Investigation on the structural, electronic and magnetic properties of ultrathin iron films grown on Cu/Si(111)

P. Castrucci

Sezione INFM-Università di Camerino

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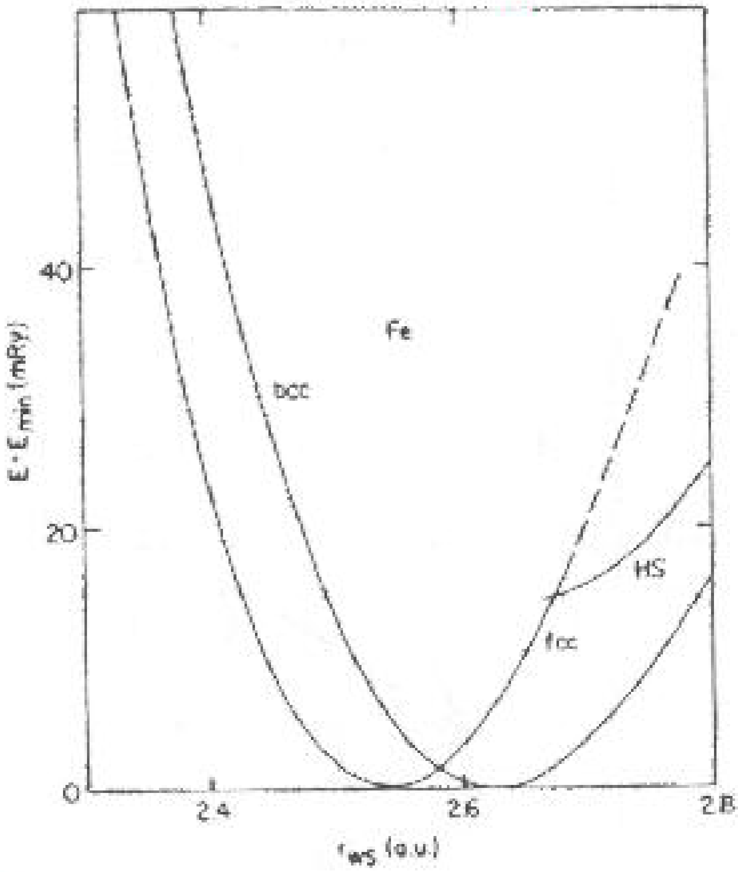
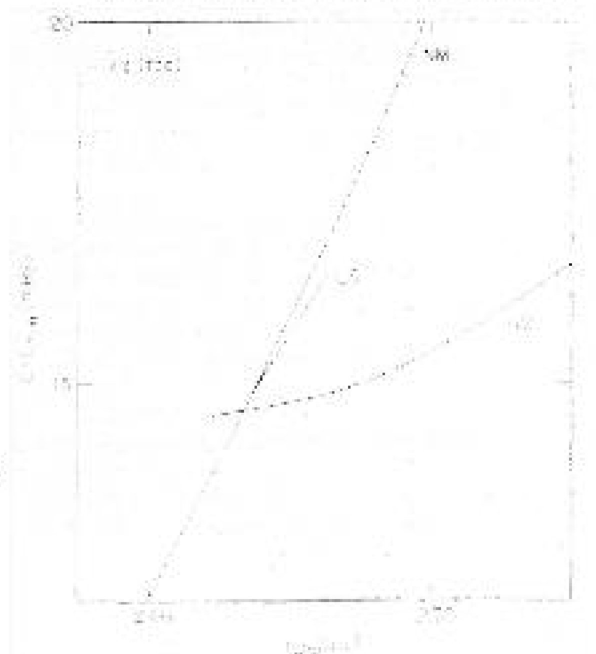
Theoretical prediction :



Total energy vs r_{WS}

by V. L. Moruzzi, P. M. Marcus, K. Schwarz, P. Mohn,

5)



- **bcc phase (α-Fe)**
  - magnetic for all the r_{WS} values

  - the most stable: r_{WS} = 2.63 a.u.

- **fcc phase (γ-Fe)**
  - different stable and metastable phases
  - NM, HS, LS

as a function of r_{WS}

In the Fe/Cu(111) case:

The fcc Fe phase occurs for thicknesses < 3 ML

What about magnetism ?

Theoretical predictions :

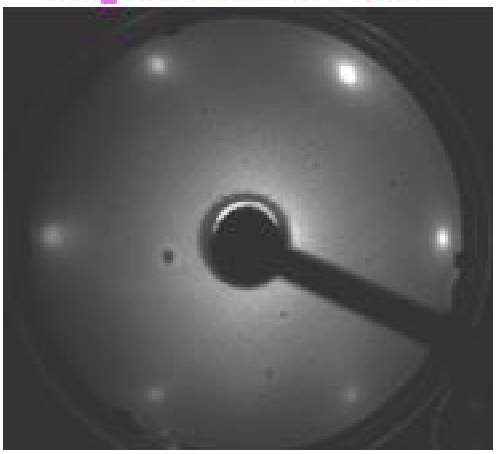
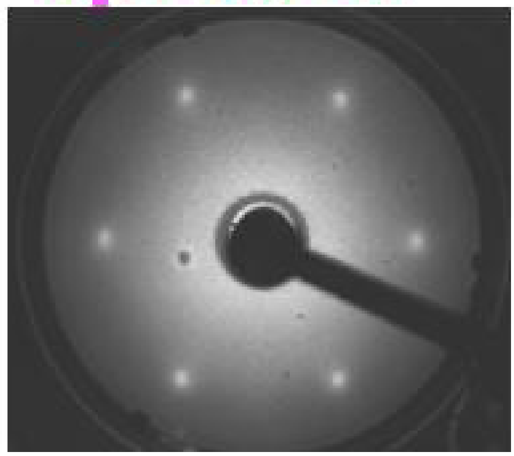
$$m = 2.79 - 2.91\ \mu_B$$

- Fe fcc lattice parameter
- ultra thin Fe film

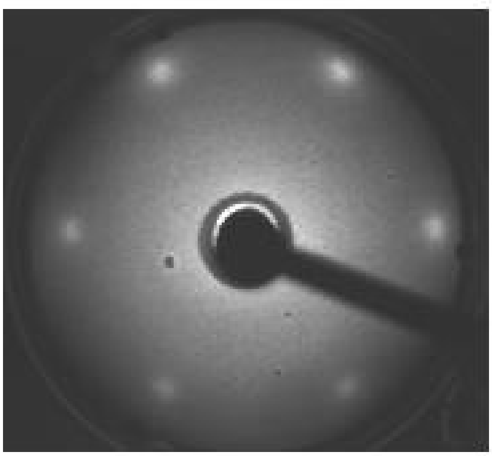
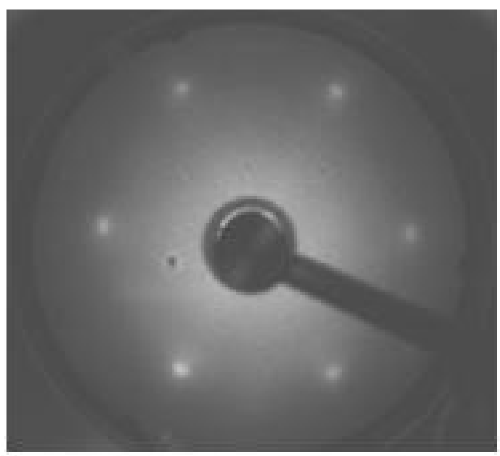
Never found experimentally

LEED images for Fe/Cu/Si(111)

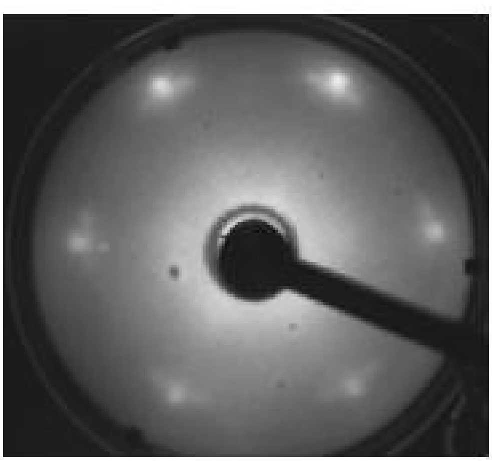
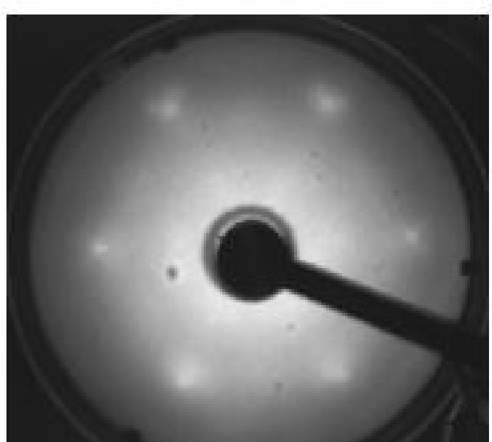
Ep = 70 eV | **Ep = 90 eV**

