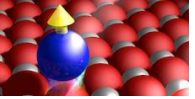
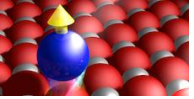


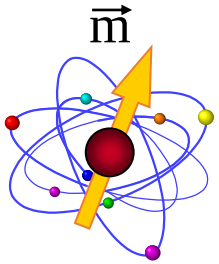
Lecture 4

Magnetic anisotropy energy

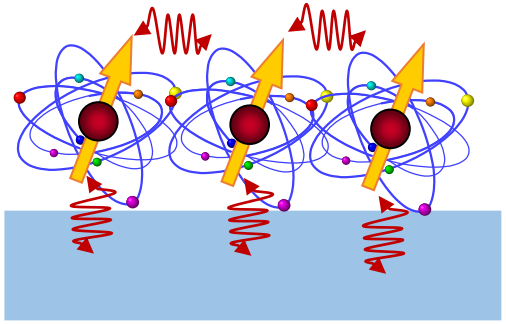
The spintronics “goose game”



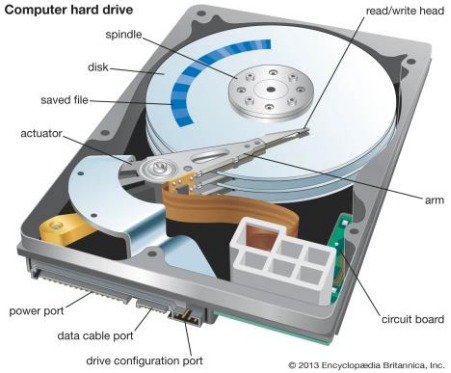
Atom magnetism

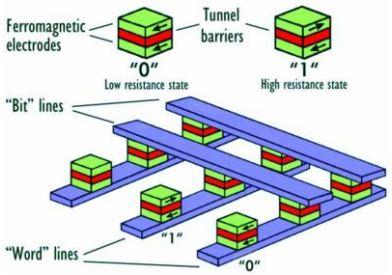


interactions between spins and with the supporting substrate

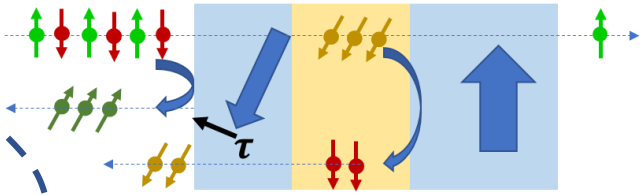


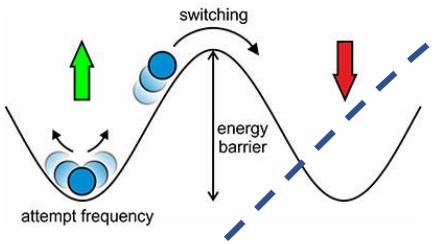
applications

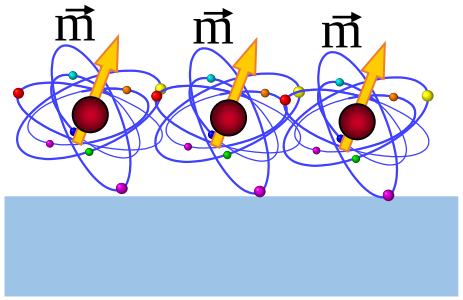




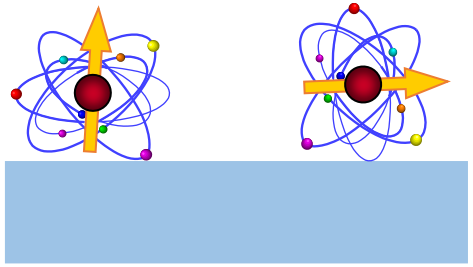
STT - SOT





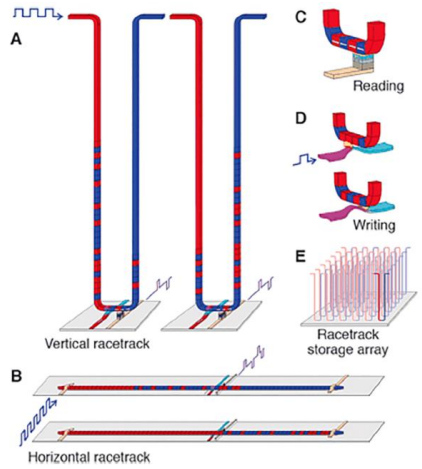


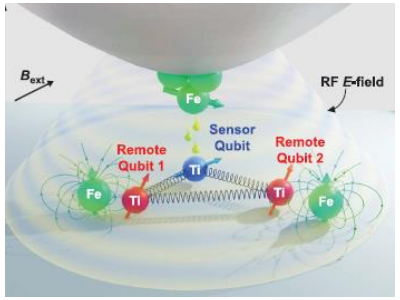
magnetic moment in a cluster and/or on a support

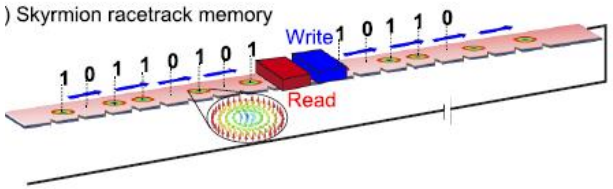


Magnetization easy axis

Future







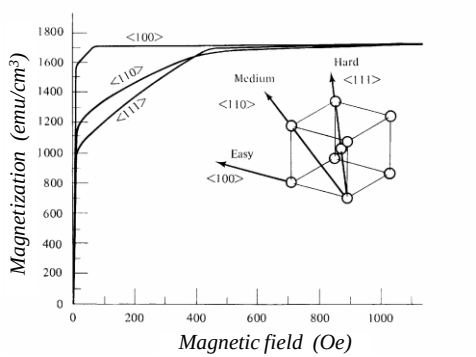
Magnetic anisotropy energy (MAE)

Bulk systems: the magnetization curve depends on the direction of the external field

Fe bcc

$K_1 = 4.8\times10^4\ J/m^3$

$= 2.4\ \mu eV/atom$

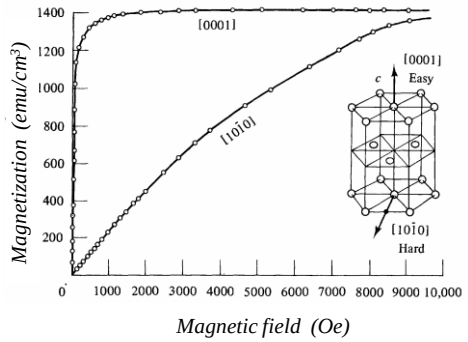


Co hcp

easy axis: (0001)

