Nanomagnetism – Part III
Atomic-scale properties

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Part I – Magnetization reversal

Part II – Techniques

Part III – Atomic-scale properties

Fundamental issues for nanomagnetism

- Is a small grain (ferro)magnetic?

  Count number of surface atoms

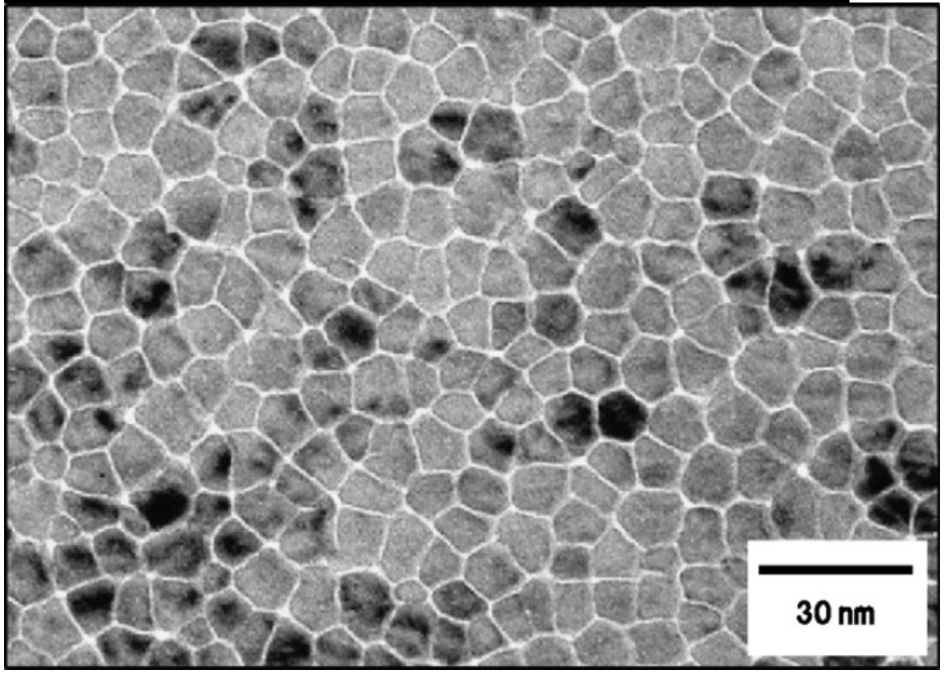
- Is a small grain stable against thermal fluctuations?

$$k_B T(300\ \mathrm{K}) \approx 4\times10^{-21}\ \mathrm{J} \approx 25\ \mathrm{meV}$$

$$100\, k_B T(300\ \mathrm{K}) \approx 2.5\ \mathrm{eV}$$

  Derive from macroscopic arguments

Magnetic grain media of current hard disks



Decades-old (yet still modern) topic

Properties of bulk Fe

(P,T) ambiant conditions

Body-Centered Cubic (bcc)

Ferromagnetic

$\approx 2.2\,\mu_B\ \text{atom}^{-1}$

$T_C = 1043\ \text{K}$

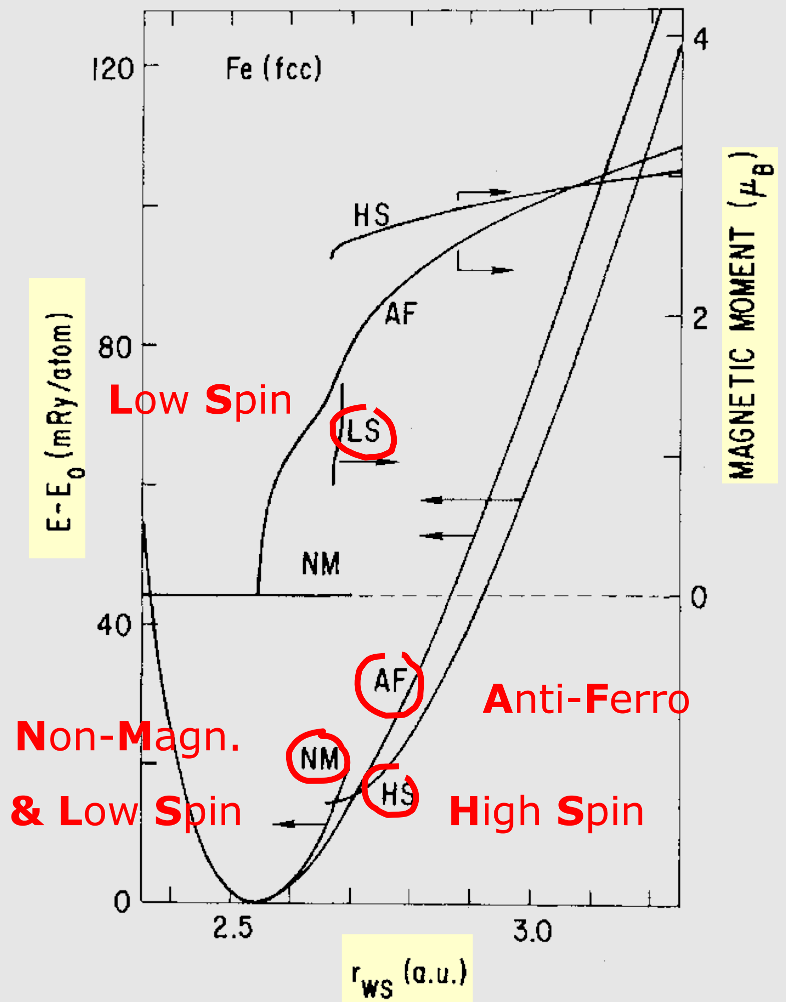
T>1185 K

Face-Centered Cubic (fcc, γ-Fe)

No magnetic order

Robustness of ferromagnetic orders

Theory: phase diagram of fcc iron (Fe)



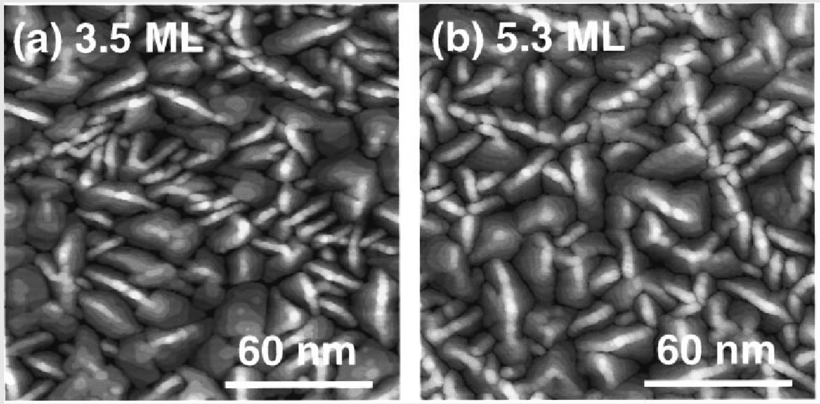
V. L. Moruzzi *et al.*, PRB39, 6957 (1989)

See also: O.K. Andersen, Physica B 86, 249 (1977)

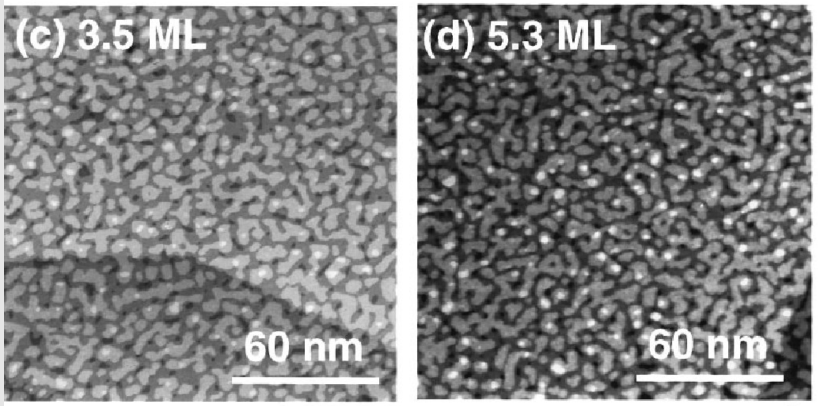
Effect of strain on the crystalline structure

Fe/Cu(001)

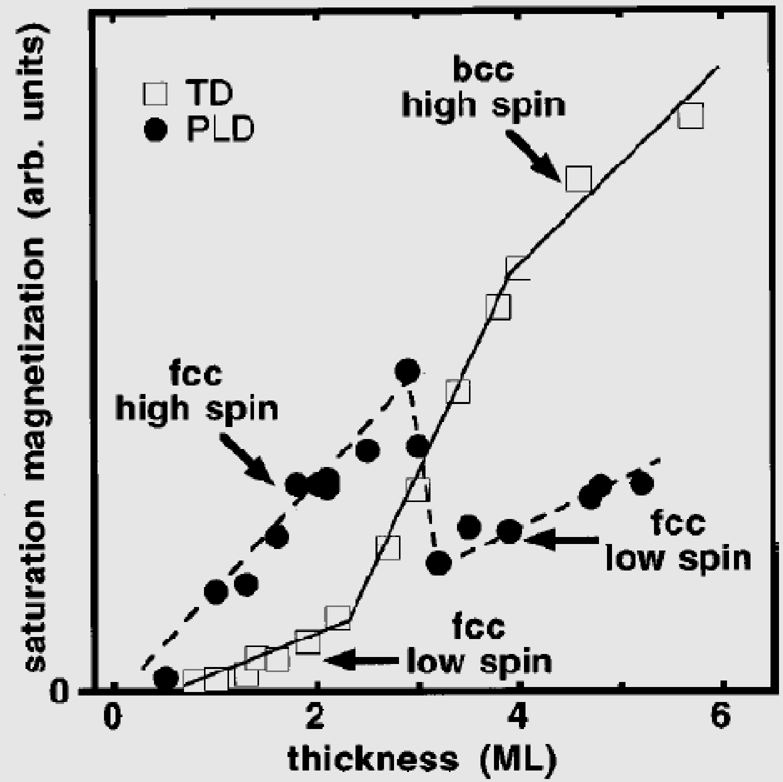
300K growth with MBE: fcc>bcc



300K growth with PLD: fcc



Magnetism of fcc Fe



High-spin and low-spin fcc phases?

