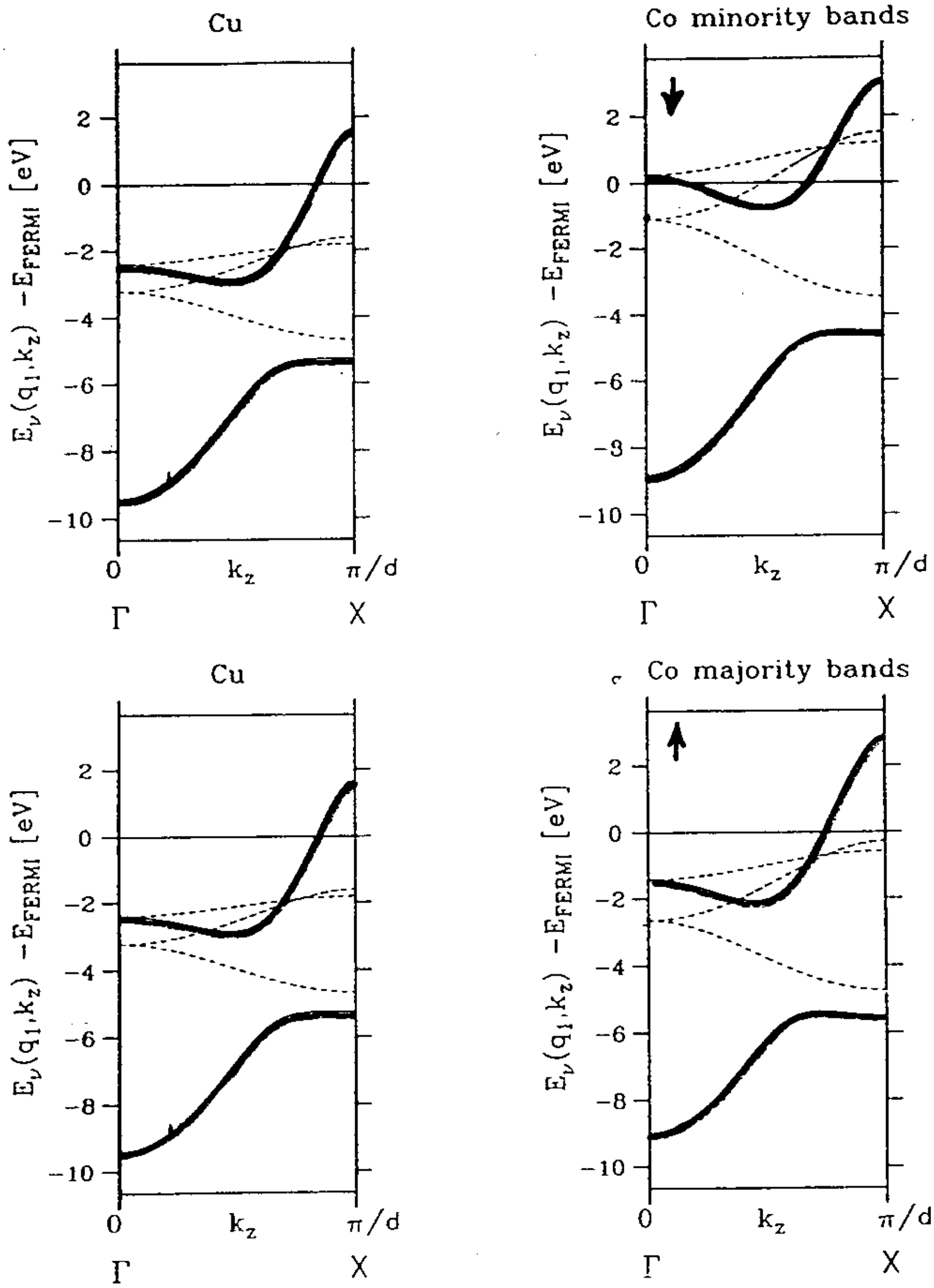
Cu / Co(100)
experimental data
Cu thickness (ML)
Binding Energy (eV)
0
5
10
15
20
25
30
2
1.5
1
0.5
0