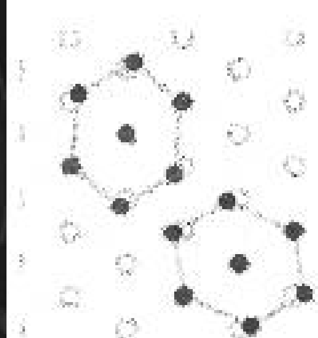
Fe 1ML

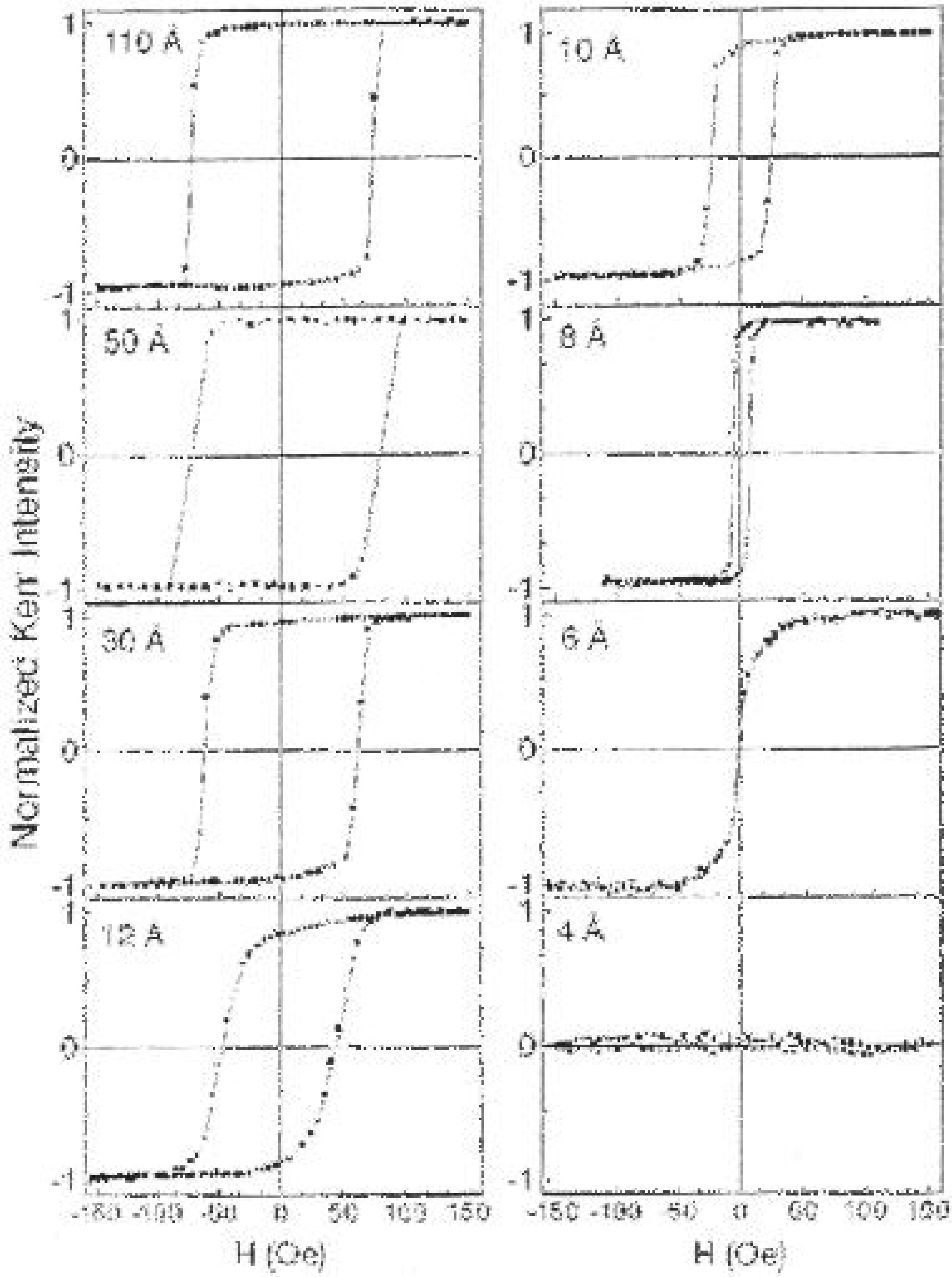
Fe 2ML

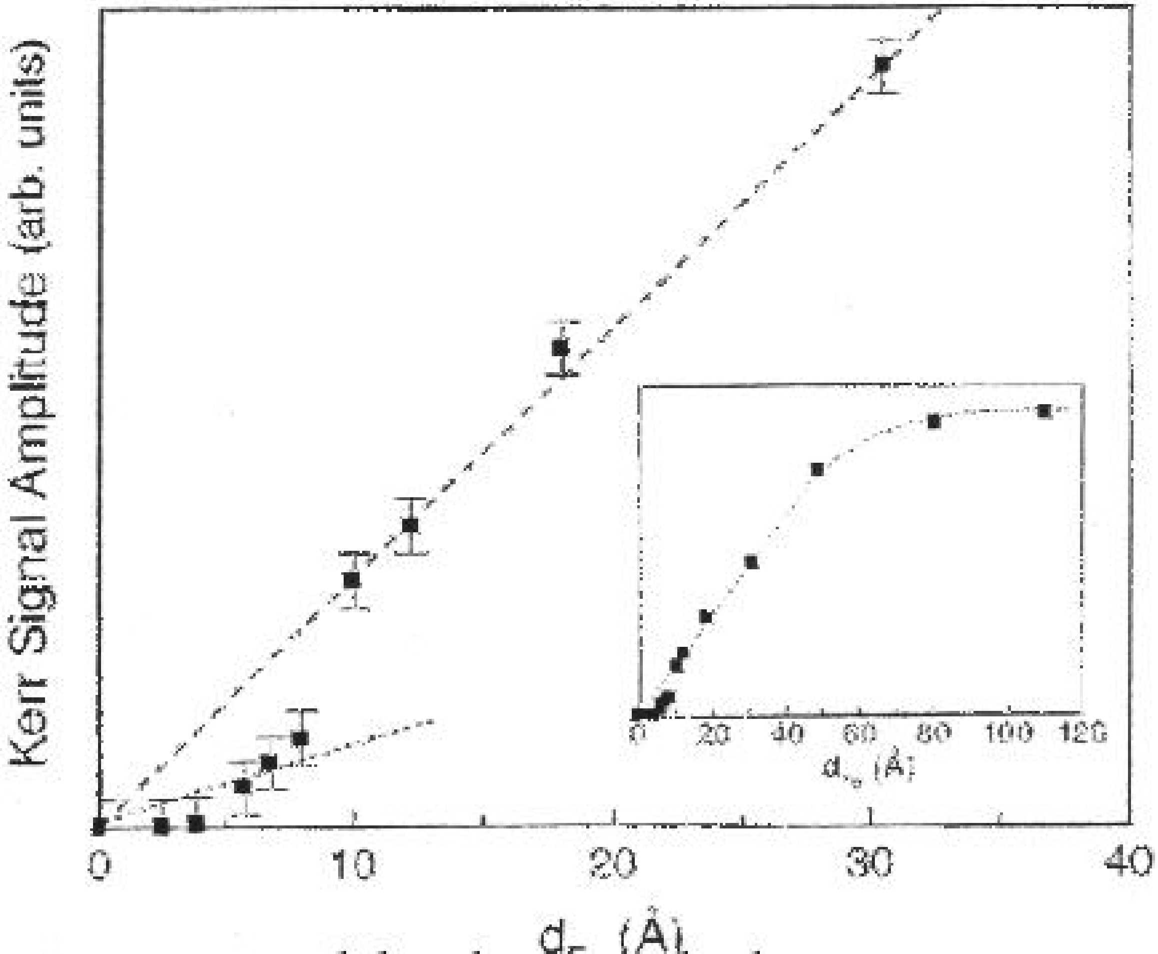
Fe 3ML



RT Longitudinal SMOKE on Cu/Fe/Cu/Si(111)