P. Ohresser et al., PRB59, 3696 (1999)

Spin-density wave antiferromagnetism

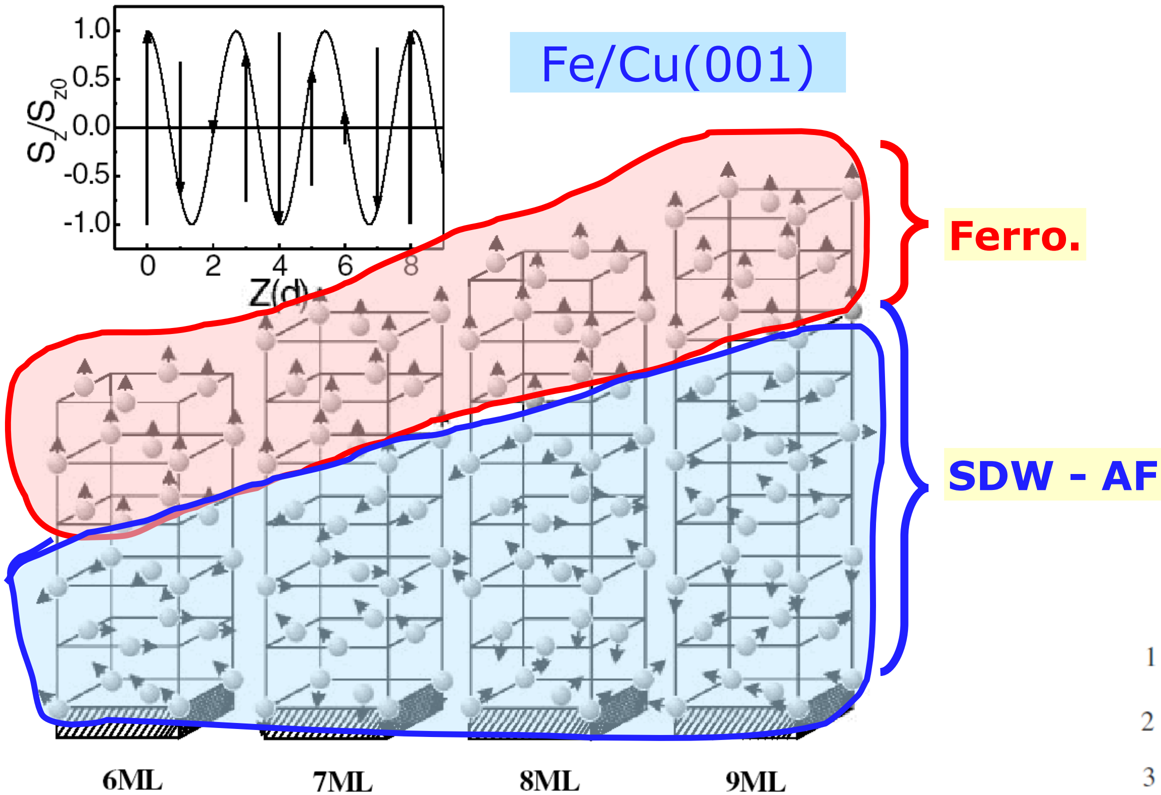
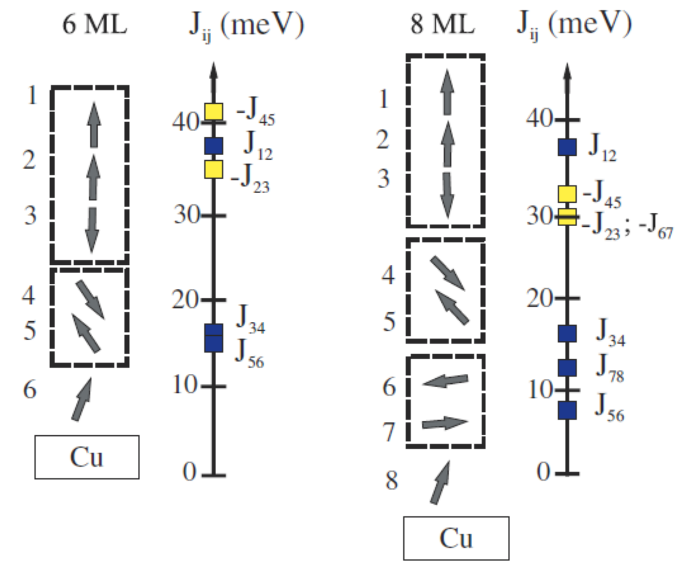


FIG. 4. Magnetic structures proposed for 6, 7, 8, and 9 ML Fe on Cu(100); the inset gives the layer dependent magnetic moments for fcc Fe along the z direction, $z(d) = 0$ corresponding to the first AFM layer. (Note: all the moments drawn here are lying in the planes parallel to the front plane of the structure section.)

D. Qian et al., PRL87, 227204(2001)

See also:
H. L. Meyerheim et al., Phys. Rev. Lett. 103, 267202 (2009)



Probing surface magnetization

Surface techniques at 0K

- Mossbauer with probe layers

Plot $m(t)$ at 0K:

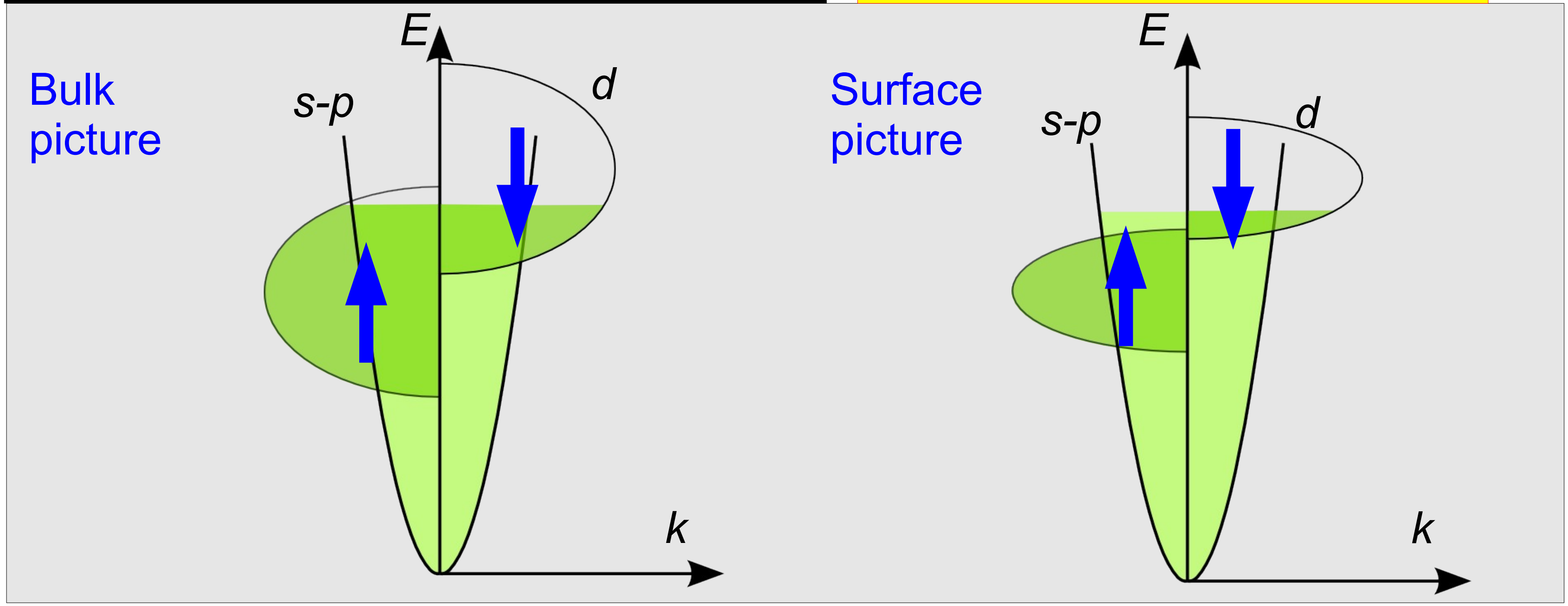
- Magnetometry
- XMCD

Some results

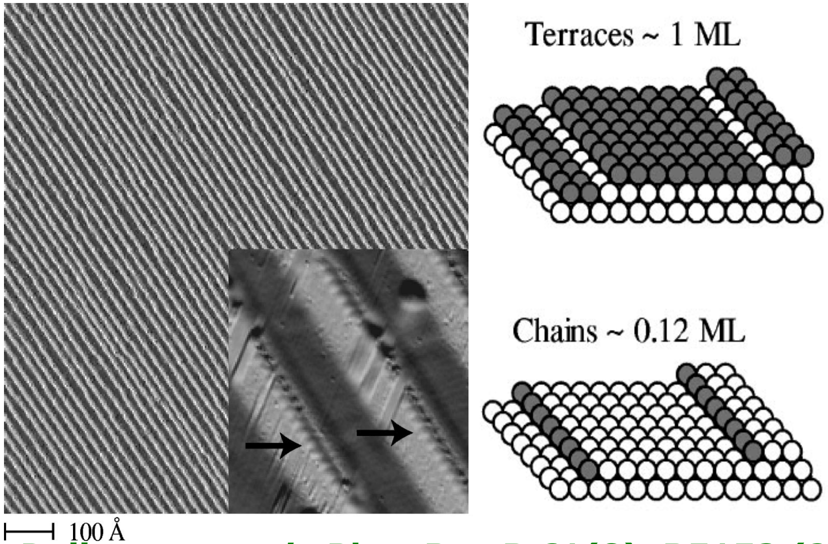
- Fe/W(110) : 0.14ml($+0.35\mu_B$)
- UHV/Fe(110); Ag/Fe(110): 0.26ml($+0.65\mu_B$)
- Cu/Ni(111): -0.5ml
- Overlayers: Pd/Ni(111)/Re(0001)

(Too) simple picture: band narrowing at surfaces

Enhanced moment at surfaces



Co/Pt(997)



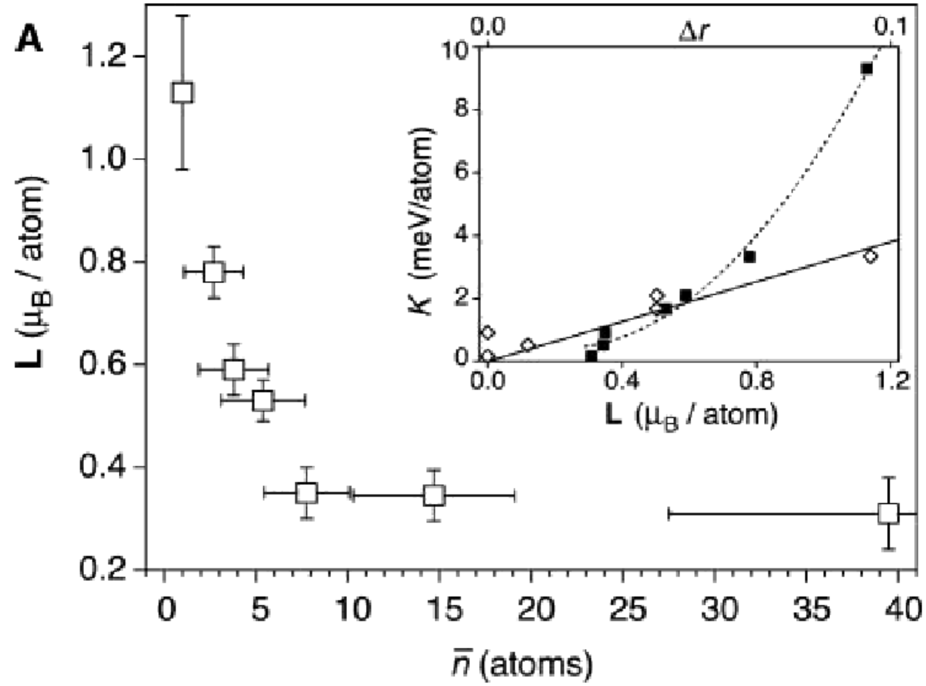
A. Dallmeyer *et al.*, Phys.Rev.B 61(8), R5153 (2000)

Conclusions

- Bulk: m_L=0.14μ_B/at.
- Surface: m_L=0.31μ_B/at.
- Bi-atomic wire: m_L=0.37μ_B/at.
- Mono-atomic wire: m_L=0.68μ_B/at.
- bi-atom: m_L=0.78μ_B/at.
- atom: m_L=1.13μ_B/at.