Theory vs. Experiment

Cu / Co(100)



BAND STRUCTURE AT $\bar{\Gamma}$



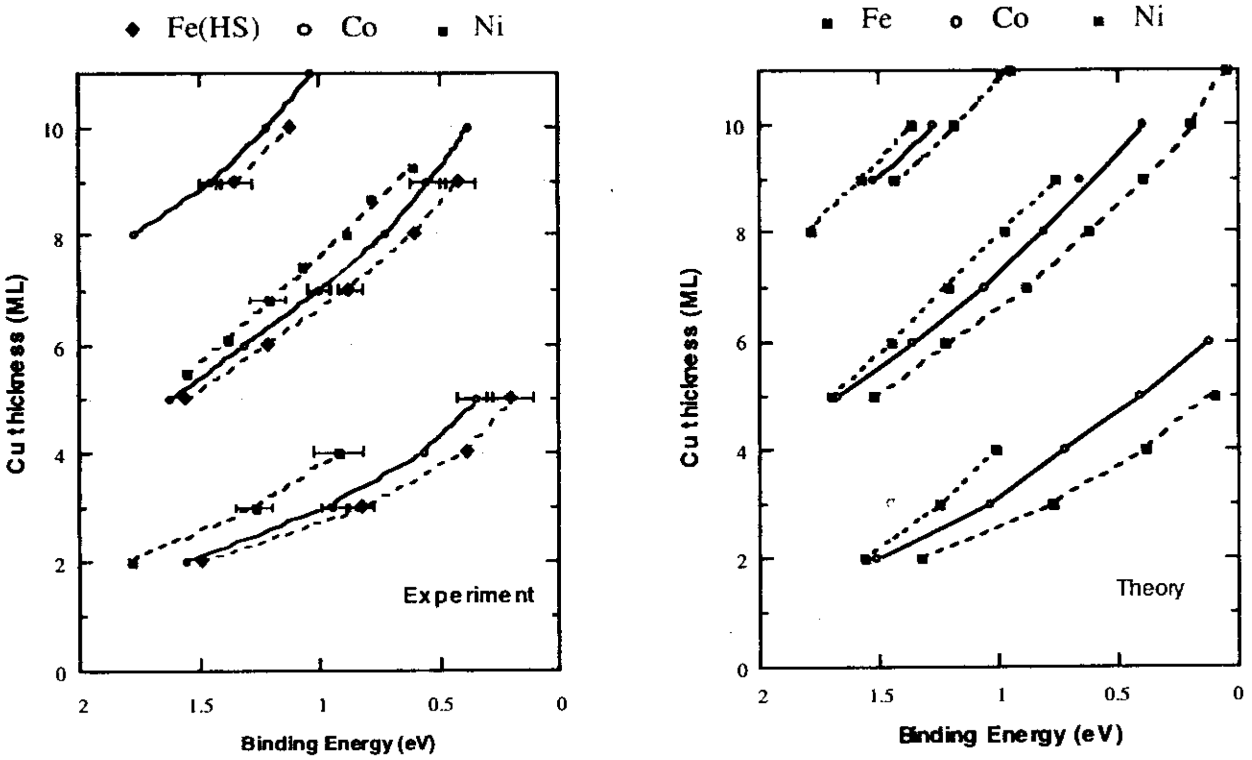
Interface reflectivity is spin dependent:

Minority-spin ====> strong reflection ====> QW

Majority-spin ====> weak reflection ====> Bloch states

Experiment and Theory

Cu films on Fe(100), Co(100), Ni(100)