$K_1 = 4.1\times10^5\ J/m^3$

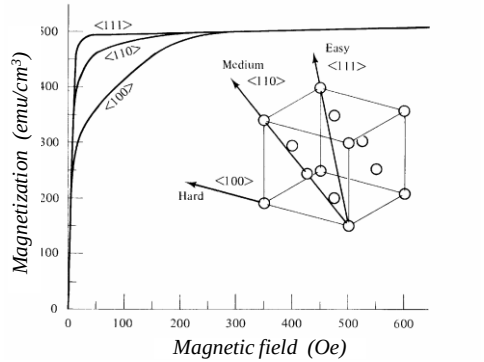
$= 45\ \mu eV/atom$



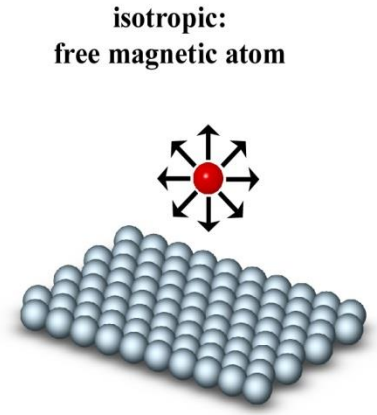
Ni fcc

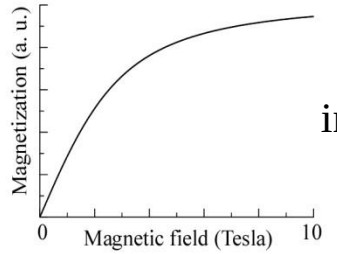
$K_1 = -5.5\times10^3\ J/m^3$

$= -0.3\ \mu eV/atom$

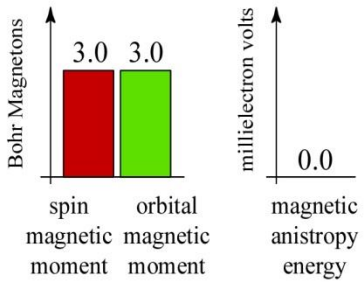


Free-standing atom: the magnetization is spatially isotropic

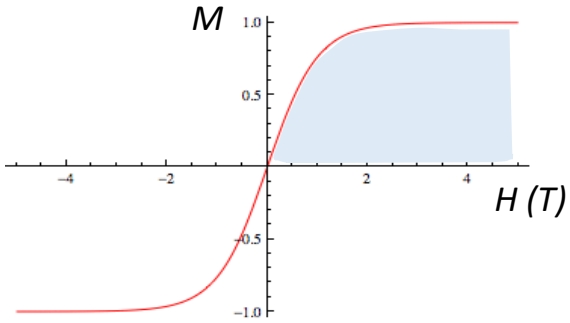




Direction independent

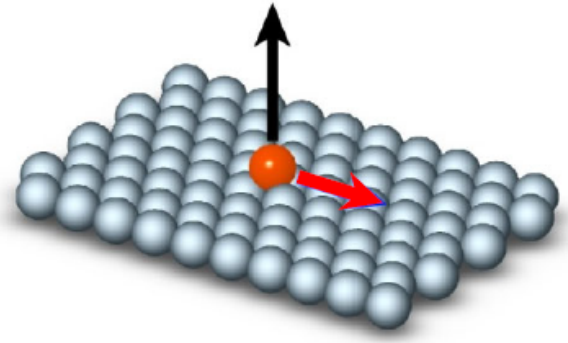


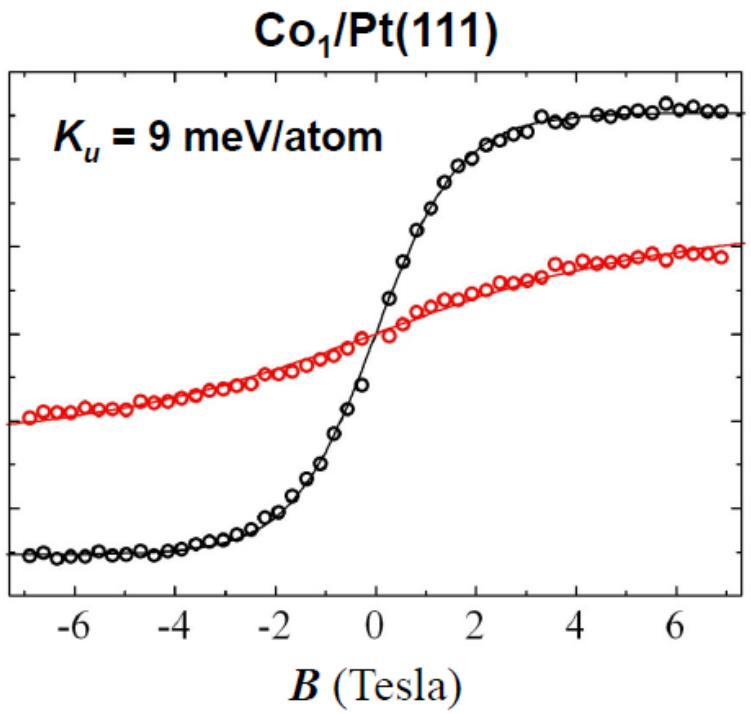
Co atoms



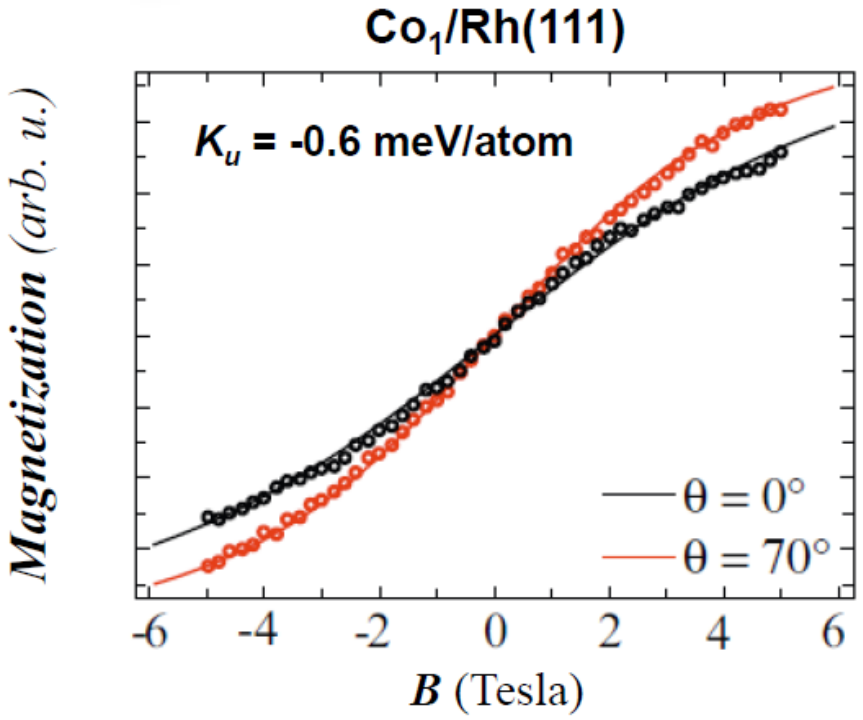
The area *MH* represents the energy stored in the system. The energy difference between two directions gives the MAE