P. Gambardella et al., Nature 416, 301 (2002)

Co/Pt(111)

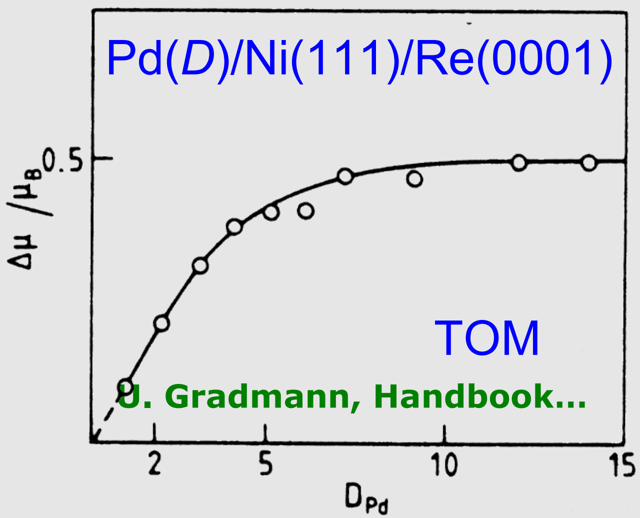


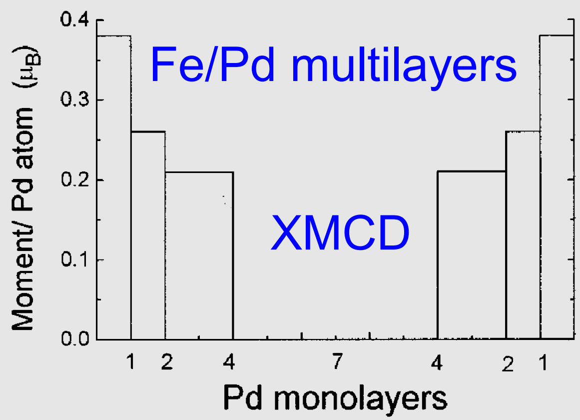
P. Gambardella et al., Science 300, 1130 (2003)

Conclusions

- From bulk to atoms: considerable **increase of orbital moment**
- **2 atoms closer to wire than 1 atom**
- **bi-atomic wire closer to surface than wire**

Exchange polarization at interfaces



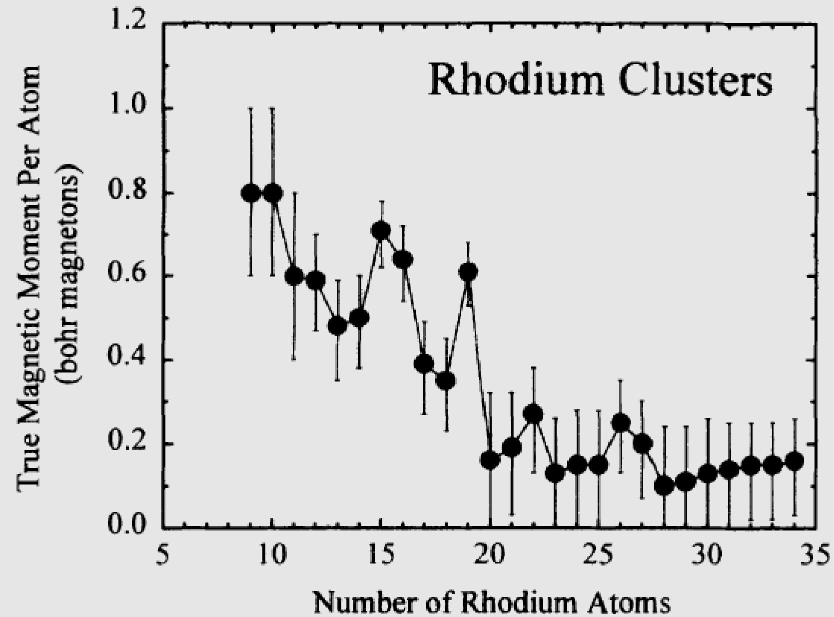


J. Vogel et al., PRB55, 3663 (1997)

Conclusion: Pd sigifnicantly polarized over several layers

Spontaneous polarization – Stoner criterieum

Small Rh(4d) clusters studied in flight (Stern-Gerlach experiment)



A. J. Cox et al., PRL71, 923 (1993)

A. J. Cox et al., PRB49, 12295 (1994)

Handwavy explanation based on Stoner criterium $I\rho_{\uparrow,\downarrow}(\epsilon_F) > 1$

Conclusion: recuced bandwidth may even drive ferromagnetism

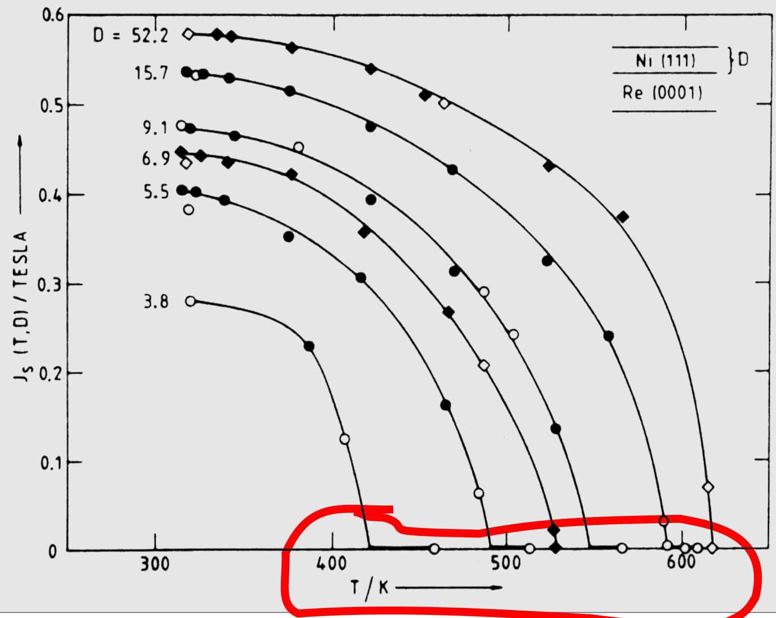
Elements of theory

- Ising (1925). No magnetic order at T>0K in 1D Ising chain.
- Bloch (1930). No magnetic order at T>OK in 2D Heisenberg.
  (spin-waves; isotropic Heisenberg)
- → N. D. Mermin, H. Wagner, PRL17, 1133 (1966)
- Onsager (1944) + Yang (1951).
  2D Ising model: Tc>0K

→ Magnetic anisotropy stabilizes ordering

Experiments

Ni(111)/Re(0001)



R. Bergholz and U. Gradmann, JMMM45, 389 (1984)

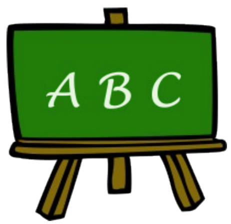
Tc interpreted with molecular field

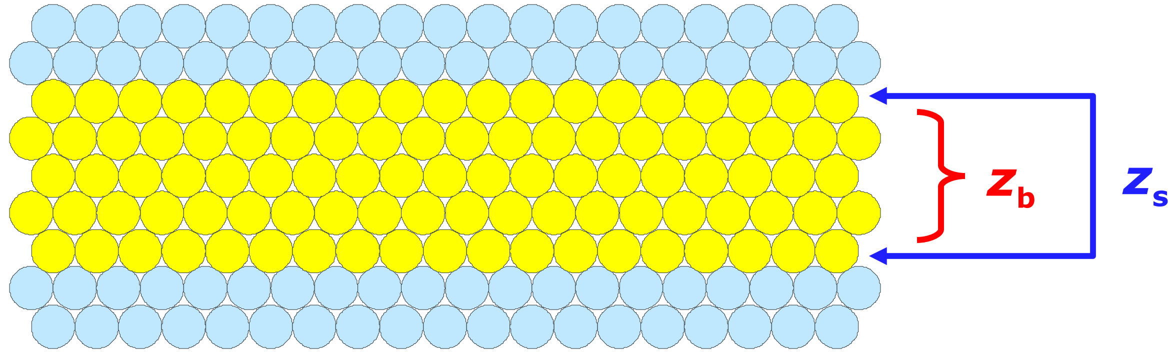
Naïve model

Molecular field

$$T_C = \frac{\mu_0 z n_{W,1} n g_J^2 \mu_B^2 J(J+1)}{3 k_B}$$

z neighbors





N atomic layers

$$\langle z \rangle = z_b - \frac{2(z_b - z_s)}{N} \Rightarrow \Delta T_C(t) \sim t^{-1}$$

Less naïve...

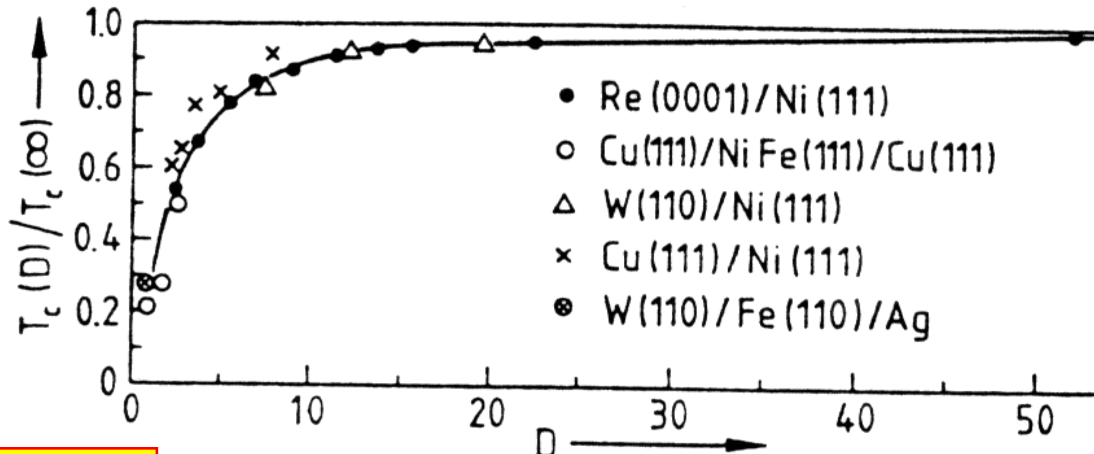
Thickness-dependant molecular field

$$\Delta T_C(t) \sim t^{-\lambda}$$

$$\lambda = 1$$

G.A.T. Allan, PRB1, 352 (1970)