No RT Polar SMOKE loops have been measured

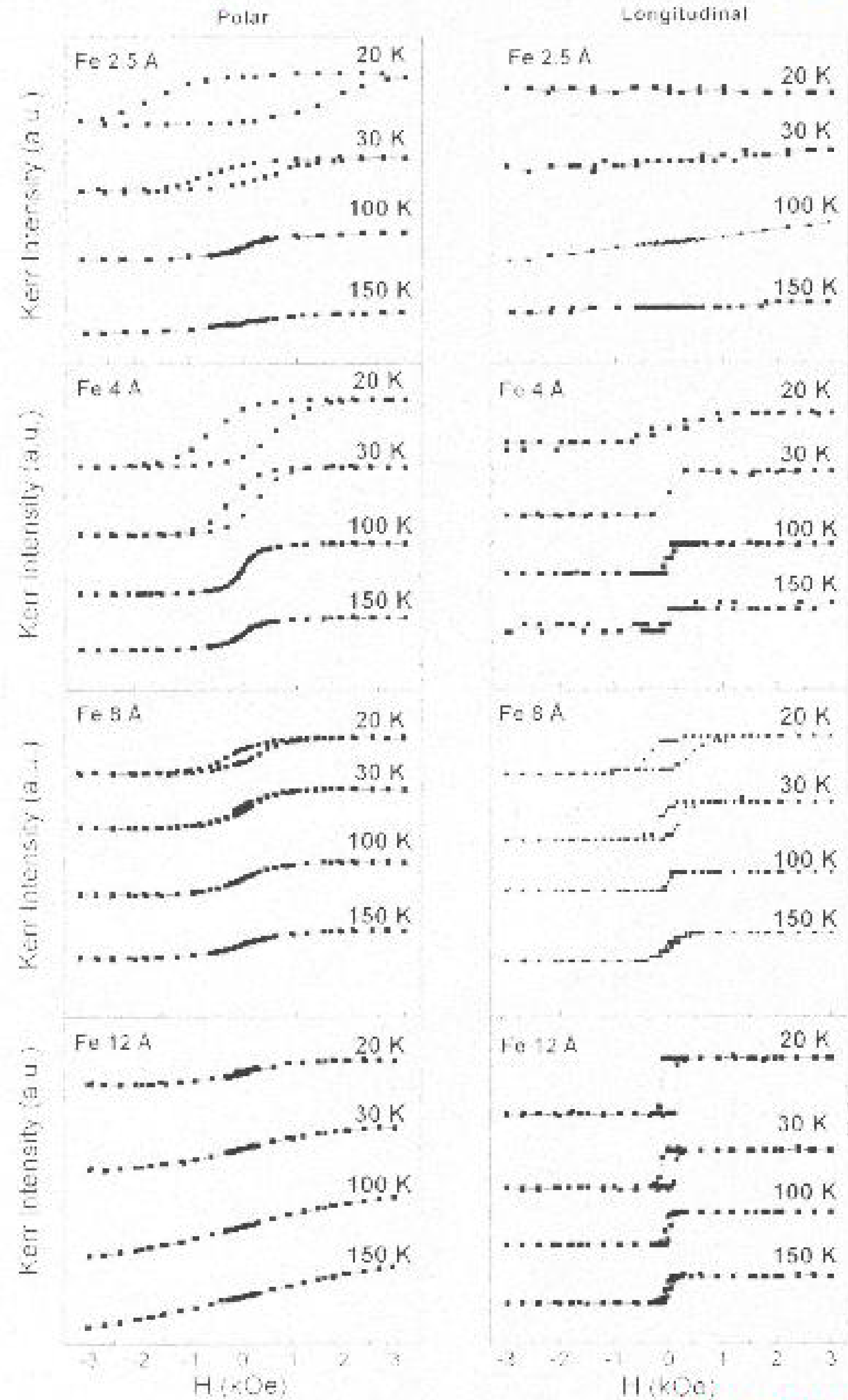


- Two roughly linear behaviours, with different slopes, can be identified, i.e. by different values of the average in-plane m.

- The slope changes for d_{Fe} = 10 Å (~ 5 ML), slightly above the fcc->bcc structural transition

- No Kerr intensity can be recorded at RT for $d_{Fe} < 6$ Å, i.e. below the fcc->bcc structural transition

SMOKE loops for Cu/Fe/Cu/Si(111) :



Summarizing SMOKE results vs T:

- For T<30K polar SMOKE loops have been detected for $d_{Fe} < 12$ Å.

- No longitudinal SMOKE loop has been measured for $d_{Fe} < 6$ Å for all the temperatures down to 20K.

- In d_{Fe} range between 8 Å and 10 Å both the in-plane (for all T) and out-of-plane (for T < 30K) magnetization directions have been detected .

⇓

No polar SMOKE loop has been recorded for T >30K and for a Fe coverage higher than 10Å

For Fe deposited amount higher than 10 Å (5 ML)

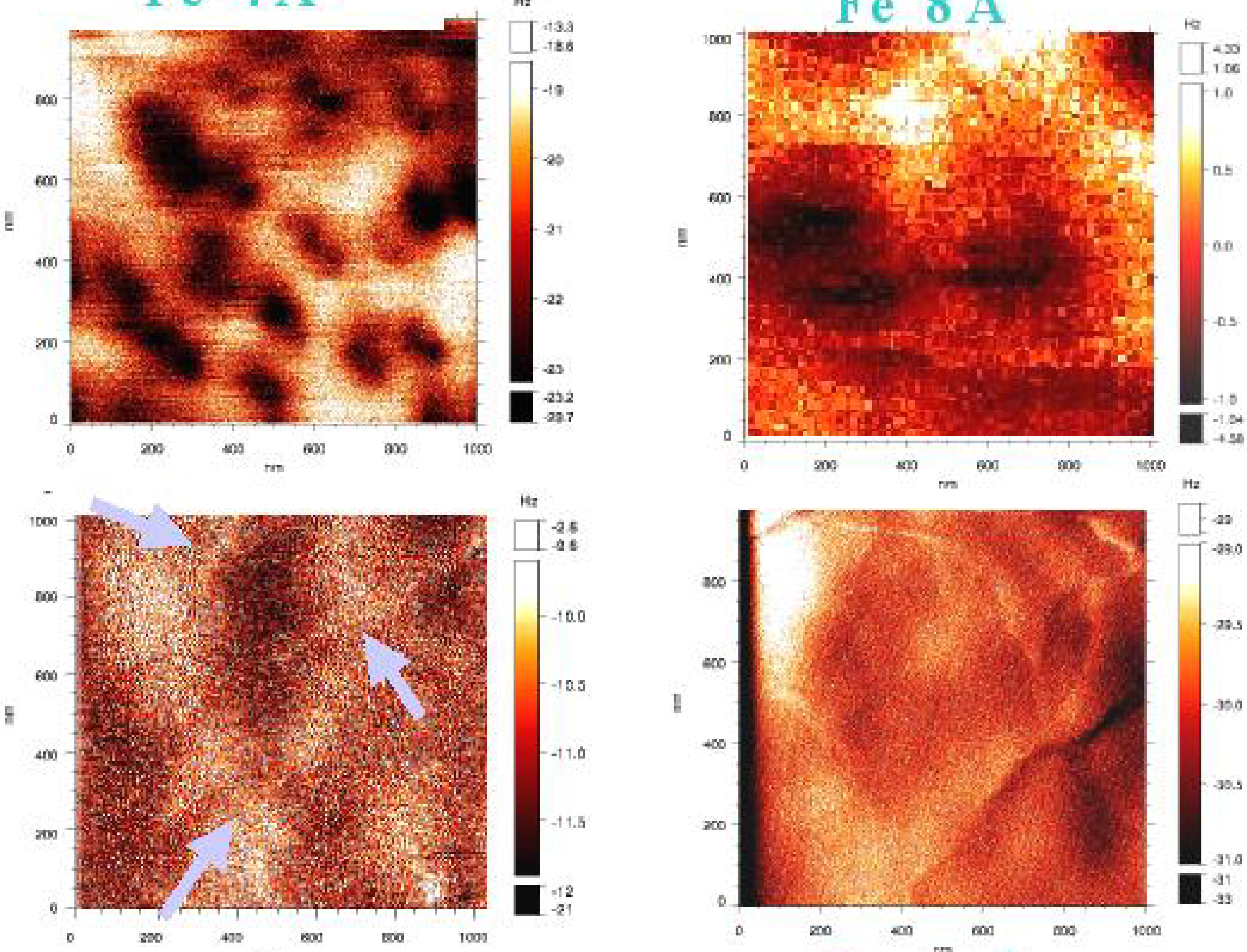
SMOKE measurements suggested:

- In-plane magnetization
- T_c well above room temperature

RT , H = 0, MFM images

Fe 4 Å

Fe 8 Å



Fe 12 Å

Fe 30 Å

- up and down out-of-plane magnetic domains. Their average size increases with d_{Fe}, up to 8 Å

- for d_{Fe} = 12 Å a coexistence of out-of-plane and in-plane magnetic domains has been detected

