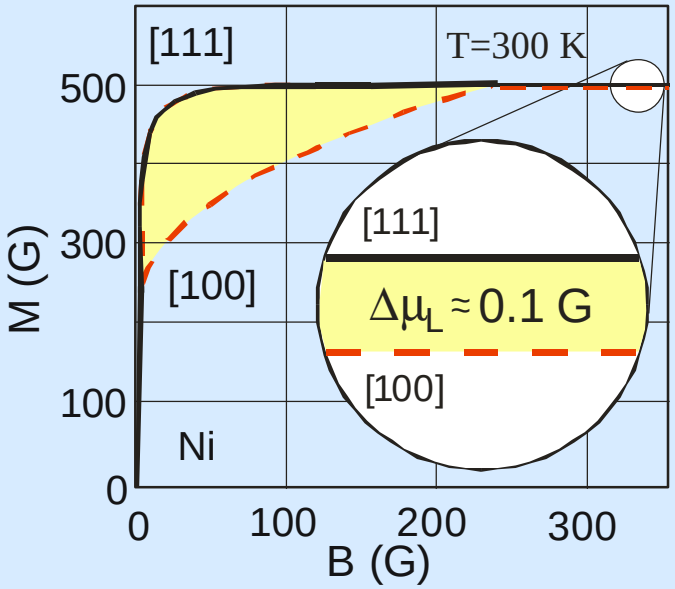
Lecture 2: Magnetic Anisotropy Energy (MAE)

1. Magnetic anisotropy energy = f(T)
2. Anisotropic magnetic moment ≠ f(T)



Characteristic energies of metallic ferromagnets

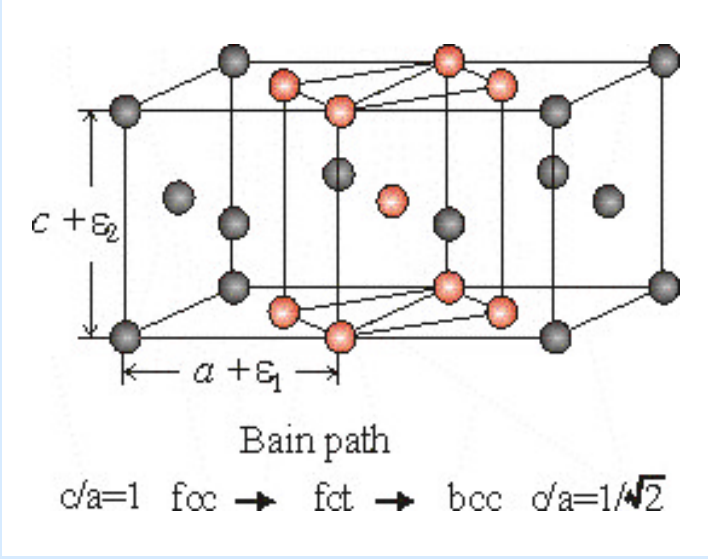
binding energy	1 - 10 eV/atom
exchange energy	10 - 10^3 meV/atom
cubic MAE (Ni)	0.2 μeV/atom
uniaxial MAE (Co)	70 μeV/atom

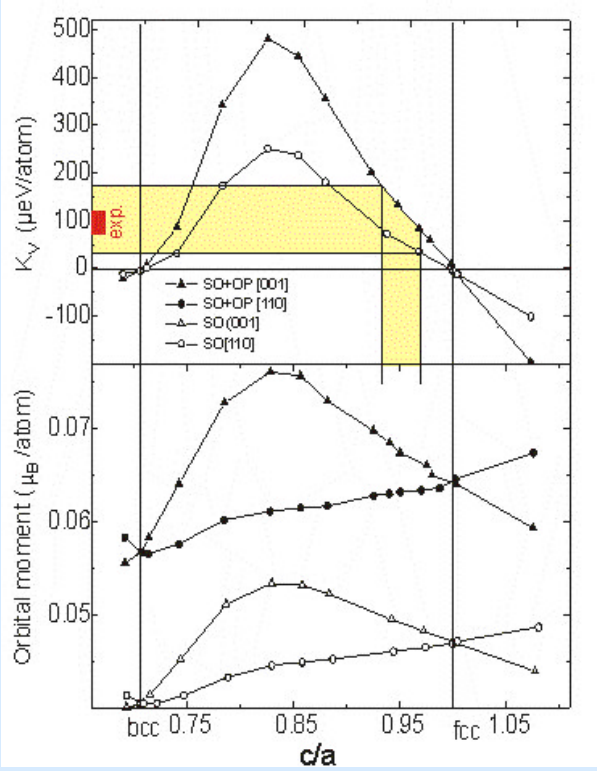
$$MAE = \int M \cdot dB \approx \frac{1}{2}\Delta M \cdot \Delta B \approx \frac{1}{2} 200 \cdot 200 G^2$$

$$MAE \approx 2 \cdot 10^4 \, erg/cm^3 \approx 0.2 \mu eV/atom$$

≈ 1μeV/atom is very small compared to
≈ 10 eV/atom total energy but all important

There are only 2 origins for MAE: 1) dipol-dipol interaction $\sim (\bar{\mu}_1 \cdot \bar{r})(\bar{\mu}_2 \cdot \bar{r})$ and
2) spin-orbit coupling ? **L S** (intrinsic K or ΔE_{band})





O. Hjortstam, K. B. et al. PRB **55**, 15026 ('97)

R. Wu et al. JMMM **170**, 103 ('97)

Structural changes by ≈ 0.05 Å increase MAE

by 2-3 orders of magnitude (~0.2→100μeV/atom)

Body-Centered-Cubic Ni and Its Magnetic Properties

C. S. Tian, D. Qian, D. Wu, R. H. He, Y. Z. Wu, W. X. Tang, L. F. Yin, Y. S. Shi, G. S. Dong, and X. F. Jin*
Surface Physics Laboratory, Fudan University, Shanghai 200433, China

X. M. Jiang,[1] F. Q. Liu,[1] H. J. Qian,[1] K. Sun,[2] L. M. Wang,[2] G. Rossi,[3] Z. Q. Qiu,[4] and J. Shi[5]
[1]*National Synchrotron Radiation Laboratory, Beijing 310027, China*
[2]*Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor Michigan 48109, USA*
[3]*Laboratorio Nazionale TASC-INFM, Strada Statale 14, km 163.5 Basovizza, I-34012 Trieste, Italy*
[4]*Department of Physics, University of California, Berkeley, California 94720, USA*
[5]*Department of Physics, University of Utah, Salt Lake City, Utah 84112, USA*
(Received 18 November 2004; published 7 April 2005)

The body-centered-cubic (bcc) phase of Ni, which does not exist in nature, has been achieved as a thin film on GaAs(001) at 170 K via molecular beam epitaxy. The bcc Ni is ferromagnetic with a Curie temperature of 456 K and possesses a magnetic moment of $0.52 \pm 0.08 \mu_B$/atom. The cubic magnetocrystalline anisotropy of bcc Ni is determined to be $+4.0 \times 10^6$ ergs $\cdot$ cm^{-3}, as opposed to -5.7×10^4 ergs $\cdot$ cm^{-3} for the naturally occurring face-centered-cubic (fcc) Ni. This sharp contrast in the magnetic anisotropy is attributed to the different electronic band structures between bcc Ni and fcc Ni, which are determined using angle-resolved photoemission with synchrotron radiation.

Free energy density of MAE, K

(intrinsic, after substraction of $2\pi M^2$)

tetragonal [e.g. Ni, Co, Fe (001) / Cu (001)]:

$E_{tetr} = -K_2\, a_z^2 - {}^1\!/_2\, K_{4\wedge}\, a_z^4 - {}^1\!/_2\, K_{4\div\div}\,(a_x^4 + a_y^4) + \ldots$ *(B.Heinrich et al.)*

$= -K_2 \cos^2\vartheta - {}^1\!/_2\, K_{4\wedge} \cos^4\vartheta - {}^1\!/_2\, K_{4\div\div}\, {}^1\!/_4\,(3+\cos 4\varphi)\sin^4\vartheta + \ldots$ *(Bab et al.)*

$= (K_2 + K_{4\wedge})\sin^2\vartheta - {}^1\!/_2\,(K_{4\wedge} + {}^3\!/_4\, K_{4\div\div})\sin^4\vartheta - {}^1\!/_8\, K_{4\div\div}\cos 4\varphi\, \sin^4\vartheta + \ldots$

$= K_2'\sin^2\vartheta + K_{4\wedge}\sin^4\vartheta + K_{4\div\div}\cos 4\varphi\, \sin^4\vartheta + \ldots$ *(traditional)*

hexagonal [e.g. Ni (111), Gd (0001) / W (110)]:

$E_{hex} = k_2 \sin^2\vartheta + {}^1\!/_2 k_{2\div\div}\cos 2\varphi \sin^2\theta + k_4 \sin^4\vartheta + k_{6\wedge}\sin^6\vartheta + k_{6\div\div}\cos 6\varphi\, \sin^6\vartheta + \ldots$