Magnetization easy axis and saturation field depend on supporting substrate





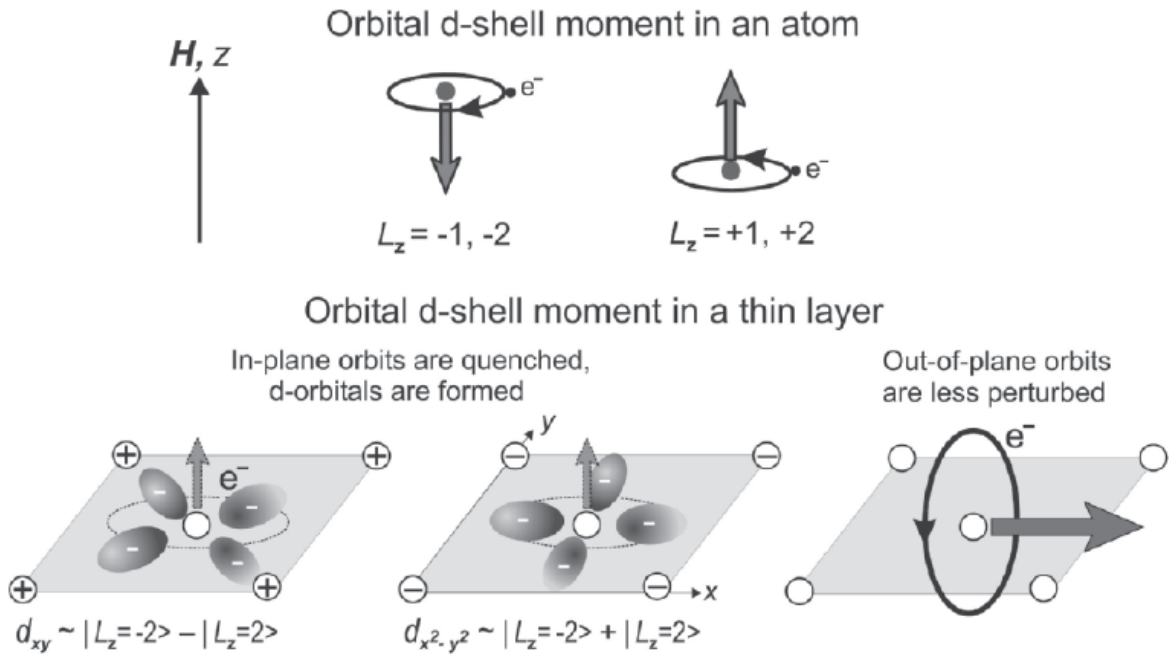
P.Gambardella et al., *Science* **300**, 1130 (2003).



A. Lehnert et al., *Phys. Rev. B* **82**, 094409 (2010)

SOC: origin of the magnetocrystalline anisotropy (K_{MCA})

See exercise: 4.1



Qualitative argument

A strong directional bond (crystal field) generates a reduction in the component of L perpendicular to the bond direction

- d electron in a free atom. Free orbital motion -> atom with maximum L_z due to Hund's rules

- atom in a plane forming bonds with neighbours atoms .

-a) in-plane orbital motion frozen by bond formation -> out-of-plane orbital moment is quenched

-b) out-of-plane orbital motion unperturbed by bonds -> in-plane orbital moment stays unquenched

→ symmetry breaking implies anisotropic orbital moments

-The spin moment S is isotropic.

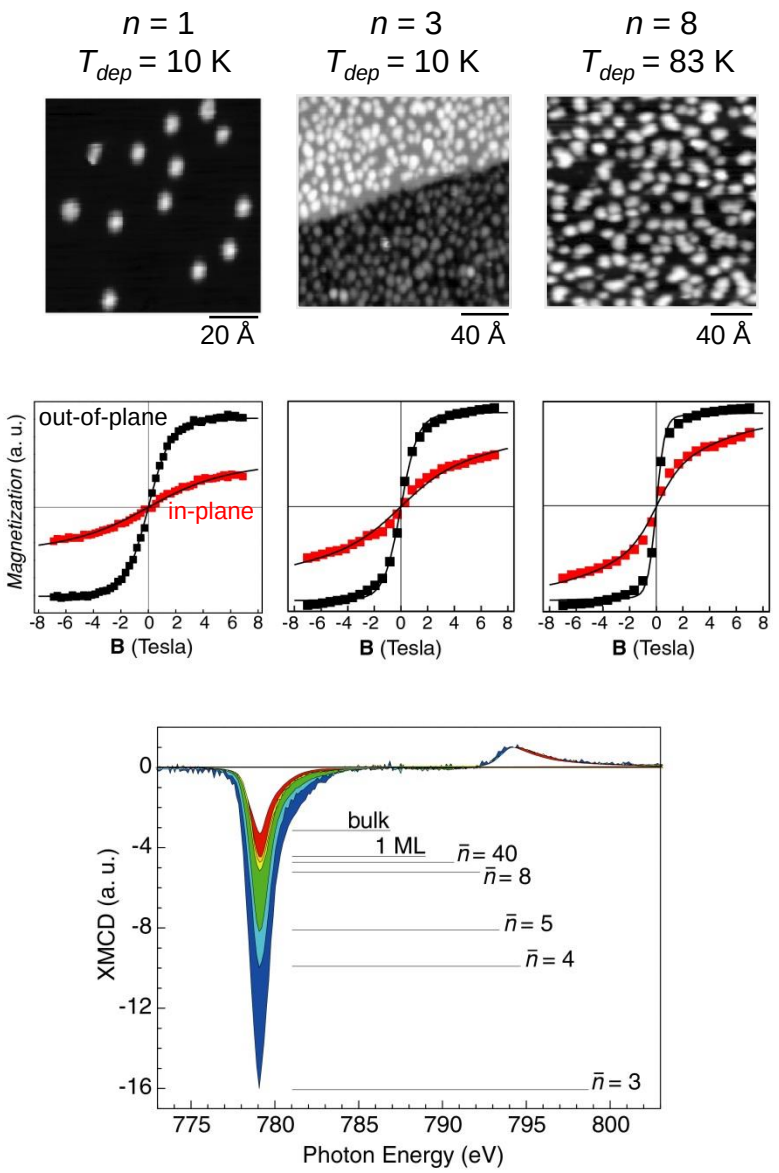
However, spin-orbit ($\lambda\, \boldsymbol{S}\cdot\boldsymbol{L}$) **locks** the spin along the spatial direction having maximum L