Investigations on the value of the magnetic moment per atom

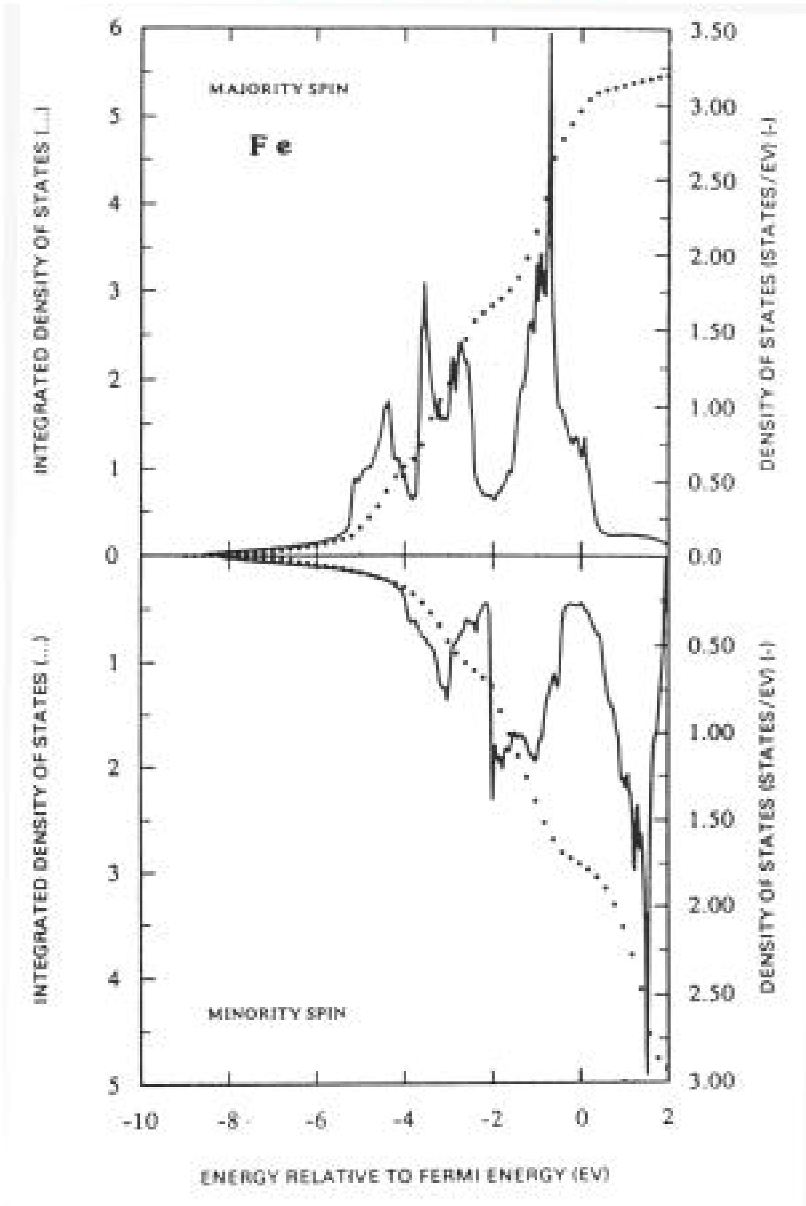
- **XAS and UPS studies**
- **Resonant magnetic scattering**

Ferromagnetism from a microscopic point of view :

- lack of balance between the number of spin up and of spin down
- correlation* between magnetic exchange splitting and magnetic moment

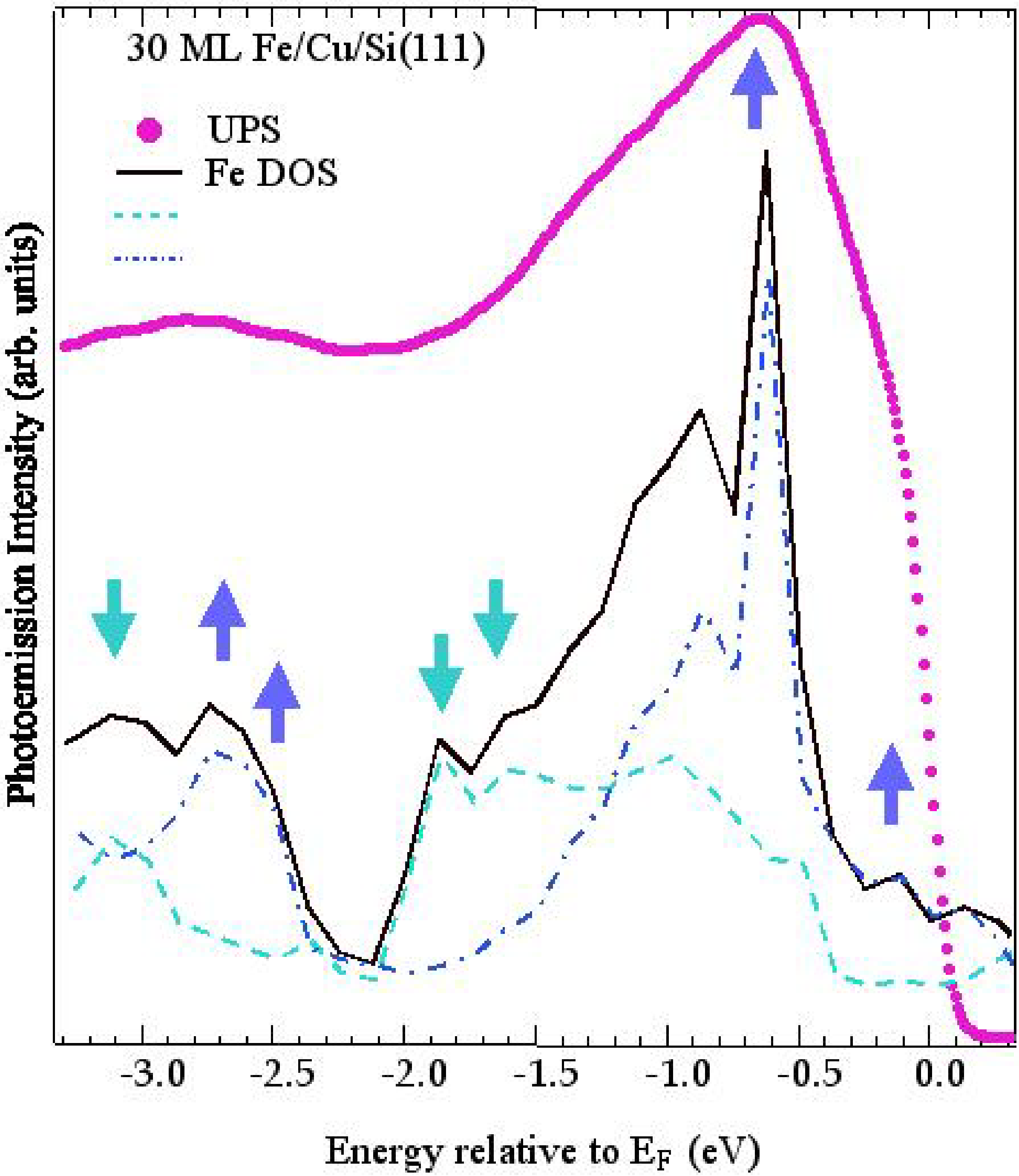
*by F. J. Himpsel, Phys. Rev. Lett. 67, 2363 (1991)

Bulk iron calculated density of states



X-ray absorption spectroscopy at Fe $L_{2,3}$ edges mainly probes the d empty density of states

