PF研究会「磁性薄膜・多層膜を究める」 Fri-Sat. 14-15, Oct 2011

深さ分解XMCD法で切り開く分子吸着Fe/Cu(001)の磁気構造

–EXAFSによる薄膜構造解析と併せて–

阿部 仁[1*], 雨宮健太[1], 酒巻真粧子[1], 香西将吾[2], 中山丈嗣[2], 近藤 寛[2]

[1]KEK-PF, [2]慶應大

*: hitoshi.abe@kek.jp

Magnetism of Fe/Cu(001) films

CO, NO on 2-4 ML

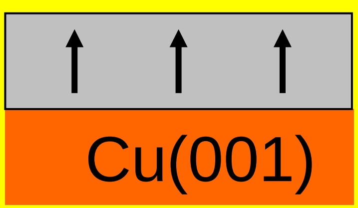
Regime Ⅰ

< 4 ML

fcc (fct)

Perpendicular

~2.4 μ_B/atom



Regime Ⅱ

5-10 ML

Surface two layers: FM

Inner layers: AFM

Regime Ⅲ

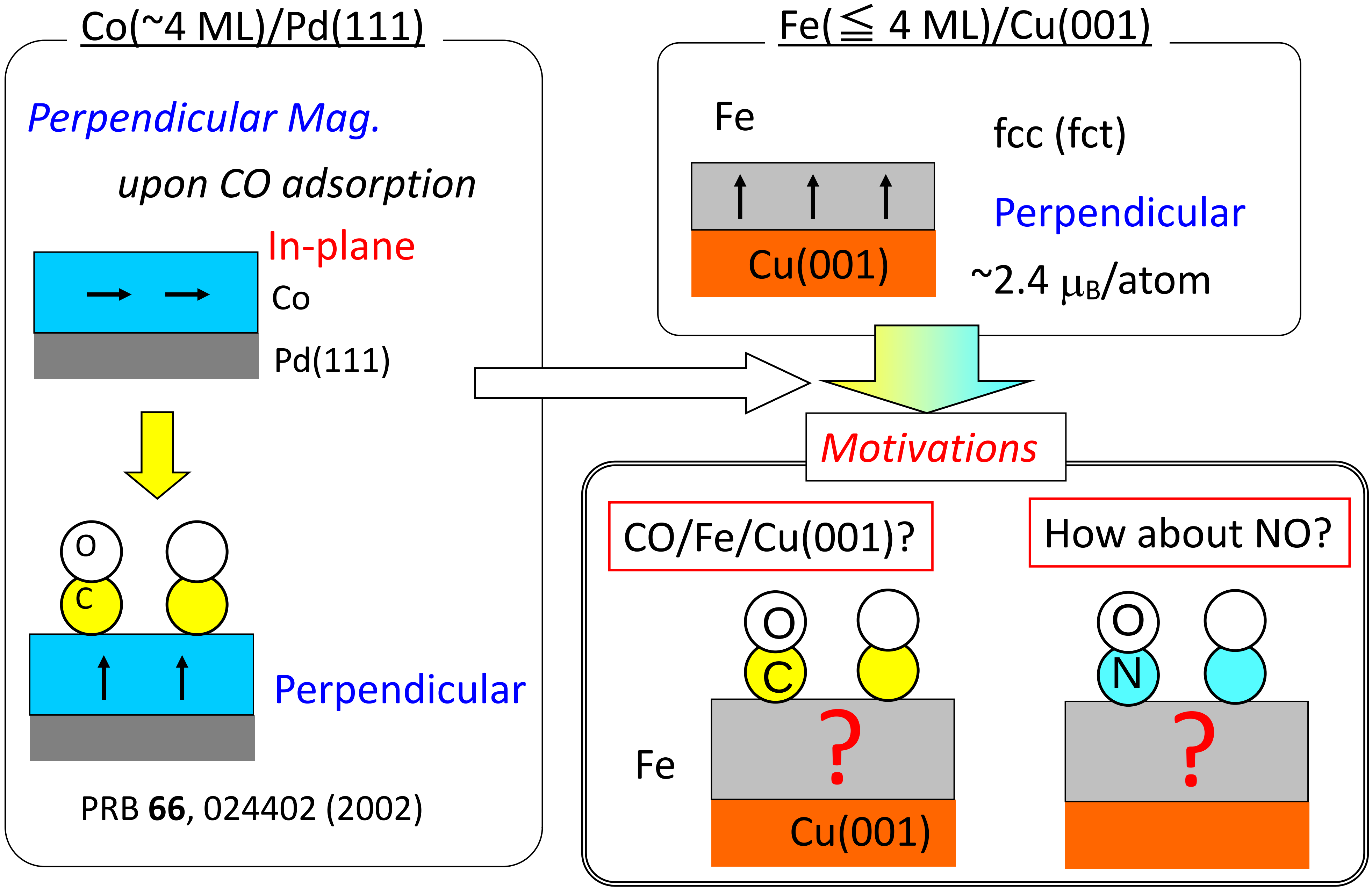
> 11 ML

bcc

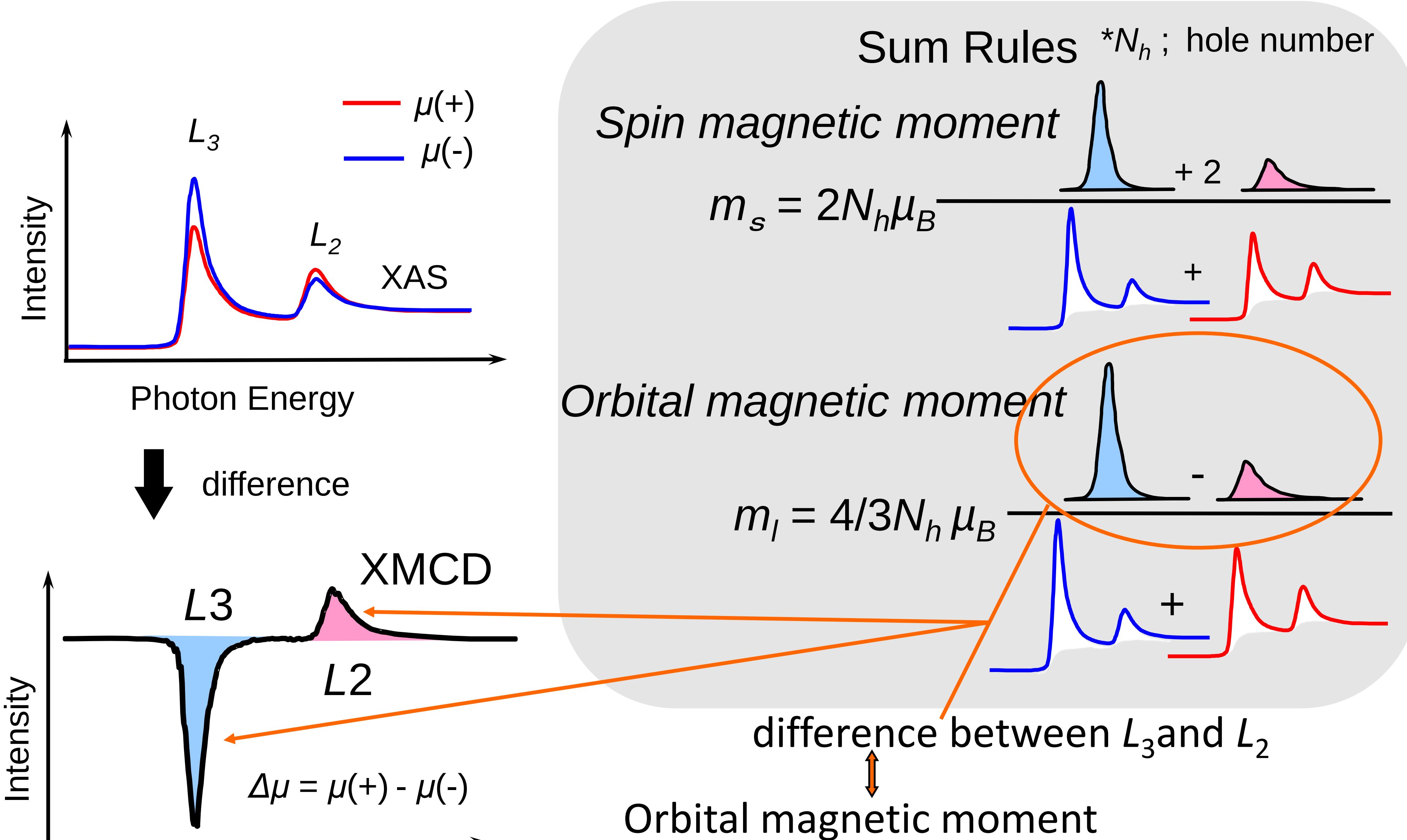
In-plane

PRL **69**, 3831 (1992), etc.