→ **easy axis of magnetization**

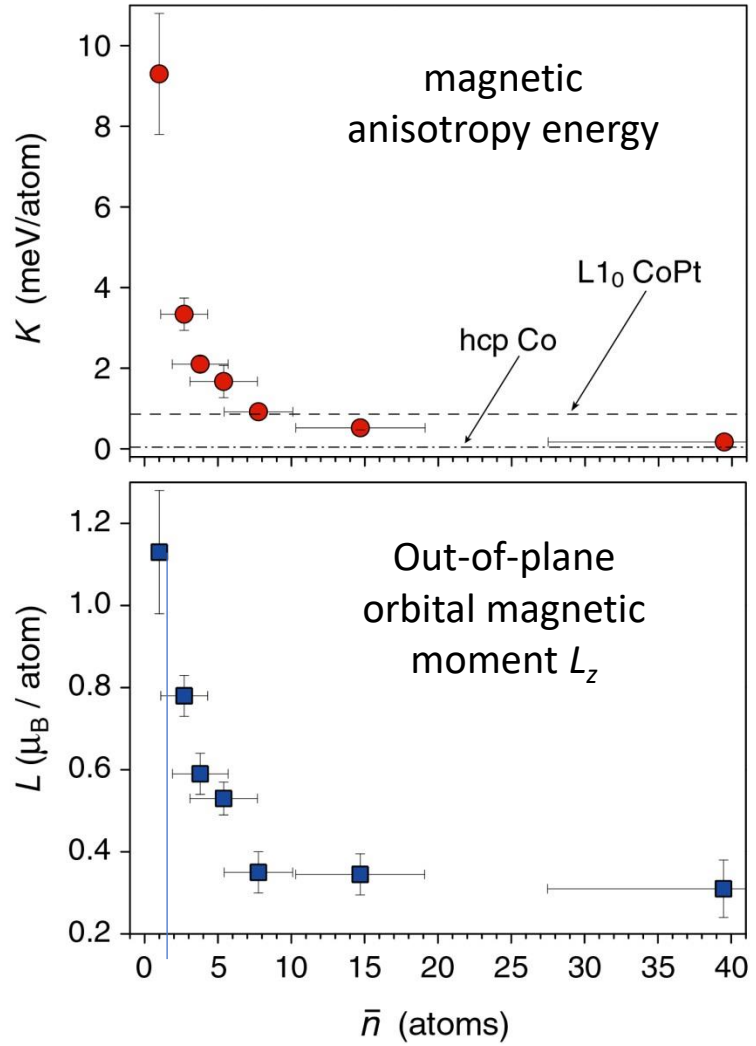
Magnetocrystalline anisotropy energy (MCA) $K_{MCA} \approx \lambda\, \boldsymbol{S}\cdot(\boldsymbol{L}_z - \boldsymbol{L}_{x,y})$

Correlation between K_{MCA} and out-of-plane L in Co_n/Pt(111)

See exercise: 4.2

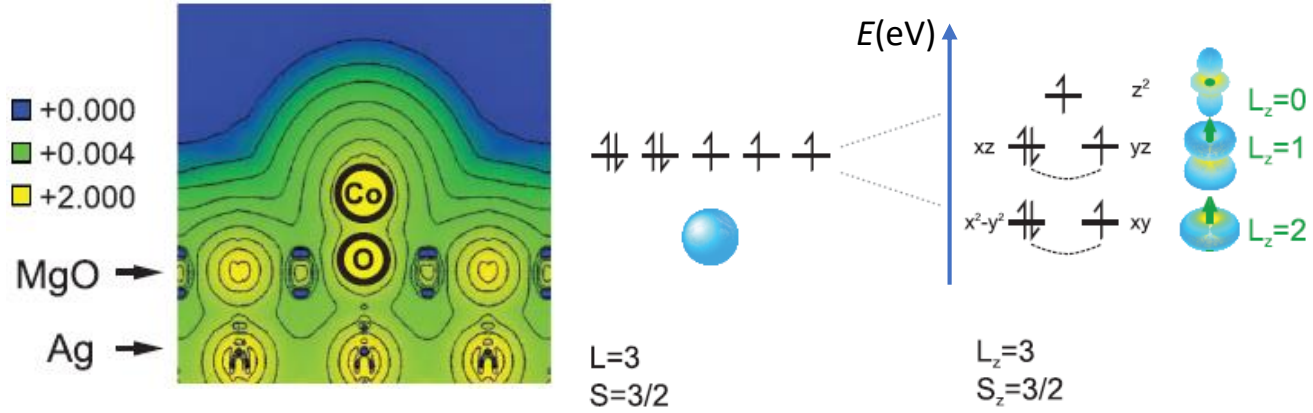


Co particles on Pt(111) with average size n



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

Reaching the MCA limit in 3d metal atoms: $Co_1/MgO(100)$



- Co atom on MgO adsorbs on top of oxygen
- strong uniaxial bond preserving atomic values of *L* and *S.*

From XMCD: $L_z = 2.9$; $S_z = 3/2$

- The uniaxial bond generates a strong out-of-plane anisotropy

$$K_{MCA} \approx \lambda \boldsymbol{S} \cdot (\boldsymbol{L}_z - \boldsymbol{L}_{x,y})$$

$$L_x(L_y) = 0$$

$$\Delta L = L_z - L_x = 3 = maximum\ value$$

$$L_z = 3$$

$$\langle d_n|L_x|d_{3z^2-r^2}\rangle = 0$$

$$\langle d_{yz}|L_x|d_{x^2-y^2}\rangle = 0$$

$$\langle d_{xz}|L_x|d_{xy}\rangle = 0$$

$L_x d_{xz} = -i\, d_{xy}$	$L_y d_{xz} = i\, d_{x^2-y^2} - i\sqrt{3}\, d_{3z^2-r^2}$	$L_z d_{xz} = i\, d_{yz}$
$L_x d_{yz} = i\sqrt{3}\, d_{3z^2-r^2} + i\, d_{x^2-y^2}$	$L_y d_{yz} = i\, d_{xy}$	$L_z d_{yz} = -i\, d_{xz}$
$L_x d_{xy} = i\, d_{xz}$	$L_y d_{xy} = -i\, d_{yz}$	$L_z d_{xy} = -i\, 2\, d_{x^2-y^2}$
$L_x d_{x^2-y^2} = -i\, d_{yz}$	$L_y d_{x^2-y^2} = -i\, d_{xz}$	$L_z d_{x^2-y^2} = i\, 2\, d_{xy}$
$L_x d_{3z^2-r^2} = -i\sqrt{3}\, d_{yz}$	$L_y d_{3z^2-r^2} = i\sqrt{3}\, d_{xz}$	$L_z d_{3z^2-r^2} = 0$

