



# Magnetic anisotropy and interlayer exchange coupling in ultrathin ferromagnets: experiment versus theory

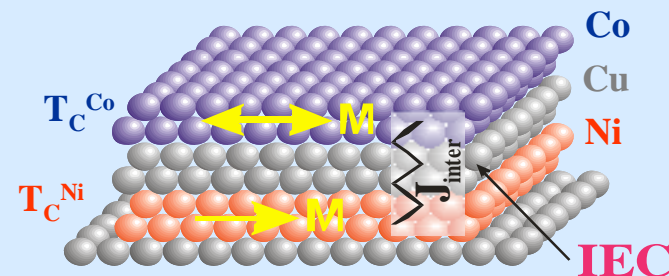
Klaus Baberschke

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Freie Universität Berlin

Arnimallee 14 D-14195 Berlin-Dahlem Germany

1. Prologue
2. **M**agnetic **A**nisotropy **E**nergy
3. **I**nterlayer **E**xchange **C**oupling and  $f(T)$
4. Summary



## 1. Prologue

Is this of interest  
for the theory?









**281. WE-Heraeus-Seminar**

**“Spin-Orbit Interaction  
and Local Structure  
in Magnetic Systems  
with Reduced Dimensions”  
June 2002 in Wandlitz**

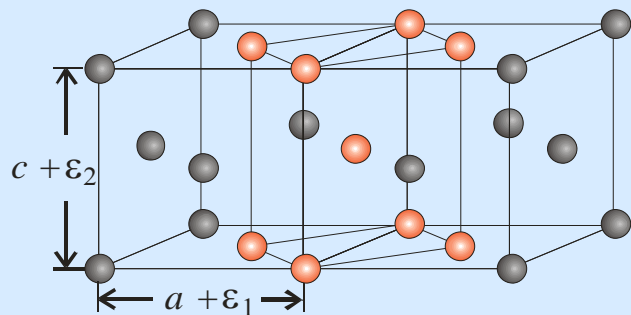
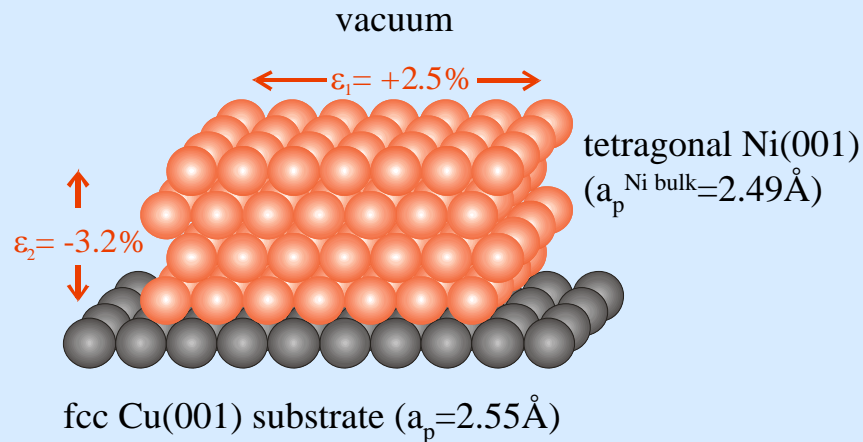