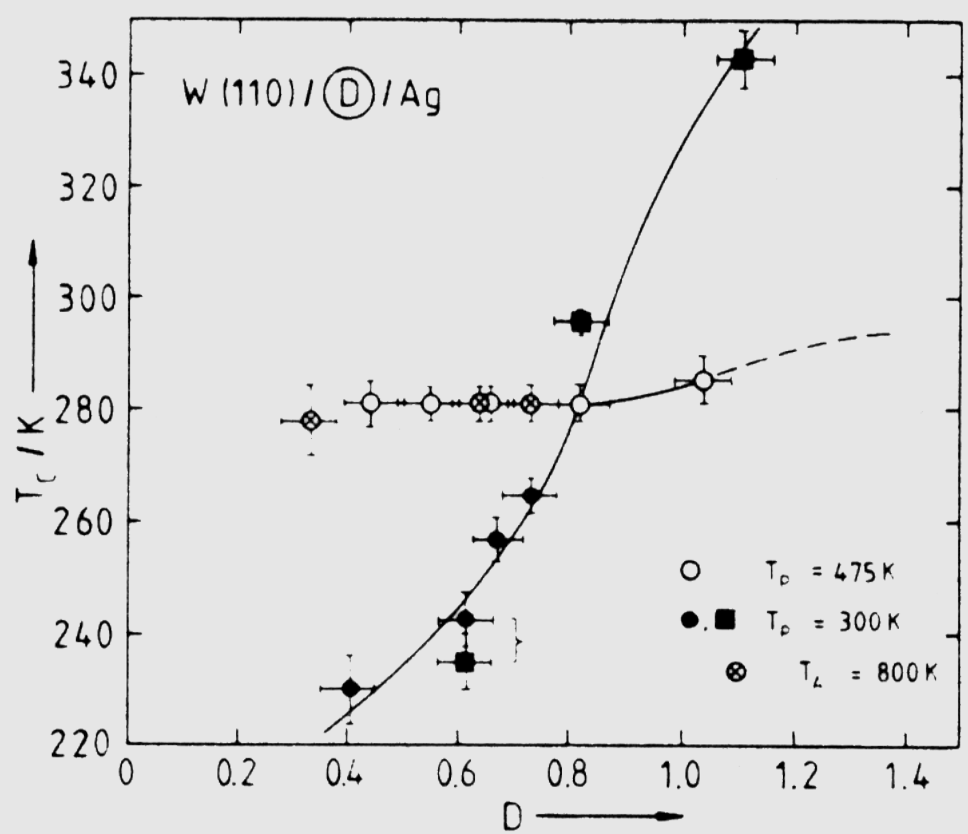
Experiments



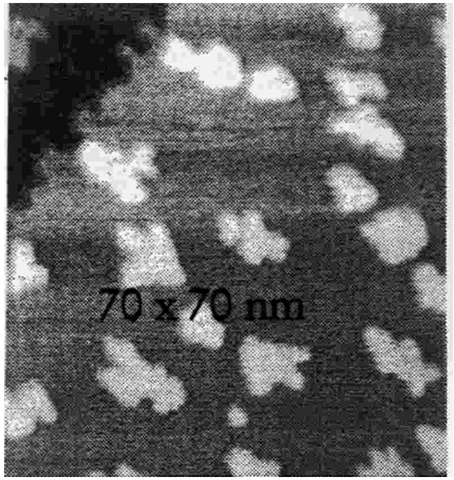
U. Gradmann,
Handbook of Magn. Mater. Vol.7, ch.1 (1993)

Conclusion:
Naïve views are roughly correct

Effect of lateral size



U. Gradmann, Handbook of Magn. Mater. 7 (1993)



H.J.Elmers *et al.*, Phys.Rev.Lett.73, 898(94)

Conclusion
Tc also depends on size of islands (lateral dimensions)

1. Ferromagnetic order in low dimensions

2. Magnetic energy anisotropy

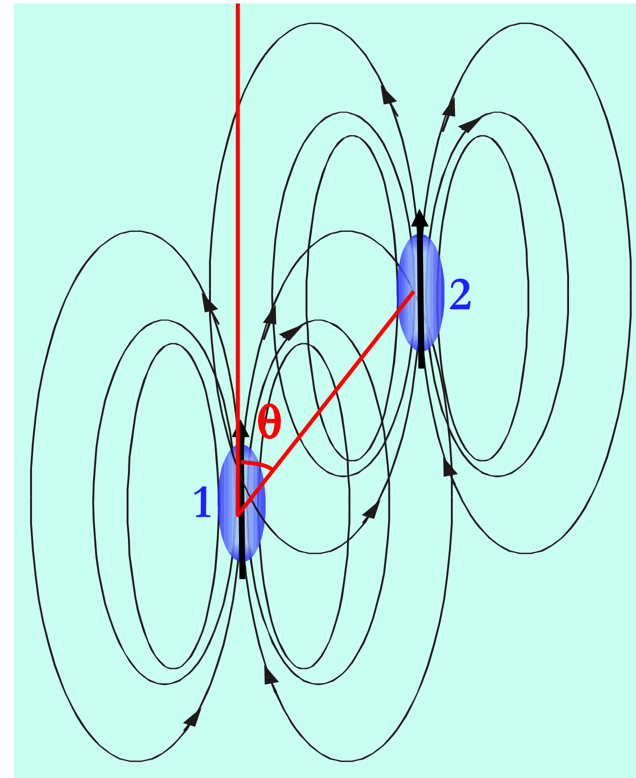
- Microscopic origins of Magnetic Anisotropy Energy (MAE)
- Surface versus magneto-elastic anisotropy
- From surfaces (2D) to atoms (0D)

3. Interfacial effects

Dipolar energy

Mutual energy of two magnetic dipoles :

$$E_{1,2} = \frac{\mu_0}{4\pi r^3}\left[\vec{\mu}_1.\vec{\mu}_2 - \frac{3}{r^2}(\vec{\mu}_1.\vec{r}).(\vec{\mu}_2.\vec{r})\right]$$



Let us assume two magnetic dipoles with vertical direction, either 'up' or 'down' :

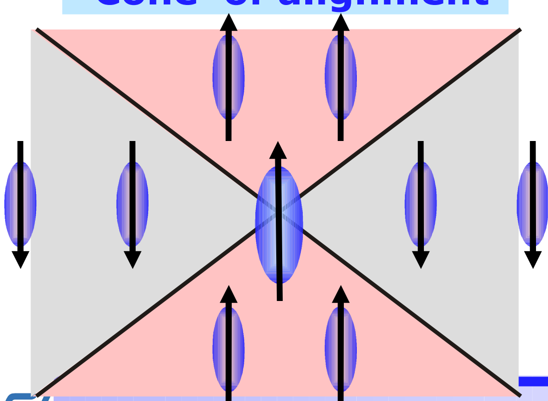
$$E_{1,2}(\theta) = \frac{\mu_0}{4\pi r^3}\mu_1\mu_2\left[1 - 3\cos^2\theta\right]$$

$$\cos^2(\theta_C) = 1/3$$

Parallel alignment is favored for $\theta < \theta_C \approx 54.74°$

Antiparallel alignment is favored for $\theta > \theta_C \approx 54.74°$

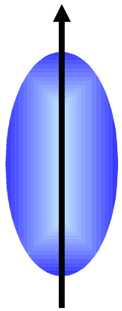
'Cone' of alignment

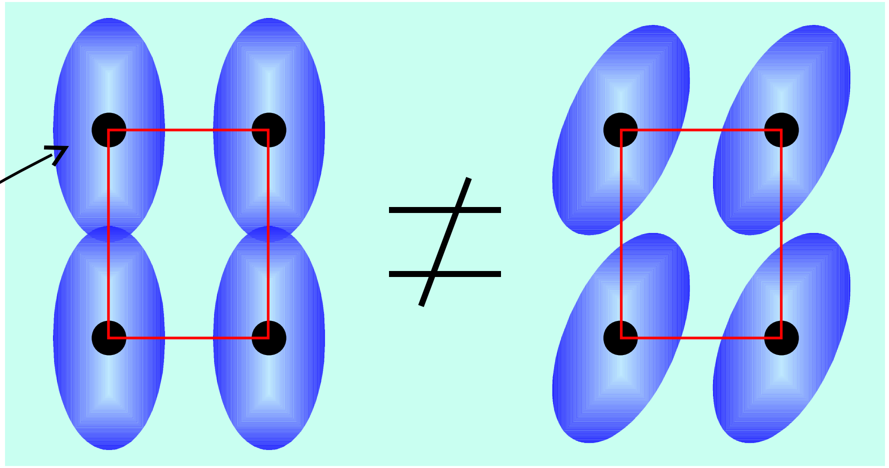


Conclusions

- Nanostructures: long axis favored
- Films: in-plane favored $e_d^z = \frac{1}{2}\mu_0 M_Z^2$

Magnetocrystalline anisotropy energy





Spin-orbit coupling ⇨ the energy of both spin and orbital moment depends on orientation

Series development on an angular basis:

Anisotropy energy **Normalized magnetization components**

$$E_{mc} = K_1 m_z^2 + K_2 m_z^4 + \dots \quad \text{Uniaxial}$$

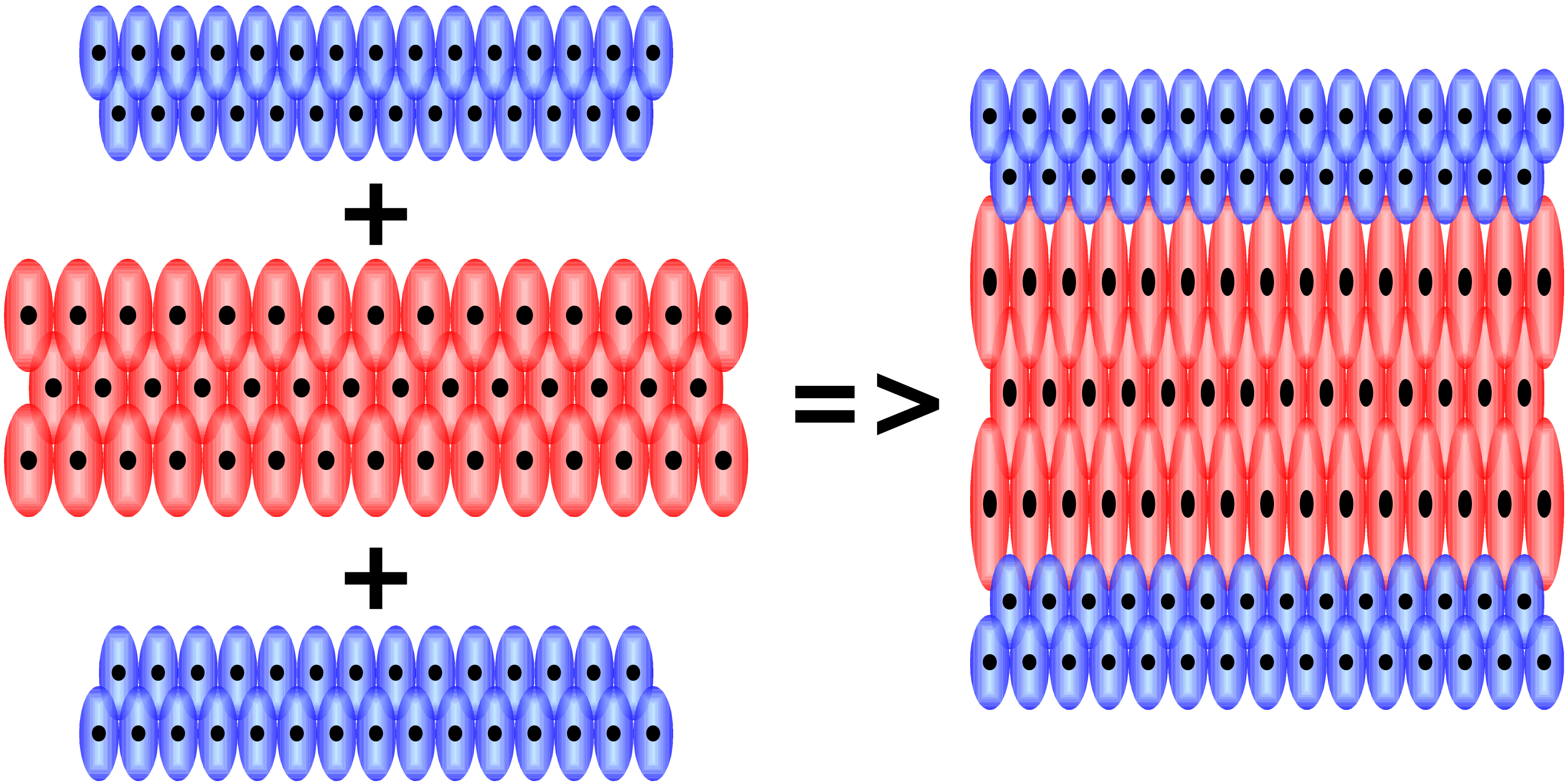
$$E_{mc} = K_4 (m_x^2 m_y^2 + m_y^2 m_z^2 + m_z^2 m_x^2) + \dots \quad \text{Cubic}$$

...