spin down



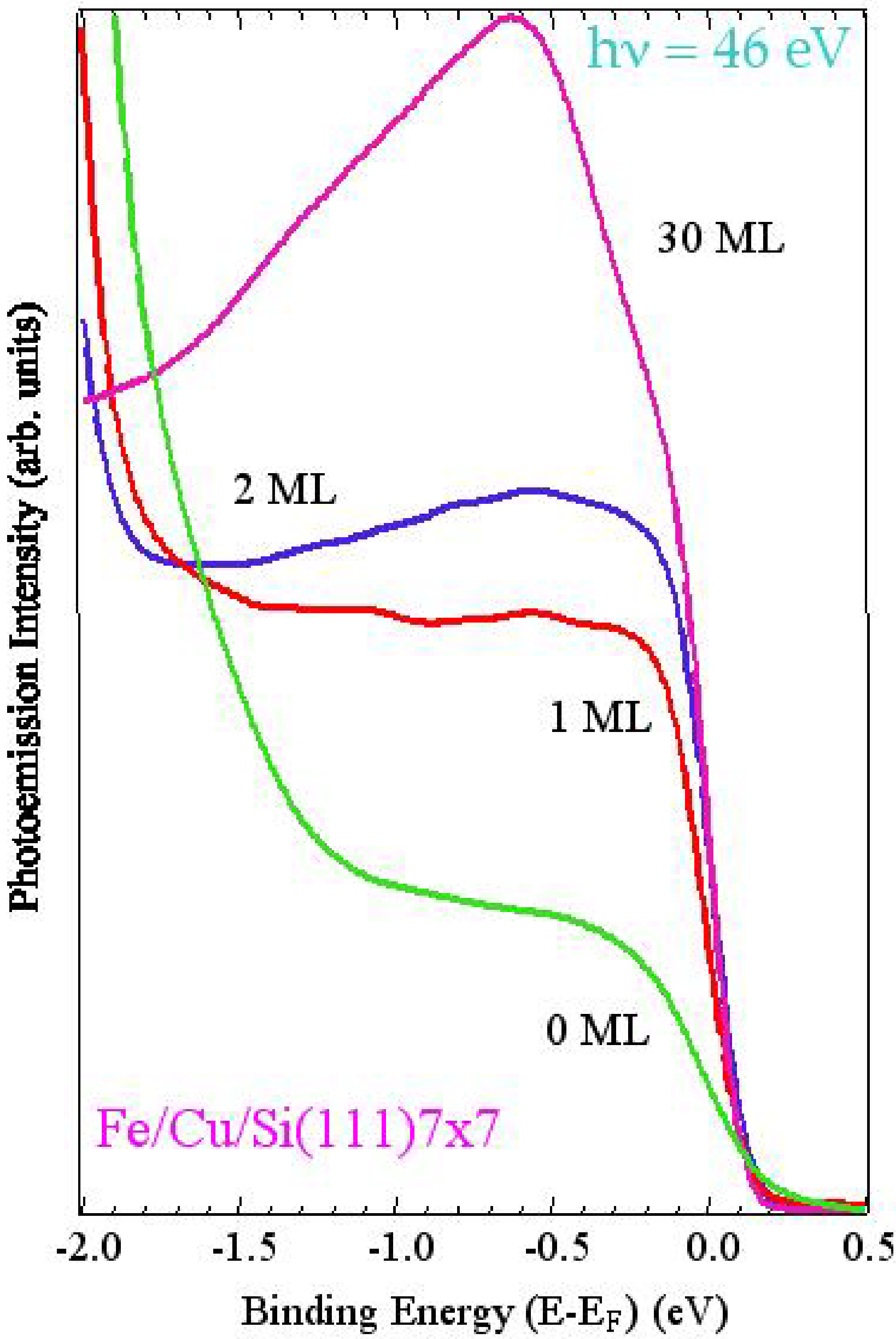
Calculated Fe DOS:

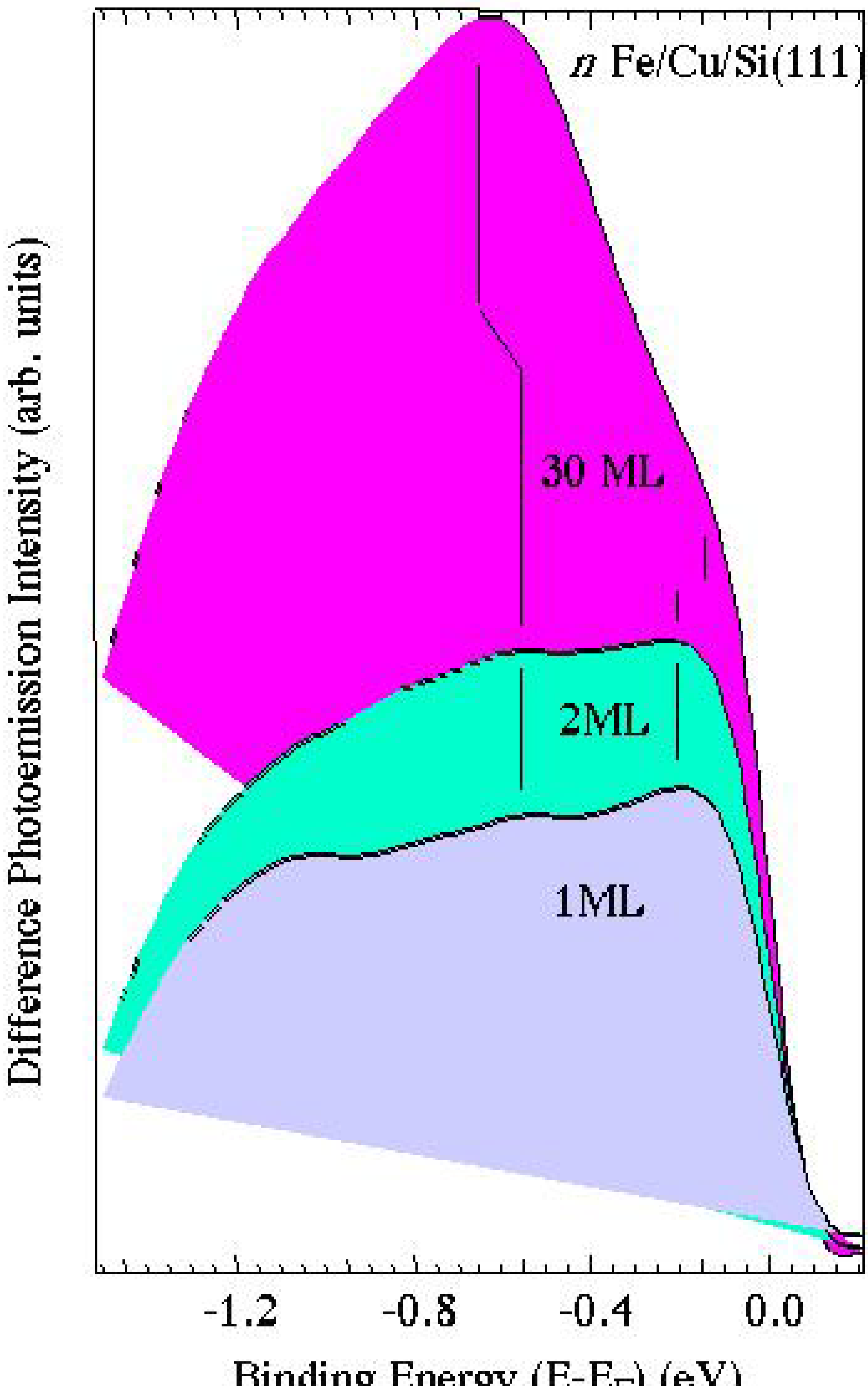
by V. L. Moruzzi, J. F. Janak, A. R. Williams

in " Calculated electronic properties of metals "