$$|\langle d_n|L_x|d_{3z^2-r^2}\rangle| = 0$$

$$|\langle d_{xy}|L_z|d_{x^2-y^2}\rangle| = 2$$

$$|\langle d_{yz}|L_z|d_{xz}\rangle| = 1$$

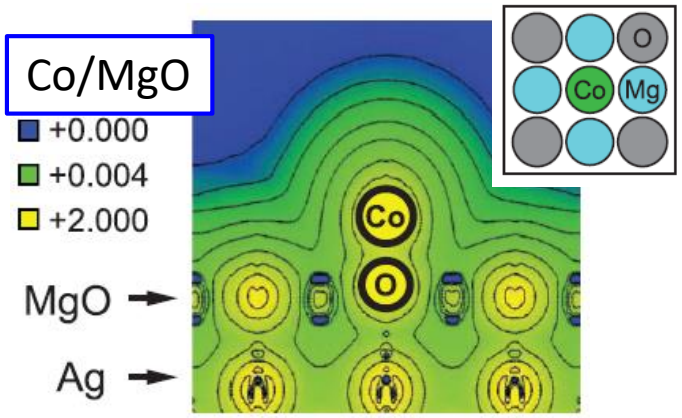
Matrix element are zero because d_{xy} and $d_{x^2-y^2}$ are not degenerate with d_{yz} and d_{xz}

Matrix element are **non** zero because d_{xy} and $d_{x^2-y^2}$ are degenerate as well as d_{yz} and d_{xz}

I. Rau *et al.*, Science **344**, 988 (2014)

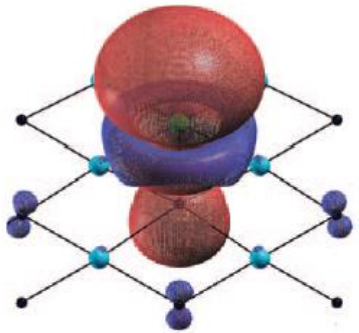
Co, Fe atoms on insulating substrates: MgO/Ag(100)

Charge distribution

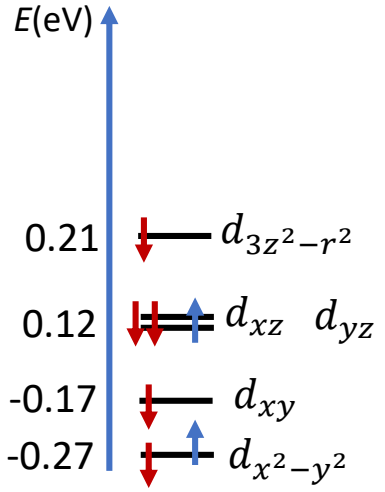


Spin distribution

Majority Minority



Axial (C_∞) crystal field



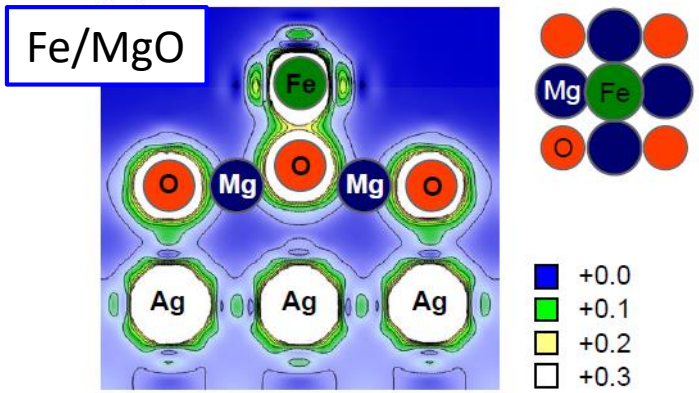
V_{ee}: $\begin{cases} L_z = 2.9 \\ S_z = 1.3 \end{cases}$

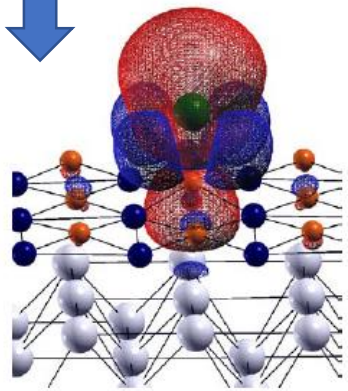
V_{ee}+ V_{SO}: $\begin{cases} L_z = 2.9 \\ S_z = 1.3 \end{cases}$

$L_{x,y} \approx 0$

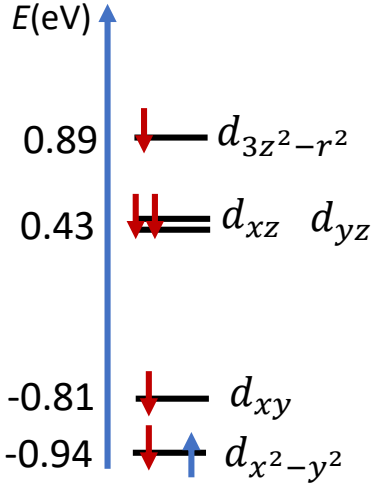
$K_{MCA} \approx 60\ meV$

Different interactions with neighbors atoms for Co and Fe





C_{4v} crystal field



V_{ee}: $\begin{cases} L_z = 0 \\ S_z = 2 \end{cases}$

V_{ee} + V_{SO}: $\begin{cases} L_z = 1.25 \\ S_z = 2 \end{cases}$

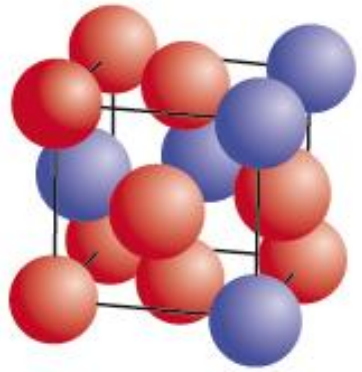
$L_{x,y} \approx 0$

$K_{MCA} \approx 20\ meV$

I.G. Rau *et al. Science* 988, **344** (2014); S. Baumann *et al.* Phys. Rev. Lett. **115**, 237202 (2015).