Alignement of magnetization is favored along given axes of the crystal

(Derived from slide of A. Thiaville - CNRS/Orsay)

Magneto-elastic anisotropy



Origin

Distortion of orbitals & crystal field

Correction to the magneto-crystalline energy

Result

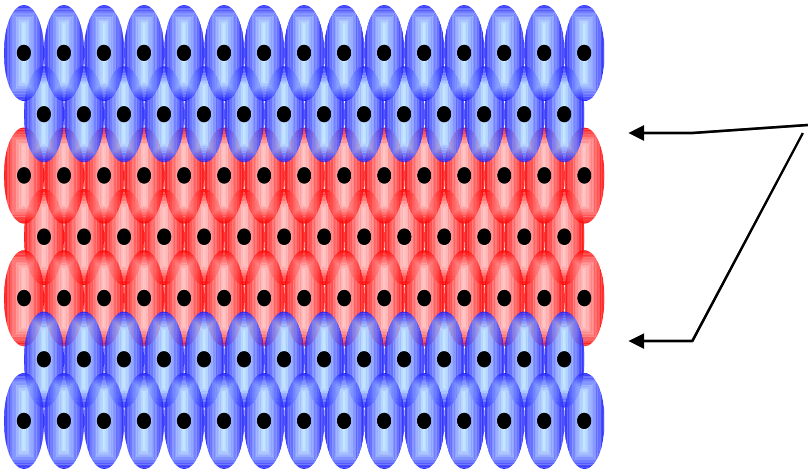
$$E_{mel} = K_{mel,1} \cos^2(\theta) + \ldots$$

$$K_{mel,i} \sim B_i \varepsilon$$

Surface anisotropy

L. Néel, J. Phys. Radium 15, 15 (1954)

« Superficial magnetic anisotropy and orientational superstructures »



Overview

Breaking of symmetry for surface/interface atoms

➡ Correction to the magneto-crystalline energy

$$E_S = K_{S,1}\cos^2(\theta) + K_{S,2}\cos^4(\theta) + \ldots$$

« This surface energy, of the order of 0.1 to 1 erg/cm2, is liable to play a significant role in the properties of ferromagnetic materials spread in elements of dimensions smaller than 100Å »

Pair model of Néel:

- Ks estimated from magneto-elastic constants
- Does not depend on interface material
- Yields order of magnitude only: correct value from experiments or calculations (precision !)

Magnetic Anisotropy Energy (MAE): Link with anisotropy of orbital moment

Theory

Perturbation theory for 3d metals:

$$MAE = \alpha \frac{\xi}{4\mu_B} \Delta \mu_L$$

P. Bruno, PRB39, 865 (1989)

μ_L does not rotate in 3d metals
-> MAE reflects cost in ξ

Covers magnetocrystalline, magnetoelastic and surface anisotropy

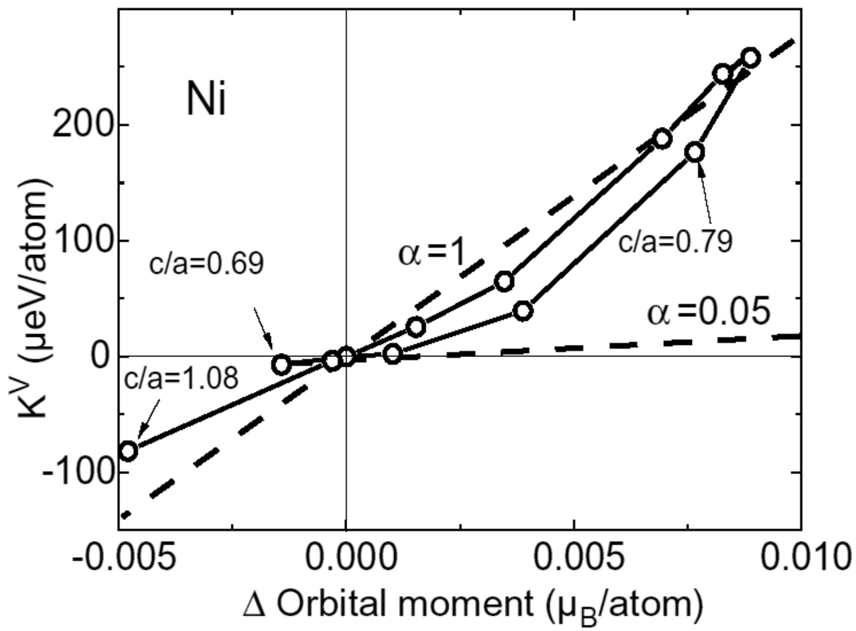
Experiments

Bulk (Fe, Ni, …)

$\Delta \mu_L \approx 10^{-4} \mu_B / atom$ ⇒ $MAE \leq 1\mu eV$

Ab initio calculations

High precision needed: $1\mu eV << 10 eV$



O. Hjortstam et al., PRB55, 15026 (1997)

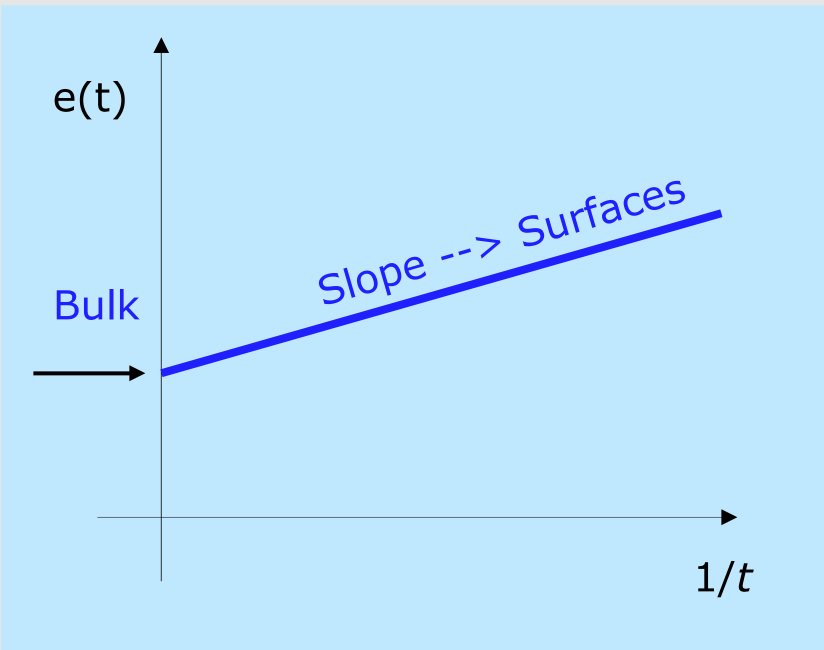
Conclusions

- Origin of MAE = anisotropy of orbital moment
- No strict linearity
- α may also depend on thickness in thin films (band structure)
  → Direct measurement of MAE preferable

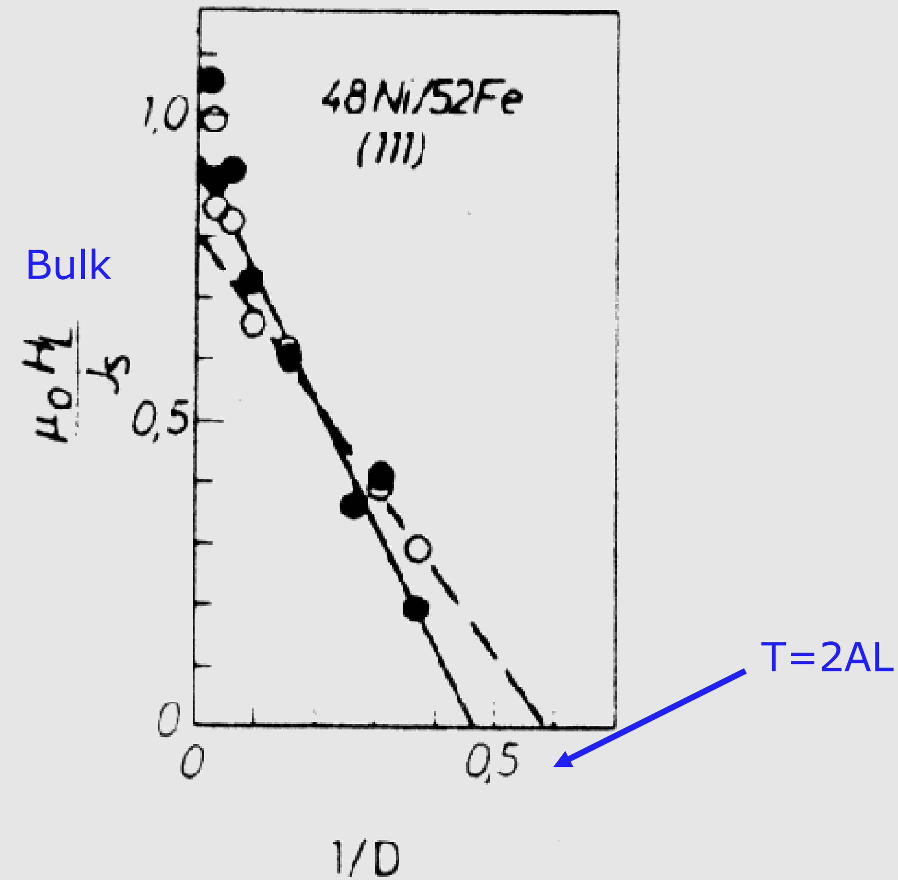
History of surface anisotropy : STEP 1 (1/t plot)

$$E_{tot}(t) = k_V t + 2k_S$$

$$\Rightarrow \quad e(t) = k_V + \frac{2k_S}{t}$$



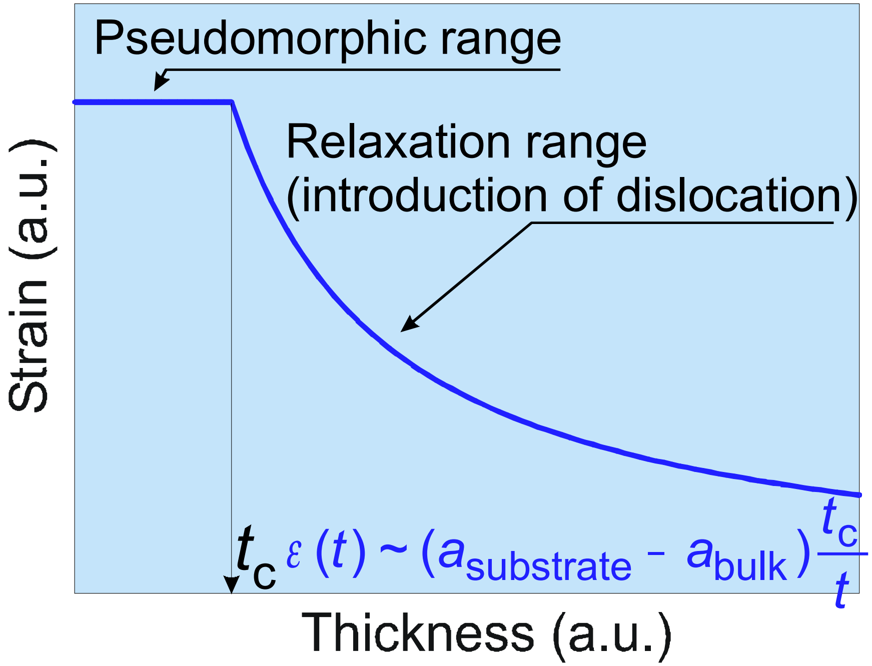
First example of perpendicular anisotropy