## 2. Magnetic Anisotropy Energy

Growth of artificial nanostructures

bcc, fcc  $\rightarrow$  tetragonal, trigonal

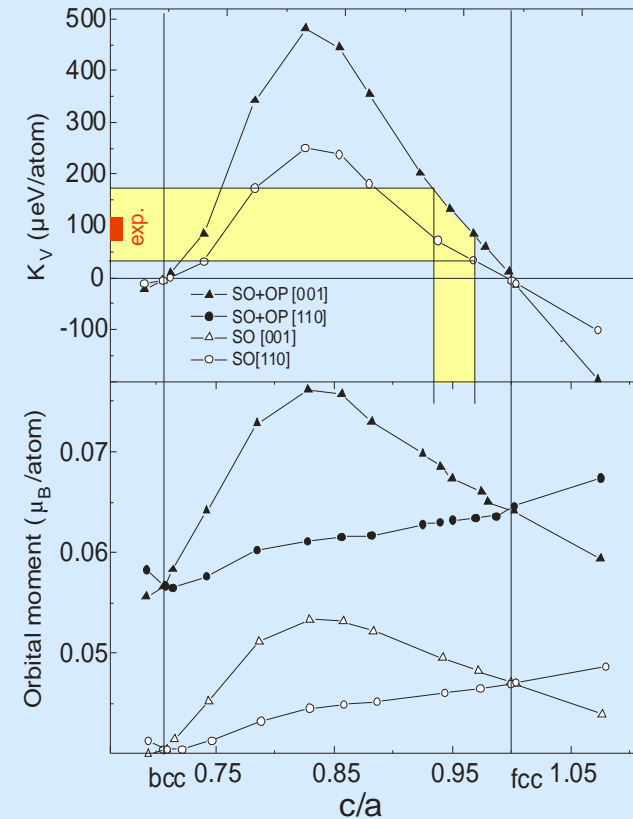


Bain path

$c/a=1$  fcc  $\rightarrow$  fct  $\rightarrow$  bcc  $c/a=1/\sqrt{2}$

Infinite sized Ni x-tal  
no surface effects

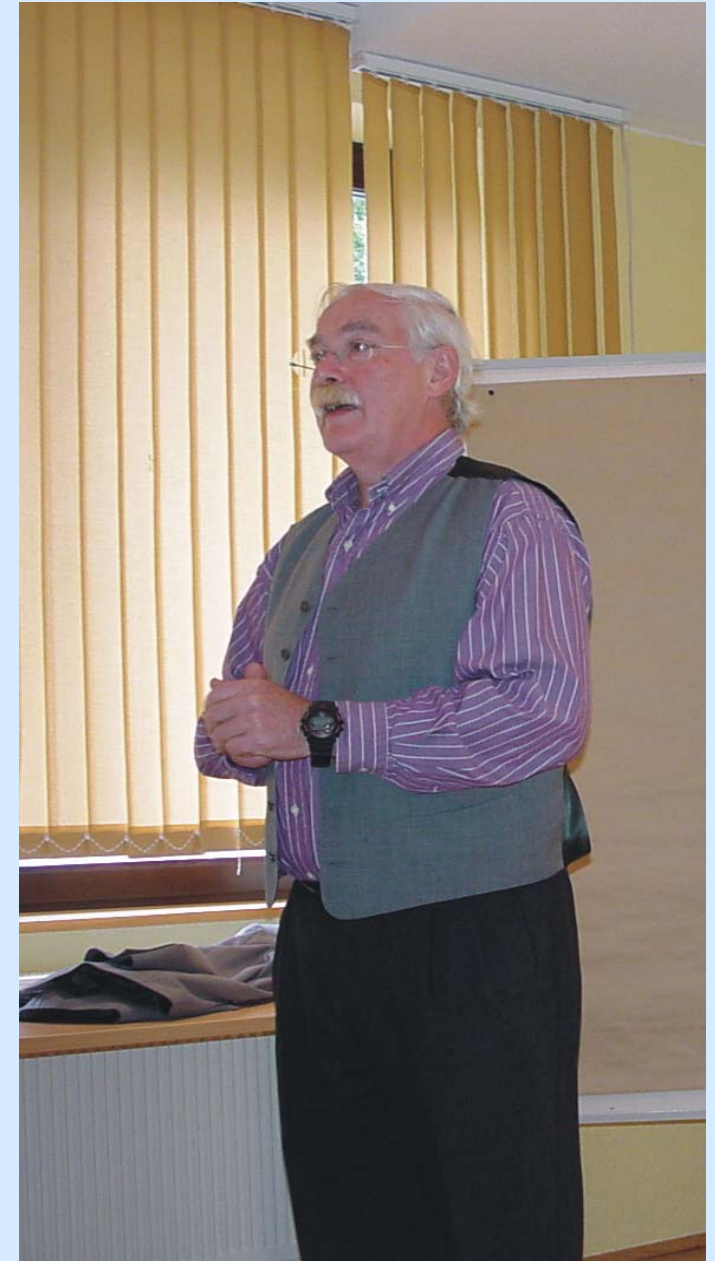
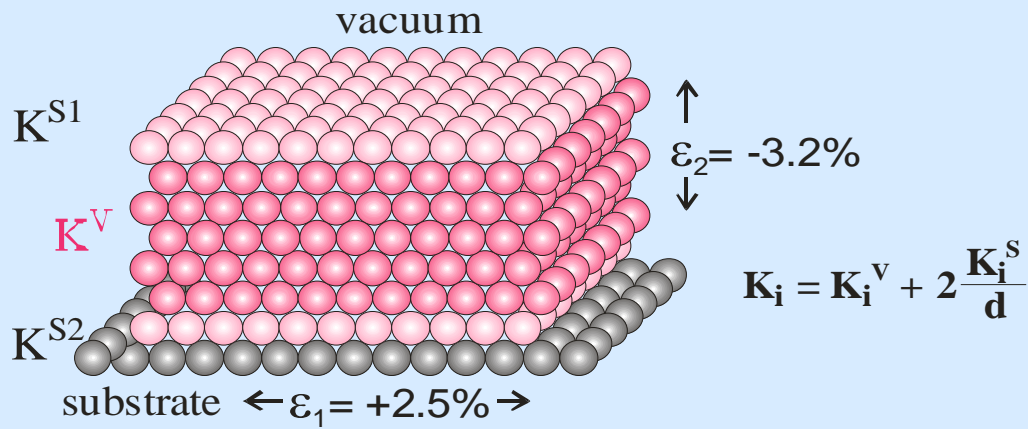
O. Hjortstam, K. B. et al. PRB **55**, 15026 ('97)



Structural changes by  $\approx 0.05 \text{ \AA}$  increase MAE  
by 2-3 orders of magnitude ( $\sim 0.2 \rightarrow 100 \mu\text{eV}/\text{atom}$ )

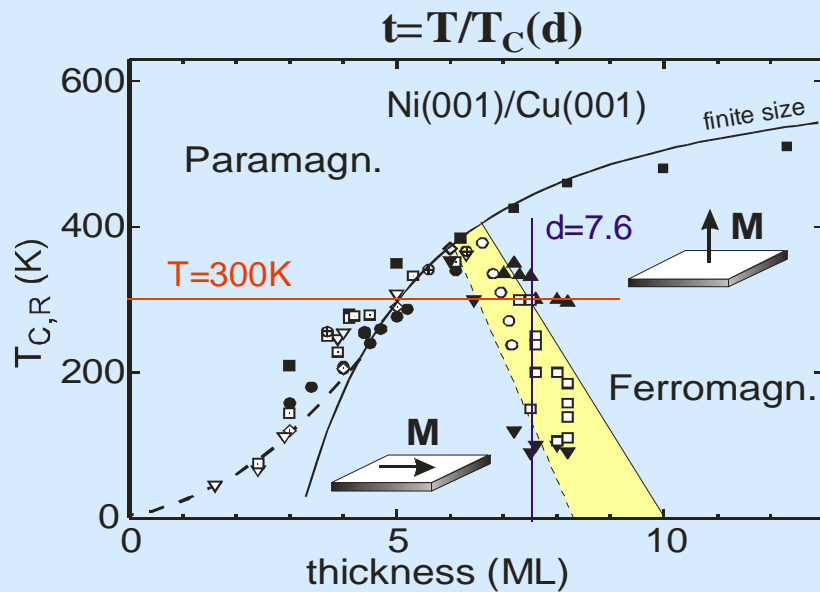
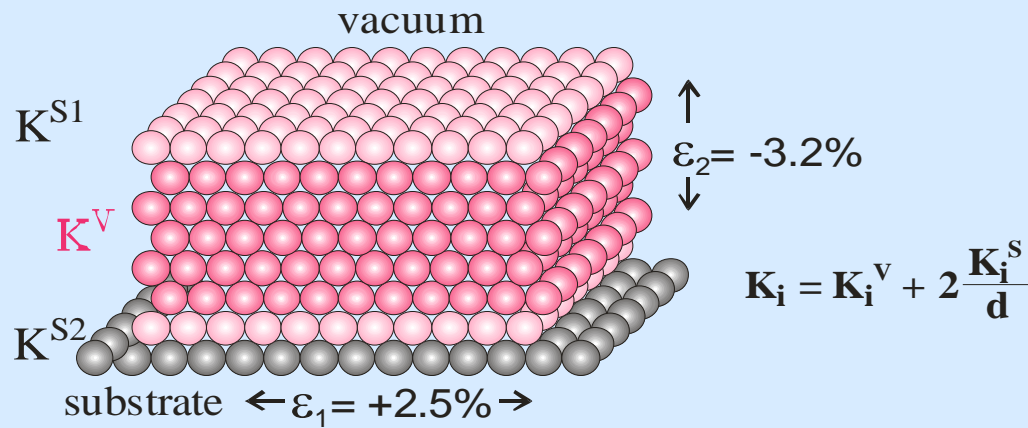
see also: R. Wu et al. JMMM **170**, 103 ('97)