Example: $L1_0$ phase in FePt alloy

Low MAE



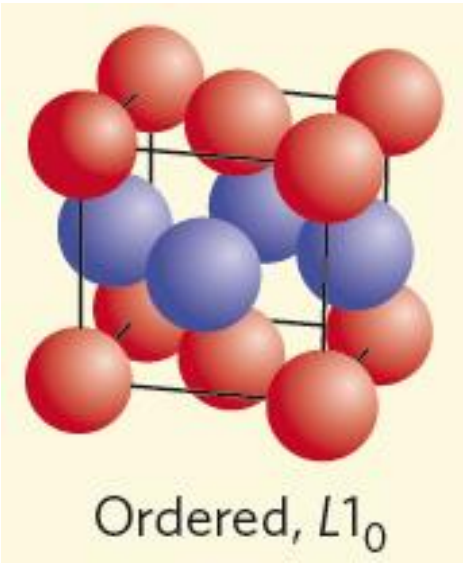
Disordered

Fe (or Co)

Pt (or Pd)

Ordering by annealing to about 600°C

High MAE

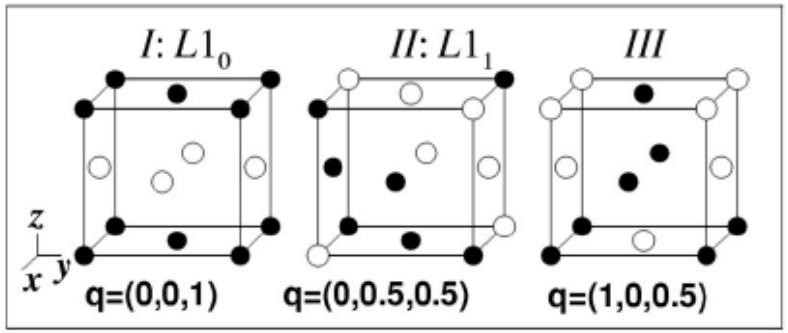


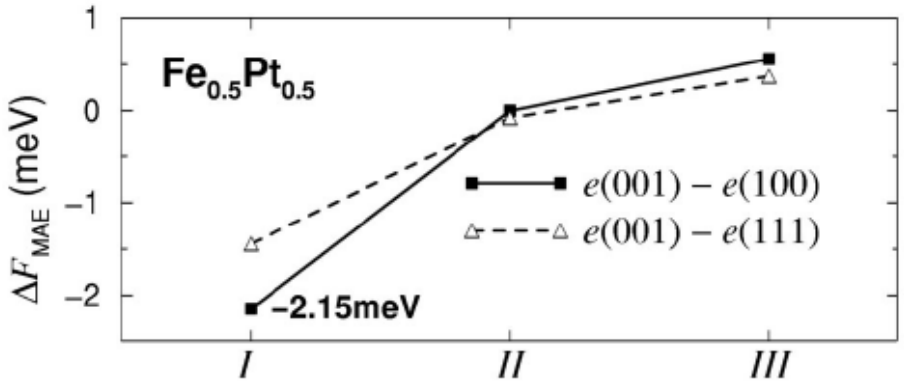
Ordered, $L1_0$

D. Alloyeau et al., Nat Mater. **8**, 940 (2009); Z.R. Day et al. Nano Lett. **1**, 443 (2001); S. Sun *et al.*, Science **287**, 1989 (2000)

S. Ostanin *et al.* J. Appl. Phys. **93**, 453 (2003); S.S.A. Razee *et al.*, Phys. Rev. Lett. **82**, 5369 (1999); J. Lyubina *et al.*, J. Phys.: Condens Matter **17**, 4157 (2005)

CF tuning of the MAE





MCA in transition metals: theory

$$H_{so} = \zeta \sum_{\mu_1,\mu_2,\sigma_1,\sigma_2} \langle \mu_2, \sigma_2 | L \cdot S | \mu_1, \sigma_1 \rangle \sum_k c^{\dagger}_{\mu_2,\sigma_2}(k) c_{\mu_1,\sigma_1}(k)$$

$|\boldsymbol{k},\mu,\sigma\rangle$ are the Bloch functions with eigenvalues $\varepsilon_{n,\sigma}(\boldsymbol{k})$

$\boldsymbol{k}$ the electron wave vector,

μ the d orbitals,

σ the spin.

$c^{\dagger}$ (c) are creation (annihilation) operators

It has to be calculated between occupied |gr> and unoccupied |ex> states

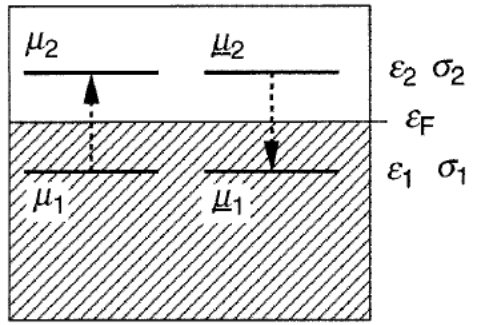
H_{so} is a one-electron operator

diagonal in $\boldsymbol{k}$ ($\boldsymbol{k}$ is conserved)

→ The excited states are unoccupied states

$$|\mathrm{ex}\rangle = c^{\dagger}_{n_2,\sigma_2}(k) c_{n_1,\sigma_1}(k) |\mathrm{gr}\rangle$$

$$\varepsilon_{n_1,\sigma_1}(k) < \varepsilon_F < \varepsilon_{n_2,\sigma_2}(k)$$



In 3d metals H_{so} ≈ 50-100 meV << band width ≈ 1-5 eV (due to the Coulomb repulsion and crystal field)

Spin-orbit can be treated as a perturbation:

- first order evaluation: the d orbitals have $L_{x,y,z} = 0$ -> $\langle \mu | H_{so} | \mu \rangle = 0$

- second order evaluation is $\neq 0$

$$\delta E = \sum_{\mathrm{ex}} \frac{\langle \mathrm{gr}|H_{so}|\mathrm{ex}\rangle \langle \mathrm{ex}|H_{so}|\mathrm{gr}\rangle}{E_{\mathrm{gr}} - E_{\mathrm{ex}}}$$

DOI 10.1088/0953-8984/10/14/012

Calculation of the spin-orbit energy

$$\delta E = -\zeta^2 \sum_{\theta} [A(\theta,\uparrow,\uparrow)\langle \underline{\mu}_1,\uparrow|\boldsymbol{L}\cdot\boldsymbol{S}|\underline{\mu}_2,\uparrow\rangle\langle\mu_2,\uparrow|\boldsymbol{L}\cdot\boldsymbol{S}|\mu_1,\uparrow\rangle$$

majority to majority state

$$+A(\theta,\downarrow,\downarrow)\langle \underline{\mu}_1,\downarrow|\boldsymbol{L}\cdot\boldsymbol{S}|\underline{\mu}_2,\downarrow\rangle\langle\mu_2,\downarrow|\boldsymbol{L}\cdot\boldsymbol{S}|\mu_1,\downarrow\rangle$$