Magnetic thin films, Molecular adsorption

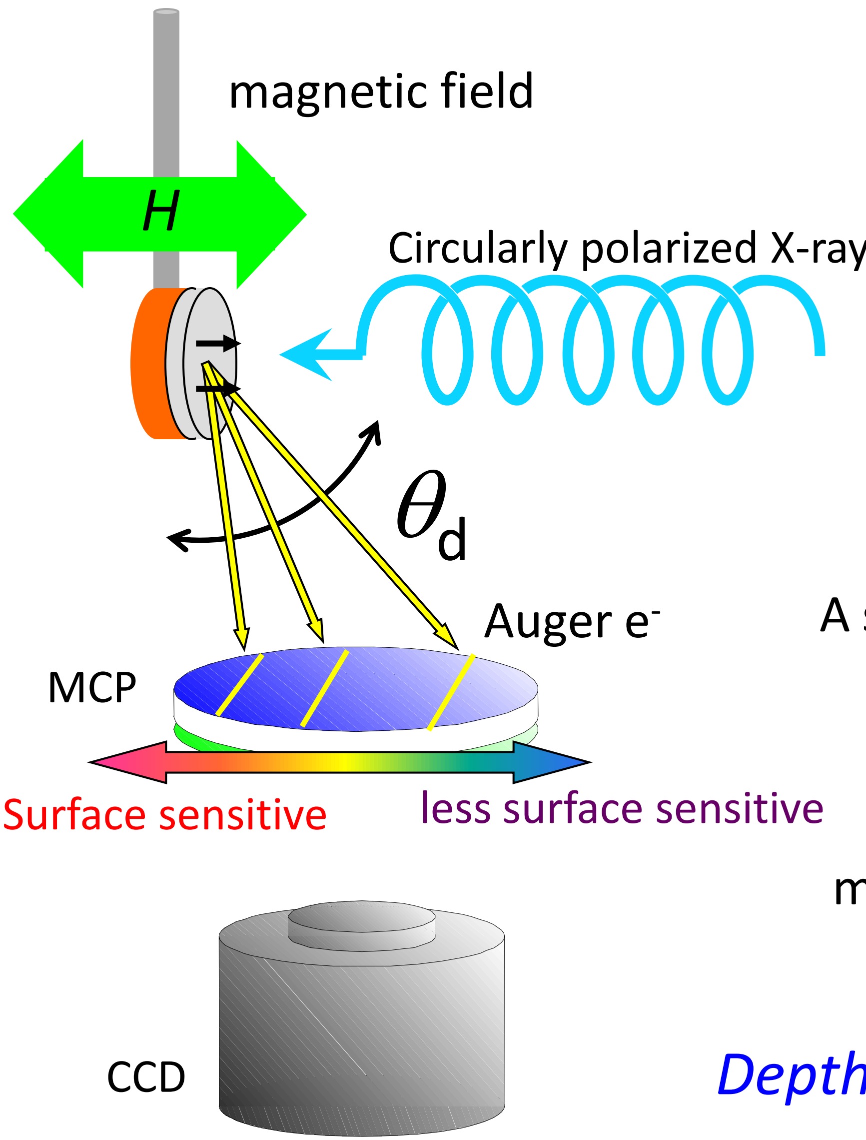


Sum rules: XMCD spectra and magnetic moments

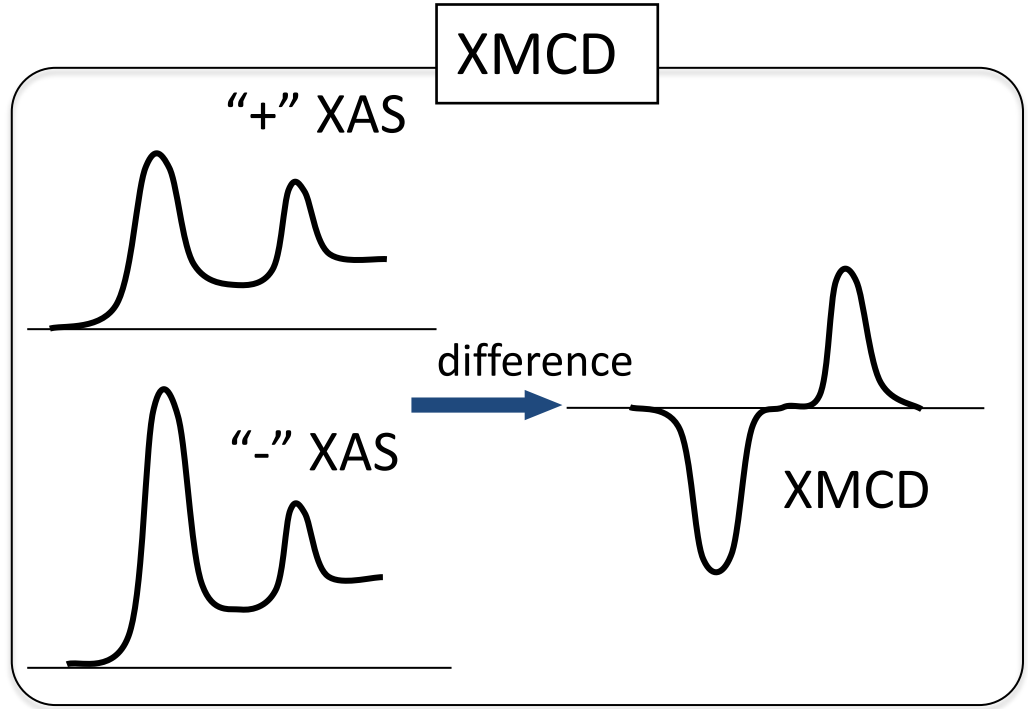


B. T. Thole, *et al.*, Phys. Rev. Lett. **68**, 1943 (1992)
P. Carra, *et al.*, Phys. Rev. Lett. **70**, 694 (1993)

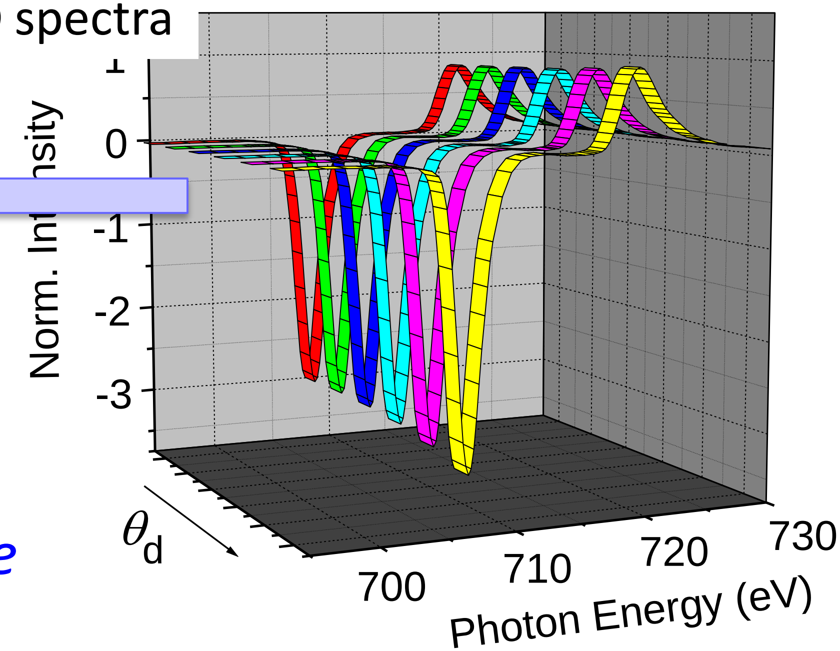
Depth-resolved XMCD



APL **84** 936-938 (2004)



A series of XMCD spectra



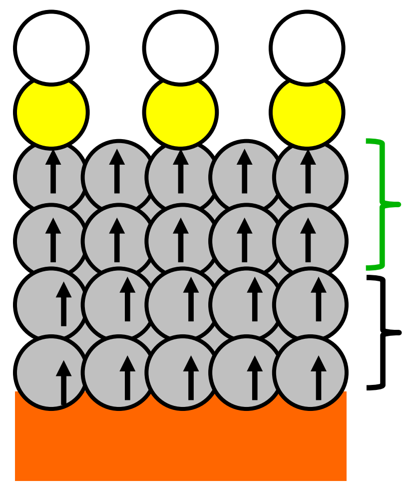
model analyses

Depth profile of magnetic structure

CO adsorption on Fe/Cu(001)

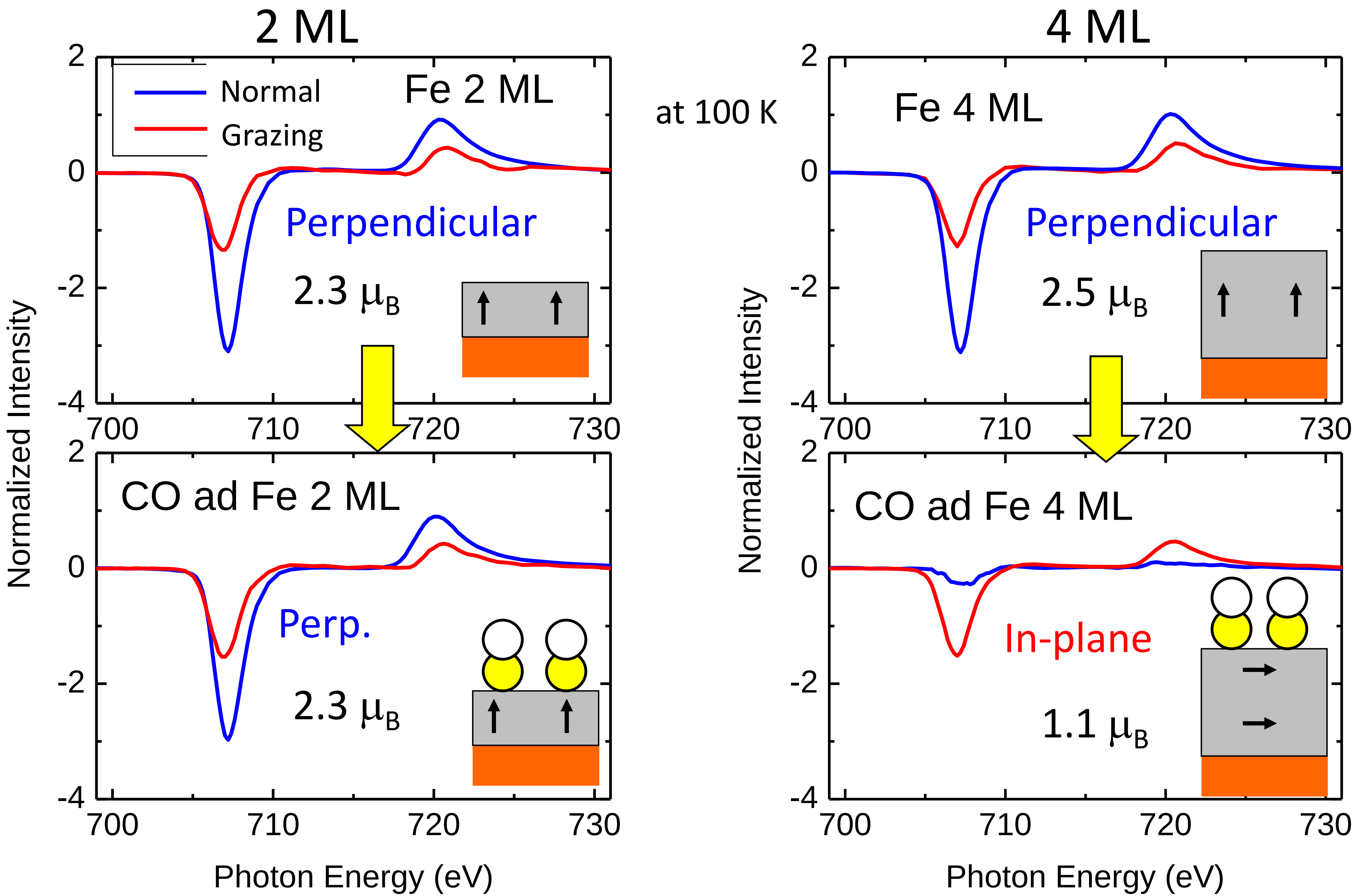
(CO molecules adsorb on atop sites.)

The magnetization of top layers disappears upon CO adsorption.



PRB **77**, 054409 (2008)

XMCD: Fe 2 and 4 ML, CO adsorption



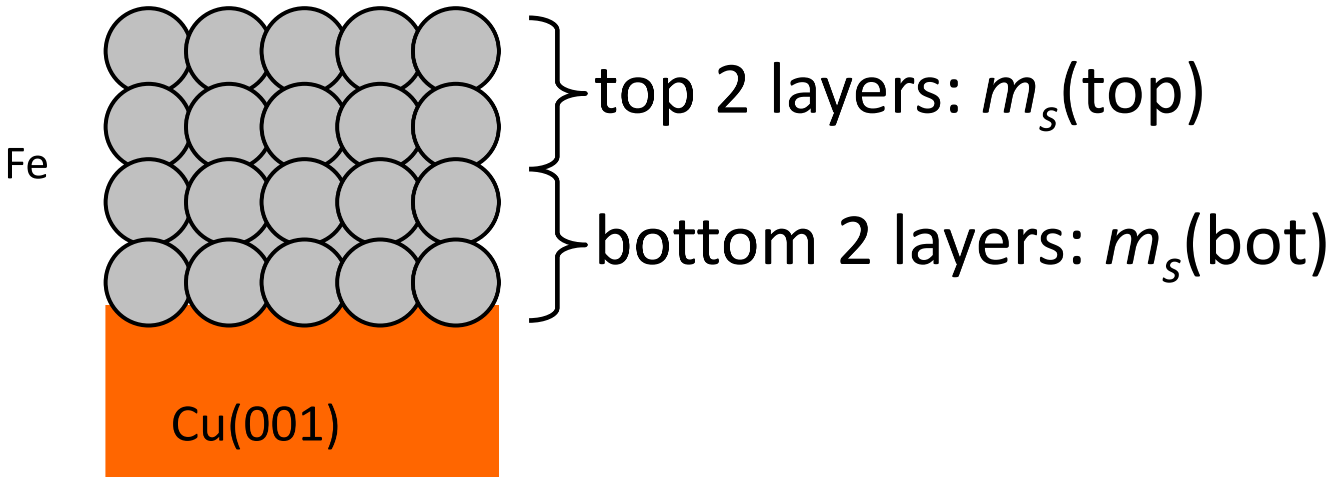
m_s^{eff} of Fe/Cu(001), CO adsorption

Fe	ML	Clean	CO ad.	
Regime I	2	2.3 μ_B, ⊥	2.3 μ_B, ⊥	No change
	3	2.4 μ_B, ⊥	1.5 μ_B, // 2/3	Mag. decrease SRT to In-plane
	4	2.5 μ_B, ⊥	1.1 μ_B, // 1/2	Mag. decrease SRT to In-plane

⊥ : Perpendicular

// : In-plane

A model to simulate the magnetic structure

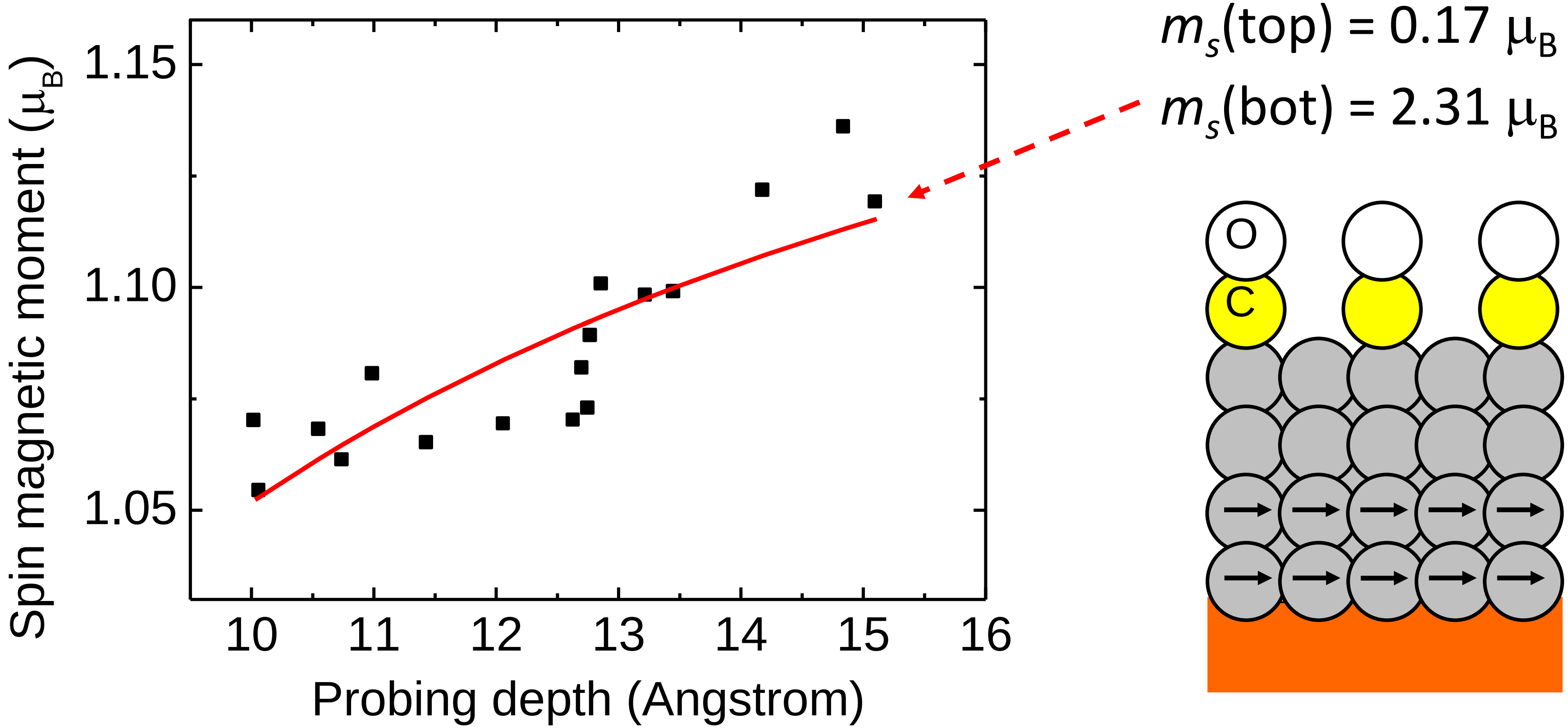


$$m_s(x) = \frac{m_s(\text{top}) \cdot \sum_{j=1}^{2} \exp\left(-{(j-1)a}/{x}\right) + m_s(\text{bot}) \cdot \sum_{j=3}^{4} \exp\left(-{(j-1)a}/{x}\right)}{\sum_{j=1}^{4} \exp\left(-{(j-1)a}/{x}\right)}$$