$K = k_2 Y_2^0 + k_{4m} Y_4^m + \ldots$ *Legendre polyn. (B. Coqblin)*

each K_i has a „volume“ and „surface“ contribution

$$K_i = K_i^v + 2K_i^s/d$$

Spin reorientation in bulk Gd

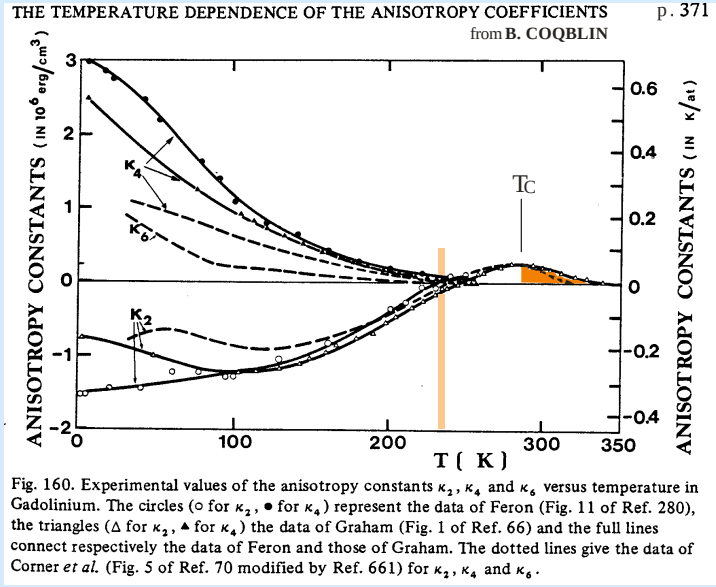


Fig. 160. Experimental values of the anisotropy constants κ_2, κ_4 and κ_6 versus temperature in Gadolinium. The circles (○ for κ_2, ● for κ_4) represent the data of Feron (Fig. 11 of Ref. 280), the triangles (Δ for κ_2, ▲ for κ_4) the data of Graham (Fig. 1 of Ref. 66) and the full lines connect respectively the data of Feron and those of Graham. The dotted lines give the data of Corner *et al.* (Fig. 5 of Ref. 70 modified by Ref. 661) for κ_2, κ_4 and κ_6.

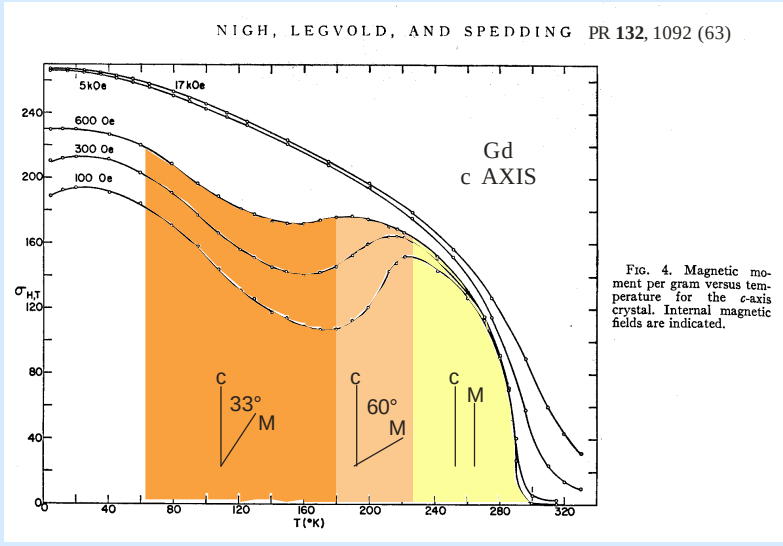


FIG. 4. Magnetic moment per gram versus temperature for the c-axis crystal. Internal magnetic fields are indicated.

Gd ist not isotropic, it has K_2, K_4, $K_6 \neq 0$

Note also finite MAE above T_C

Spin reorientation in bulk Ni und Co

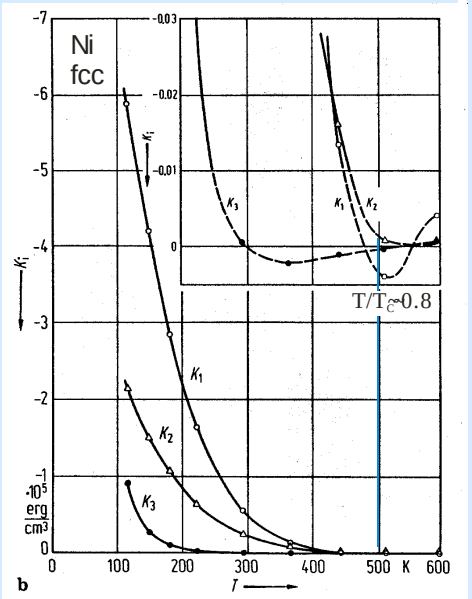


Fig. 7. Temperature dependence of magnetocrystalline anisotropy constants of Ni. (a) K_1. *1*: [68 F 1], *2*: [74 T 1], *3*: [77 B 2], *4*: [77 O 1]. Solid line: calculation [77 O 1]. (b) K_1, K_2, and K_3. Accuracy of data is considerably reduced near T_C: dashed lines in the insert [68 A 1]. (c) K_3. *1* and *2*: [76 A 1], *3*: [69 F 2], *4*: [77 B 2]. Solid line is to guide the eye through confidence limits [76 A 1].

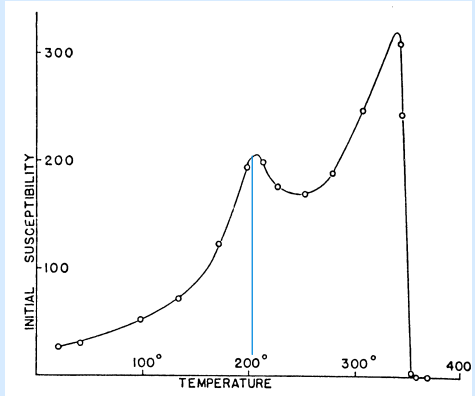


FIG. 6. The variation of the initial susceptibility with temperature in nickel.

SRT for hcp Co

$\sin\theta = (K_2/2K_4)^{1/2}$

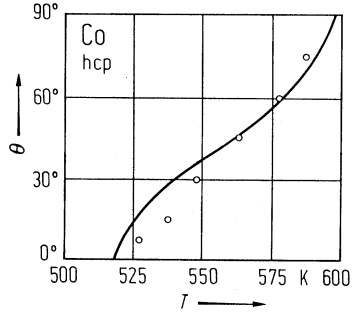
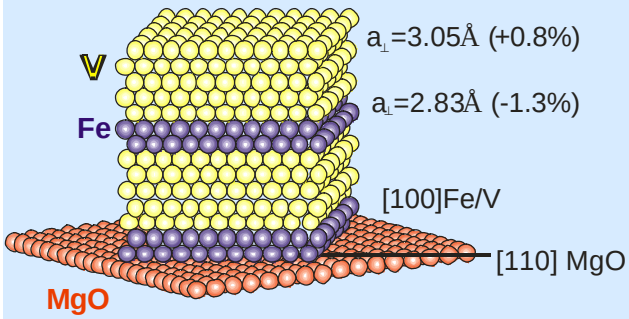


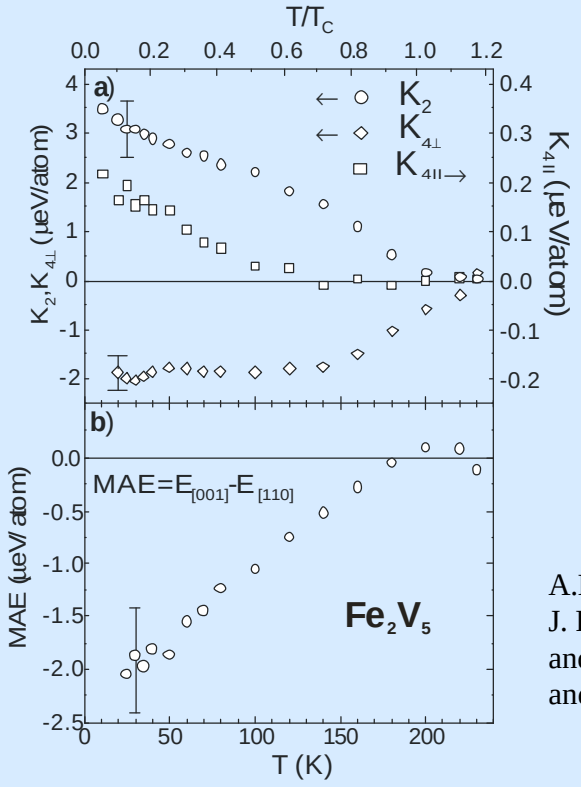
Fig. 5. Temperature dependence of the angle θ between the direction of spontaneous magnetization and the *c* axis of a single crystal of hcp Co [61 B 5]. Points: data. Curve: calculated from $\sin\theta = (-K_1/2K_2)^{1/2}$.