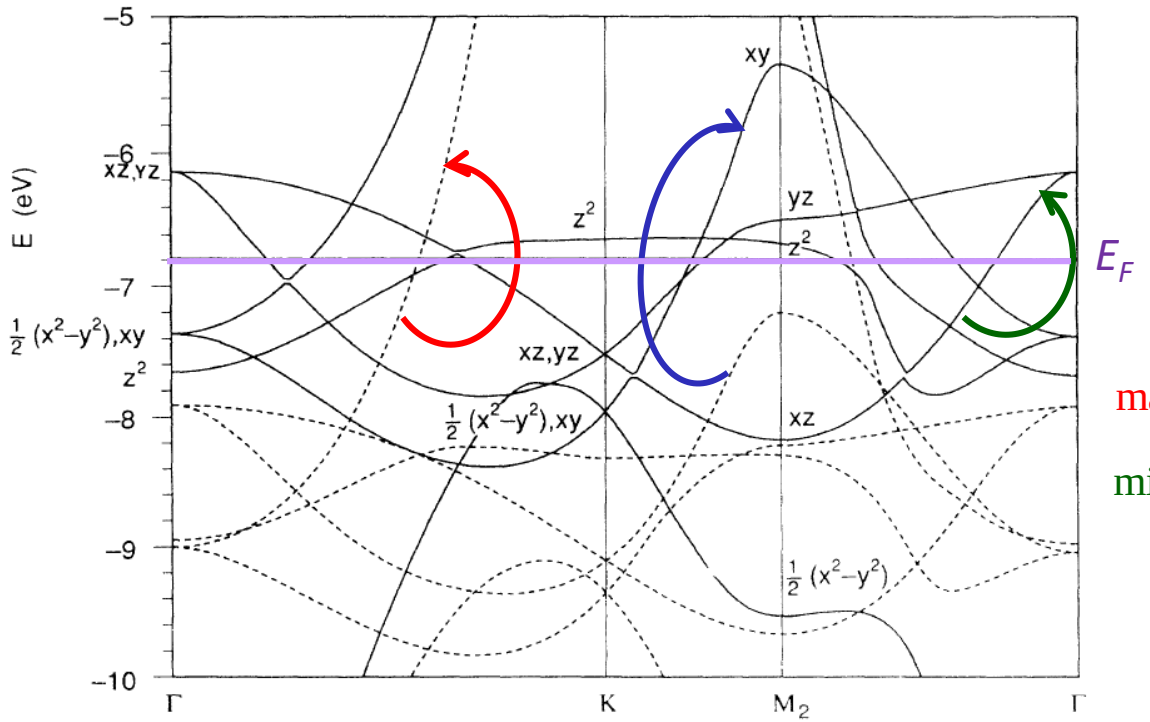
minority to minority state

$$-A(\theta,\uparrow,\downarrow)\langle \underline{\mu}_1,\uparrow|\boldsymbol{L}\cdot\boldsymbol{S}|\underline{\mu}_2,\downarrow\rangle\langle\mu_2,\downarrow|\boldsymbol{L}\cdot\boldsymbol{S}|\mu_1,\uparrow\rangle$$

$$-A(\theta,\downarrow,\uparrow)\langle \underline{\mu}_1,\downarrow|\boldsymbol{L}\cdot\boldsymbol{S}|\underline{\mu}_2,\uparrow\rangle\langle\mu_2,\uparrow|\boldsymbol{L}\cdot\boldsymbol{S}|\mu_1,\downarrow\rangle]$$

spin-flip transitions

$$A(\theta,\sigma_1,\sigma_2) \equiv \int_{\varepsilon_1<\varepsilon_F<\varepsilon_2} \frac{d\varepsilon_1\, d\varepsilon_2}{\varepsilon_2-\varepsilon_1} \sum_k n_{\mu_1,\underline{\mu}_1,\sigma_1}(k,\varepsilon_1) n_{\mu_2,\underline{\mu}_2,\sigma_2}(k,\varepsilon_2) \qquad \theta = \mu_1, \underline{\mu}_1, \mu_2, \underline{\mu}_2$$



majority spin (dashed)
minority spin (solid)

majority to majority state

minority to minority state

Spin-flip transitions

G.H.O. Daalderop *al.* Phys. Rev. B **50**, 9989 (1994)

Magnetocrystalline anisotropy energy (K_{mc})

$$\delta E \approx -\frac{1}{4}\zeta\, \boldsymbol{S}\cdot\left(\boldsymbol{L}^{\downarrow}-\boldsymbol{L}^{\uparrow}\right)+\frac{\zeta^2}{\Delta E_{exc}}\left[\frac{21}{2}\boldsymbol{S}\cdot\boldsymbol{T}+2(S_zL_z)^2\right]$$

Majority to majority
Minority to minority

Spin-flip transitions

ΔE_{exc} is the exchange splitting between majority and minority states

$$\boldsymbol{T}=\hat{\boldsymbol{S}}-3\hat{r}(\hat{r}\cdot\boldsymbol{S})$$

Magnetic dipole -> Anisotropy of the spin moment (for ex. due to an anisotropy of the electron charge distribution)

$$K_{MCA}=\delta E(H\parallel z)-\delta E(H\parallel x,y)$$

K_{MCA} = energy difference between two magnetization directions

If majority states are completely full ($L^{\uparrow}=0$)

$$K_{MCA}\approx\frac{\zeta}{4}\boldsymbol{S}\cdot\Delta L_{z,x(y)}+O\left(\frac{\zeta^2}{\Delta E_{exc}}\right)$$