# “volume”, “surface” and “interface” MAE



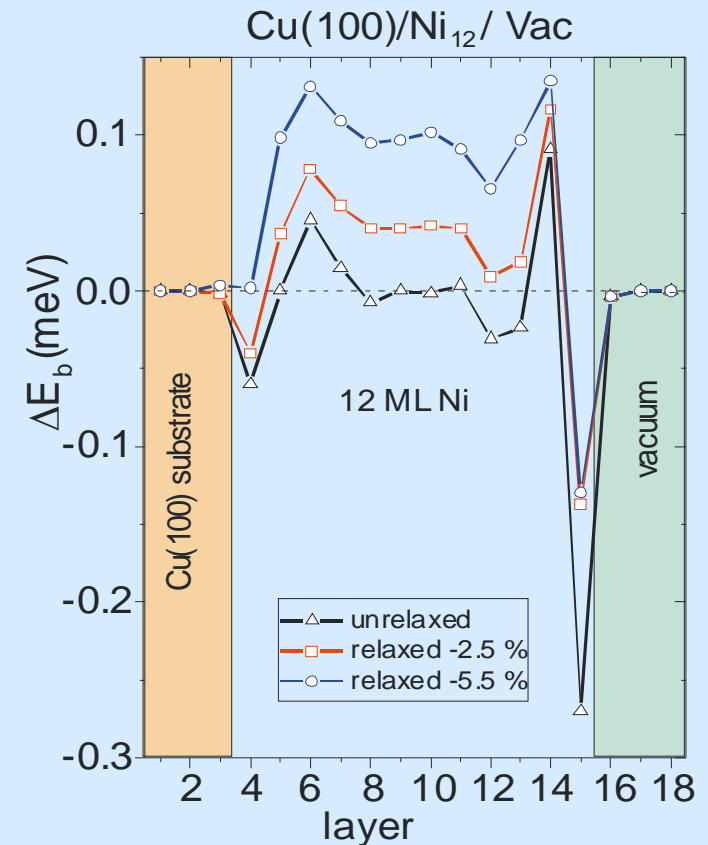


# “volume”, “surface” and “interface” MAE



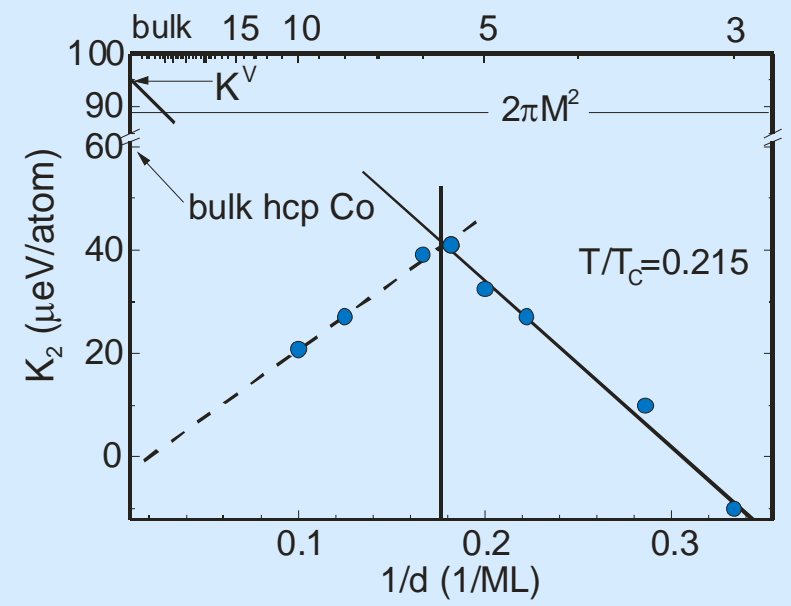
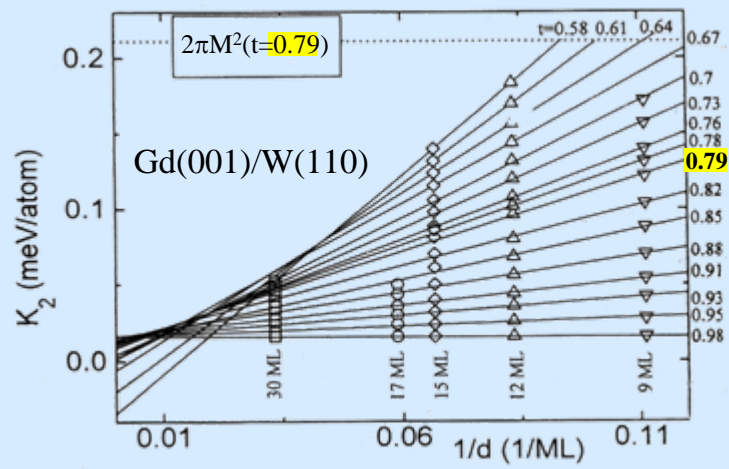
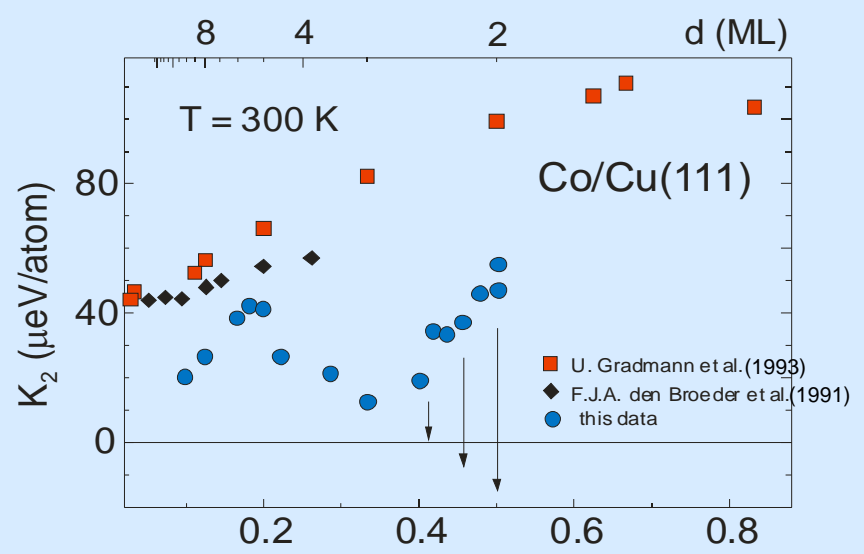
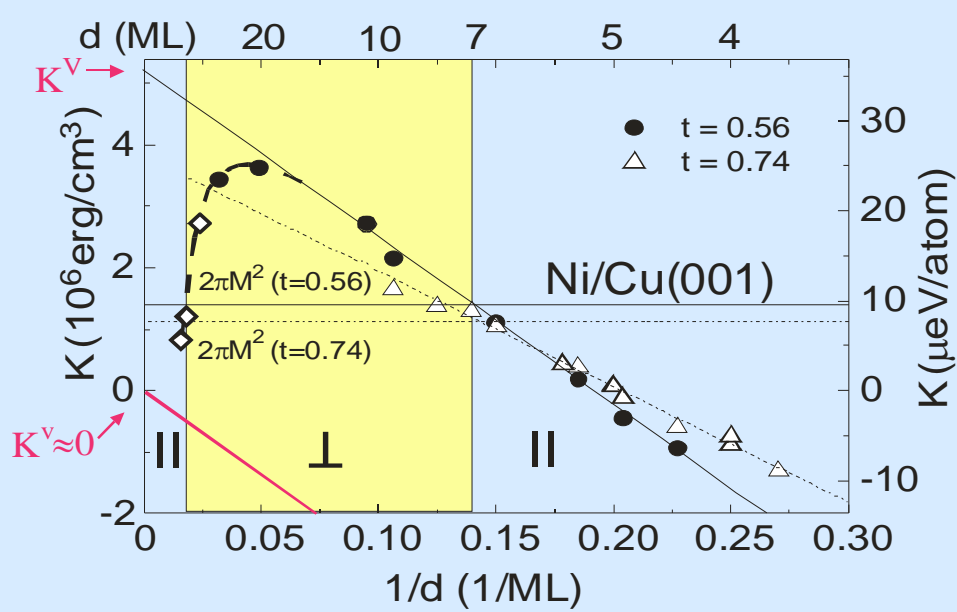
P. Poulopoulos and K. B.  
J. Phys.: Condens. Matter **11**, 9495 (1999)