Spin magnetic moment to be observed at the probing depth x

a: interlayer distance

The depth profile of m_s of CO/Fe(4 ML)/Cu(001)

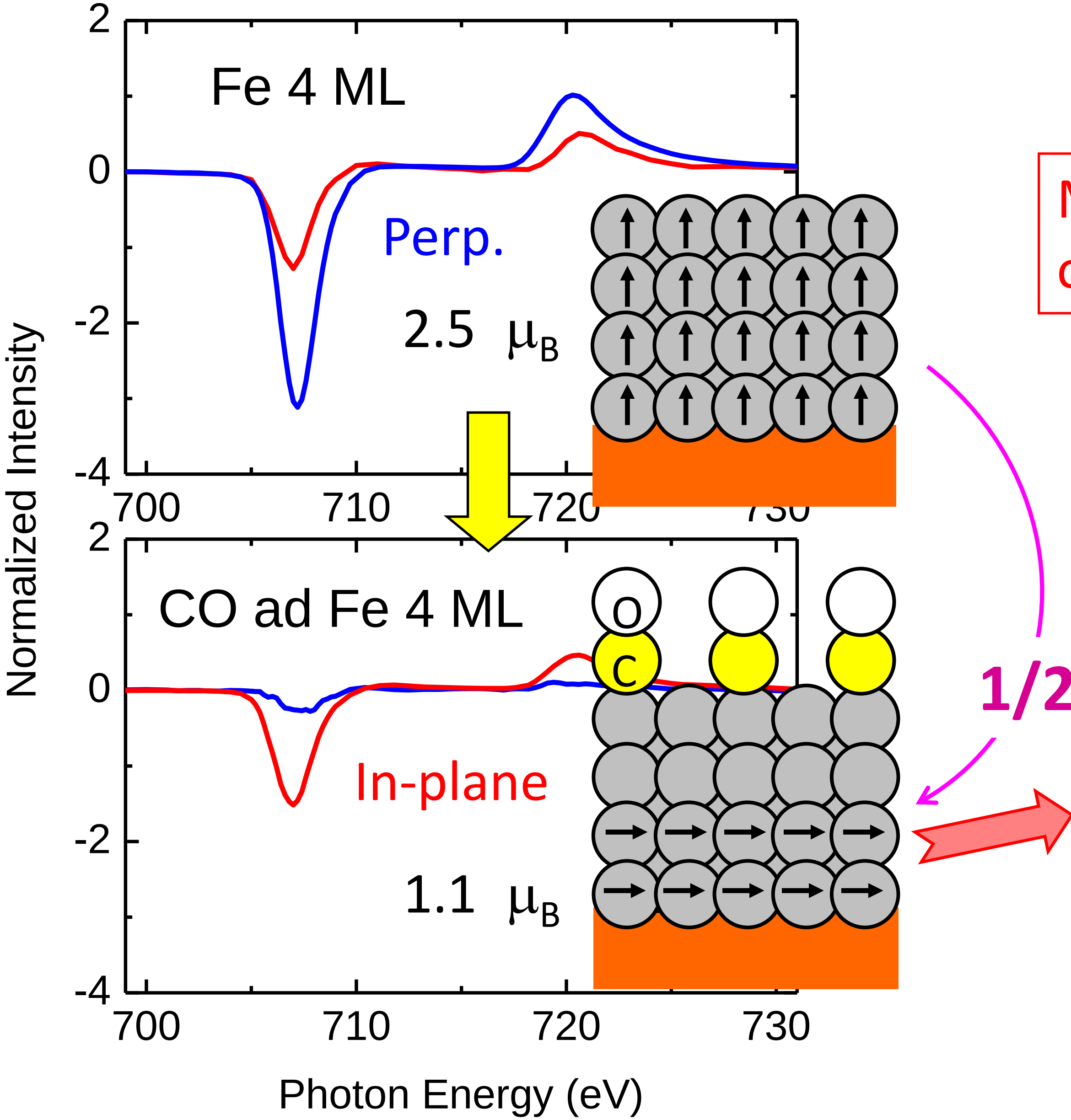


The top two layers magnetization disappeared.

PRB **77**, 054409 (2008)

XMCD: Fe 4 ML, CO adsorption

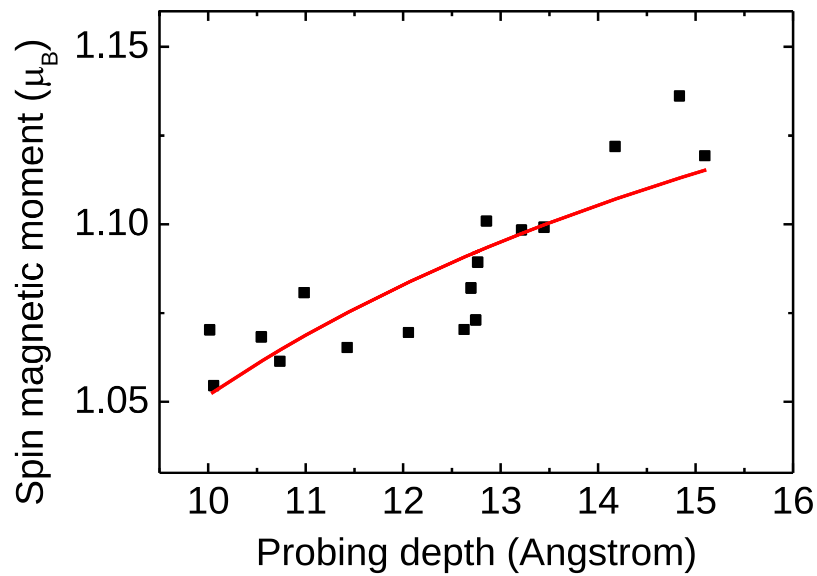
at ~120 K



Magnetization disappearance of surface two layers

m_s(top) = 0.17 μ_B

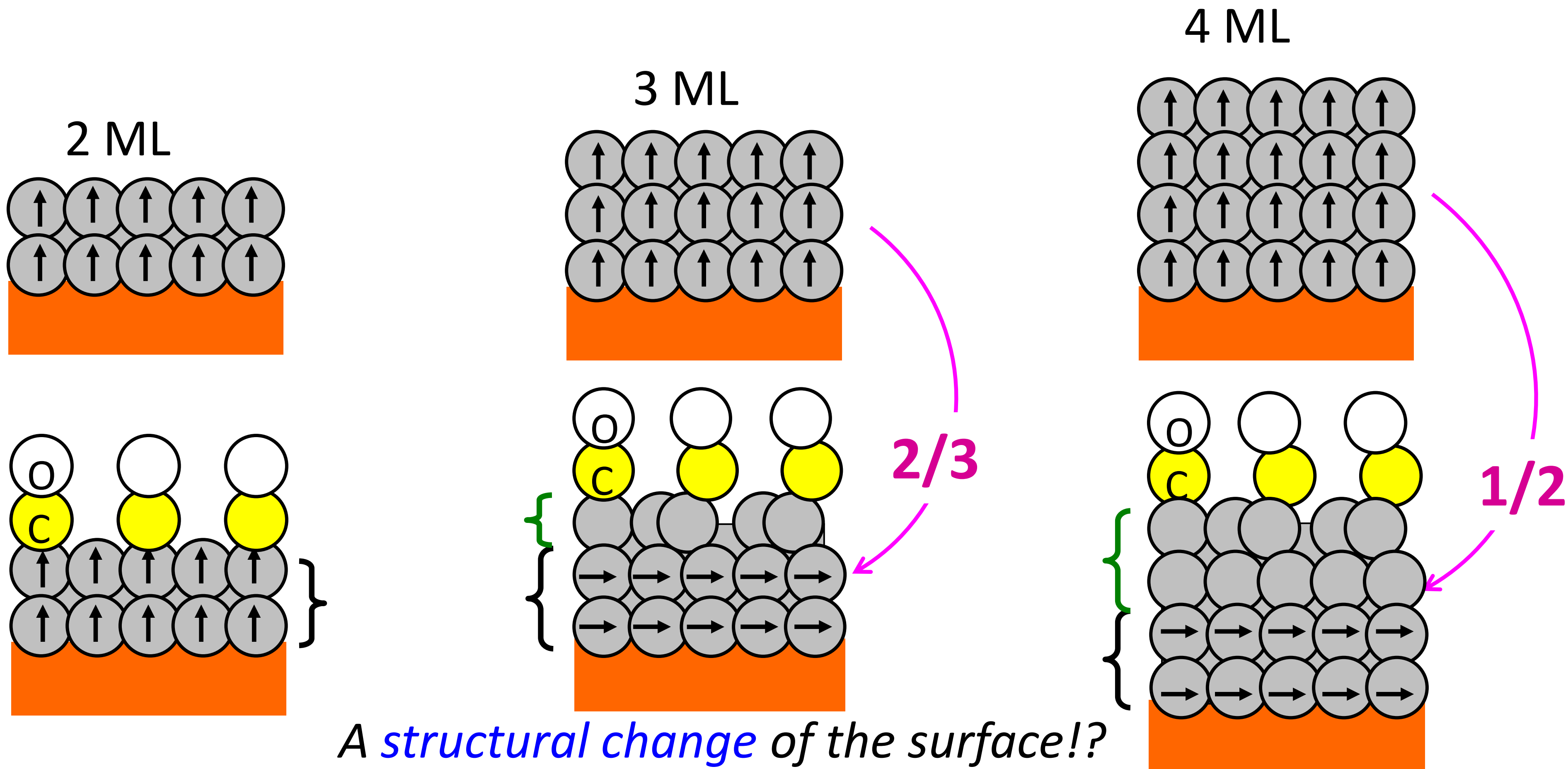
m_s(bot) = 2.31 μ_B



PRB **77**, 054409 (2008)

Apparent magnetization decrease

1. Cu(001) keeps the magnetization of adjacent Fe two layers.
2. Adsorbed CO vanishes the magnetization of top two layers at most.



A ***structural change*** *of the surface!?*

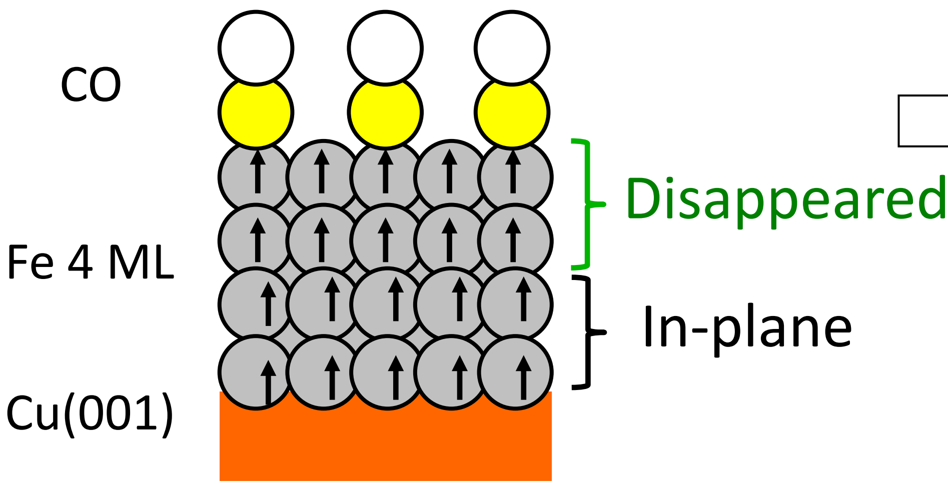
EXAFS experiment.