Pergamon Press, 1978

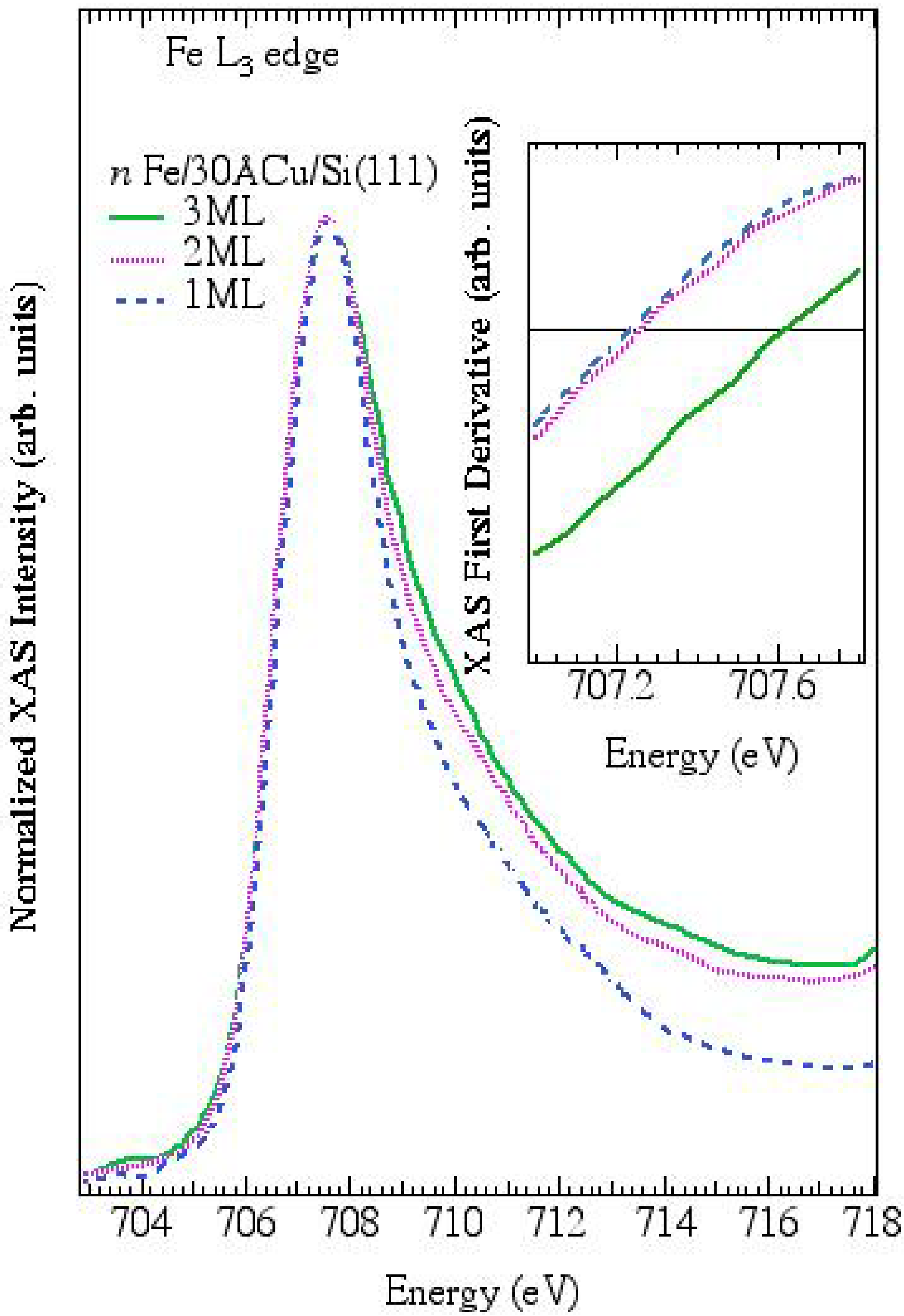
UPS valence band spectra





n Fe/Cu/Si(111)
30 ML
2ML
1ML
Difference Photoemission Intensity (arb. units)
-1.2
-0.8
-0.4
0.0
Binding Energy (E-E$_F$) (eV)

X-ray absorption spectra at Fe L_3 edge



UPS results (± 0.02 eV) :

- 30 ML Fe
  -0.65 eV, -0.15 eV
- 2 ML Fe
  -0.55 eV, -0.20 eV
- 1 ML Fe
  -0.55 eV, -0.20 eV

XAS results (± 0.1 eV) :

- 3 ML Fe
  707.6 eV
- 2 ML Fe
  702.2 eV
- 1 ML Fe
  707.2 eV

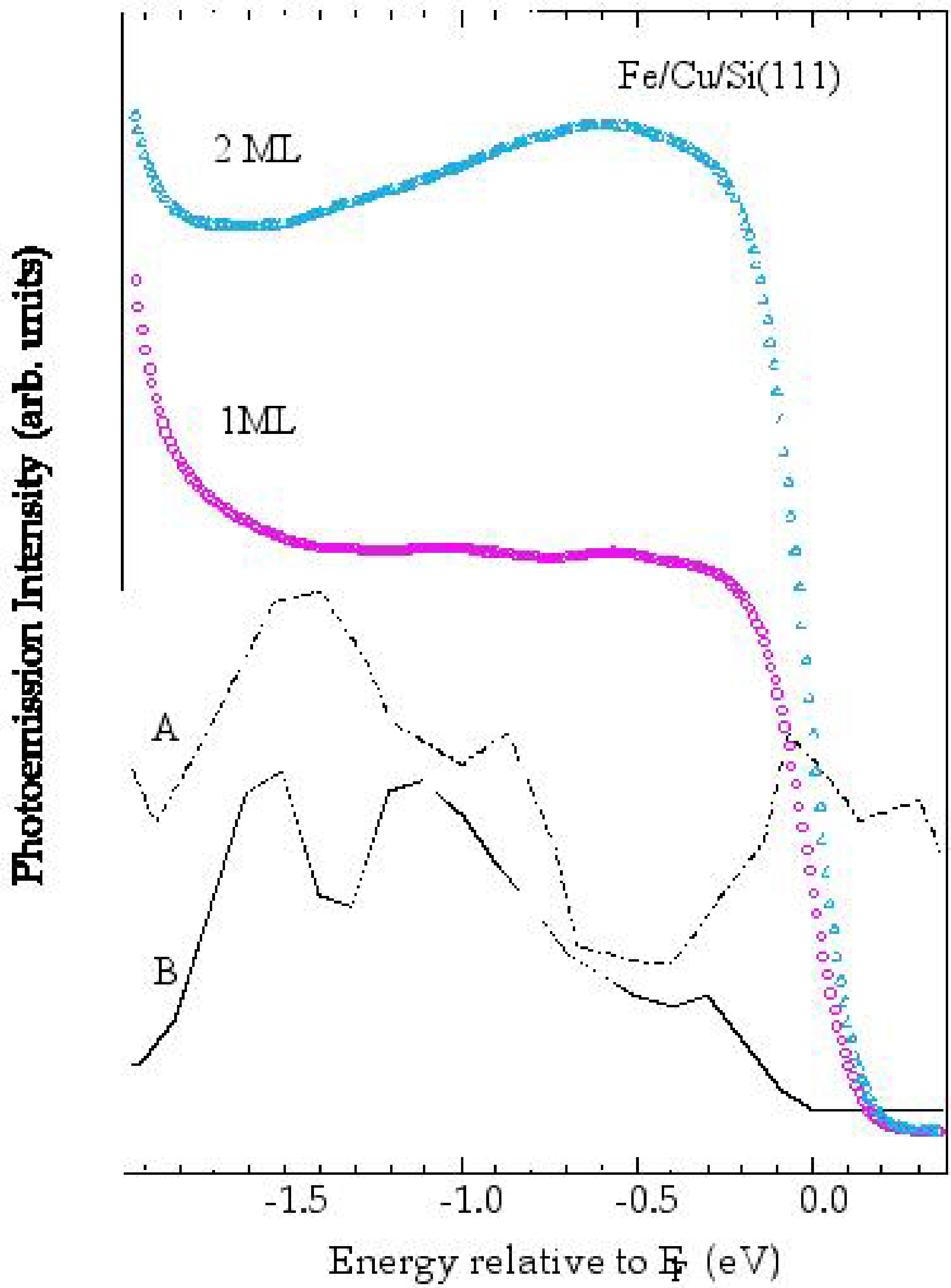
Experimentally :

For the Fe fcc phase (given by LEED)

- lowering of the exchange splitting with thickness decreasing

- exchange splitting value lower than that of Fe bcc bulk (few tenths of eV)

$$m_{\gamma\text{-Fe}} \lessapprox m_{\alpha\text{-Fe}}$$



A,B → m=2.7–2.9 μ_B

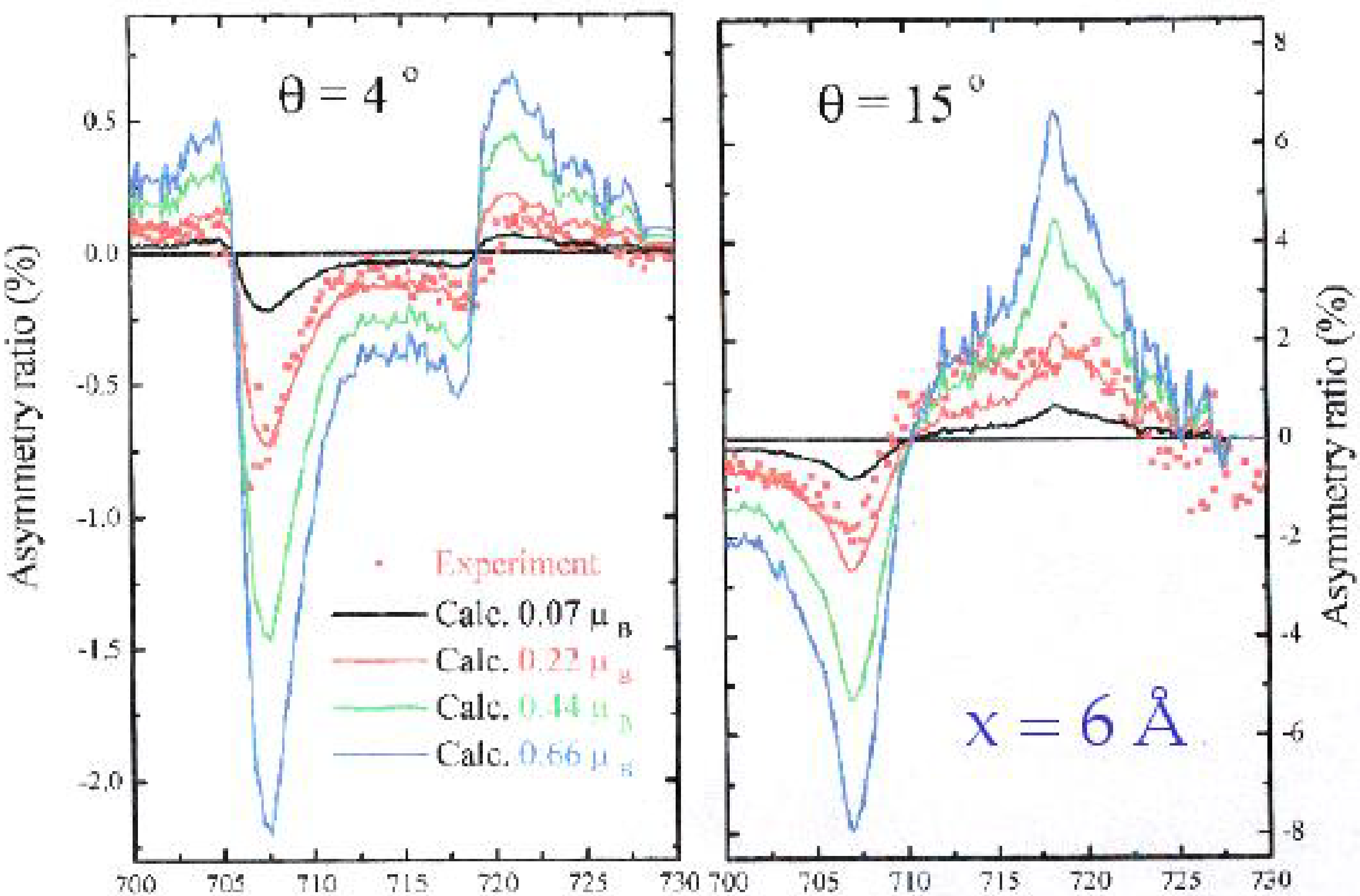
A : S. Ohnishi *et al.*
Phys. Rev. B 28, 6741 (1983)