C. Uiberacker et al.  
Phys. Rev. Lett. **82**, 1289 (1999)



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



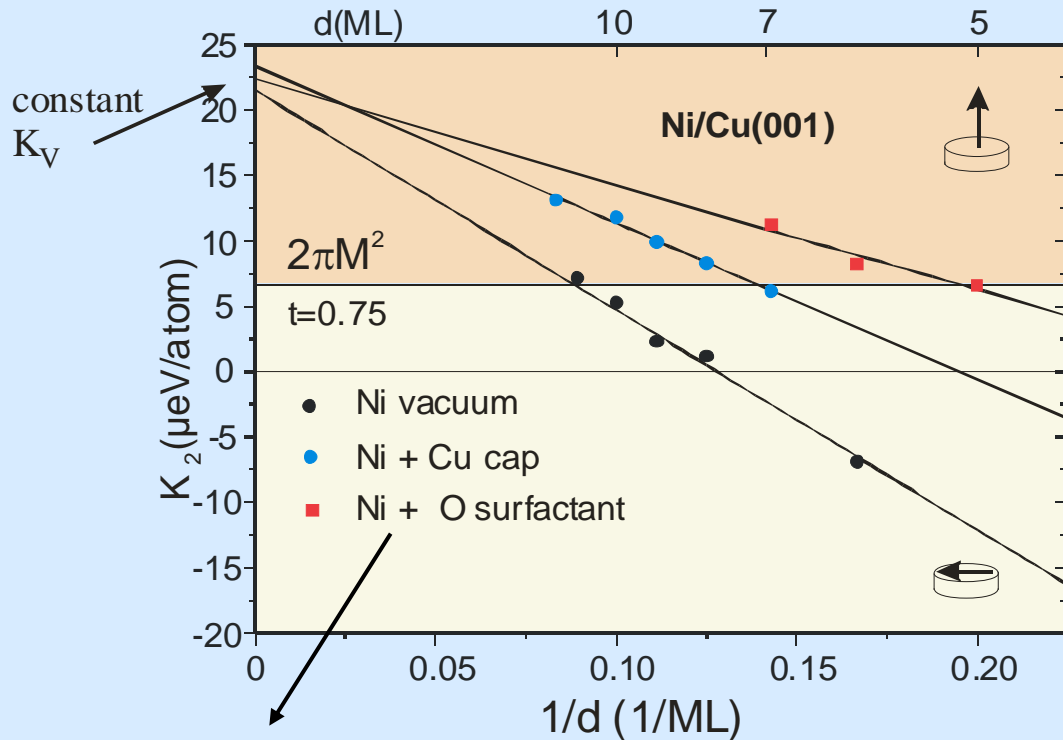


G. André et al., Surface Science **326**, 275 (1995)  
 K. B. and M. Farle, J. Appl. Phys. **81**, 5038 (1997)

M. Farle et al., Surf. Sci. **439**, 146 (1999)

In a proper analysis, taking  $T/T_C(d)$  in consideration, we always find a linear  $K=K_V+2K_S/d$  dependence.  
 A departure from this “Néel argument” indicates changes in the x-tal structure

## Manipulation of surface MAE, $K_S$ by adsorbed molecules, metal cap and surfactant growth



Interface	$K_S$ ( $\mu\text{eV}/\text{atom}$ )	$d_C$ (ML)
Ni/vacuum	-107	10.8
Ni/Cu	-59	7.6
Ni/CO (van Dijken et al.)	-81	7.3
Ni/H <sub>2</sub> (van Dijken et al.)	-70	6.8
Ni/O (surfactant)	-17	4.9

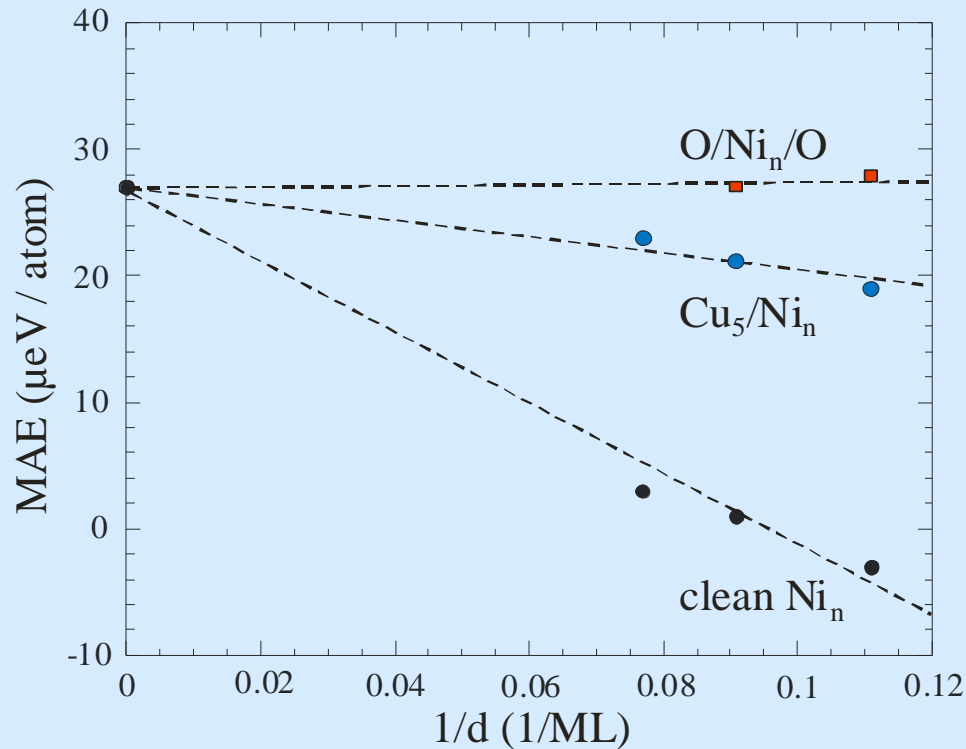
Changes of  $K_S$  shift  
the spin reorientation transition  $d_C$

J. Lindner et al. Surf. Sci. Lett. **523**, L65 (2003)

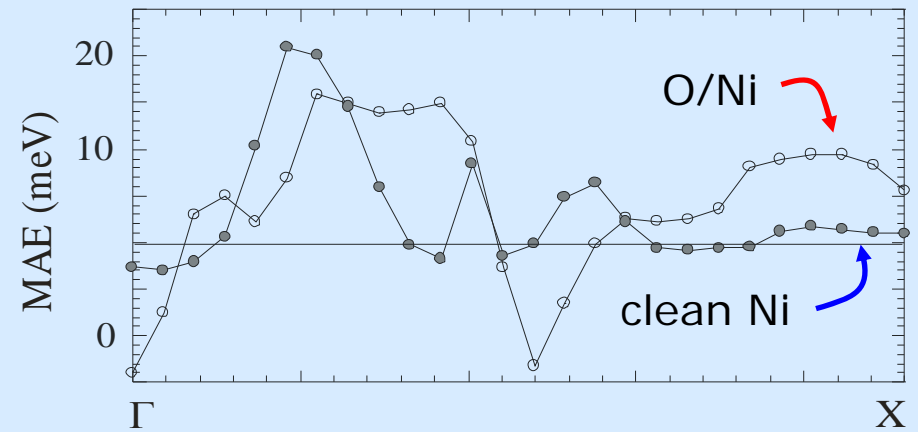
K. B. *Handbook of Magnetism and Advanced Magnetic Materials*, Vol. 3  
Ed. Kronmüller and Parkin, 2007 John Wiley & Sons, Ltd.