Motivation: to reveal film structures by EXAFS

to discuss ***the relationship*** *between* ***the anomalous magnetism*** *and* ***the structure***

the result of depth-resolved XMCD

magnetization vanishment of top two layers

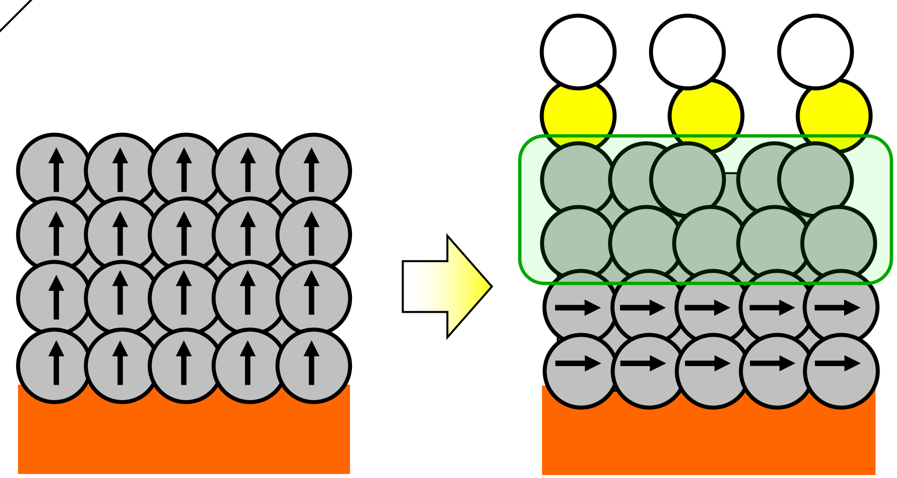


PRB **77**, 054409 (2008)

Surf-EXAFS measurements

to study **the structure of the films**

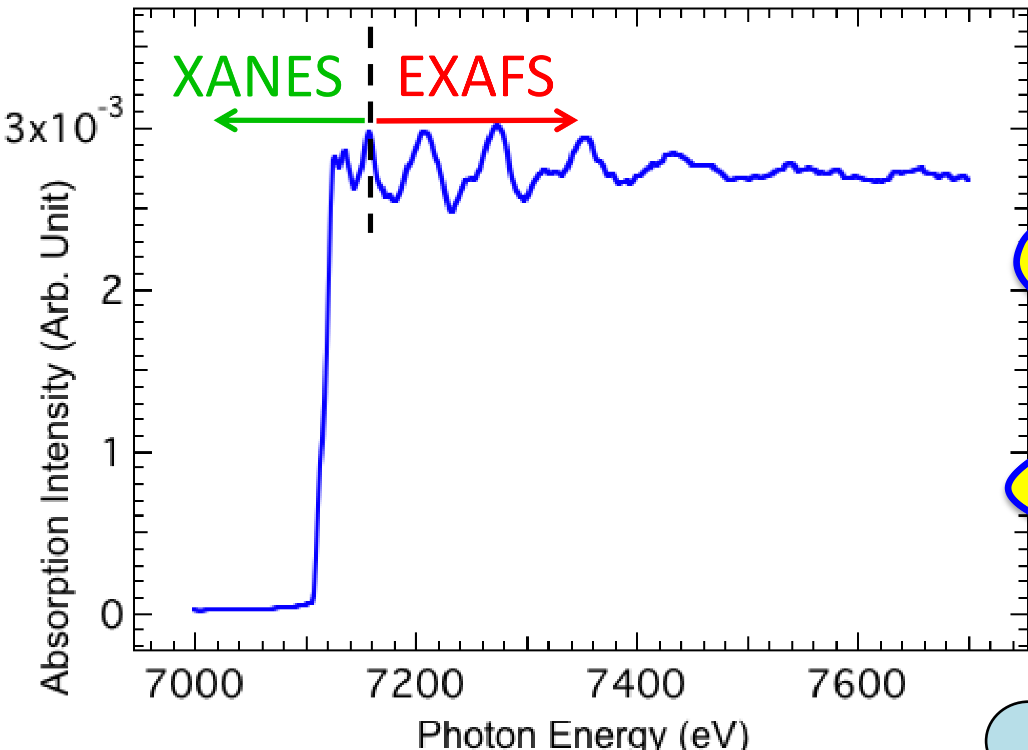
Structural change!?



about EXAFS

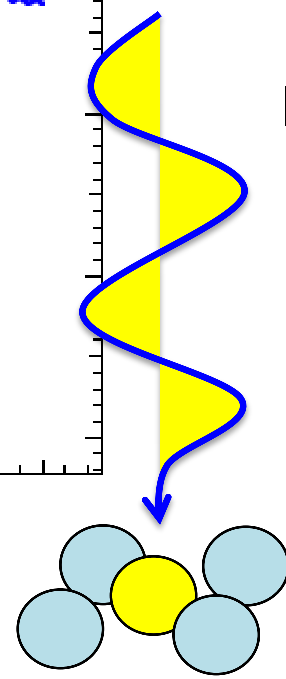
XAFS (X-ray Absorption Fine Structure)

- XANES (X-ray Absorption Near Edge Structure)
- EXAFS (Extended X-ray Absorption Fine Structure)



Element specificity

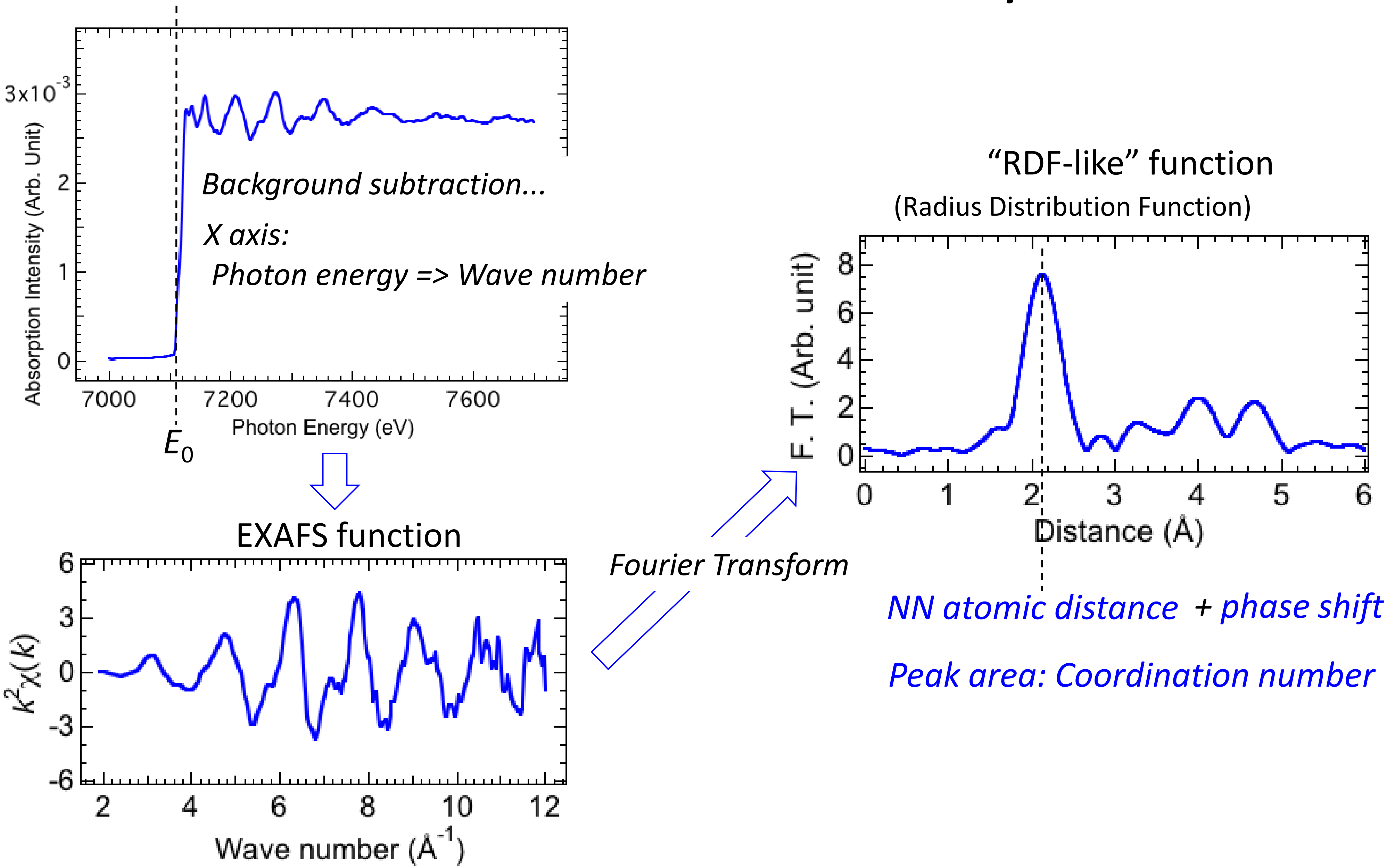
Direct observation of Crystalline anisotropy
(based on polarization dependence)



Local structure

- Coordination number
- Bond length
- Debye-Wallar factor, etc.