LB III, 19a, p.45

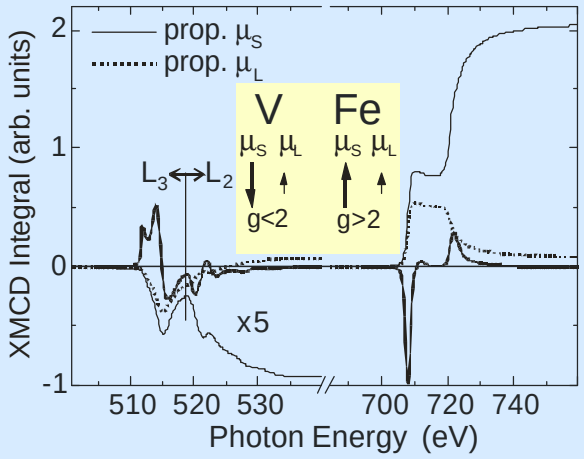
At the extremal value of K_2 a reorientation and second maximum in χ appears

Ferromagnetic resonance on $Fe_n/V_m(001)$ superlattices

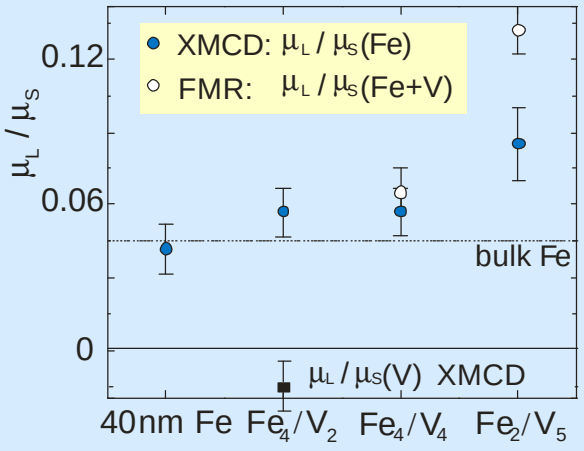




XMCD



FMR



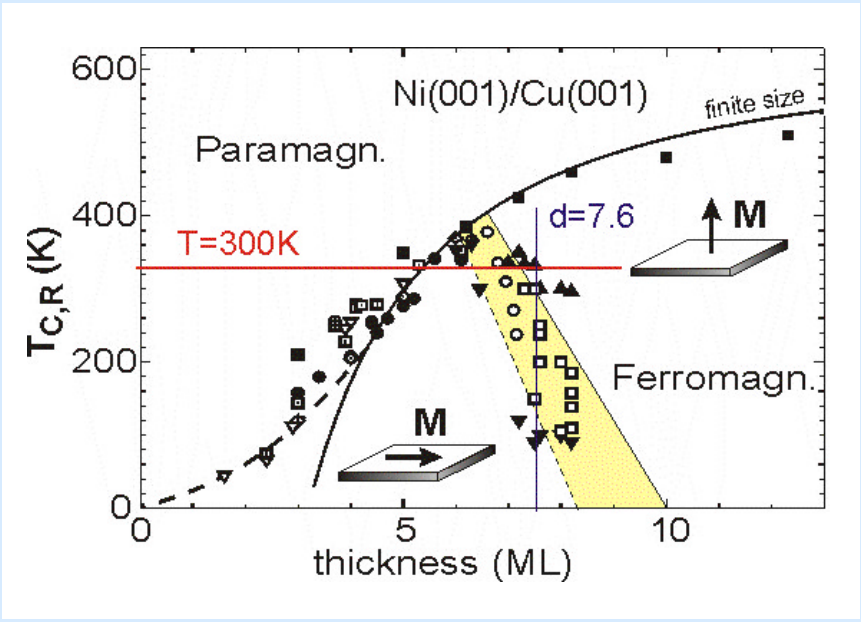
$$\frac{\mu_L}{\mu_S} = \frac{g-2}{2}$$ (Kittel'49)

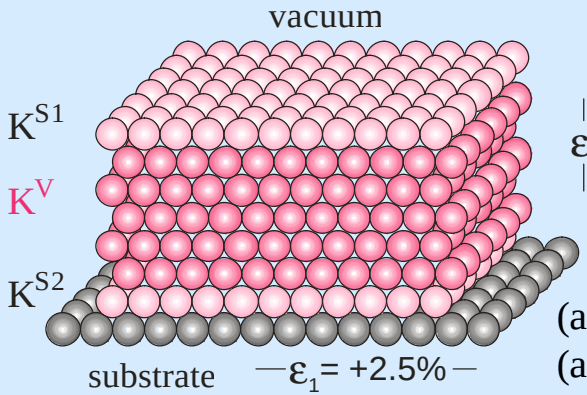
In solids g and μ_L are tensors

bcc (001) Fe_2/V_5 superlattice					
$g_{\parallel}$	$g_{\perp}$	μ_L/μ_S	$\mu_L(\mu_B)$	$\mu_S(\mu_B)$	MAE μeV/atom
2.264	2.268	0.133	0.215	1.62	-2.0
bcc Fe-bulk					
2.09	2.09	0.045	0.10	2.13	-1.4

A.N. Anisimov et al.
J. Phys. C **9**, 10581 (1997)
and PRL **82**, 2390 (1999)
and Europhys. Lett. **49**, 658 (2000)

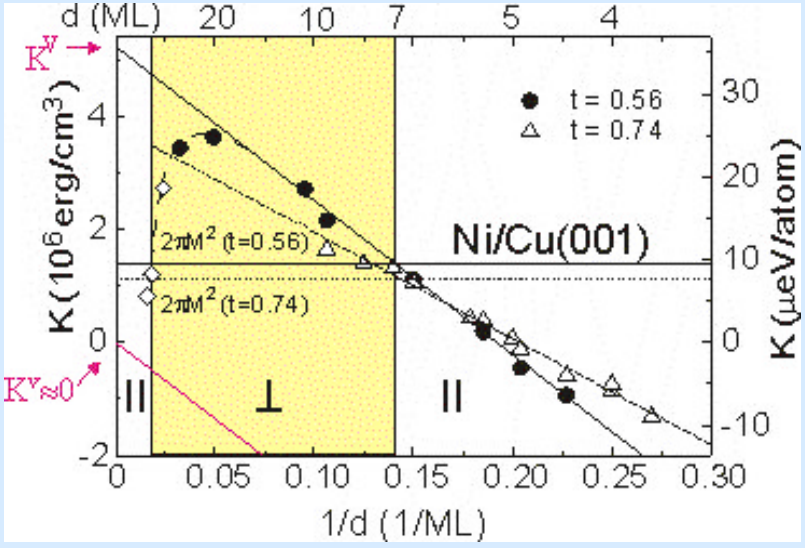
For thin films the Curie temperature can be manipulated





$$K_i = K_i^V + 2\frac{K_i^S}{d} \qquad t=T/T_C(d)$$

P. Poulopoulos and K. B.
J. Phys.: Condens. Matter **11**, 9495 (1999)



Free energy density of MAE, K

(intrinsic, after substraction of $2\pi M^2$)

tetragonal [e.g. Ni, Co, Fe (001) / Cu (001)]:

$E_{tetr} = -K_2\, a_z^2 - \frac{1}{2} K_{4\wedge}\, a_z^4 - \frac{1}{2} K_{4\div\div} (a_x^4 + a_y^4) + \ldots$ *(B.Heinrich et al.)*

$= -K_2 \cos^2\theta - \frac{1}{2} K_{4\wedge} \cos^4\theta - \frac{1}{2} K_{4\div\div} \frac{1}{4} (3+\cos 4\varphi) \sin^4\theta + \ldots$ *(Bab et al.)*

$= (K_2 + K_{4\wedge}) \sin^2\theta - \frac{1}{2} (K_{4\wedge} + \frac{3}{4} K_{4\div\div}) \sin^4\theta - \frac{1}{8} K_{4\div\div} \cos 4\varphi \sin^4\theta + \ldots$

$= K_2' \sin^2\theta + K_{4\wedge} \sin^4\theta + K_{4\div\div} \cos 4\varphi \sin^4\theta + \ldots$ *(traditional)*

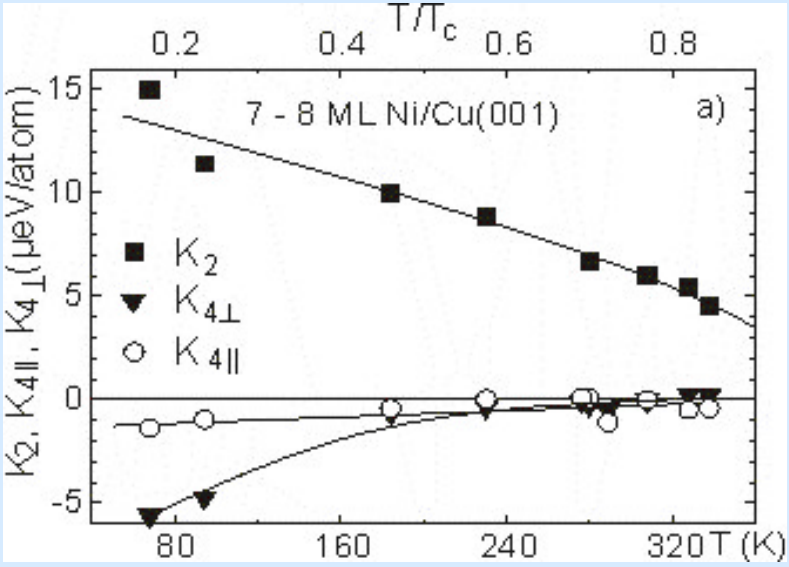
hexagonal [e.g. Ni (111), Gd (0001) / W (110)]:

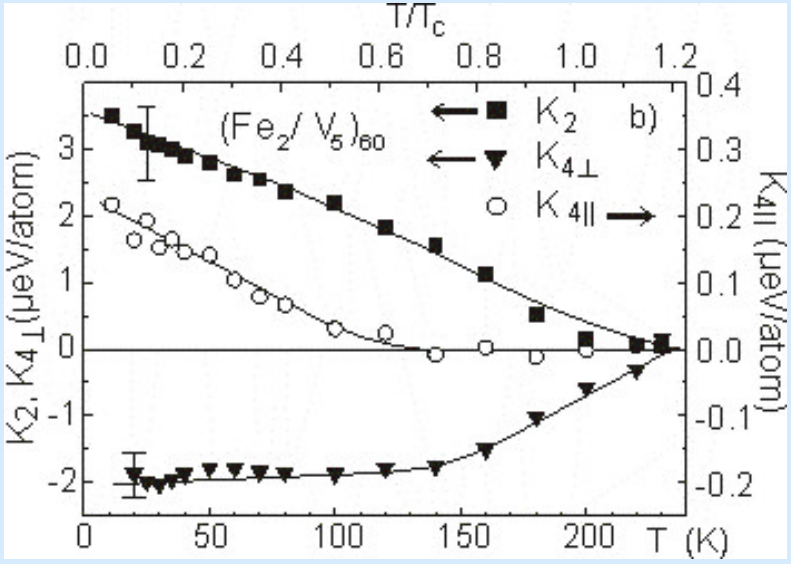
$E_{hex} = k_2 \sin^2\theta + \frac{1}{2} k_{2\div\div} \cos 2\varphi \sin^2\theta + k_4 \sin^4\theta + k_{6\wedge} \sin^6\theta + k_{6\div\div} \cos 6\varphi \sin^6\theta + \ldots$

$K = k_2 Y_2^0 + k_{4m} Y_4^m + \ldots$ *Legendre polyn. (B. Coqblin)*

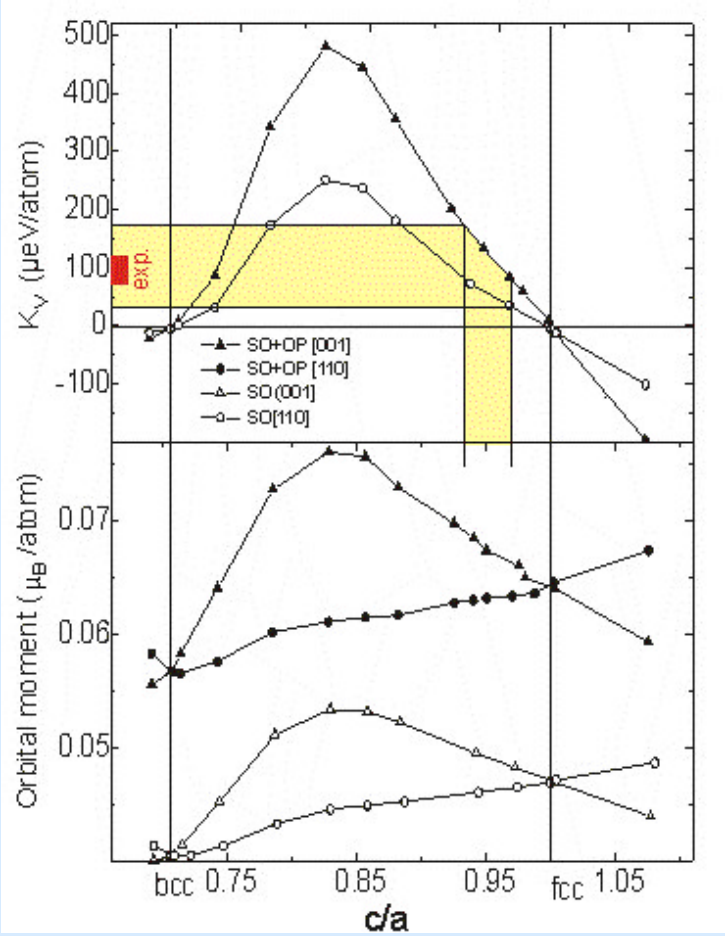
each K_i has a „volume“ and „surface“ contribution

$$K_i = K_i^v + 2K_i^s/d$$

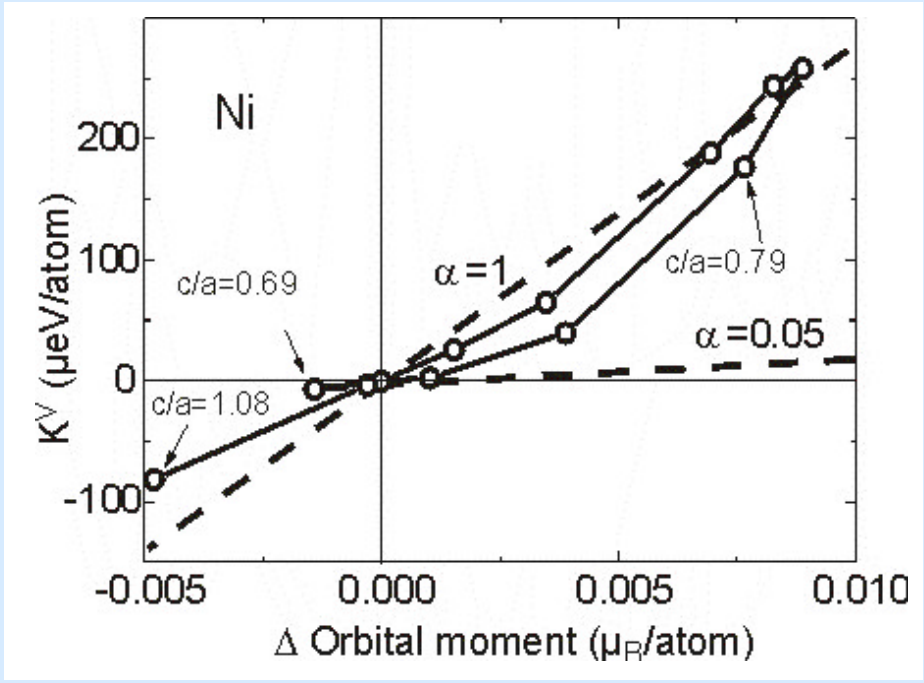

T/Tc
0.2
0.4
0.6
0.8
7 - 8 ML Ni/Cu(001)
a)
K2
K4⊥
K4||
K2, K4||, K4⊥ (μeV/atom)
15
10
5
0
-5
80
160
240
320
T (K)


T/Tc
0.0
0.2
0.4
0.6
0.8
1.0
1.2
(Fe2/ V5)60
b)
K2
K4⊥
K4||
K2, K4⊥ (μeV/atom)
K4|| (μeV/atom)
3
2
1
0
-1
-2
0.4
0.3
0.2
0.1
0.0
-0.1
-0.2
0
50
100
150
200
T (K)

2b *ab initio* calculations



O. Hjortstam, K. B. et al. PRB **55**, 15026 ('97)



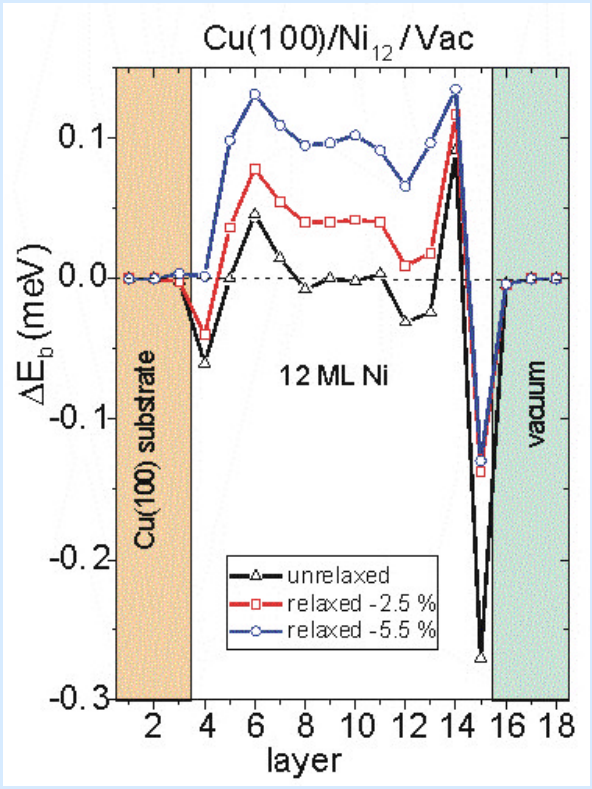
$$g_{II} - g_{\perp} = g_e \lambda (\Lambda_{\perp} - \Lambda_{II})$$