# Results of ab initio calculations

R. Q. Wu & coworkers



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

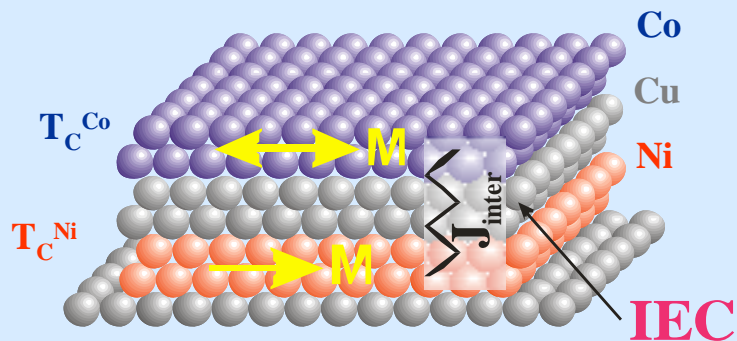


O-induced surface state seen in the vicinity of  $\bar{X}$ -point is responsible for change in **MAE**

for details see *Phys. Rev. Lett.* **92**, 147202 (2004)

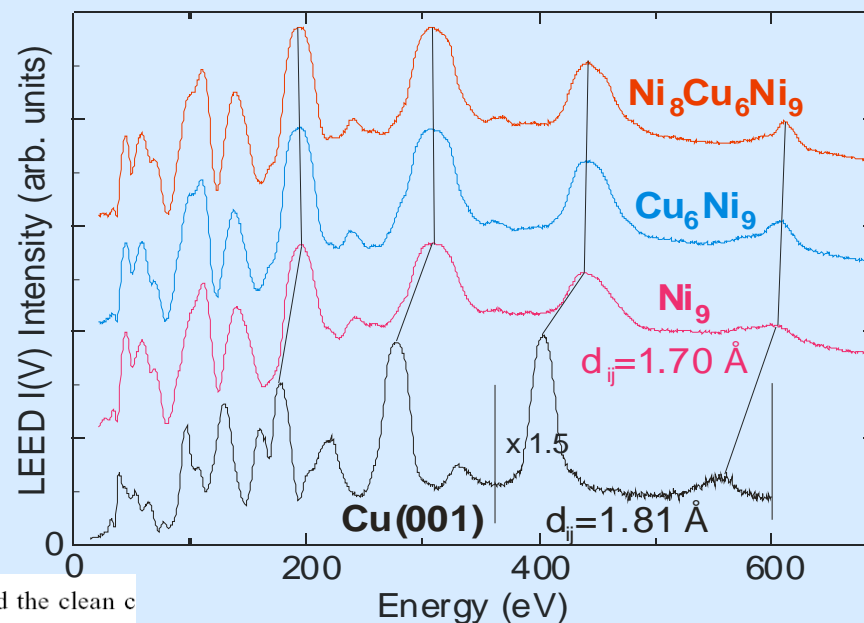


### 3. Interlayer Exchange Coupling and $f(T)$



W. Platow et al. PRB **59**, 12641 (1999)

full trilayer grows in fct structure



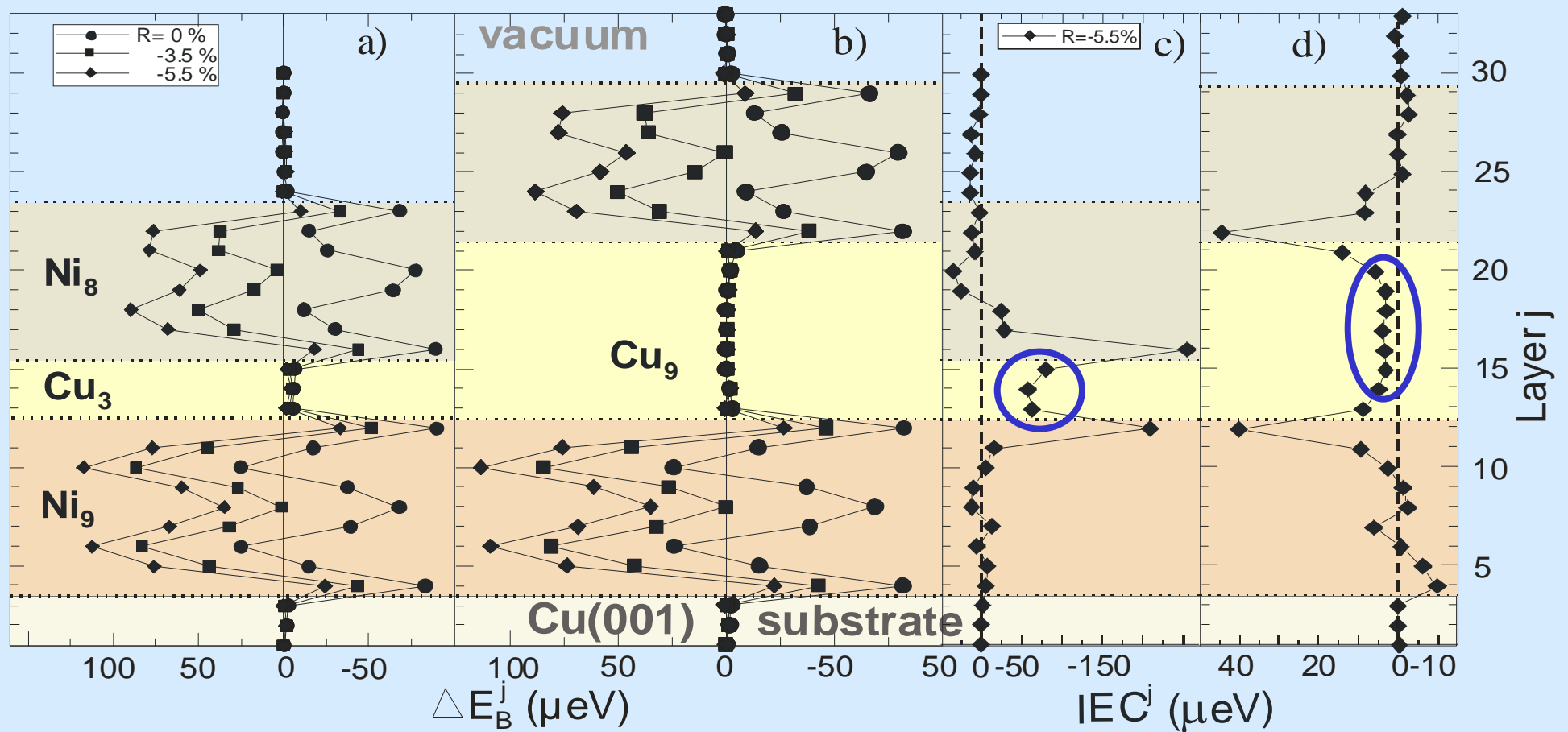
R. Nünthel, PhD Thesis FUB 2003

TABLE I. Best-fit structural data for the nickel films of different thickness and the clean c