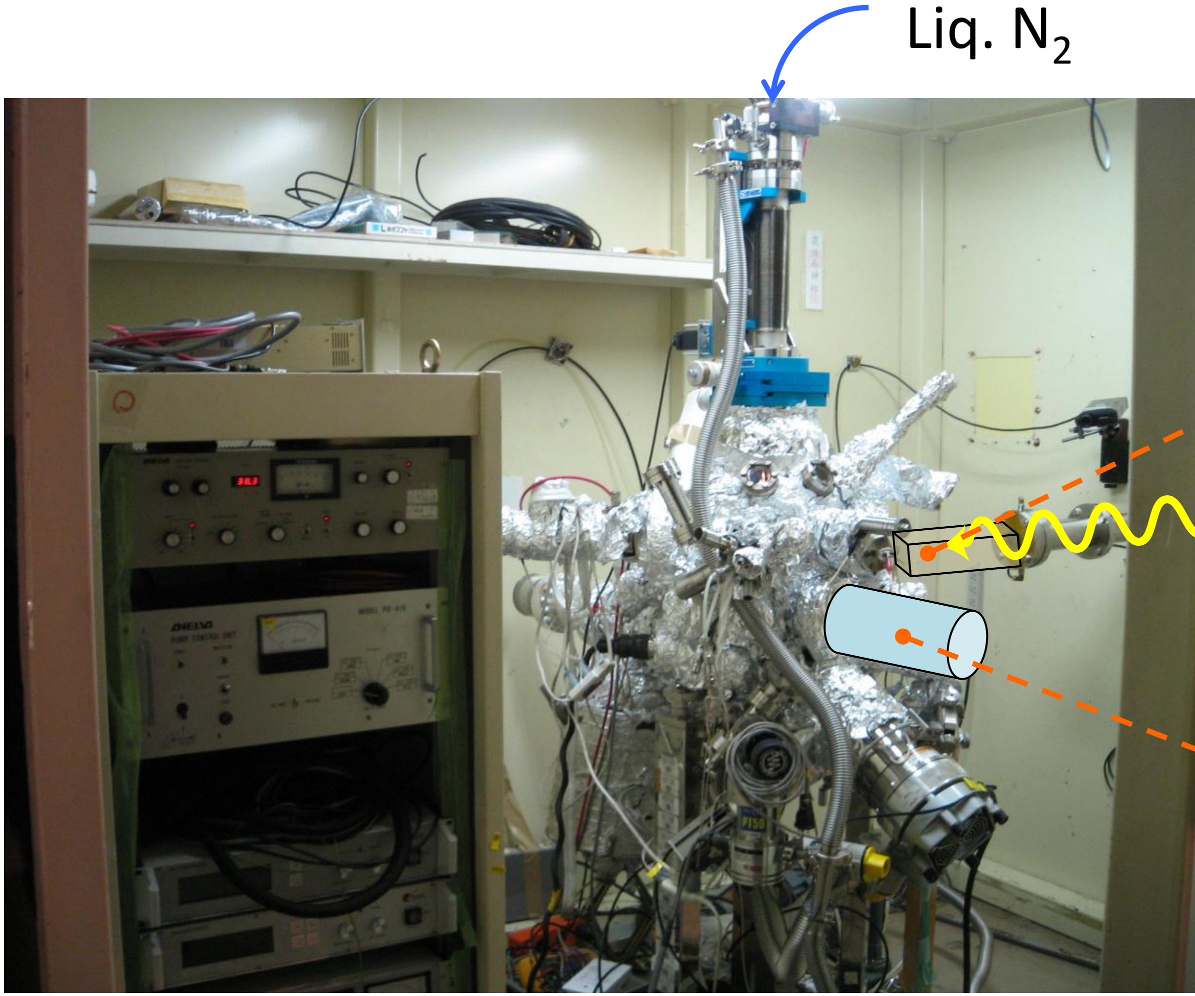
Procedure of EXAFS Analysis



Fluorescence yield EXAFS experiment

to study the structures of the films

at PF BL-7C

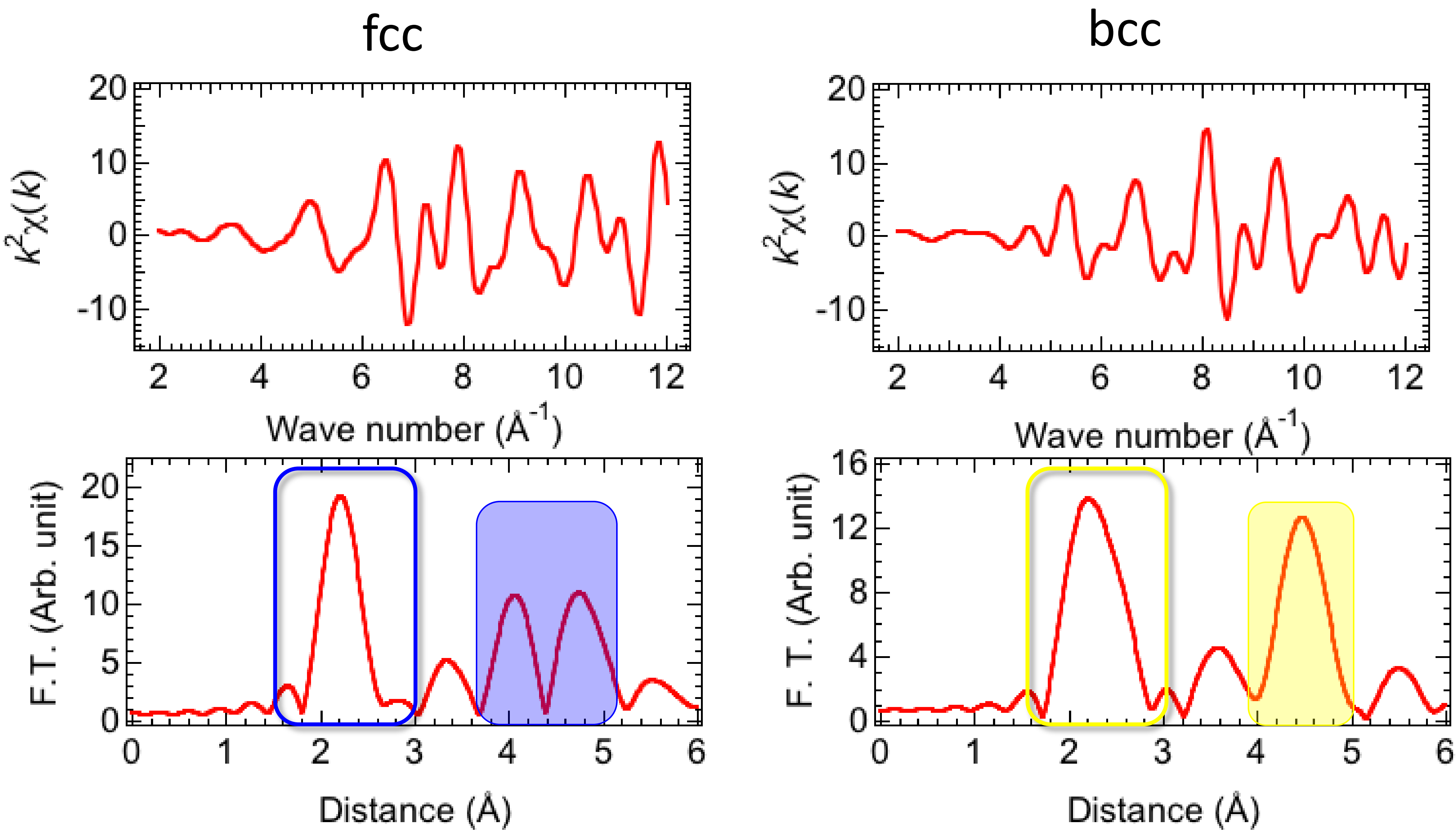


Fe *K*-edge EXAFS

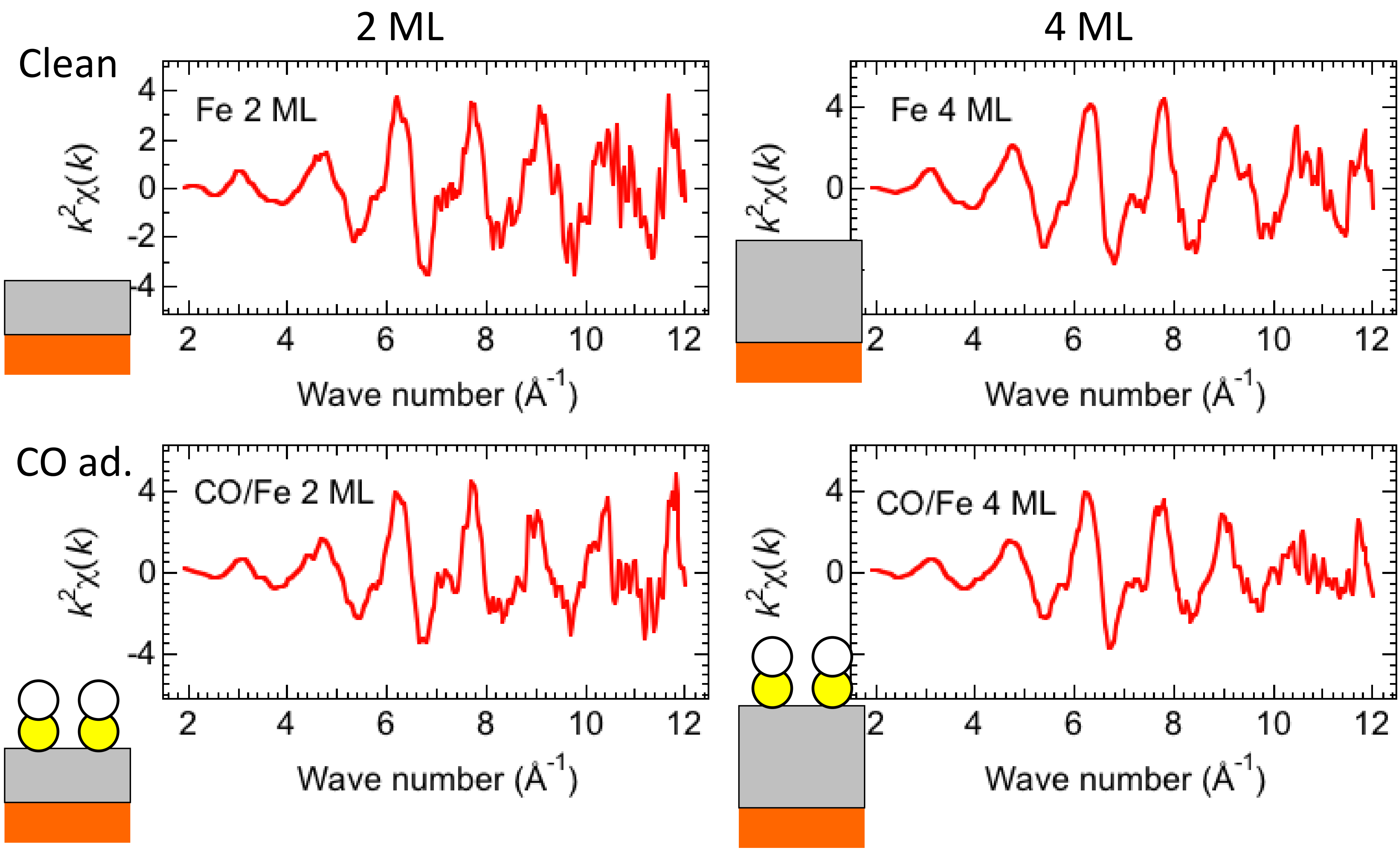
CO/Fe(2, 4 ML)/Cu(001)

NO/Fe(2, 4 ML)/Cu(001)

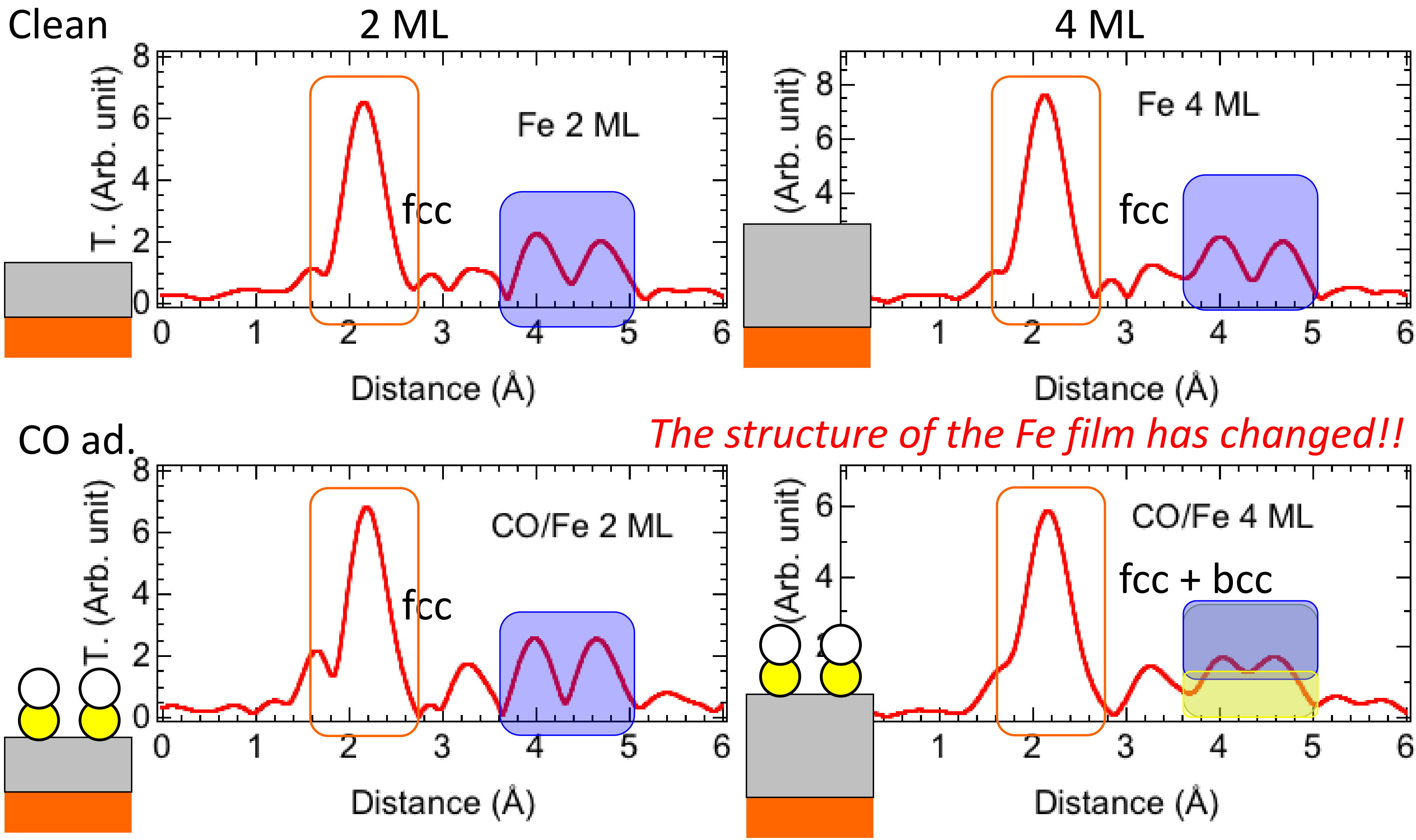
Fe-*K* EXAFS, FEFF simulation



Obtained EXAFS functions



Fourier Transforms of $\chi(k)$



Curve fit for Fe 2 ML, CO-ad.

Sample	model	CN	Radius	R-factor	Conclusion
Fe 2ML	fcc	4.61	2.55	0.038	fcc
	bcc	3.56	2.49	0.205	
	fcc & bcc	4.30	2.55	0.019	
		0.31	2.47		
CO/Fe 2 ML	fcc	4.52	2.56	0.116	fcc
	bcc	3.30	2.50	0.231	
	fcc & bcc	4.43	2.56	0.091	
		2.04	2.38		

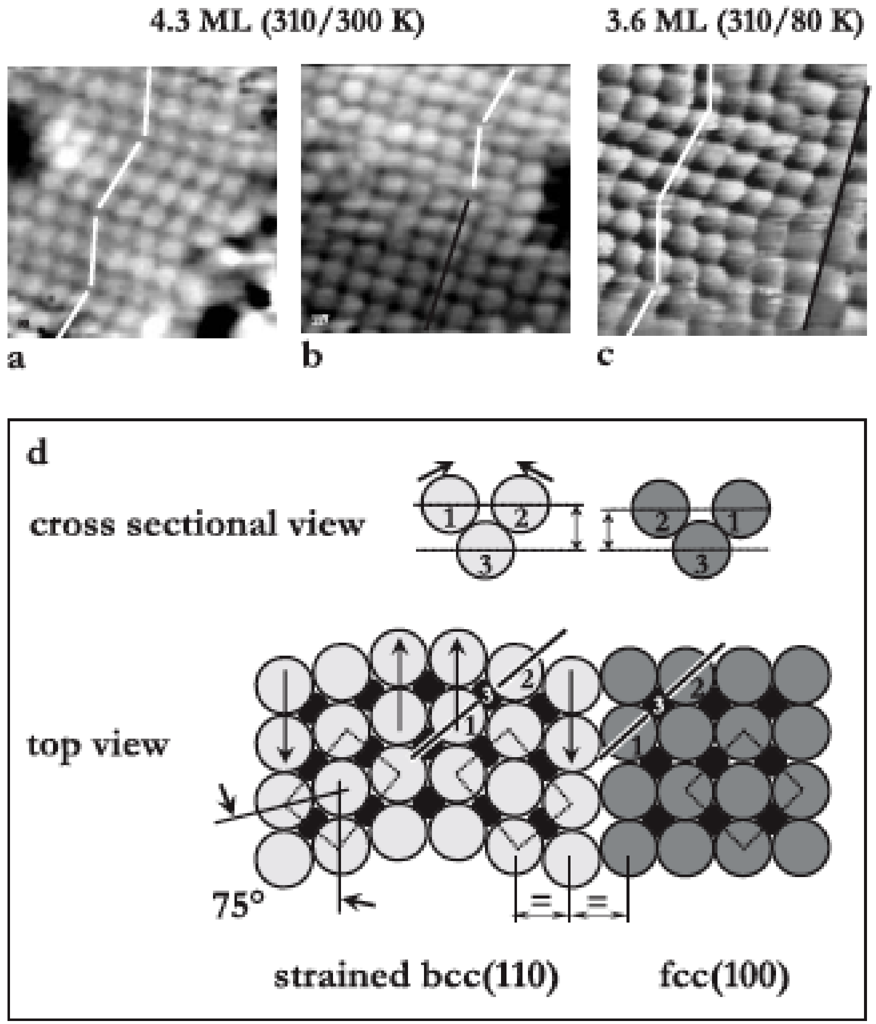
too short (2.38)

Curve fit for Fe 4 ML, CO-ad.