anisotropic μ_L ↔ MAE

$$MAE \propto \frac{X_{LS}}{4\mu_B} \Delta\mu_L$$

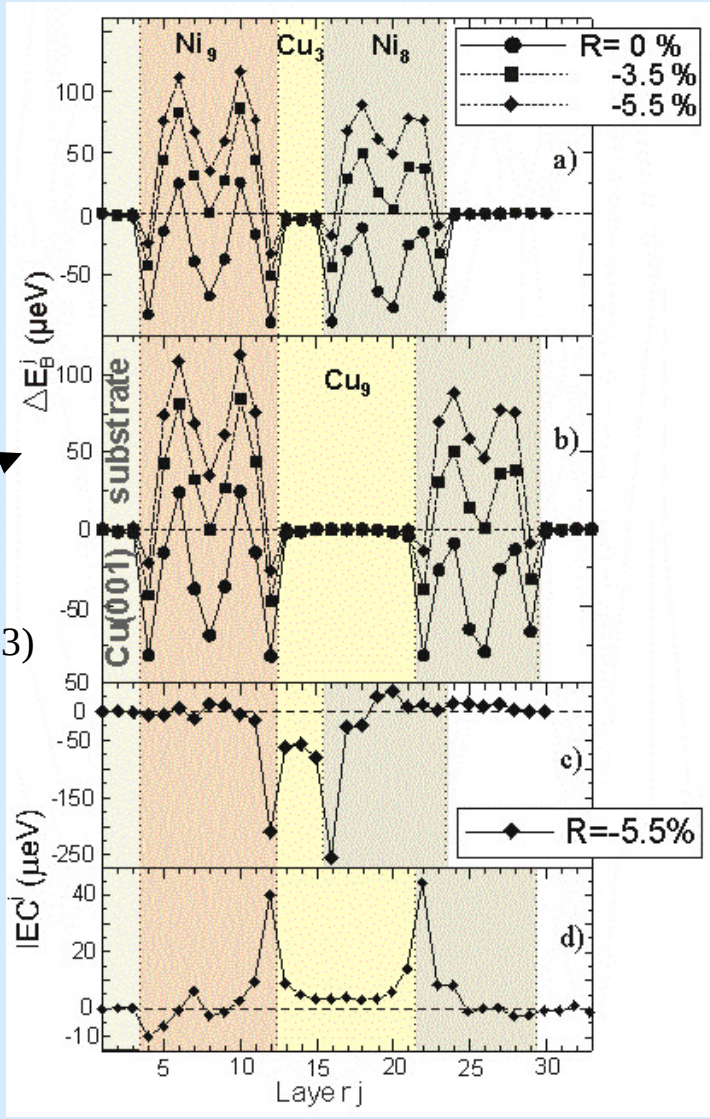
SP-KKR calculation for rigit fcc and relaxed fct structures

layer resolved $\Delta E_b = \Sigma K_i$ at T=0

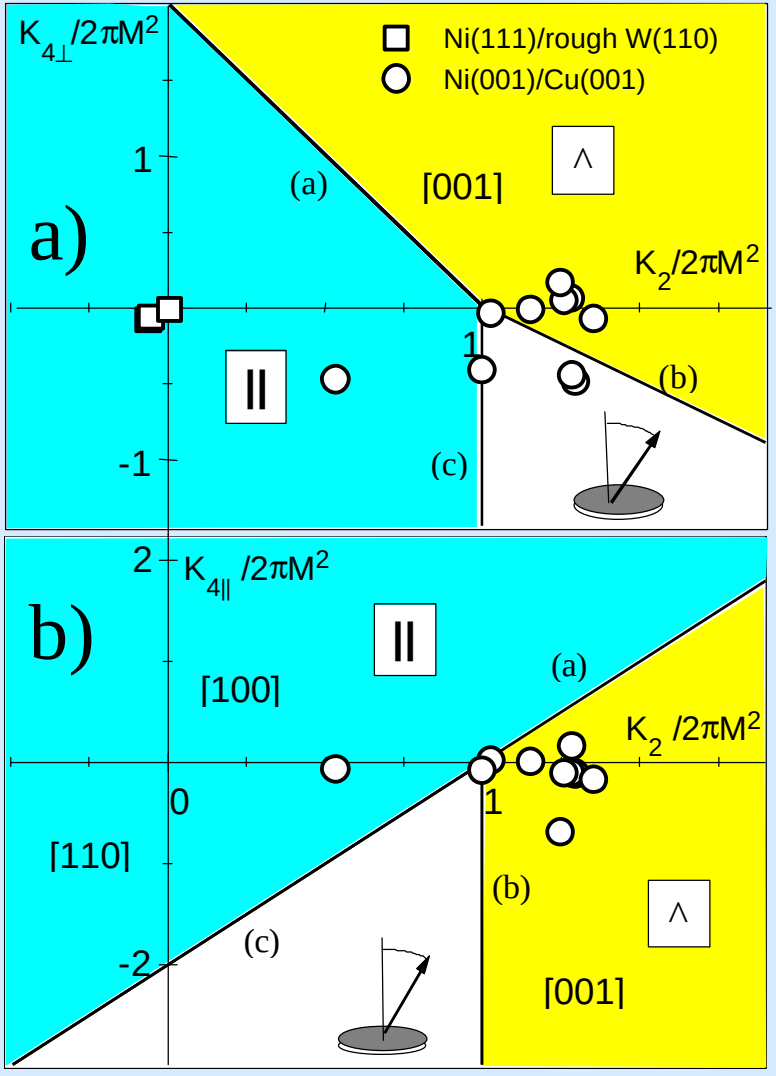


C. Uiberacker et al., PRL **82**, 1289 (1999)

R. Hammerling et al., PRB **68**, 092406 (2003)



The surface and interface MAE are certainly large (L. Néel, 1954) but count only for one layer each. The inner part (volume) of a nano-structure will overcome this, because they count for n-2 layers.



A. Berghaus, M. Farle, Yi Li, K. Baberschke
Absolute determ. of the mag. anisotropy of ultrathin Gd and Ni/W(110).
Second Intern. Workshop on the Magnetic Properties of Low-Dimensional Systems.
San Luis Potosi, Mexico, Proc. in Physics **50**, 61 (1989)

M. Farle et al., PRB **55**, 3708 (1997)

Only with $K_4 \neq 0$a continues SRT is possible!

Do not use $K_{eff} = 2\pi M^2 - K_i$ …
because f(T) and f'(T) are different.
Use the ratio $K_i / 2\pi M^2 \Rightarrow f(T) / f'(T)$

Oxygen surfactant assisted growth: a new procedure to prepare ferromagnetic ultrathin films

VOLUME 92, NUMBER 14 PHYSICAL REVIEW LETTERS week ending 9 APRIL 2004

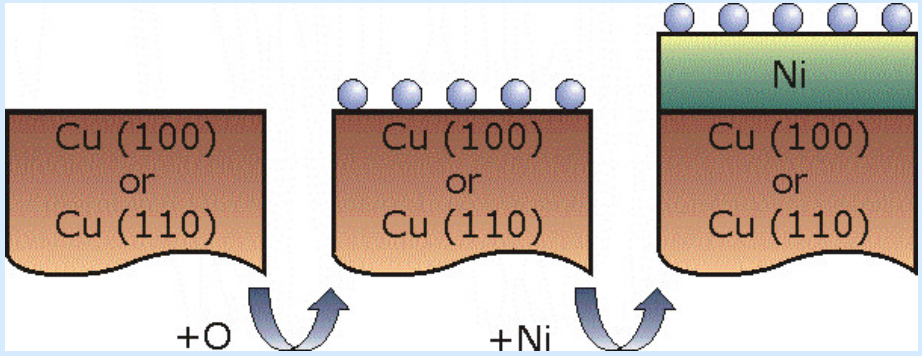
Manipulation of Spin Reorientation Transition by Oxygen Surfactant Growth: A Combined Theoretical and Experimental Approach

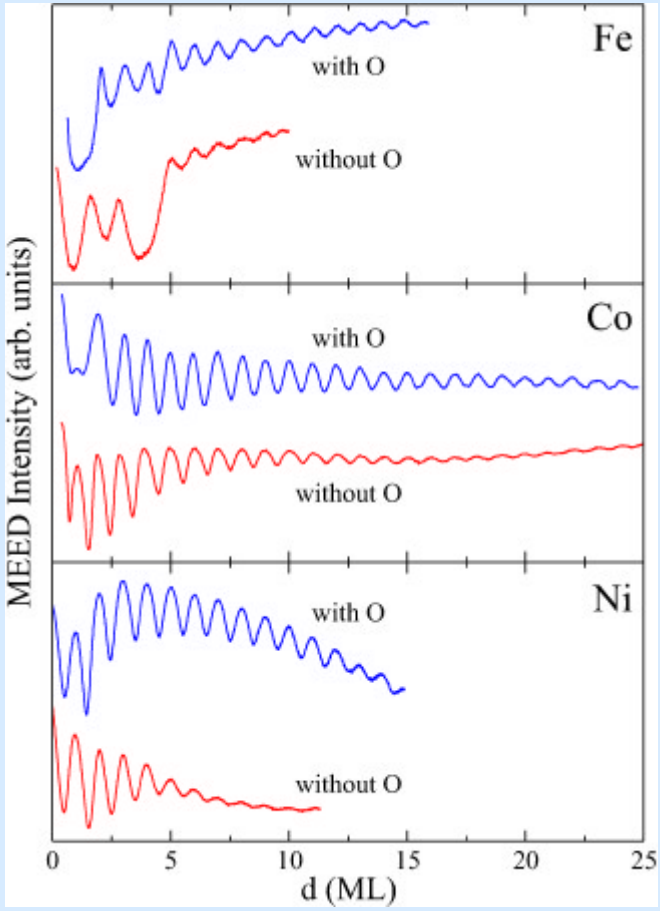
Jisang Hong and R. Q. Wu
Department of Physics and Astronomy, University of California, Irvine, California 92697, USA