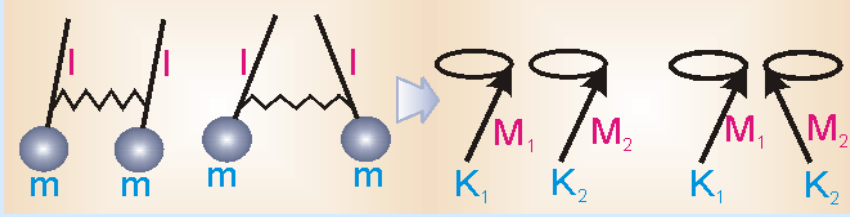
Parameter	0 ML	1 ML	2 ML	3 ML	4 ML	5 ML
$d_{12}$ (Å)	$1.755^{+0.011}_{-0.007}$	$1.720^{+0.014}_{-0.018}$	$1.715^{+0.015}_{-0.015}$	$1.725^{+0.022}_{-0.016}$	$1.705^{+0.015}_{-0.011}$	$1.675^{+0.012}_{-0.014}$
$d_{23}$ (Å)	$1.805^{+0.006}_{-0.011}$	$1.770^{+0.012}_{-0.014}$	$1.720^{+0.011}_{-0.011}$	$1.710^{+0.012}_{-0.009}$	$1.705^{+0.011}_{-0.013}$	$1.710^{+0.010}_{-0.014}$
$d_{34}$ (Å)	$1.800 \pm 0.010$	$1.795^{+0.012}_{-0.012}$	$1.775^{+0.014}_{-0.021}$	$1.715^{+0.024}_{-0.017}$	$1.71^{+0.014}_{-0.016}$	$1.700^{+0.014}_{-0.014}$
$d_{45}$ (Å)	$1.790 \pm 0.013$	$1.800^{+0.017}_{-0.014}$	$1.790^{+0.028}_{-0.015}$	$1.760^{+0.028}_{-0.017}$	$1.72^{+0.024}_{-0.017}$	$1.715^{+0.014}_{-0.014}$
$d_{56}$ (Å)	$1.800^{+0.010}_{-0.009}$	$1.790^{+0.020}_{-0.017}$	$1.800^{+0.028}_{-0.028}$	$1.790^{+0.021}_{-0.022}$	$1.76^{+0.033}_{-0.022}$	$1.730^{+0.018}_{-0.025}$
$d_b$ (Å)	1.790	1.79	1.79	1.79	1.77	1.70
$\Delta E$ (eV)	2270	2070	2220	2090	1450	2120
$R_p$	0.085	0.093	0.170	0.138	0.096	0.111

# SP-KKR calculation for $\Delta E_{\text{band}}$ and IEC for rigid fcc and relaxed fct structures

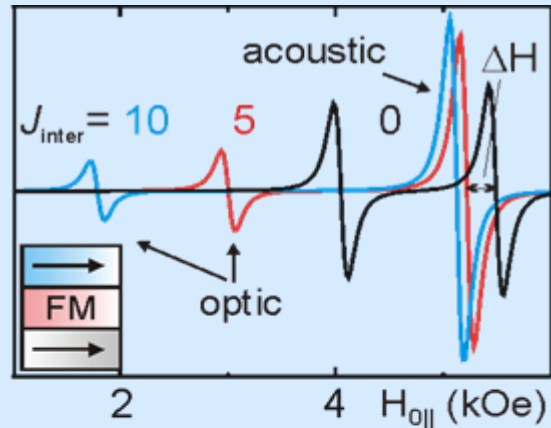
R. Hammerling, P. Weinberger et al., PRB **68**, 092406 (2003)



# *in-situ* FMR in coupled films

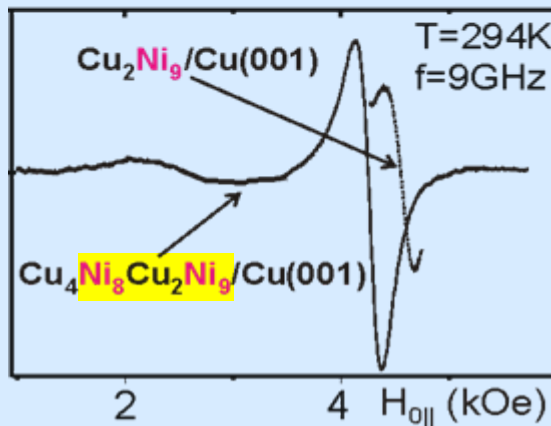


Advantage: **FM and AFM**  
IEC =>  $f(T)$  in  $\mu\text{eV}/\text{particle}$

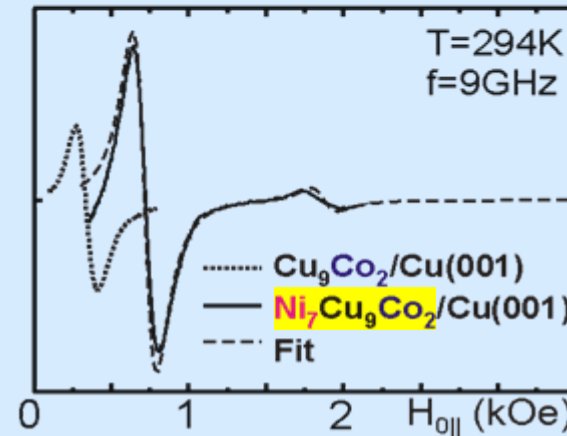
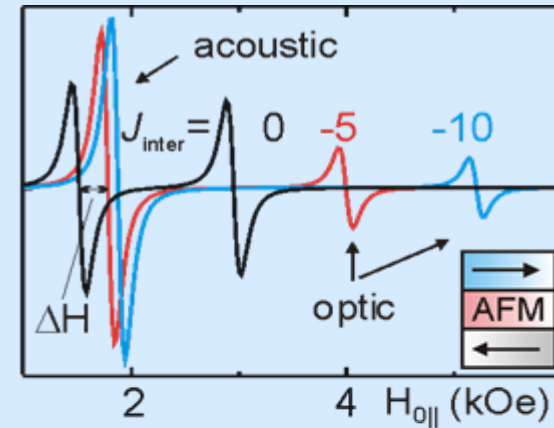


theory

**FMR**



*in-situ*  
UHV-experiment



J. Lindner, K. B. Topical Rev., J. Phys. Condens. Matter **15**, R193-R232 (2003)



# Interlayer exchange coupling and its T-dependence.

P. Bruno, PRB **52**, 411 (1995); V. Drchal et al. PRB **60**, 9588 (1999)

$$J_{\text{inter}} = J_{\text{inter},0} \left[ \frac{T/T_0}{\sinh(T/T_0)} \right] \quad T_0 = \hbar v_F / 2\pi k_B d$$