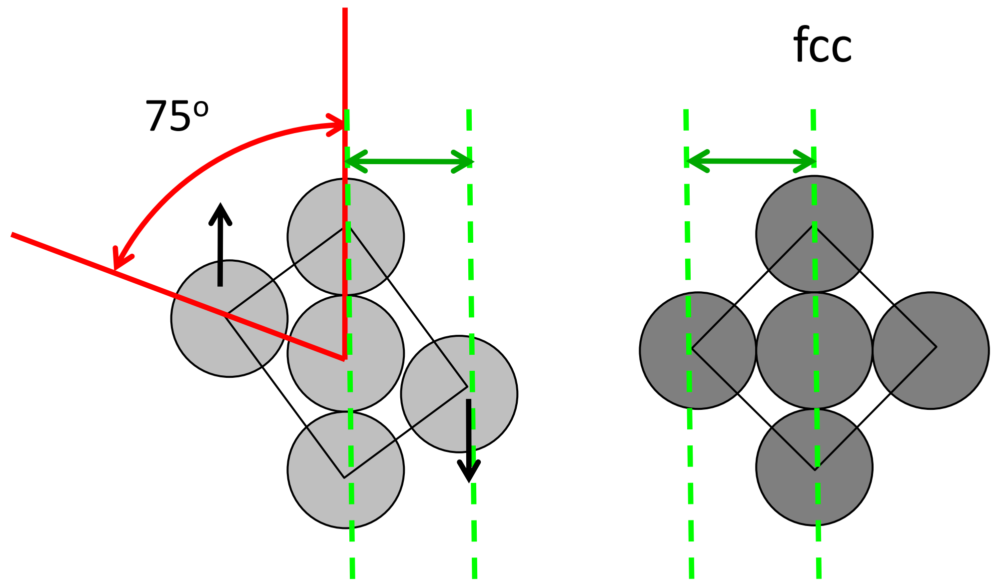
Sample	model	CN	Radius	R-factor	Conclusion
Fe 4ML	fcc	6.51	2.53	0.061	fcc
	bcc	5.78	2.48	0.207	
	fcc & bcc	5.12	2.53	0.036	
		1.96	2.51		
CO/Fe 4 ML	fcc	6.56	2.55	0.124	fcc + bcc
	bcc	6.72	2.49	0.183	
	fcc & bcc	4.08	2.56	0.074	
		3.00	2.47		

Strained bcc structure observed by STM

Fe/Cu(001)



bcc-like structure; “strained bcc”

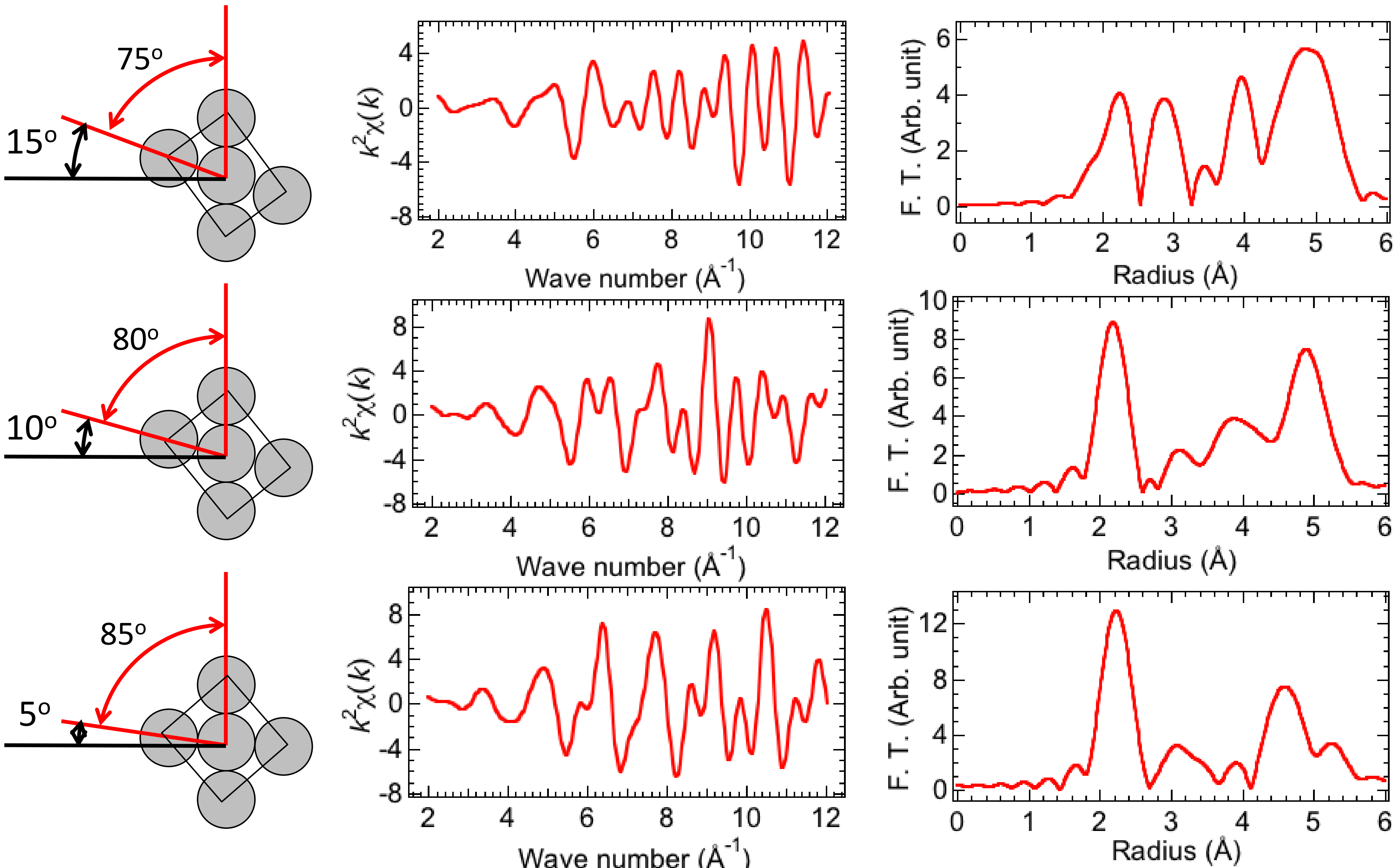


bonding angle 75°

(shear angle 15°)

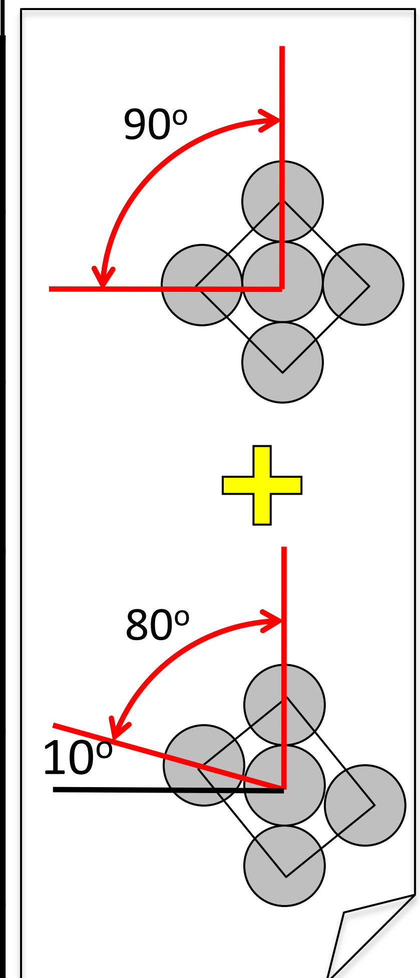
A. Biedermann, *et al.*, Appl. Phys. A **78**, 807–816 (2004)

strained bcc: models, $k^2\chi(k)$, FT



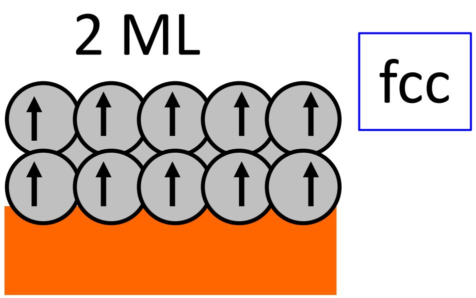
CO/Fe(4 ML)/Cu(001) curve fit results

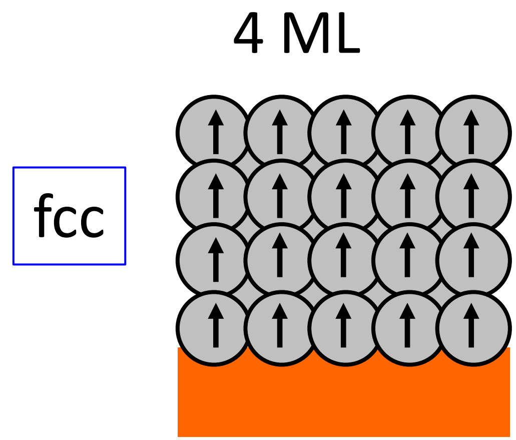
geometry	model	CN	Radius	R-factor
NI(90°)	fcc + strained bcc(**15°**)	5.53	2.548	0.042
		1.23	2.558	
	fcc + strained bcc(**10°**)	4.69	2.555	0.023
		1.73	2.652	
	fcc + strained bcc(**5°**)	4.74	2.555	0.023
		1.53	2.588	
GI(30°)	fcc + strained bcc(**15°**)	3.77	2.569	0.011
		0.97	2.798	
	fcc + strained bcc(**10°**)	3.74	2.563	0.014
		1.95	2.697	
	fcc + strained bcc(**5°**)	Not converged		



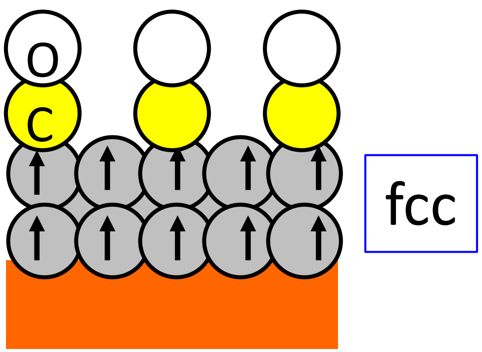
Possible model of structures of the films

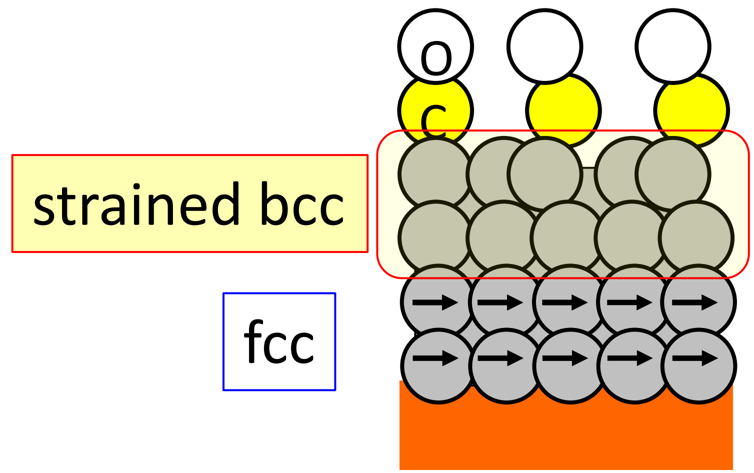
Before CO ad. : fcc





<u>Probably Changed to be fcc + strained bcc</u>





...though further precise analyses are required.