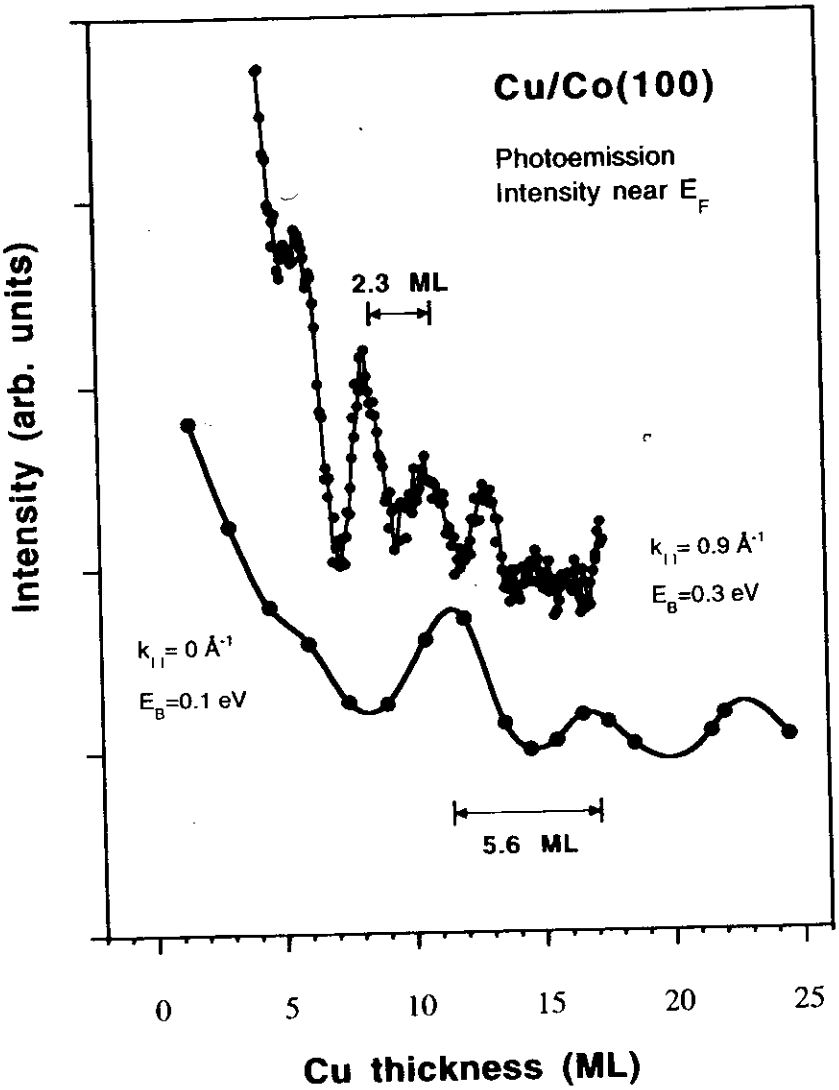


Binding energy of spind-down quantum well states ⟶ **Phase shift in the interface reflection**