B : O. Hjortstam *et al.*
Phys. Rev. B 53, 9240 (1996)

Resonant magnetic scattering at 2p Fe edge

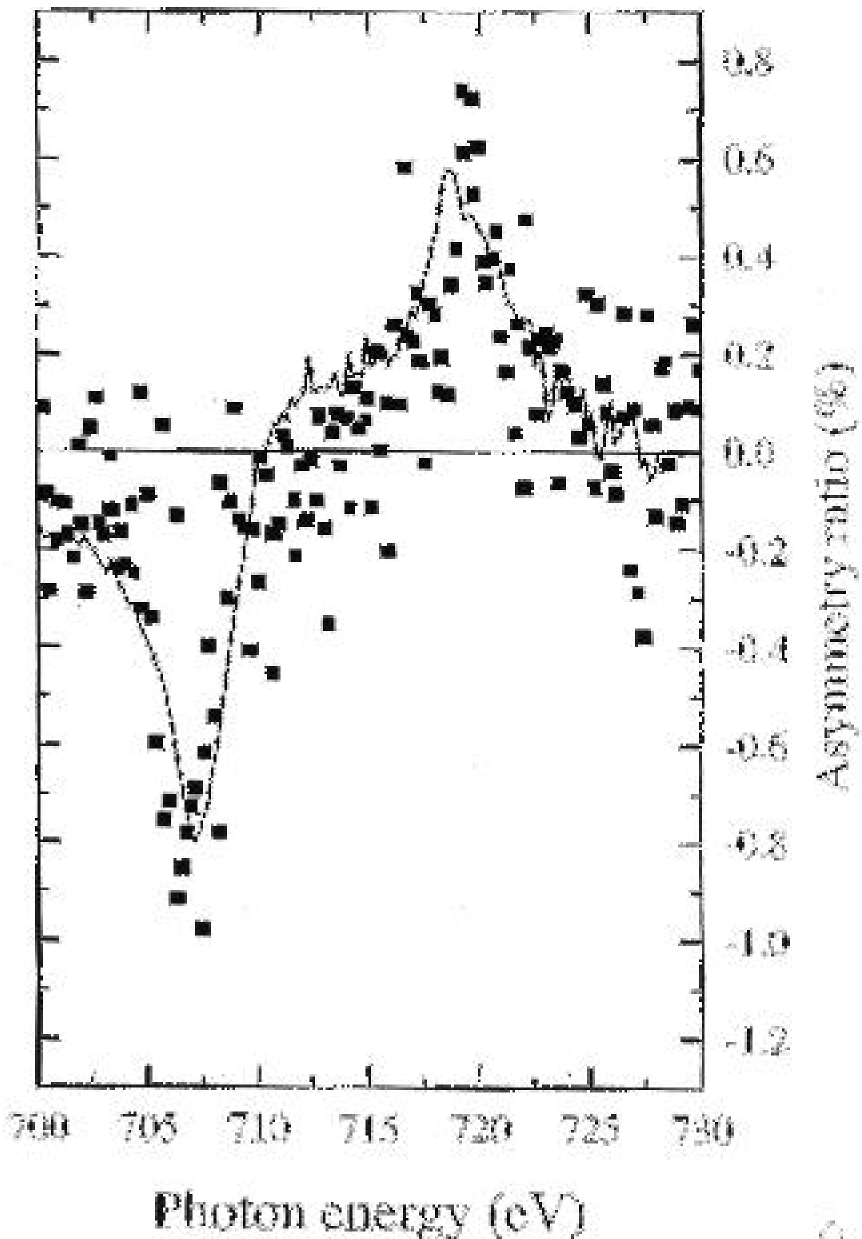
RT, In-plane H field

$Cu/Fe_x/Cu/Si(111)$



Best fit obtained for $m = 0.20\ \mu_B$

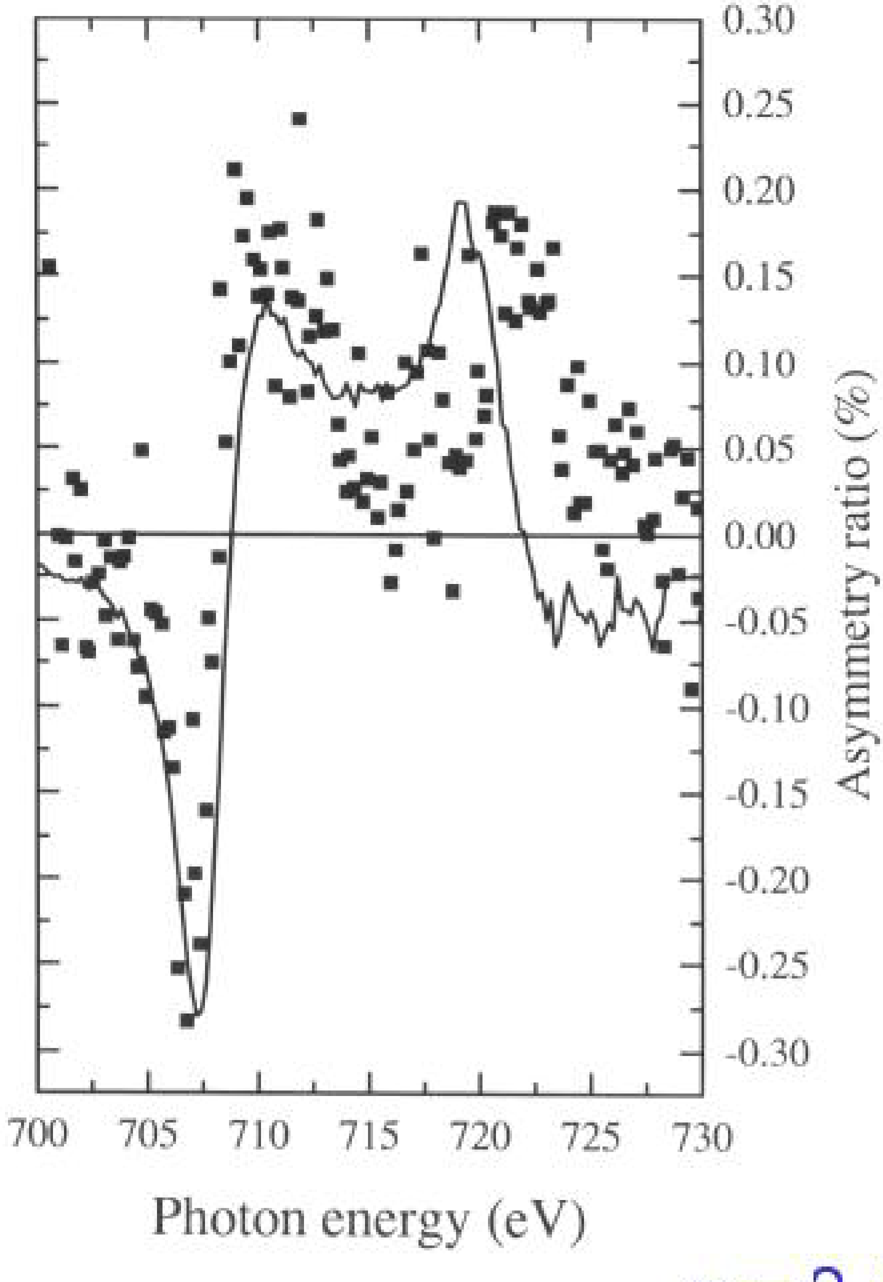
Cu/Fe_x/Cu/Si(111)