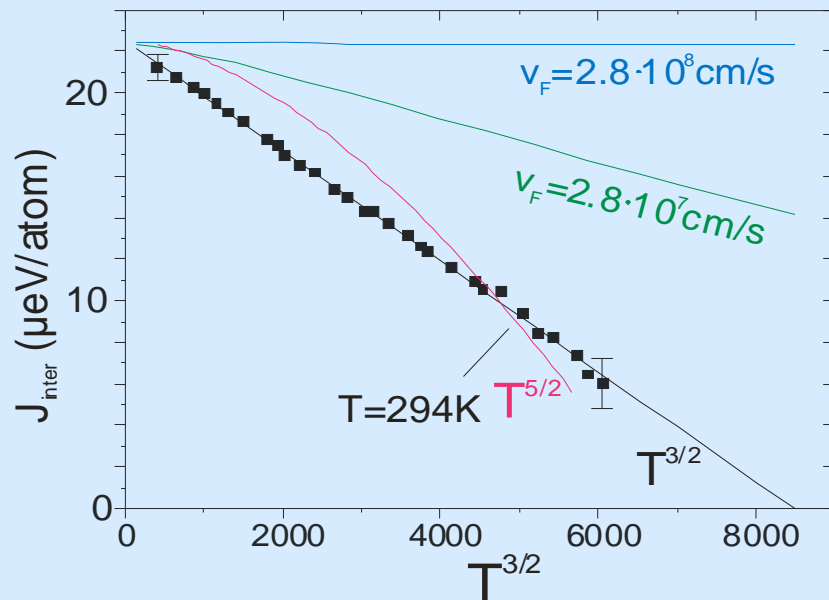
N.S. Almeida et al. PRL **75**, 733 (1995)

$$J_{\text{inter}} = J_{\text{inter},0} [1 - (T/T_C)^{3/2}]$$

**Ni<sub>7</sub>Cu<sub>9</sub>Co<sub>2</sub>/Cu(001)**

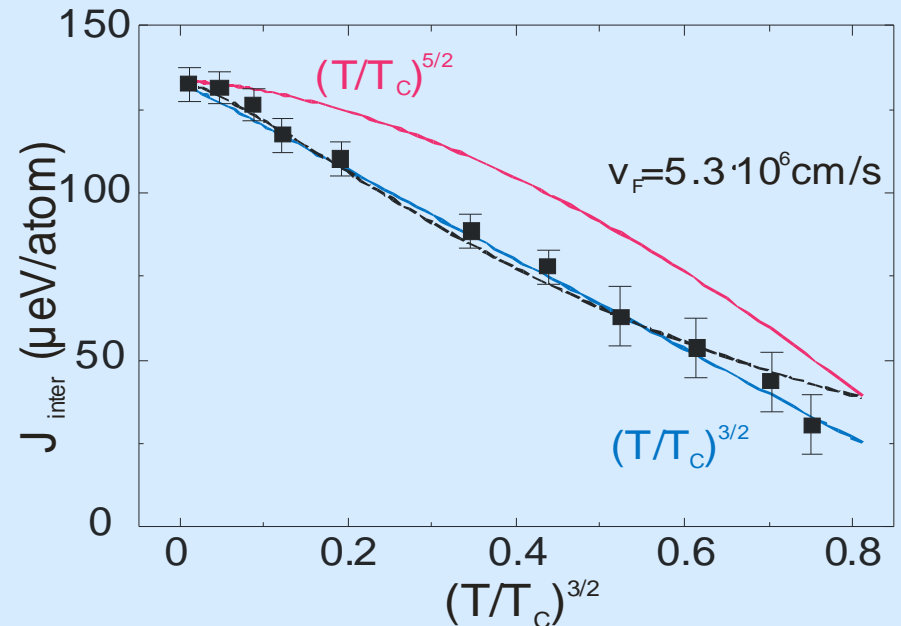
J. Lindner et al.  
PRL **88**, 167206 (2002)

T=55K - 332K



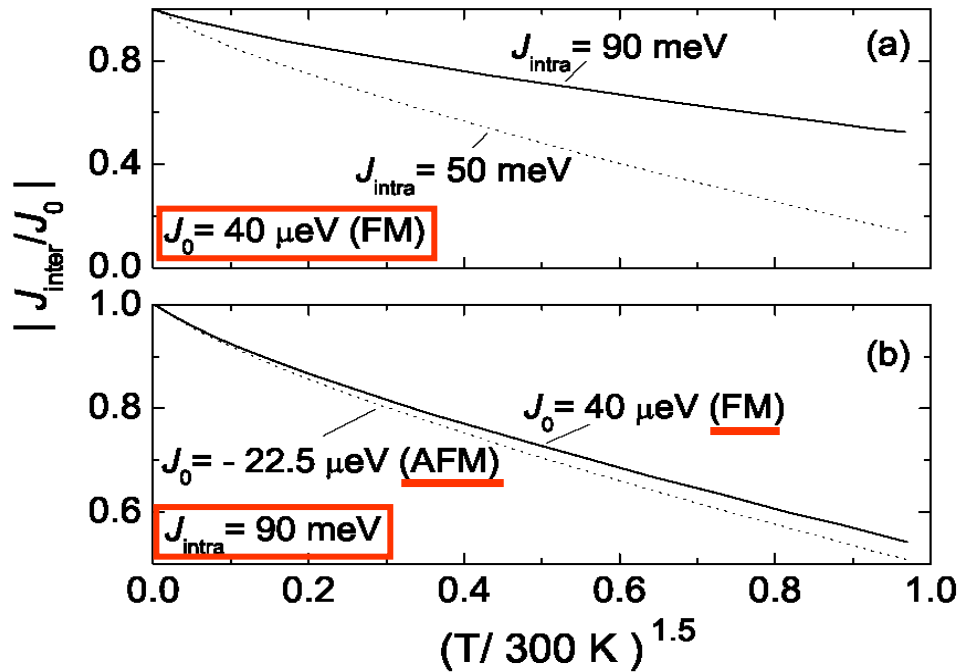
**(Fe<sub>2</sub>V<sub>5</sub>)<sub>50</sub>**