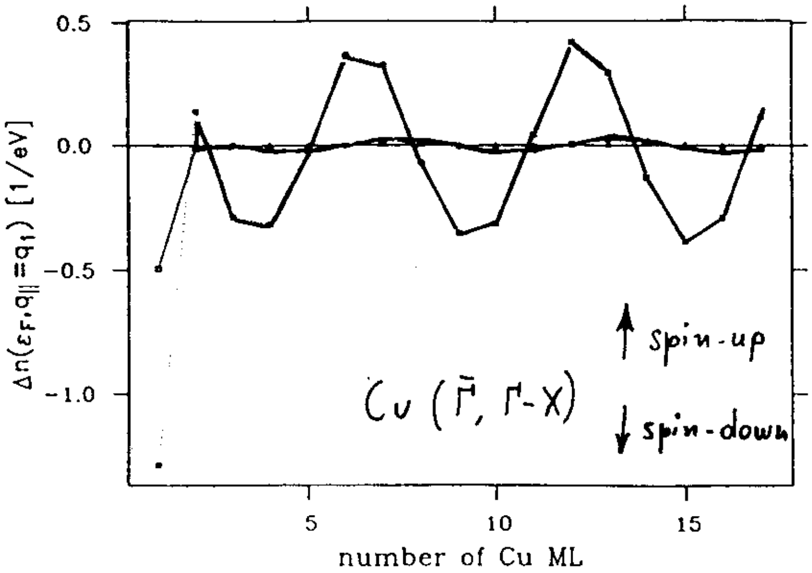
$$2kd + \Phi_i + \Phi_v = 2n\pi$$

R. Kläsges et al. (1998)

Long- and short-period oscillation near E_F in Cu/Co(100)

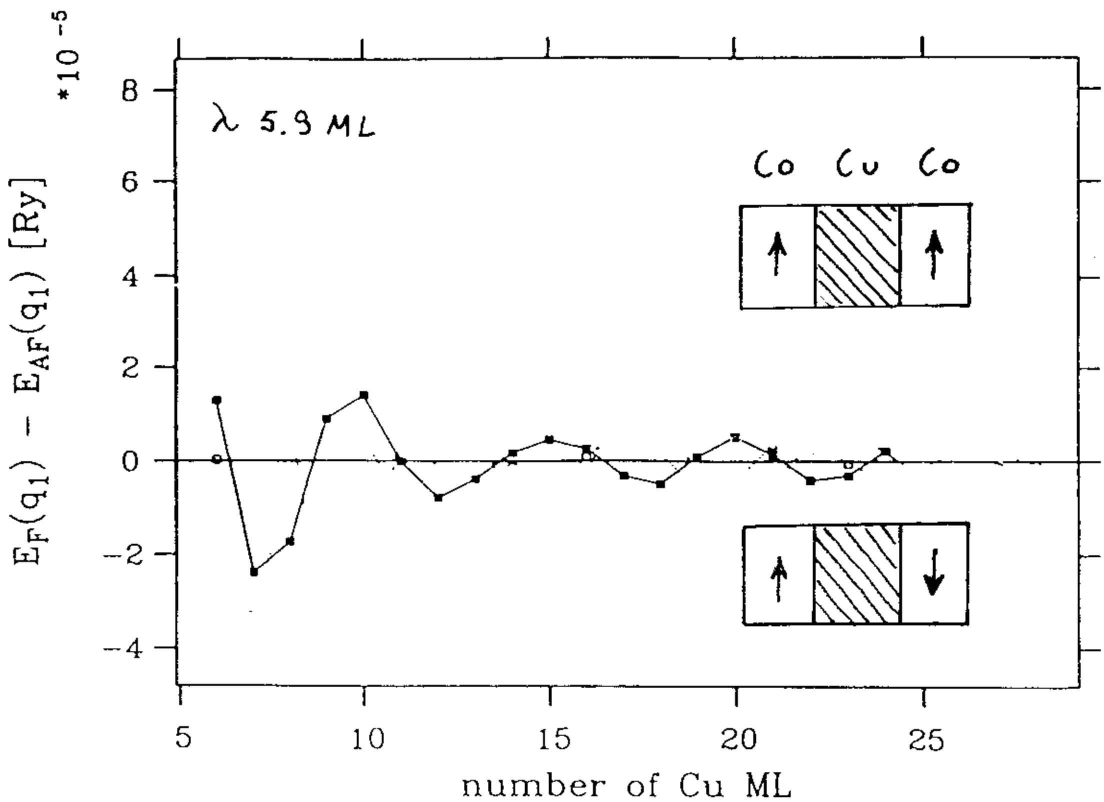


Change of the Partial Density of States at E_F



Exchange Coupling

11 Co / n Cu / 11 Co



L. Nordström et al., PRB 50, 13058 (95)

Spin- Polarized QW States ⇔ Oscillatory Exchange Coupling