J. Lindner,* E. Kosubek, and K. Baberschke
Institut für Experimentalphysik, Freie Universitat Berlin, Arnimallee 14, D-14195 Berlin-Dahlem, Germany
(Received 6 August 2003; published 5 April 2004)

- oxygen acts as surfactant for Fe, Co and Ni films on Cu(100)
- change of magnetic anisotropy by surfactant
- induced magnetic moment of surfactant

Improved growth by oxygen surfactant

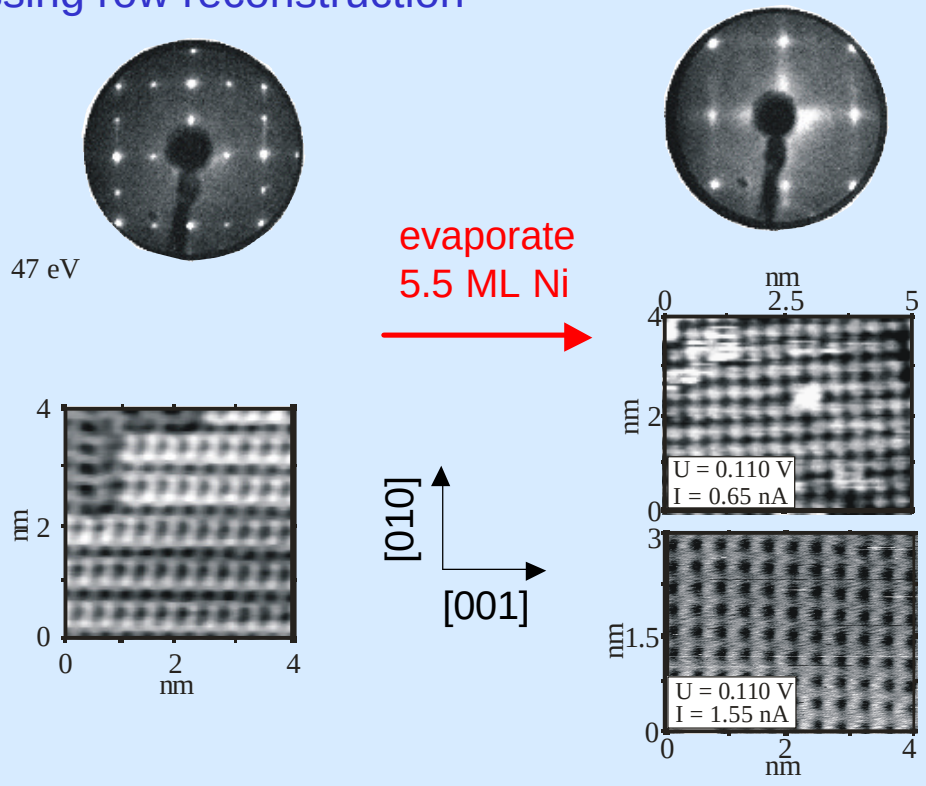


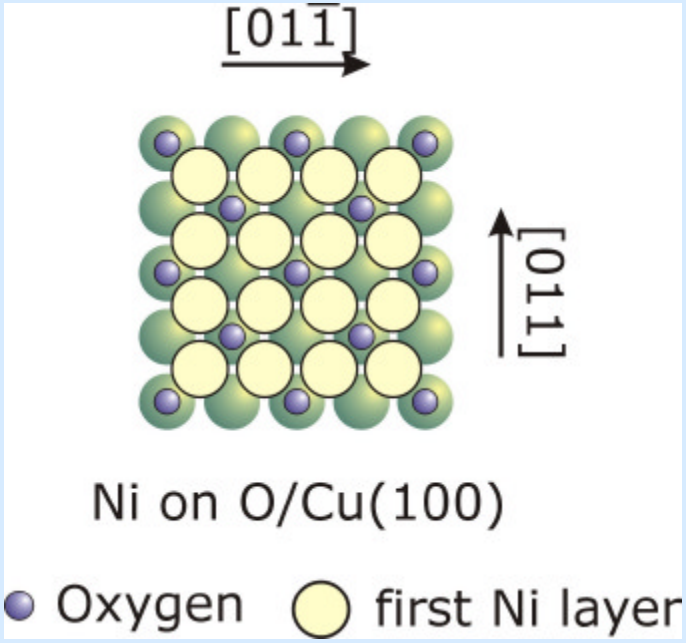


C. Sorg et al., *Surf. Sci.* **565**, 197-205 (2004)
M. Farle, *Surf. Sci. Perspectives* **575**, 1-2 (2005)

O($\sqrt{2} \times 2\sqrt{2}$)R45°/Cu(100) missing row reconstruction

c(2×2)O/Ni/Cu(100)

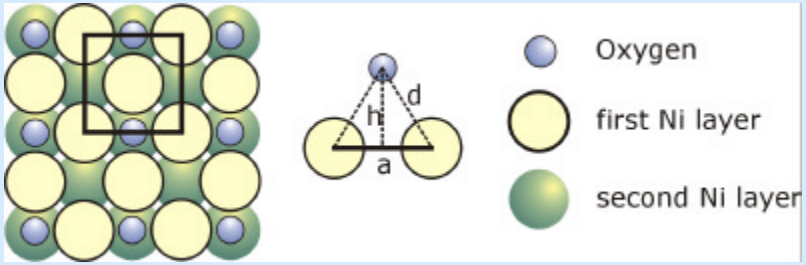




from AES ⇒ oxygen floats on top of Ni film

R. Nünthel et al., *Surf. Sci.* **531**, 53-67 (2003)

Local structure: Surface EXAFS Ni on O/Cu(100)



R_{nn}= (1.85±0.03) Å

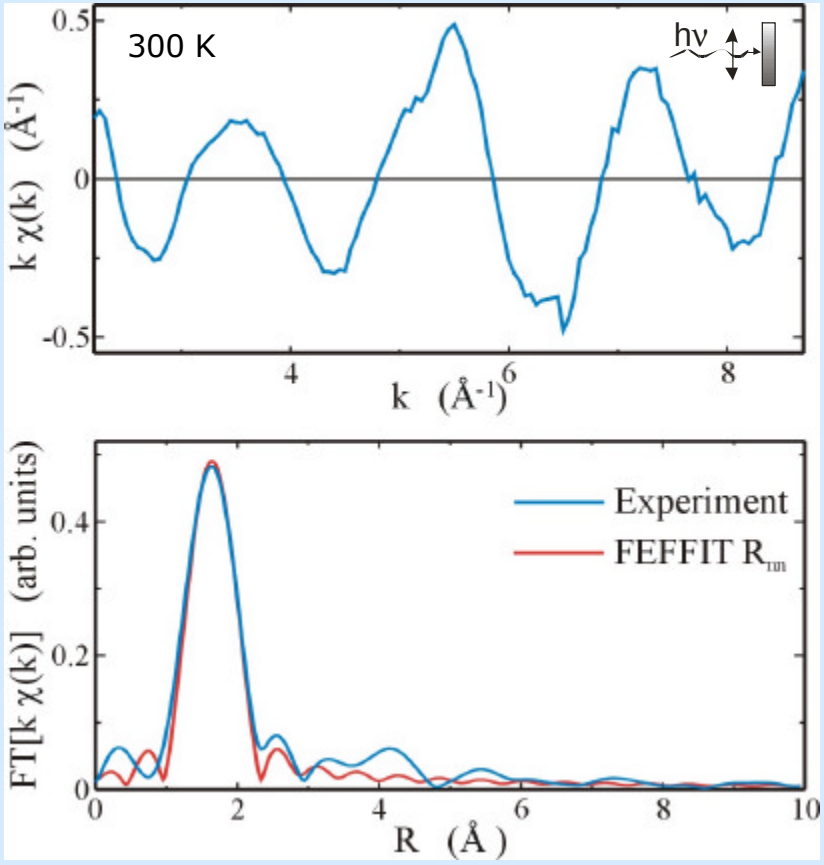
h = 0.41 Å

Comparison to theory (T.S. Rahman):