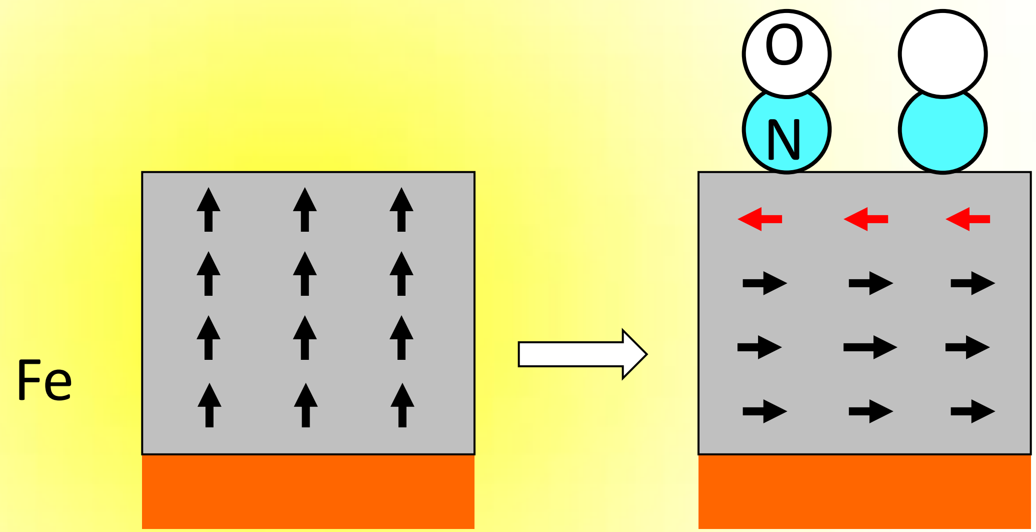
Before going to our EXAFS results of CO/Fe/Cu(001)...,

NO adsorption on Fe/Cu(001)

Antiferromagnetic coupling at the surface

Conventional XMCD
Depth-resolved XMCD

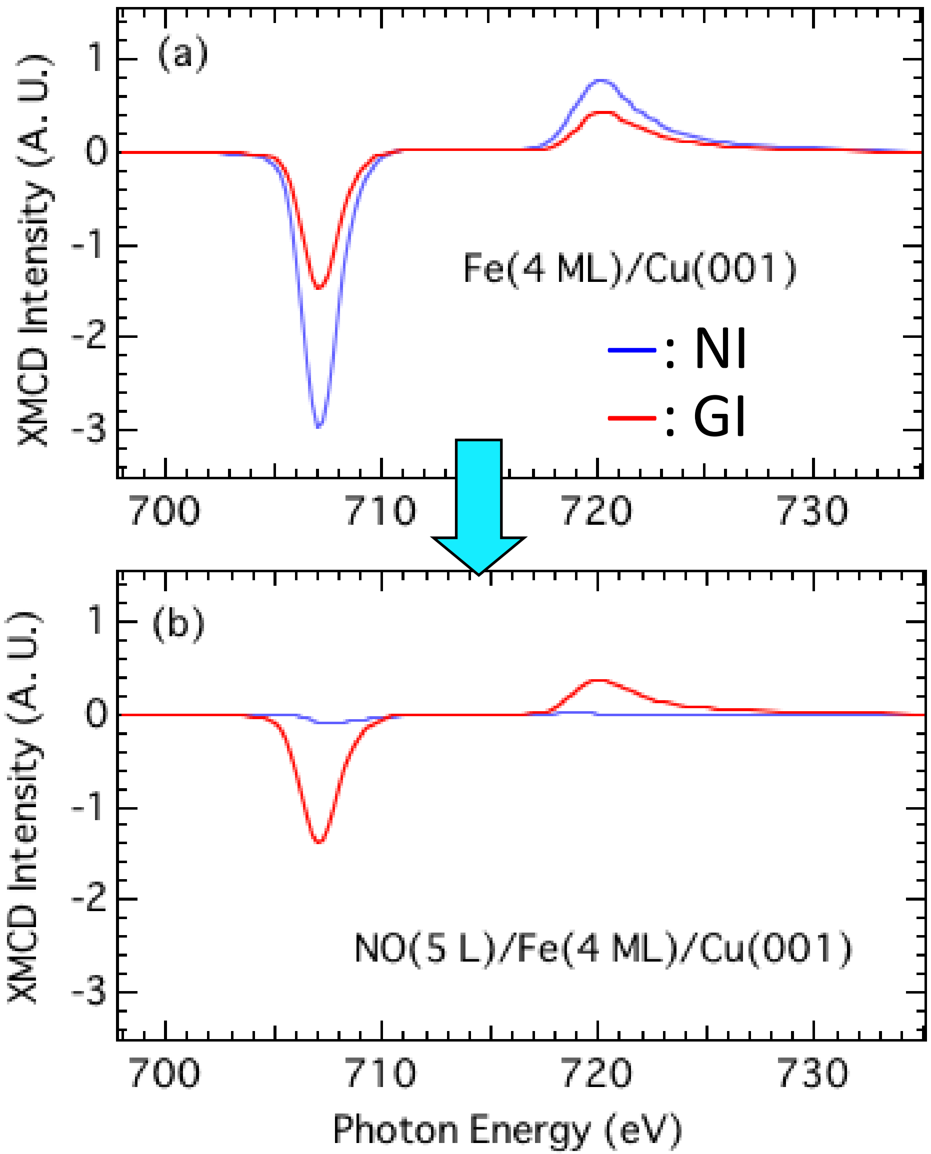
At 100-120 K

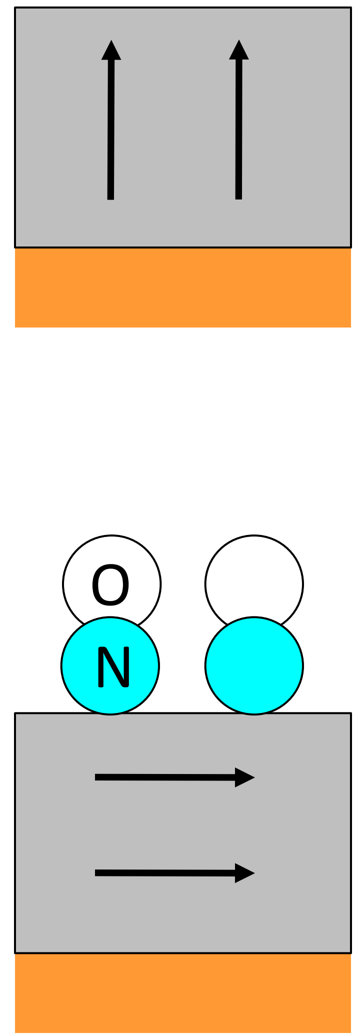


To investigate the magnetic properties

NO: Linear hetero-diatomic molecule, as same as CO
One more electron than CO
=> may affect on electronic structure more

NO adsorption on Fe(4 ML)/Cu(001)





Perpendicular

2.5 μ_B

1/2

In-plane

1.2 μ_B

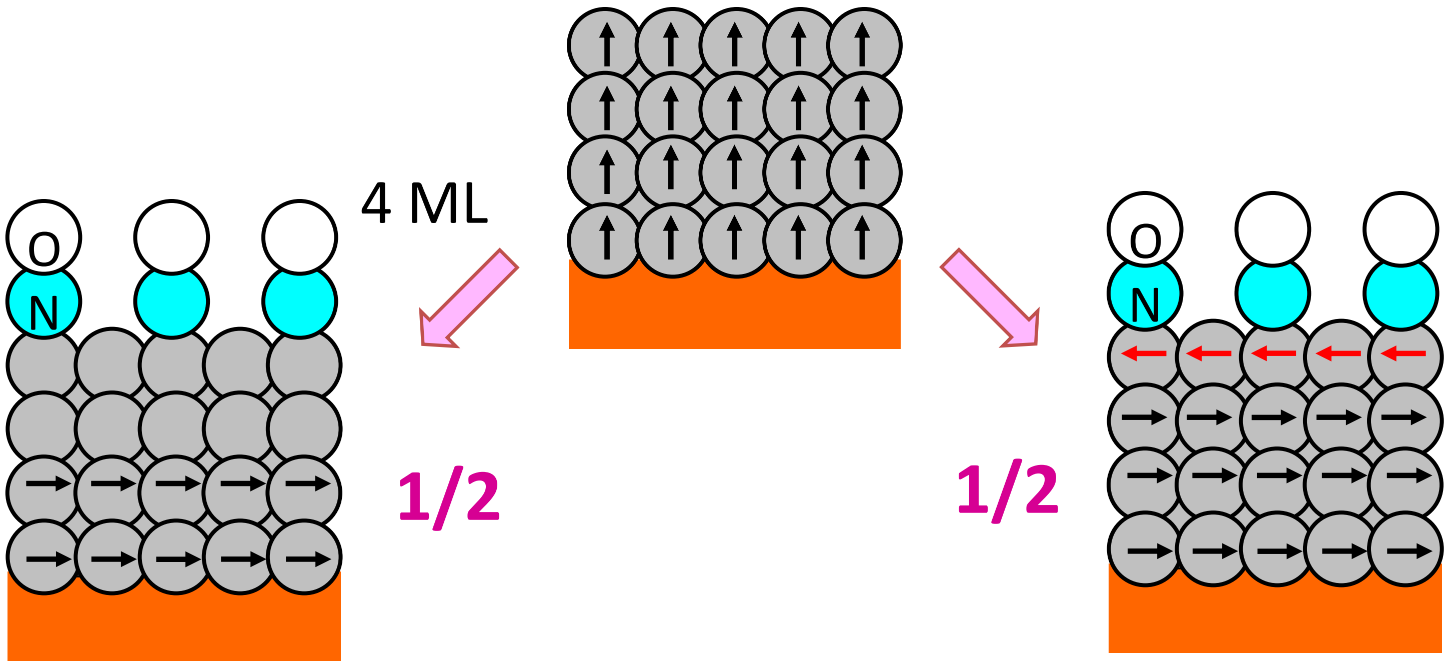
m_s^{eff} of Fe/Cu(001), NO adsorption

ML	Clean	NO ad	cf. CO ad
2	2.5 μ_B, ⊥	~0 μ_B	2.3 μ_B
3	2.5 μ_B, ⊥	0.9 μ_B, // **1/3**	1.5 μ_B (2/3)
4	2.5 μ_B, ⊥	1.2 μ_B, // **1/2**	1.2 μ_B (1/2)

The results are similar to the CO's case but not the same.

⊥ : Perpendicular
// : In-plane

Possible models to express the decrease



Model 1: **Demagnetized model**,
The magnetization of the surface two layers disappears.

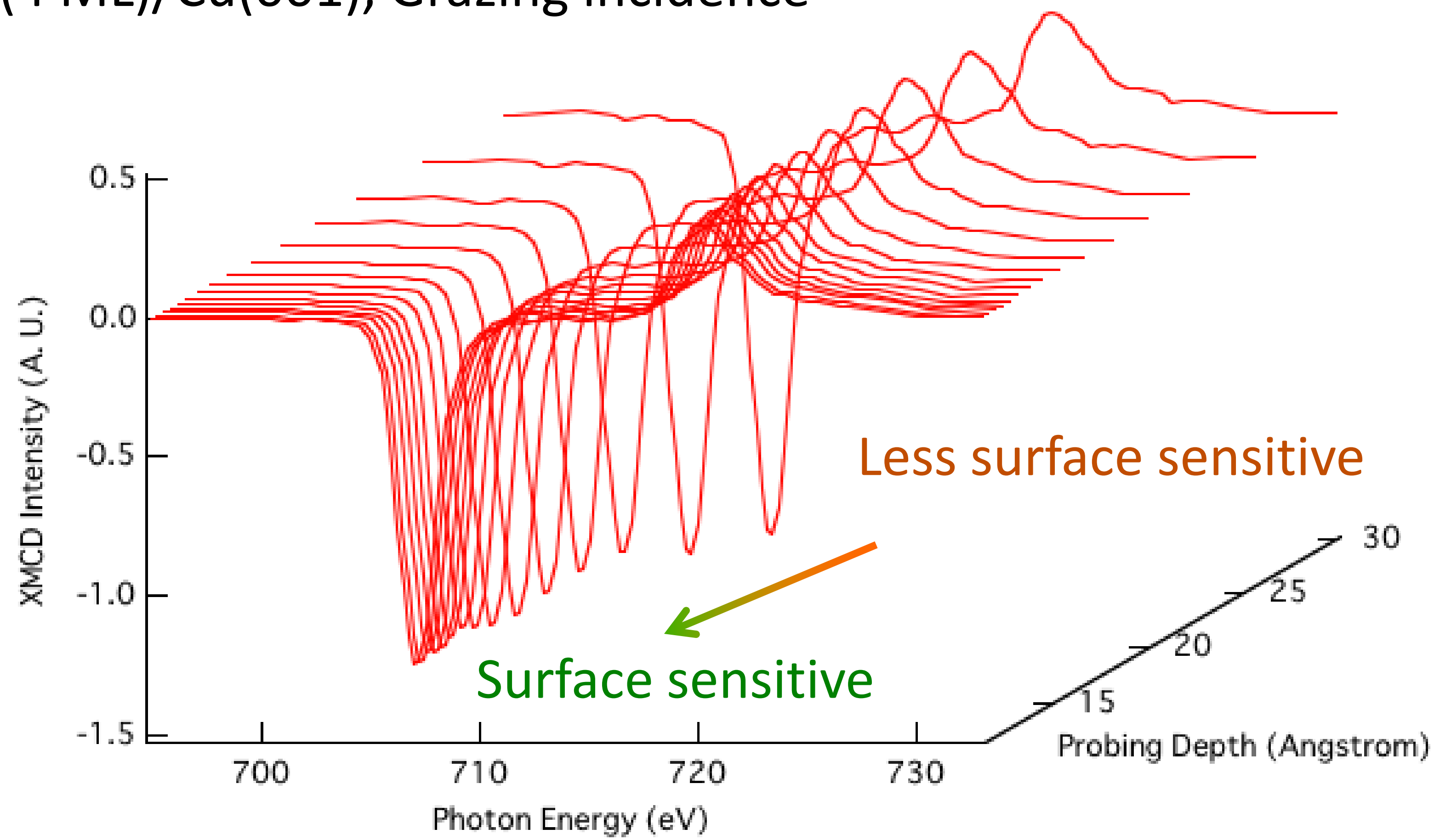
Model 2: **AFM coupling model**,
Antiferromagnetic between the surface two layers
(The topmost layer: opposite direction.)