x = 4 Å

Best fit obtained for $m = 0.10\ \mu_B$

Cu/Fe_x/Cu/Si(111)



x = 2 Å

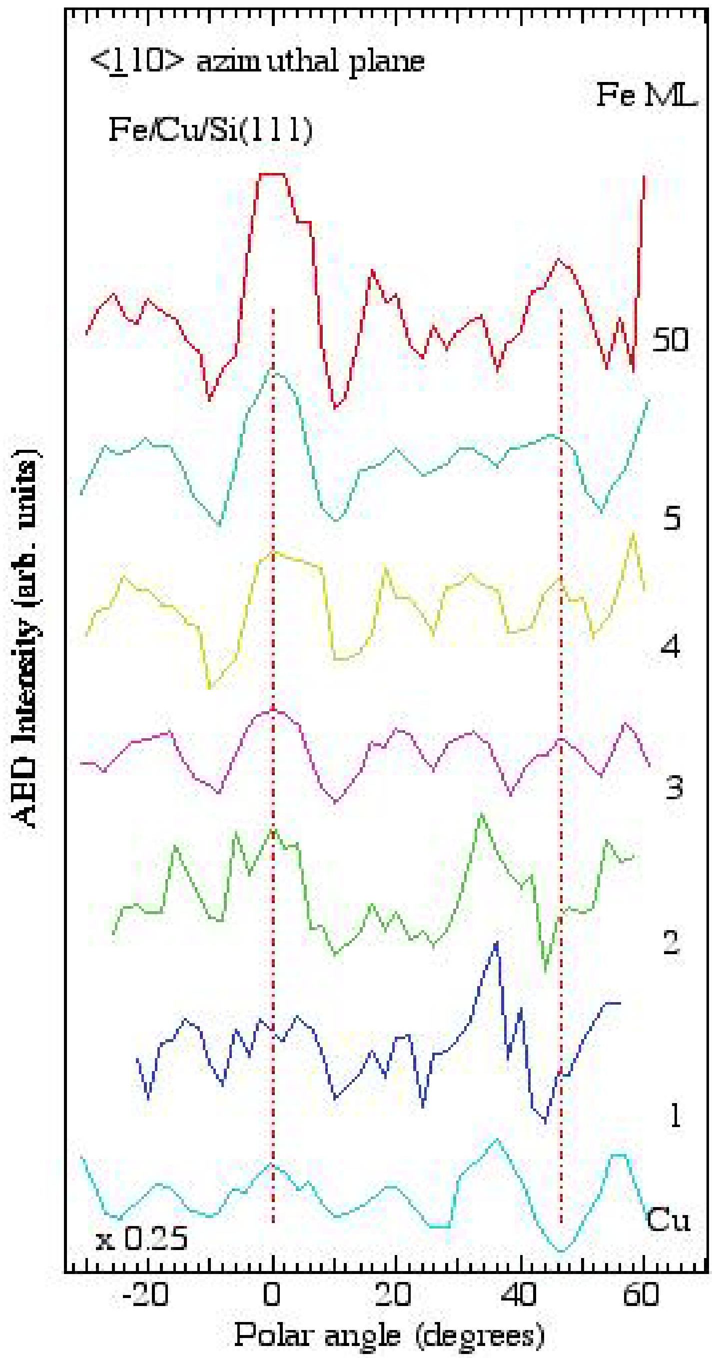
Best fit obtained for $m = 0.05\ \mu_B$

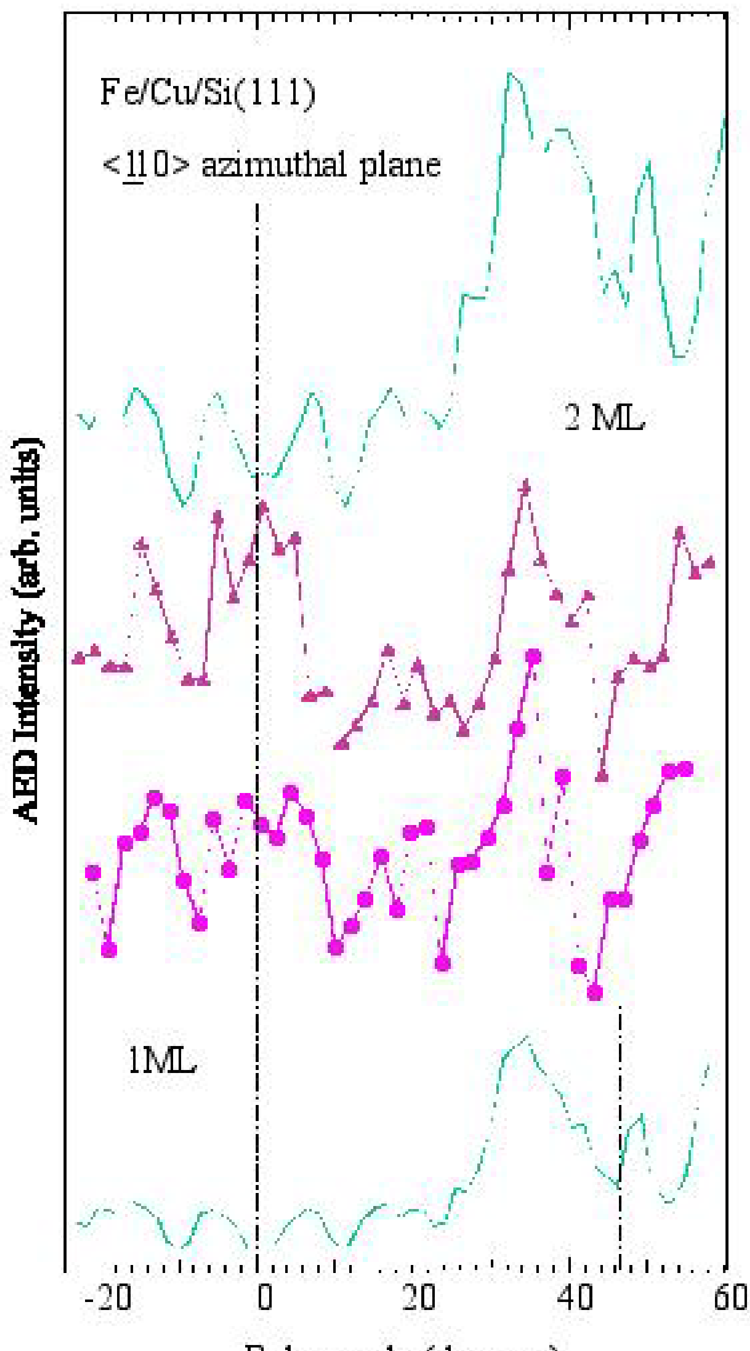
What about structural information?

Polar angular Auger electron diffraction patterns :

- sample rotation in front of the CMA
- azimuthal plane identified by LEED images
- peak-to-peak intensity of Fe $L_{2,3VV}$ and/or Cu $L_{2,3VV}$
- Auger spectra
  - collected in first derivative mode
  - measured vs polar angle
- primary electron beam of 1500 eV

AED patterns





Fe/Cu/Si(111)
<110> azimuthal plane
2 ML
1ML
AED Intensity (arb. units)
-20
0
20
40
60
Polar angle (degrees)

In summary by AED analysis :

- presence of bcc structural phase even for 1 ML Fe equivalent coverage

- bi-tri layers fcc arranged platelets and/or intermixing processes cannot be completely excluded

- assessment at 2.5-3 ML the nominal thickness at which most of Fe prefer to arrange in a bcc structural phase

In Summary :

Fe (Å)	2	4	6	8	12	20
LEED	fcc	fcc	fcc→bcc	bcc	bcc	bcc
$M_{//}$ (μ_B)(RT)	0.05	0.10	0.20			2.20
SMOKE(RT)	No	No	No	//	//-*Hi*	//-*Hi*
SMOKE(LT)	⊥	⊥	⊥	⊥-//	//	//
MFM (RT)		⊥		⊥	⊥-//	//

- Coexistence of fcc and bcc phase
- Is the fcc superparamagnetic ?