R_{nn}= 1.87 Å

h = 0.44 Å

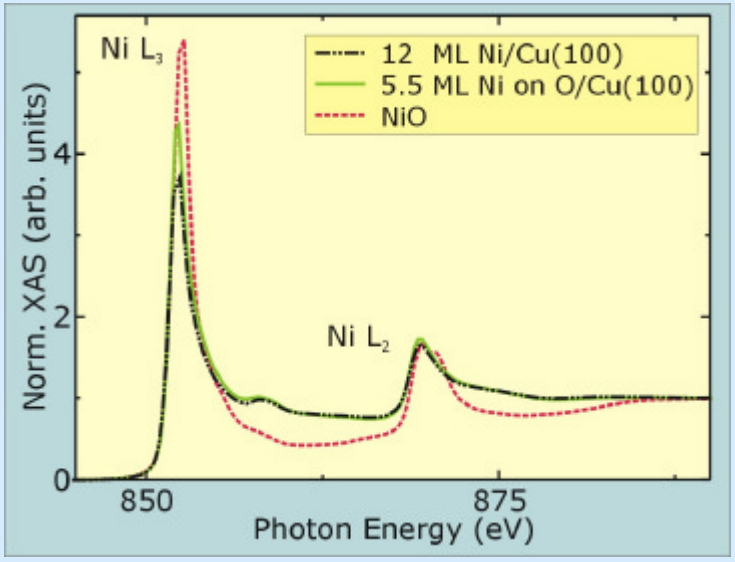
oxygen K-edge SEXAFS



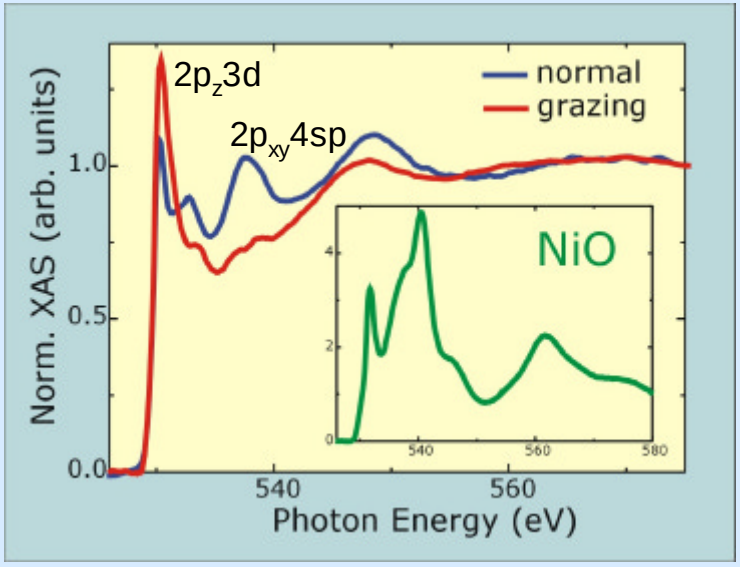
R. Nünthel et al., *Surf. Sci.* **531**, 53-67 (2003)

Electronic structure from X-ray absorption spectroscopy

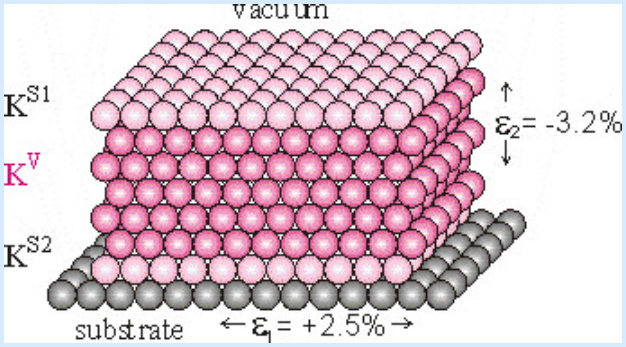
Ni $L_{2,3}$-edge



O K-edge



NEXAFS ⇒ no bulklike NiO is formed

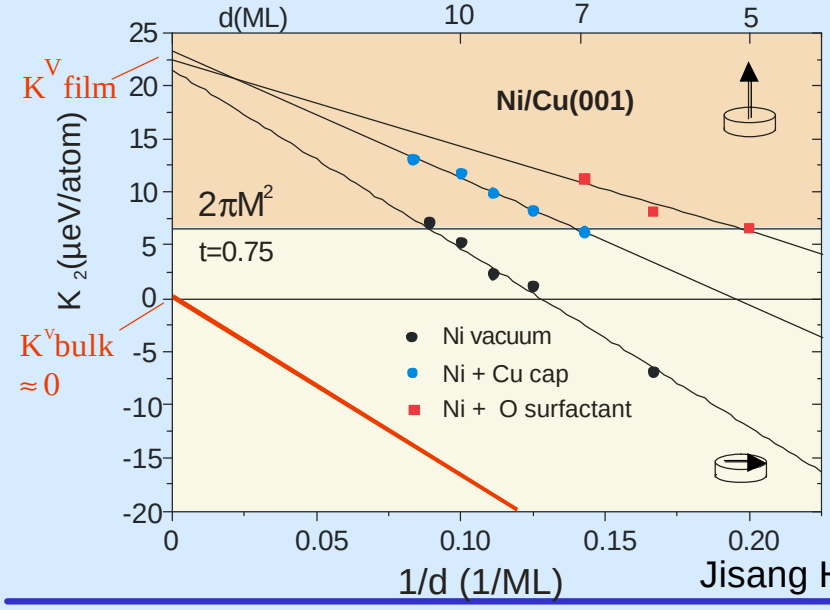


Interface	K_s (μeV/atom)	d_c (ML)
Ni/vacuum	-107	10.8
Ni/Cu	-59	7.6
Ni/CO (van Dijken et al.)	-81	7.3
Ni/H_2 (van Dijken et al.)	-70	6.8
Ni/O (surfactant)	-17	4.9

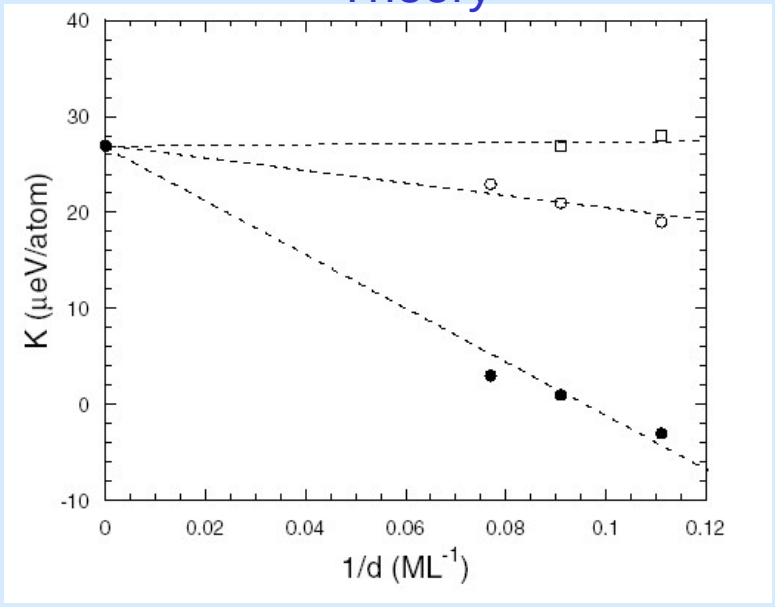
$$F \sim \left(2pM^2 - K_{2\perp}\right)\cos^2 q$$

$$K = K^V + \frac{K^{S1} + K^{S2}}{d}$$

Experiment



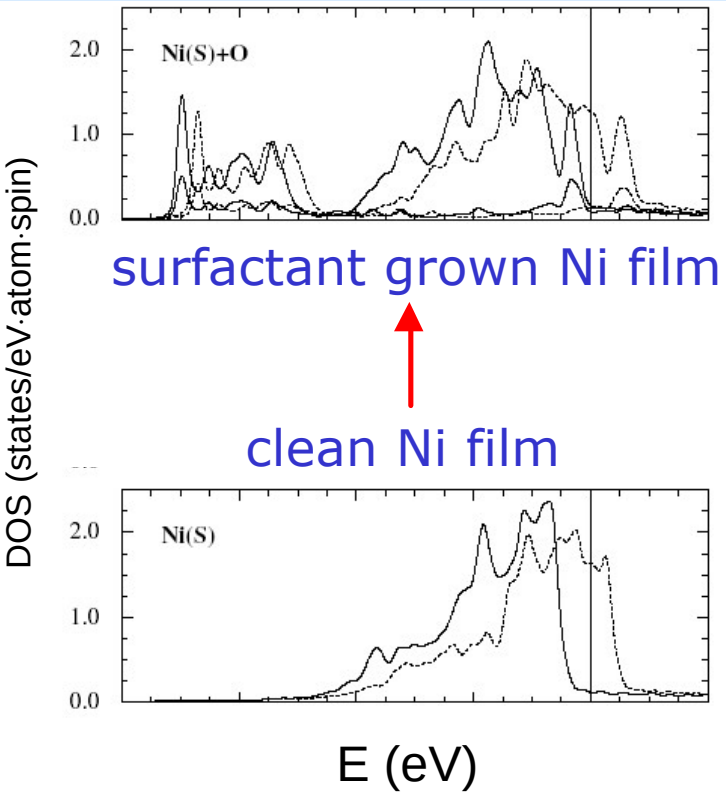
Theory



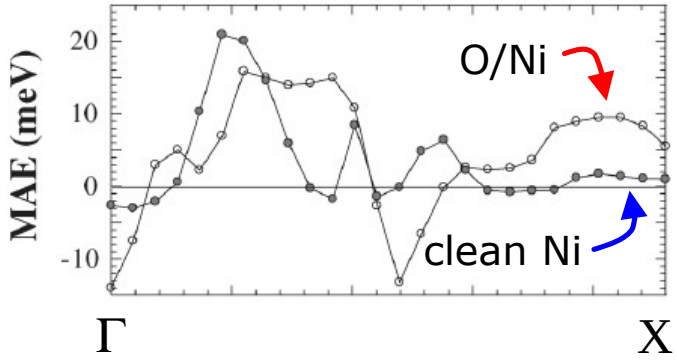
Jisang Hong et al., *Phys. Rev. Lett.* **92**, 147202-1 (2004)