Which is true?

A turn of the depth-resolved XMCD method!!

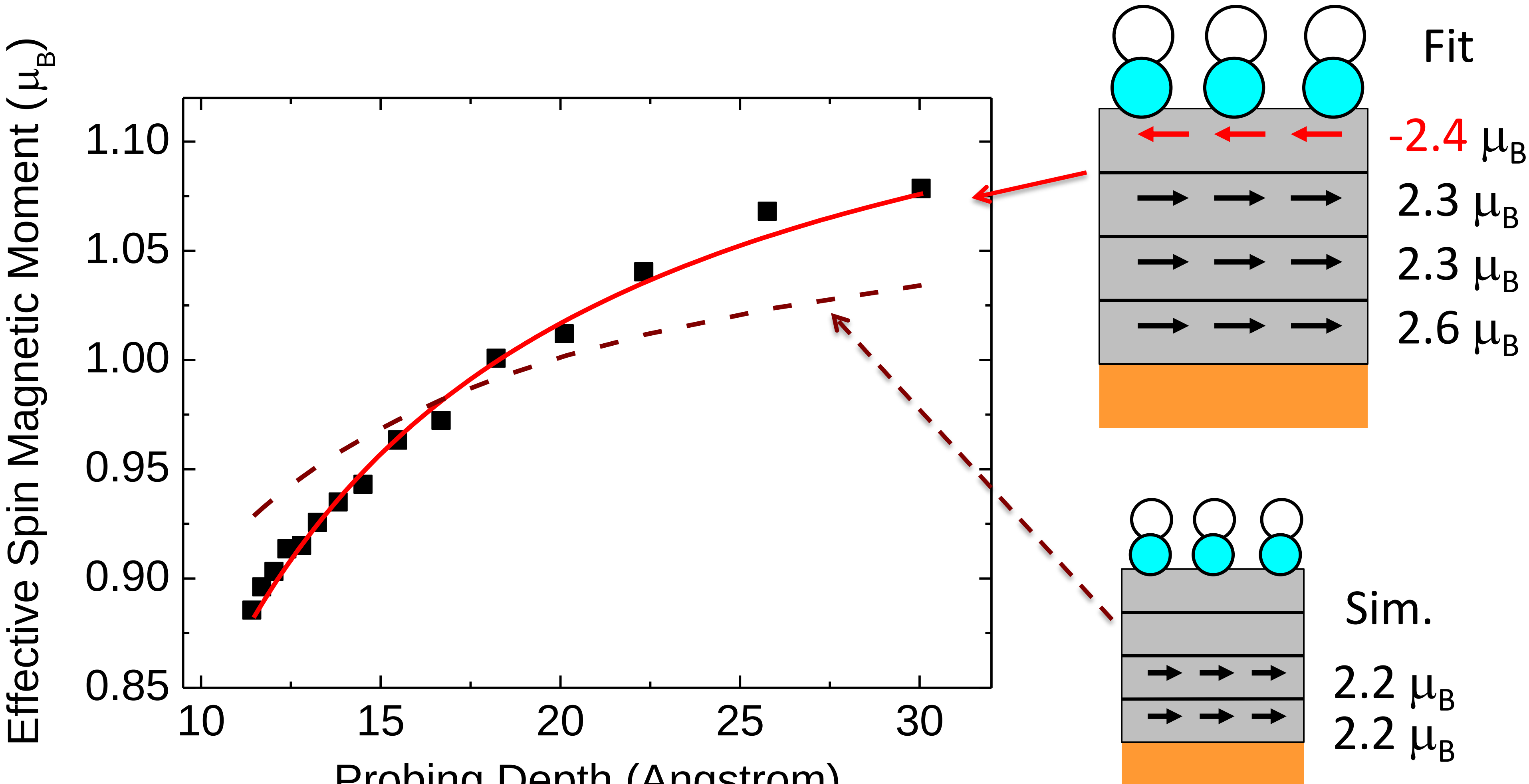
Probing depth dependence of the XMCD spectra

NO/Fe(4 ML)/Cu(001), Grazing incidence



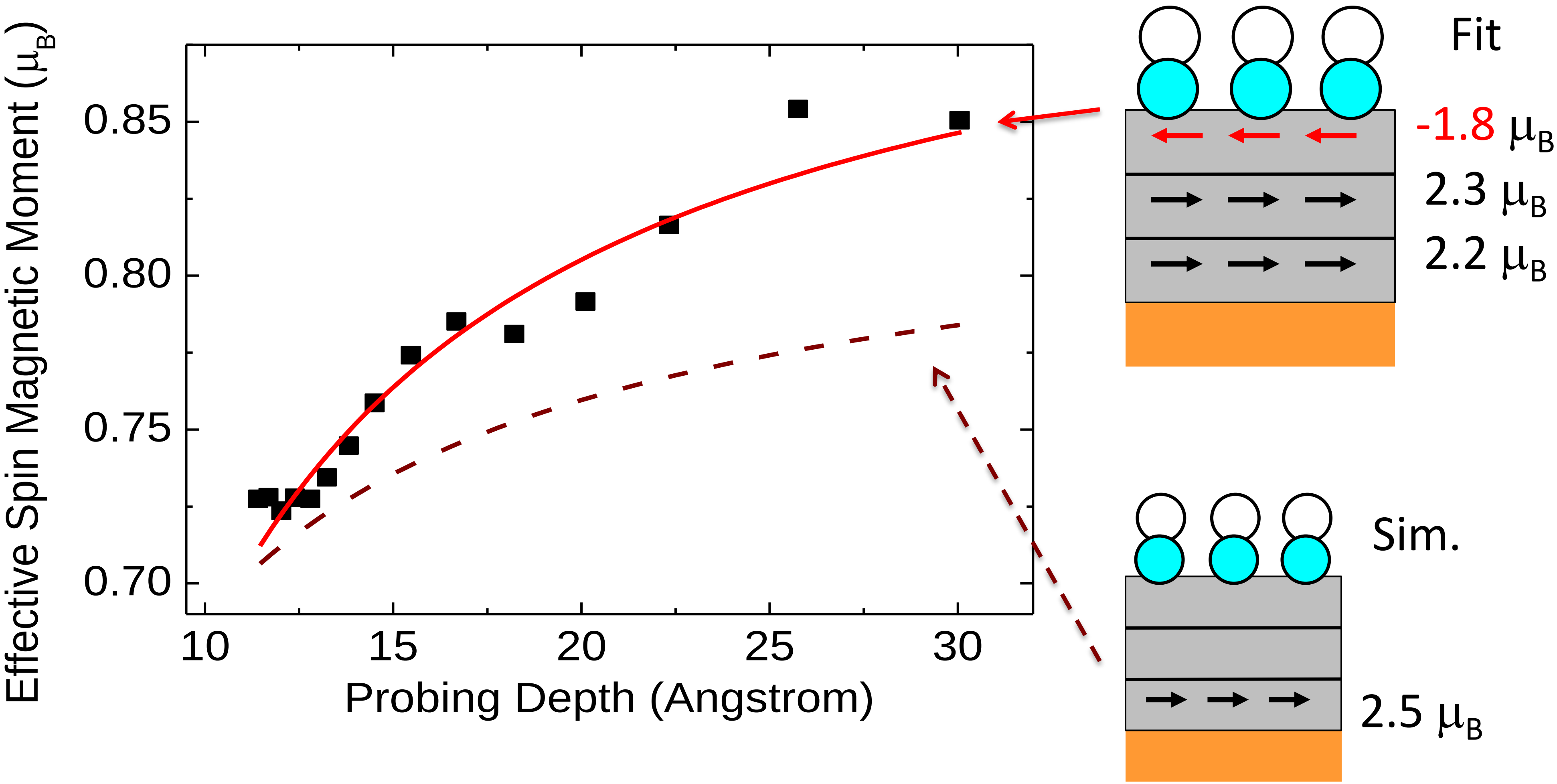
Obtained m_s^{eff} , NO/Fe(4 ML)/Cu(001)

m_s^{eff} of the NO-ad topmost layer: Opposite direction



Obtained m_s^{eff}, NO/Fe(3 ML)/Cu(001)

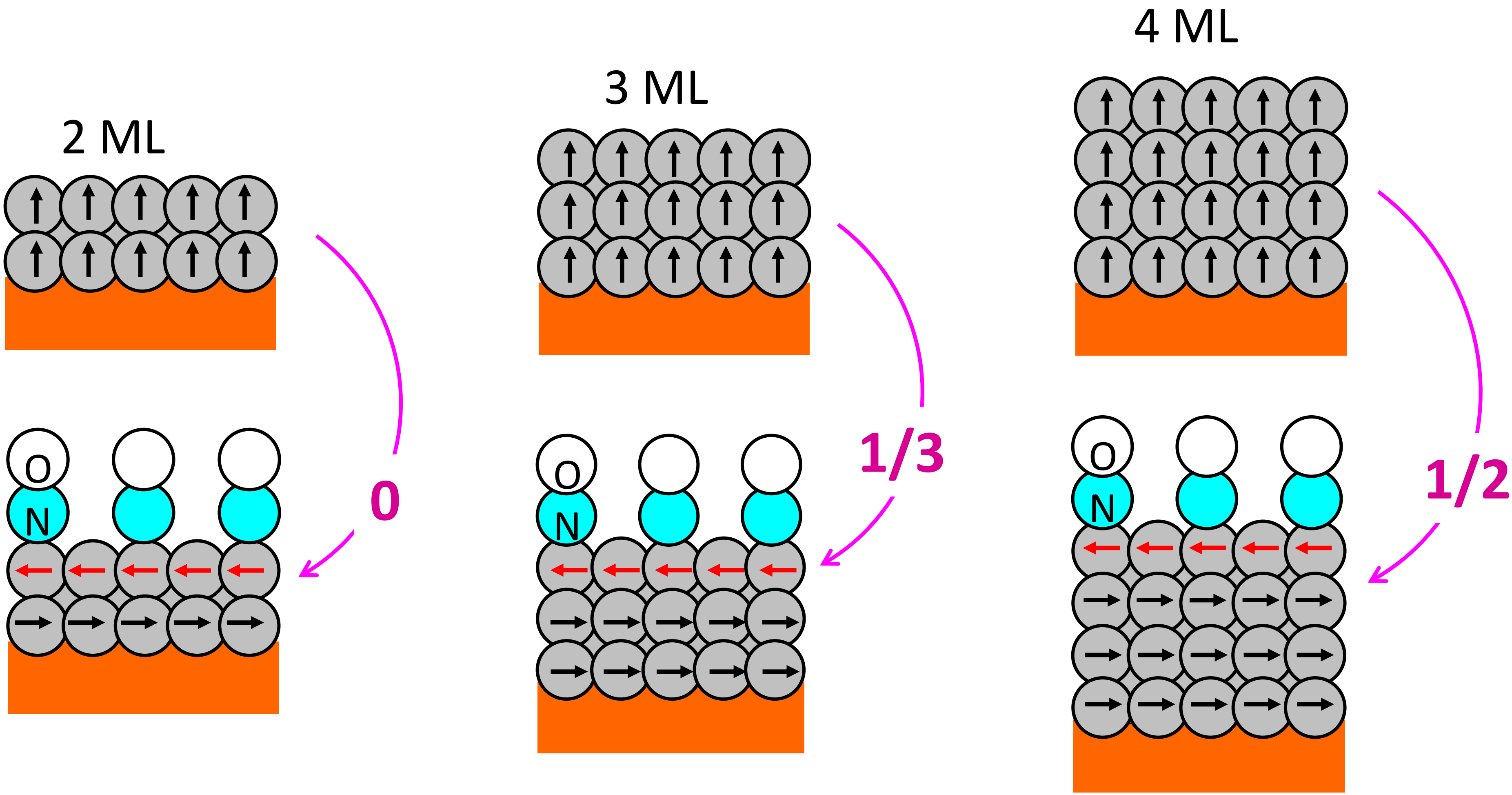
m_s^{eff} of the NO-ad topmost layer: Opposite direction



The reason of the apparent decrease of magnetization

The topmost spin aligns in the opposite direction.

(Antiferromagnetic coupling between the top two layers)



Summary

Anomalous surface magnetic states and their structure

NO or CO adsorption: SRT to in-plane magnetization

- Adsorbed CO demagnetizes the top layer(s) of Fe/Cu(001).
- The surface of CO/Fe(4 ML)/Cu(001) probably changed from fcc to strained-bcc structure.

- The m_s^{eff} of Fe topmost layer aligns in the opposite direction to that of the other layers upon NO adsorption.

  (Antiferromagnetic coupling in the surface two layers)