T=15K - 252K, T<sub>C</sub>=305K



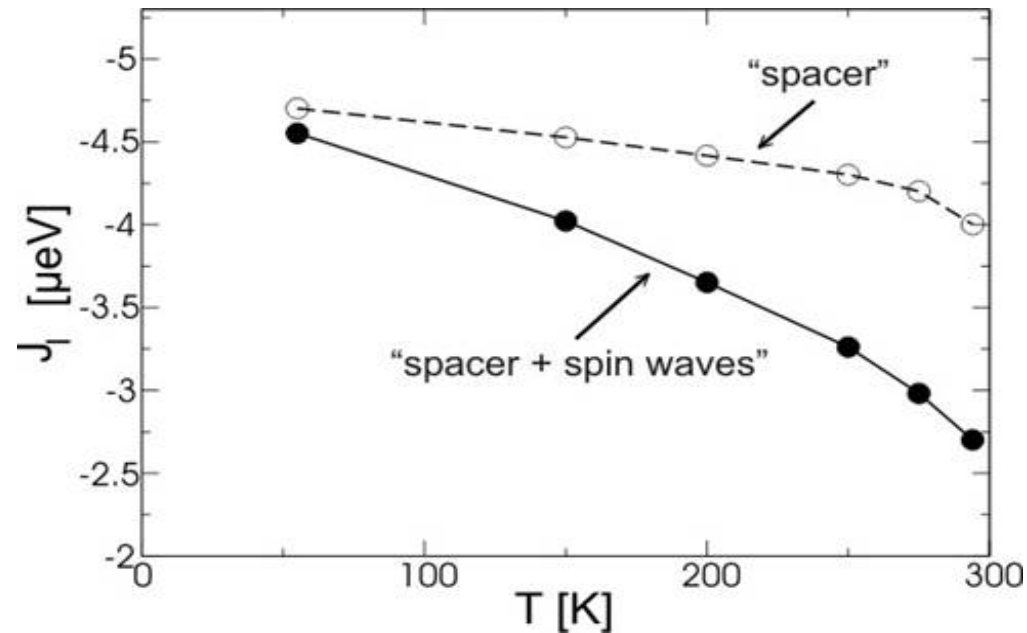
All contributions due to the spacer, interface and magnetic layers, nevertheless give an effective power law dependence on the temperature:

$$J(T) \approx 1 - AT^n, \quad n \approx 1.5 \quad (1)$$



## T dependence of IEC

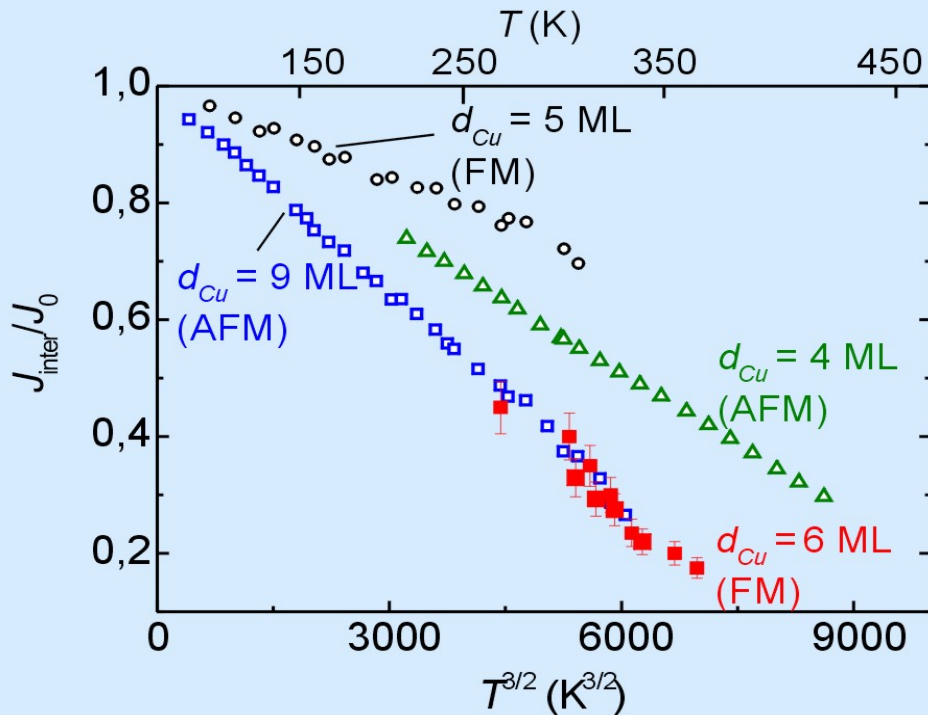
S. Schwieger et al., PRL **98**, 57205 (2007)



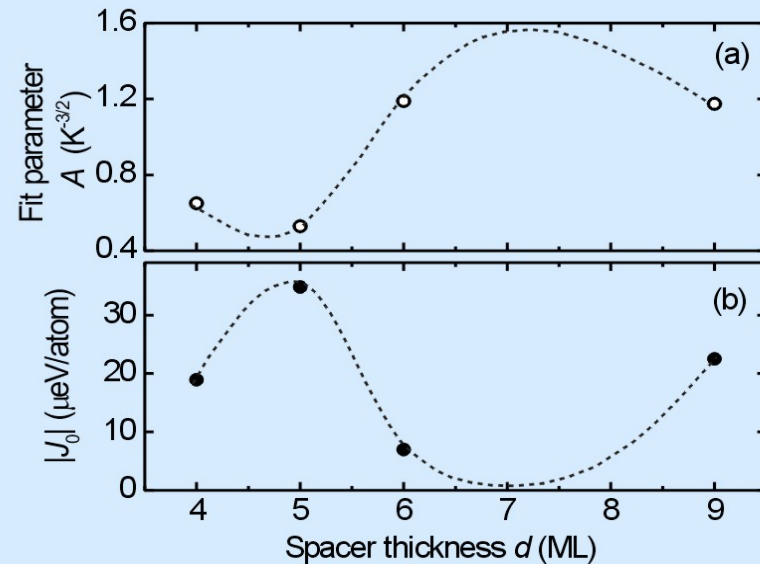
# The dominant role of thermal magnon excitation in the temperature dependence of the interlayer exchange coupling: experimental verification

S. S. Kalarickal,\* X. Y. Xu,<sup>†</sup> K. Lenz, W. Kuch, and K. Baberschke<sup>‡</sup>  
*Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany*

PRB 75, 224429 (2007)



$$J(T) \approx 1 - A(d)T^n, \text{ with } n \approx 1.5$$



- $A(d) \neq \text{const.}$
- $A(d) \neq \text{linear function}$
- $A(d) \approx \text{osc. function}$

- (interface)
- (electronic bandstructure)
- (spin wave excitation)



#### 4. Summary: **Very fruitful collaboration between theory and experiment.**

Theory can disentangle various mechanisms ( $K^s$ ,  $K^v$ , layer-by-layer, spin waves or band structure, etc.)

Experiment needs no muffin tin radius, is full-relativistic (anisotropy depends on orbital magnetism)

For details see: K. B. in Vol. 3 *Handbook of Magnetism and Advanced Magnetic Materials*,  
Ed. Kronmüller and Parkin, 2007 John Wiley & Sons, Ltd.

**Theory:** H. Ebert, LMU; J.J. Rehr, UW; O. Eriksson UU; P. Weinberger, TU Vienna;

R. Wu, D.L. Mills, UCI; P. Jensen + K.H. Bennemann, FUB; W. Nolting, HUB



[www.physik.fu-berlin.de/~bab](http://www.physik.fu-berlin.de/~bab)

**Thanks to my former coworkers:** S. Kalarickal, X. Xu, K. Lenz, J. Lindner, E. Kosubek, H. Wende, C. Sorg, F. Wilhelm, A. Scherz, a. o.

**Support:**  
BMBF, DFG