Results of ab initio calculations

Density of states



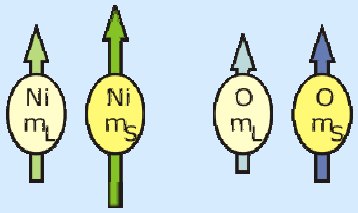
MAE along $\bar{\Gamma}\bar{X}$ axis



- DOS shows that topmost Ni moment is basically unchanged
- O-induced surface state seen in the vicinity of $\bar{X}$-point is responsible for change in MAE
- theory reveals induced moment in surfactant oxygen

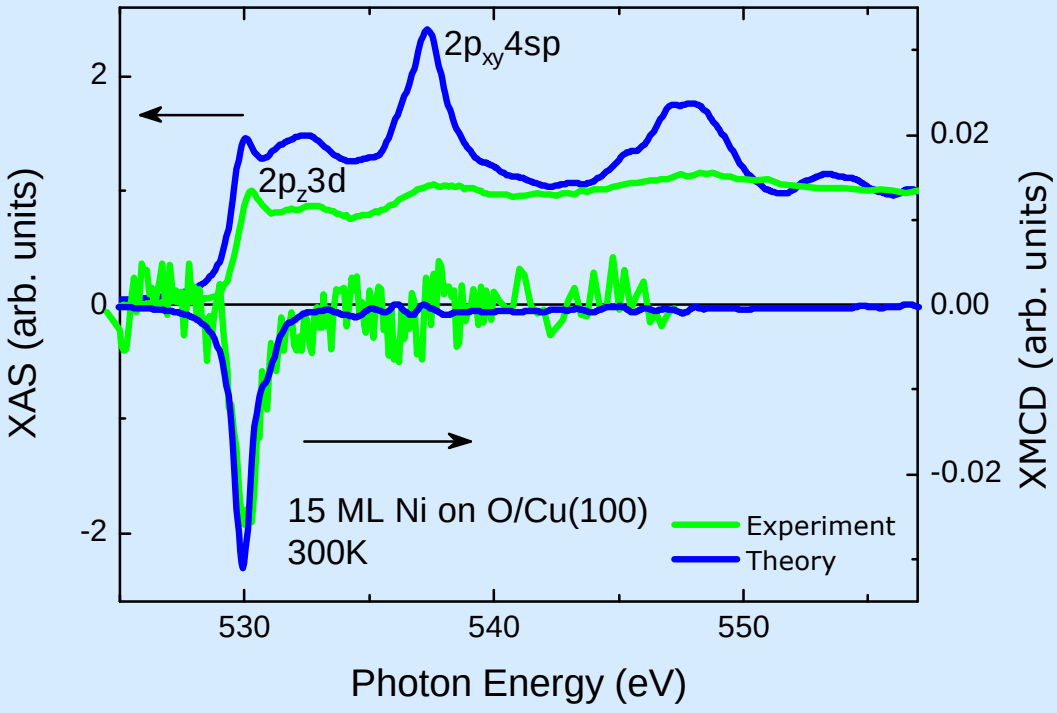
Jisang Hong et al., *Phys. Rev. Lett.* **92**, 147202-1 (2004)

Induced magnetism in oxygen: Ni on O/Cu(100)



oxygen K-edge XMCD → orbital moment μ_L

BESSY: UE56/2-PGM2



theory: Ruqian Wu (UC Irvine):

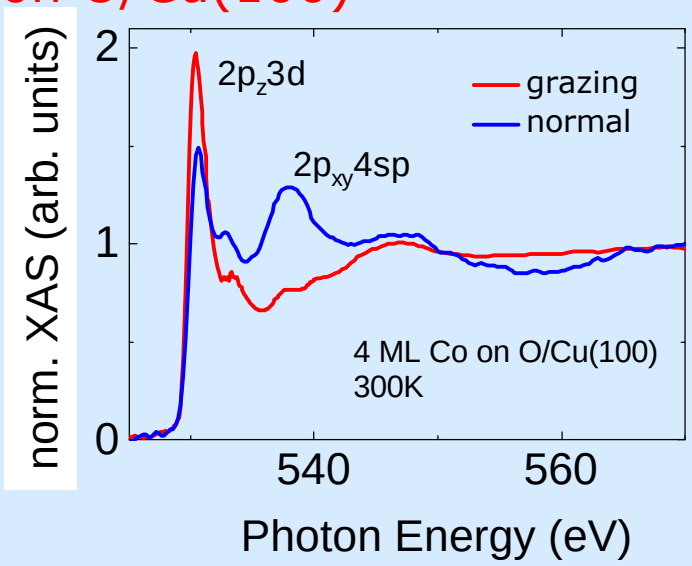
induced moments in oxygen:

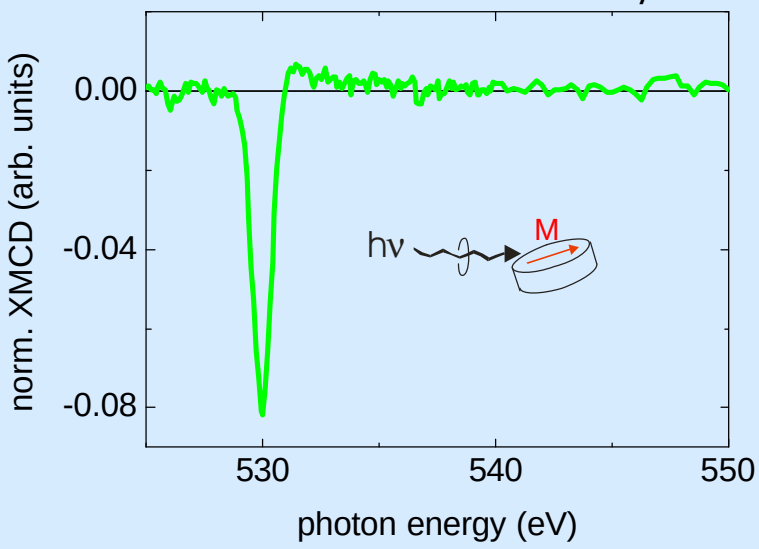
$\mu_S = 0.053\ \mu_B$
$\mu_L = 0.0021\ \mu_B$

Induced magnetism in oxygen: Co and Fe films

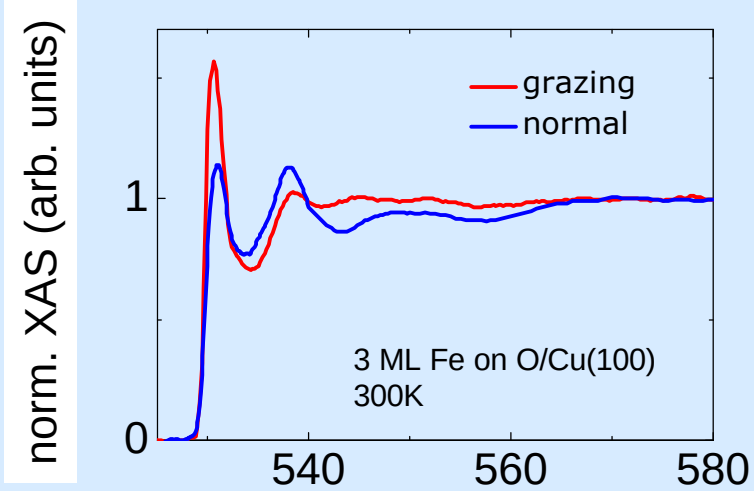
Co on O/Cu(100)

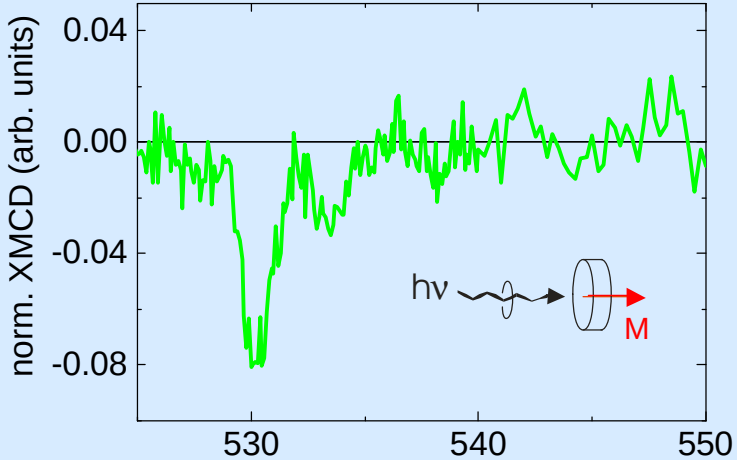
BESSY: UE56/2-PGM2





Fe on O/Cu(100)





Conclusion

- spin reorientation transition changes dramatically with surfactant
  $\rightarrow$ surface anisotropy is strongly reduced in magnitude
- Fe, Co and Ni induce magnetic moment in surfactant
- fair agreement with *ab initio* calculations