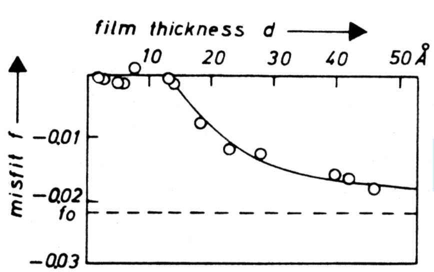
U. Gradmann and J. Müller,
Phys. Status Solidi 27, 313 (1968)

2. Magnetic anisotropy – Surface anisotropy

Structural relaxation



W. A. Jesser et al., Phys. Stat. Sol. 19, 95 (1967)



Co/Cu(111)

U. Gradmann, Appl. Phys.3, 161 (1974)

Effect on anisotropy

Magneto-elastic anisotropy:

$$k_{mel} \sim B_{mel}\varepsilon$$

Strain relaxation regime:

$$k(t) = k_{bulk} + \alpha B_{mel} / t$$

Conclusion:

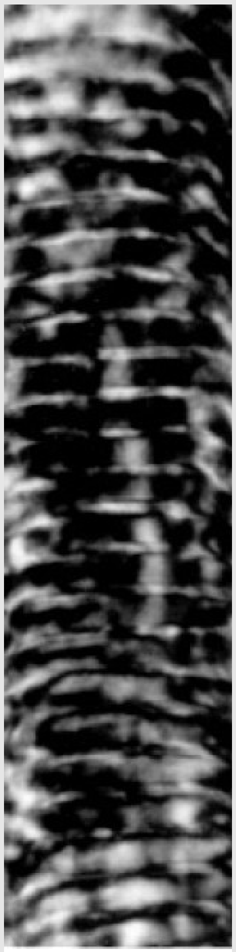
Mixing of surface and magneto-elastic contributions

$$e(t) = k_V + \frac{2k_S}{t}$$

C. Chappert and P. Bruno., JAP64, 5736 (1988)

Main use in applications : perpendicular magnetic anisotropy

Materials and geometry

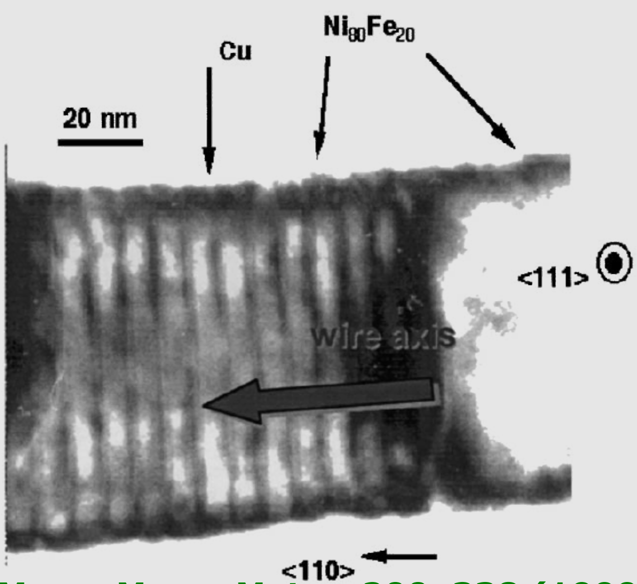


Interfacial elements with large spin-orbit: Pt, Au, Pd

Often: multilayers

Co/Au film

M. T. Johnson et al., Rep. Prog. Phys. 59, 1409 (1996)

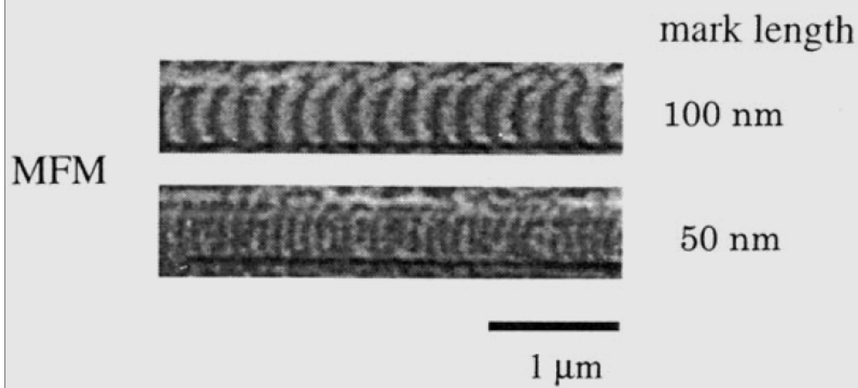


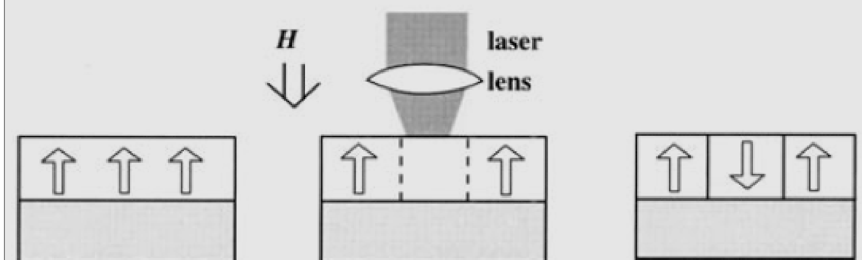
A. Fert et al., J. Magn. Magn. Mater. 200, 338 (1999)

Magneto-optical recording

Why: large magneto-optical response

Material: 3D-Rare-Earth based



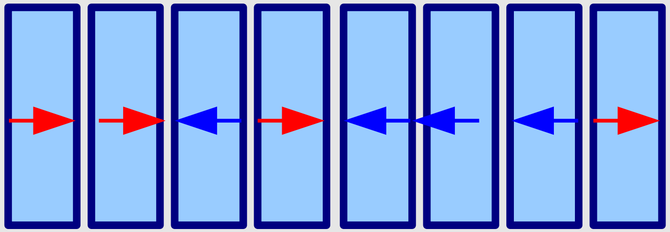


S. Tsunashima, J. Phys. D 34, R87 (2001)

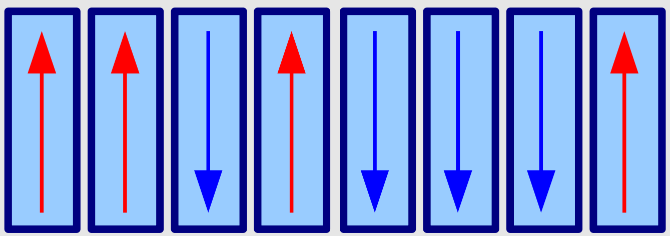
Main use in applications : perpendicular magnetic anisotropy

Decreased dipolar coupling in HDD media

Longitudinal recording (1956 -)



Perpendicular recording (2005 -)



S. N. Piramanayagam, J. Appl. Phys. 102, 011301 (2007)

⇨ High anisotropy with low spread angle

⇨ Reduced intra- and inter-grain dipolar coupling

See lecture: Laurent RANNO

Enhanced anisotropy for solid-state memories

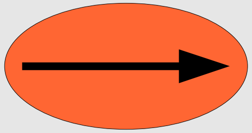
Concerns MRAM: Magnetic Random Access Memories

C. Chappert et al., The emergence of spin electronics in data storage, Nat. Mater. 6, 813 (2007)

Reminder for the thermal stability fo small flat elements:

$$H_c = \frac{2K}{\mu_0 M_s}\left(1-\sqrt{\frac{25 k_B T}{KV}}\right)$$

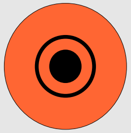
⇨ In-plane magnetization



$$K = N \times \frac{1}{2}\mu_0 M_s^2$$

Issue: N is small with flat elements

⇨ Perpendicular magnetization



$$K \approx \frac{1}{2}\mu_0 M_s^2$$

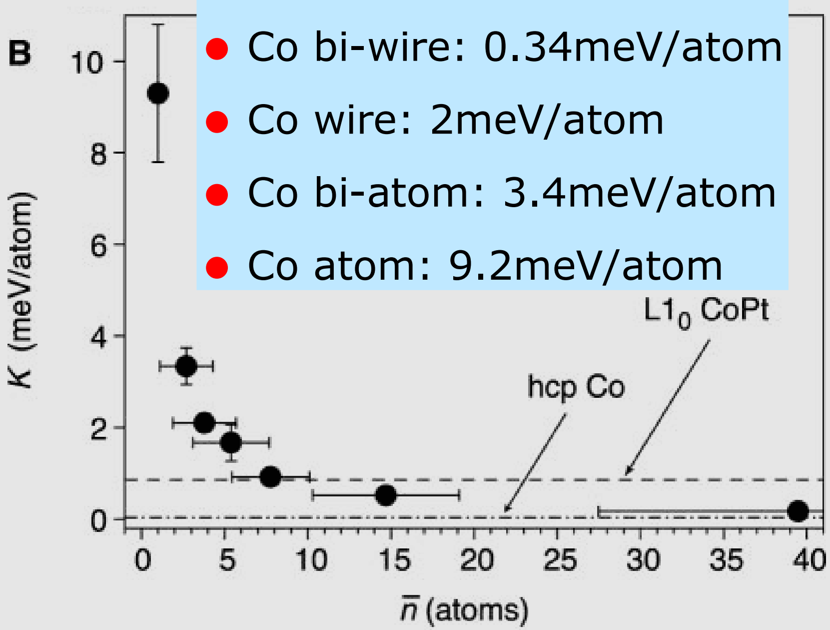
From surfaces (2D) to wires (1D) and atoms (0D)

Method

- XMCD
- Fit magnetization curves

Magnetic Anisotropy Energy

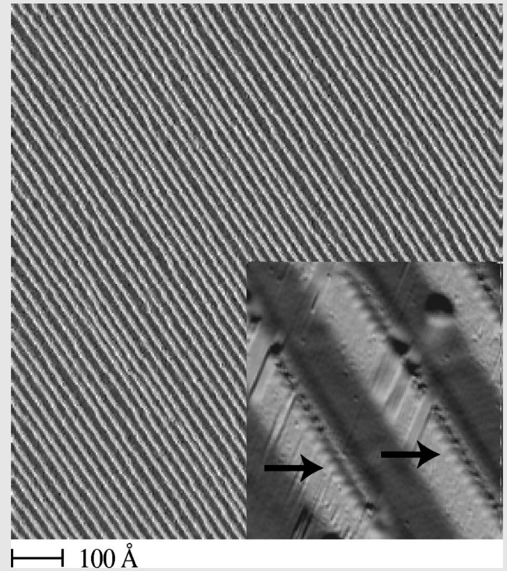
- Bulk Co: 40μeV/atom
- Co ML: 140μeV/atom
- Co bi-wire: 0.34meV/atom
- Co wire: 2meV/atom
- Co bi-atom: 3.4meV/atom
- Co atom: 9.2meV/atom



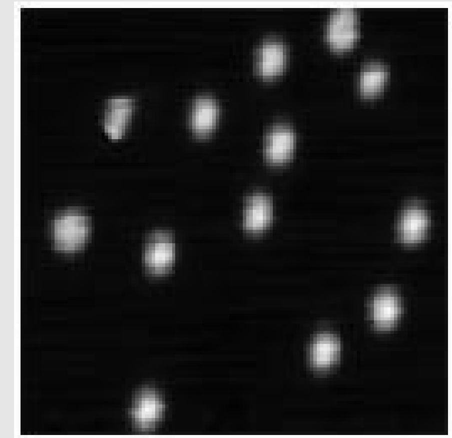
P. Gambardella *et al.*, Nature 416, 301 (2002)

P. Gambardella et al., Science 300, 1130 (2003)

Views of the model systems



STM, 8.5nm, 5.5K

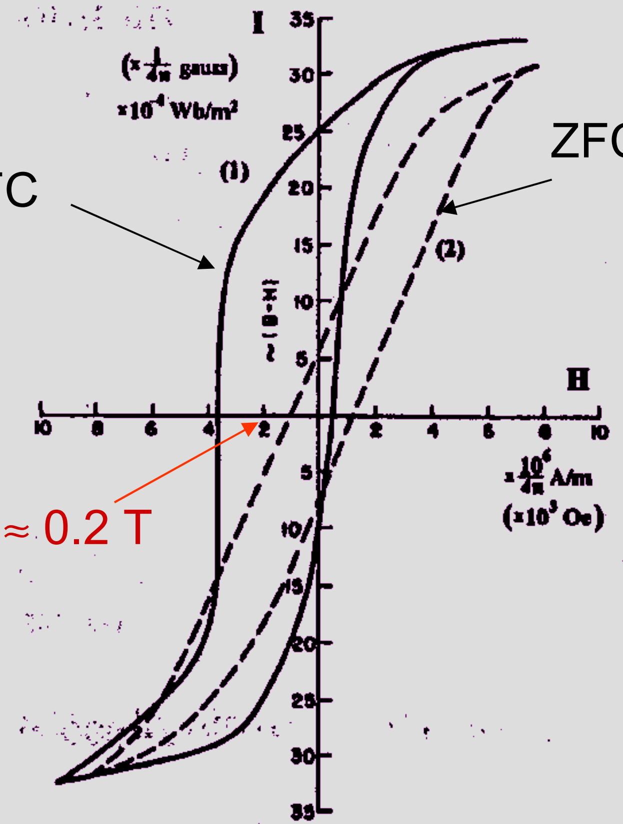


Conclusions:

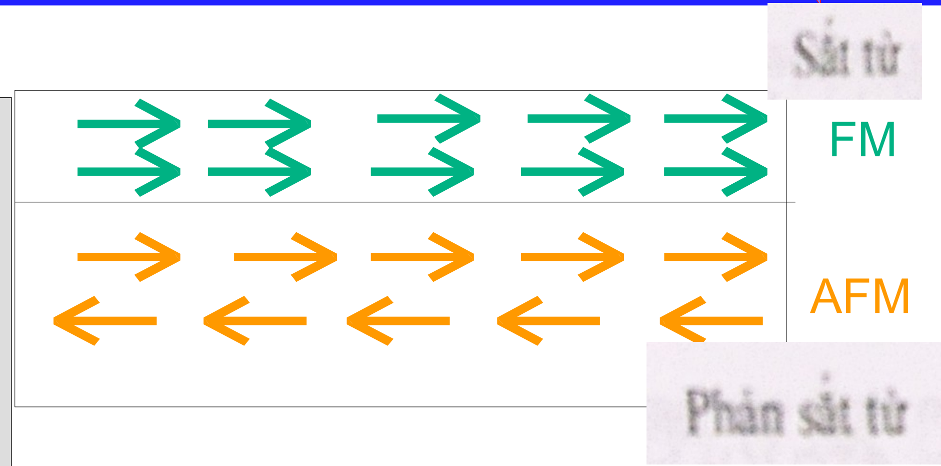
- Model systems to highlight trends in applied materials
- Anisotropy per atom increases in low dimensions
- The TOTAL anisotropy decreases → Not thermally stable

Seminal studies

Oxidized Co nanoparticles



Meiklejohn and Bean,
Phys. Rev. 102, 1413 (1956),
Phys. Rev. 105, 904, (1957)



Field-cooled hysteresis loops:

- **Increased coercivity**
- **Shifted in field**

Exchange bias
J. Nogués and Ivan K. Schuller
J. Magn. Magn. Mater. 192 (1999) 203

Exchange anisotropy—a review
A E Berkowitz and K Takano
J. Magn. Magn. Mater. 200 (1999)

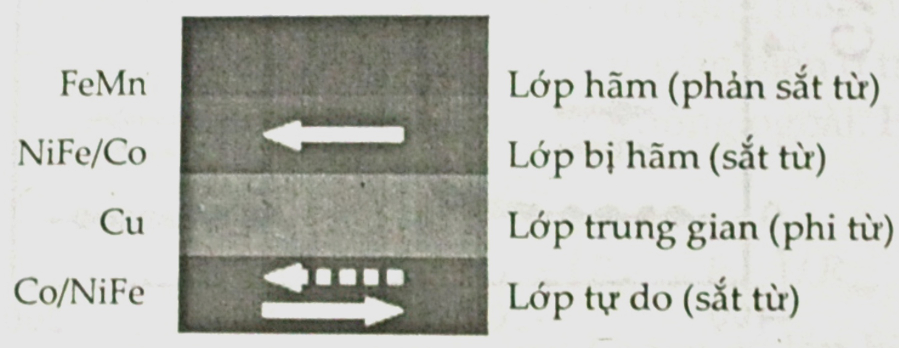
Increase coercivity of layers

Crude approximation for thin layers:

$$H_{F-AF} \approx H_F \left(1 + \frac{K_{AF} t_{AF}}{K_F t_F} \right)$$

Application

Concept of spin-valve in magneto-resistive elements

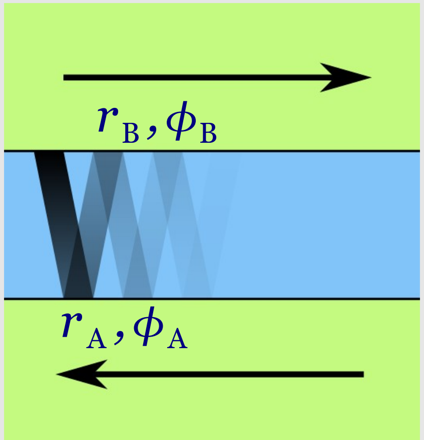


B. Diény et al., Phys. Rev. B 43, 1297 (1991)

- ⇨ Sensors
- ⇨ Memory cells
- ⇨ Etc.

The physics

Spin-dependent quantum confinement in the spacer layer



Forth & back phase shift

$$\Delta\phi = qt + \phi_A + \phi_B$$

Spin-independent

$$q = k^+ - k^-$$

Spin-dependent

$$r_A, \phi_A, r_B, \phi_B$$

Figures

Constructive and destructive interferences

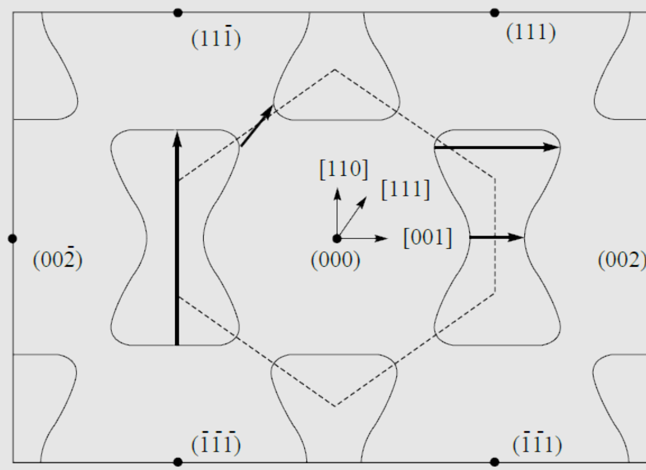
⇨ Maxima and minima of $n(\epsilon)$

Coupling strength:

$$E_S = J(t)\cos\theta \quad \text{in } J/m^2$$

$$\theta = \langle m_1, m_2 \rangle$$

with: $J(t) = \dfrac{A}{t^2}\sin(q_\alpha t + \Psi)$



P. Bruno, J. Phys. Condens. Matter 11, 9403 (1999)

Element	Structure	A_1 (Å)	ΔA_1 (Å)	J_1 (erg/cm²)	P (Å)	r_{ws} (Å)
Ti	hcp	No Coupling				2.89
V	bcc	9	3	0.1	9	2.62
Cr	bcc	7	7	.24	18	2.50
Mn	complex cubic					2.24
Fe	bcc	Ferro-Magnet				2.48
Co	hcp	Ferro-Magnet				2.50
Ni	fcc	Ferro-Magnet				2.49
Cu	fcc	8	3	0.3	10	2.56
Zr	hcp	No Coupling				3.17
Nb	bcc	9.5	2.5	.02	*	2.86
Mo	bcc	5.2	3	.12	11	2.72
Tc	hcp					2.71
Ru	hcp	3	3	5	11	2.65
Rh	fcc	7.9	3	1.6	9	2.69
Pd	fcc	No Coupling				2.75
Ag	fcc	No Coupling				2.89
Hf	hcp	No Coupling				3.13
Ta	bcc	7	2	.01	*	2.86
W	bcc	5.5	3	.03	*	2.74
Re	hcp	4.2	3.5	.41	10	2.74
Os	hcp					2.68
Ir	fcc	4	3	1.85	9	2.71
Pt	fcc	No Coupling				2.77
Au	fcc	No Coupling				2.88

fcc bcc hcp complex cubic

Element: A_1 (Å), ΔA_1 (Å), J_1 (erg/cm²), P (Å), r_{ws} (Å)

$$J(t)=\frac{A}{t^2}\sin\left(\frac{2\pi t}{P}+\Psi\right)$$

Illustration of coupling strength

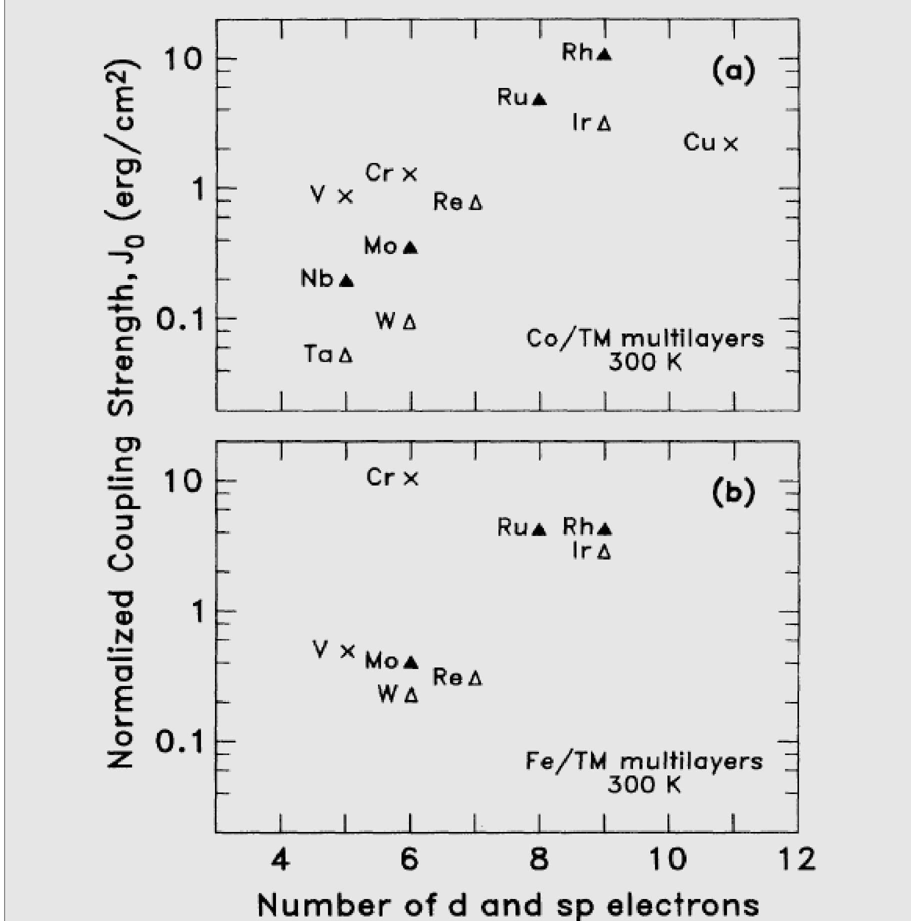
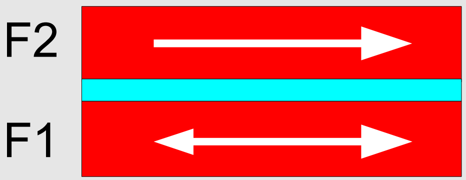


FIG. 3. Dependence of the normalized exchange coupling constant on the 3*d*, 4*d* and 5*d* transition metals in (a) Co/TM and (b) Fe/TM multilayers.

Note: *J*(*t*) extrapolated for t=3Å

S. S. P. Parkin, Phys. Rev. Lett. 67, 3598 (1991)

Synthetic Ferrimagnets (SyF) – Crude description



Hypothesis:

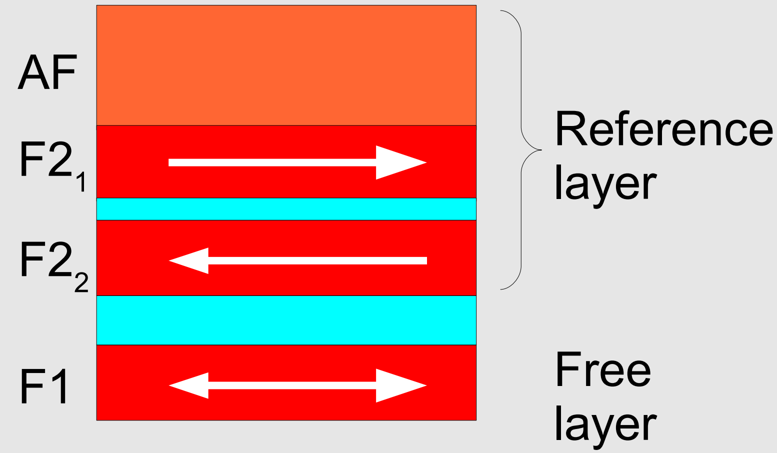
- Two layers rigidly coupled
- Reversal modes unchanged
- Neglect dipolar coupling

$$M=\frac{\left|e_1 M_1 - e_2 M_2\right|}{e_1+e_2} \qquad K=\frac{e_1 K_1 + e_2 K_2}{e_1+e_2}$$

$$H_c=\frac{e_1 M_1 H_{c,1} + e_2 M_2 H_{c,2}}{\left|e_1 M_1 - e_2 M_2\right|}$$

What use?

- Increase coercivity of pinned layers
- Decrease intra- and inter- dot dipolar coupling



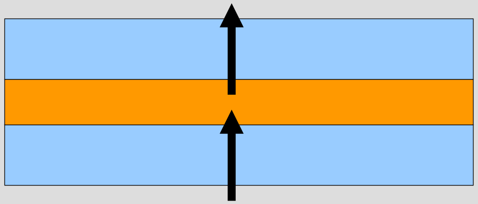
Practical aspects

- Ru spacer layer (largest effect)
- Control thickness within a few Angströms !

Stacked dots : dipolar

In-plane magnetization

Out-of-plane magnetization



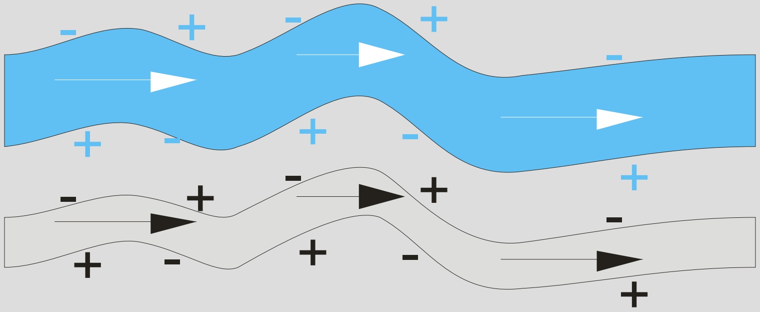
Hint:

An upper bound for the dipolar coupling is the self demagnetizing field

Notice: similar situation as for RKKY coupling

Stacked dots : orange-peel coupling

In-plane magnetization



Always parallel coupling

L. Néel, C. R. Acad. Sci. 255, 1676 (1962)

(valid only for thick films)

J. C. S. Kools et al., J. Appl. Phys. 85, 4466 (1999)

(valid for any films)

Out-of-plane magnetization

May be parallel or antiparallel

J. Moritz et al., Europhys. Lett. 65, 123 (2004)

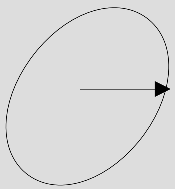
Upper bound for dipolar fields in 2D

Estimation of an upper range of dipolar field in a 2D system

$$\|\mathbf{H}_\mathrm{d}(R)\| \leq \oint \frac{2\pi\, r\mathrm{d}r}{r^3}$$

Integration

Local dipole: $1/r^3$

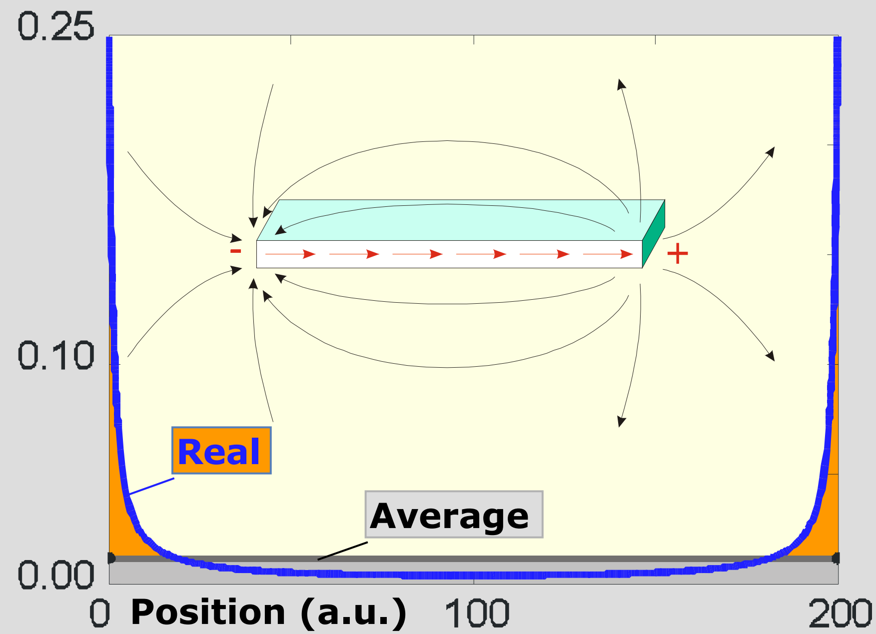


$$\|\mathbf{H}_\mathrm{d}(R)\| \leq \mathrm{Cte} + 1/R$$

Convergence with finite radius (typically thickness)

Non-homogeneity of dipolar fields in 2D

Example: flat stripe with thickness/height = 0.0125



- Dipolar fields are weak and short-ranged in 2D or even lower-dimensionality systems
- Dipolar fields can be highly non-homogeneous in anisotropic systems like 2D
- Consequences on dot's non-homogenous state, magnetization reversal, collective effects etc.

Moment and anisotropy of ultrathin films

U. Gradmann, Handbook of magnetic materials vol. 7, K. H.K. Buschow Ed., Elsevier, Magnetism of transition metal films, 1 (1993)

M. Farle, Ferromagnetic resonance of ultrathin metallic layers, Rep. Prog. Phys. 61, 755 (1998)

P. Poulopoulos et al., K. Baberschke, Magnetism in thin films, J. Phys.: Condens. Matter 11, 9495 (1999)

H. J. Elmers, Ferromagnetic Monolayers, Int. J. Mod. Phys. B 9 (24), 3115 (1995)

O. Fruchart, Epitaxial self-organization: from surfaces to magnetic materials, C. R. Phys. 6, 61 (2005)

O. Fruchart et al., Magnetism in reduced dimensions, C. R. Phys. 6, 921 (2005)

Perpendicular anisotropy

M. T. Johnson et al., Magnetic anisotropy in metallic multilayers, Rep. Prog. Phys. 59, 1409 (1996)

Exchange-bias

J. Nogues et al., I. K. Schuller, Exchange bias, J. Magn. Magn. Mater 192 (2), 203 (1999).

Magneto-elasticity in thin films

D. Sander, The correlation between mechanical stress and magnetic anisotropy in ultrathin films, Rep. Prog. Phys. 62, 809 (1999)

Theory (misc)

T. Asada et al., G. Bihlmayer, S. Handschuh, S. Heinze, P. Kurz, S. Blügel, First-principles theory of ultrathin magnetic films, J. Phys.: Condens. Matter 11, 9347 (1999)

F. J. Himpsel et al., Magnetic Nanostructures, Adv. Phys. 47 (4), 511 (1998)

P. Bruno, Theory of interlayer exchange interactions in magnetic multilayers, J. Phys.: Condens. Matter 11, 9403 (1999)

F. E. Gabaly et al., Noble metal capping effects on the spin-reorientation transitions of Co/Ru(0001), N. J. Phys. 10, 073024 (2008)

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- **[2009]** Magnetic field, Origin of magnetism, Spin and orbital magnetic moments, Crystal field, Magnetism of free electrons - Paramagnetism etc.: **JOHN MICHAEL COEY**, *TCD-Dublin, Ireland*. [Abstract pt.1 | pt.2] [Slides pt.1 | pt.2 | pt.3-4]
- **[2007]** Fundamental properties: **EKKES BRÜCK**, , *Amsterdam, The Netherlands* [Abstract | Slides pt.1 | Slides pt.2]
- **[2005]** Basis and magnetic materials: **K.H. MÜLLER** [Abstract | Slides (2.2MB)]
- **[2003]** Magnetism of matter - Basic interactions and magnetization processes: **D. GIVORD** [Abstract | Slides]

Exchange, magnetic ordering, magnetic anisotropy

Exchange and magnetic ordering

- **[2009]** Exchange interactions: exchange, super-exchange, RKKY, Stoner ferromagnetism: **TOMASZ DIETL**, *Warsaw, Poland*. [Abstract | Slides]
- **[2009]** Magnetic Order: different types, dimensionality effects, number of components (Ising, XY, Heisenberg): **PETER DE CHATEL**, *Amsterdam, The Netherlands*. [Abstract | Slides]
- **[2009]** Magnetism at finite temperature: molecular field, phase transitions: **CLAUDINE LACROIX**, *Institut Néel - Grenoble, France* [Slides].

Magnetic anisotropy

- **[2009]** Magnetic anisotropy and how it can be controlled: **DIRK SANDER**, *MPI-Halle, Germany*. [Abstract | Slides]

Low-dimensional and surface magnetism

- **[2003]** Low dimensional magnetism - experiments: **O. FRUCHART** [Abstract | Slides]
- **[2003]** Low dimensional magnetism : the role of the electronic structure: **H. DREYSSÉ** [Content | Abstract]
- **[2003]** From the atom to magnetic nanoparticles: **E. BONET** [Abstract | Slides]

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- Magnetization processes
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I. Overview of self-organization processes