P. Bruno, PRB **39**, 865 (1989);
G. van der Laan, JPCM **10**, 3239 (1998).

Frequently

$$K_{MCA}=\alpha\frac{\zeta}{4}S\cdot\Delta L$$

$$\alpha\approx 0.1\ -\ 0.25$$

J. Stöhr, J. Magn. Magn. Mater **200**, 470 (1999);

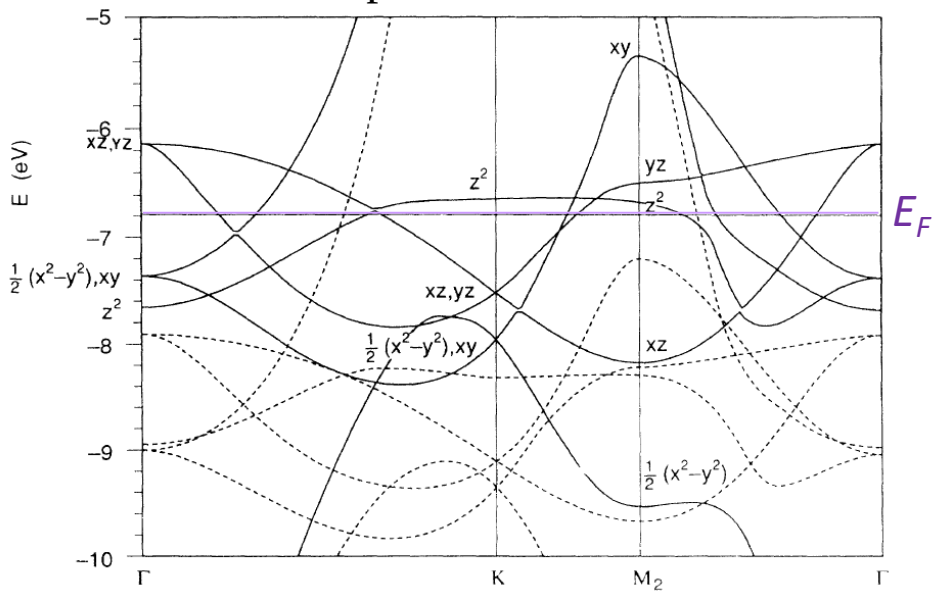
In thin film and nanostructures, the factor α is necessary to find a good agreement between XMCD and other magnetometer measurements. Discrepancy probably due to spin-flip term and not perfectly spin-split bands

Magnetocrystalline anisotropy *vs.* band structure

G.H.O. Daalderop *al.* Phys. Rev. B **50**, 9989 (1994)

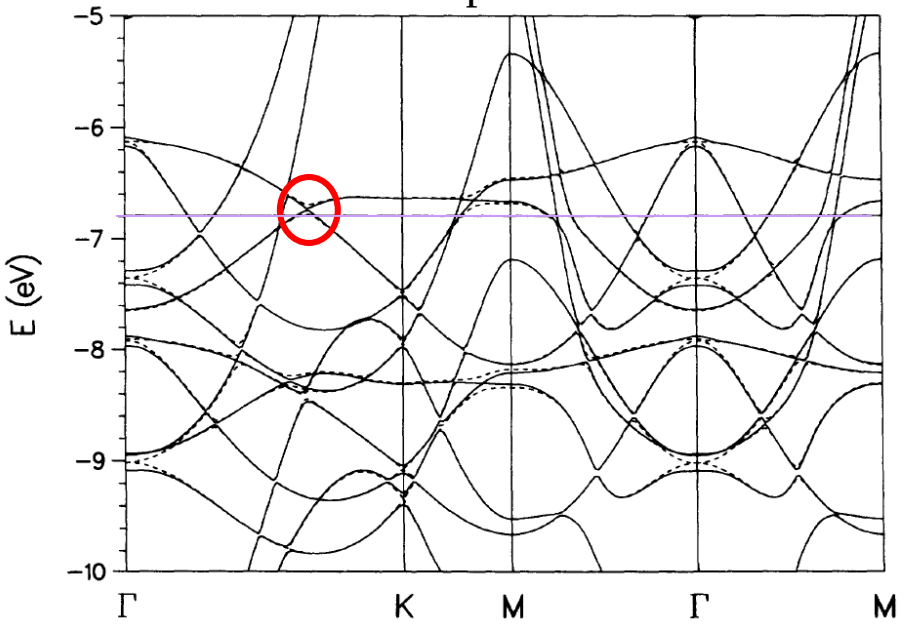
Free-standing Co monolayer

Spin-orbit off



Majority spin (dashed) and minority spin (solid)

Spin-orbit on



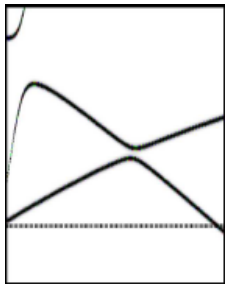
S // z (solid) and S // x (dashed)

Hot spot (red circle)

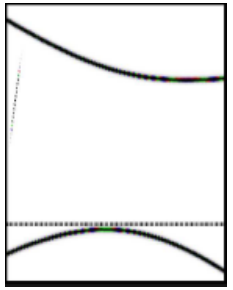
Magnetization easy axis = axis corresponding to the lowest energy (*x* in the present case)

Hot spot:
Degenerate states close to E_F
can give huge contributions
to the MAE

H // z

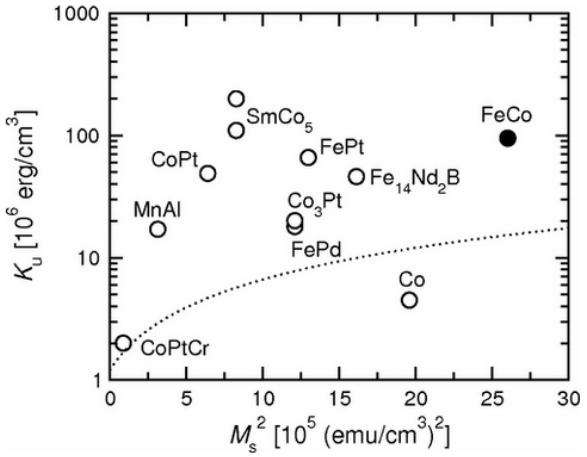


H // x



Spin-orbit splits the degenerate states in such a way that one state is shifted below E_F and the second one is shifted above E_F when H // x

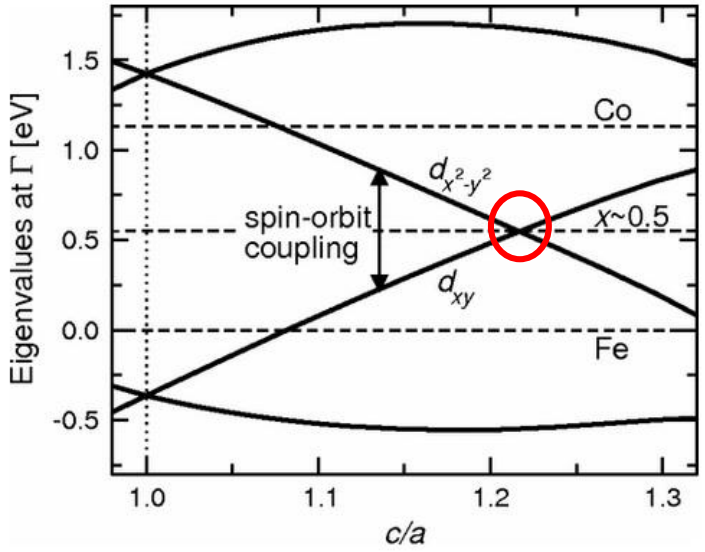
Ex.: FeCo bulk



FeCo bcc -> K_{MCA}= 1-2 μeV/atom

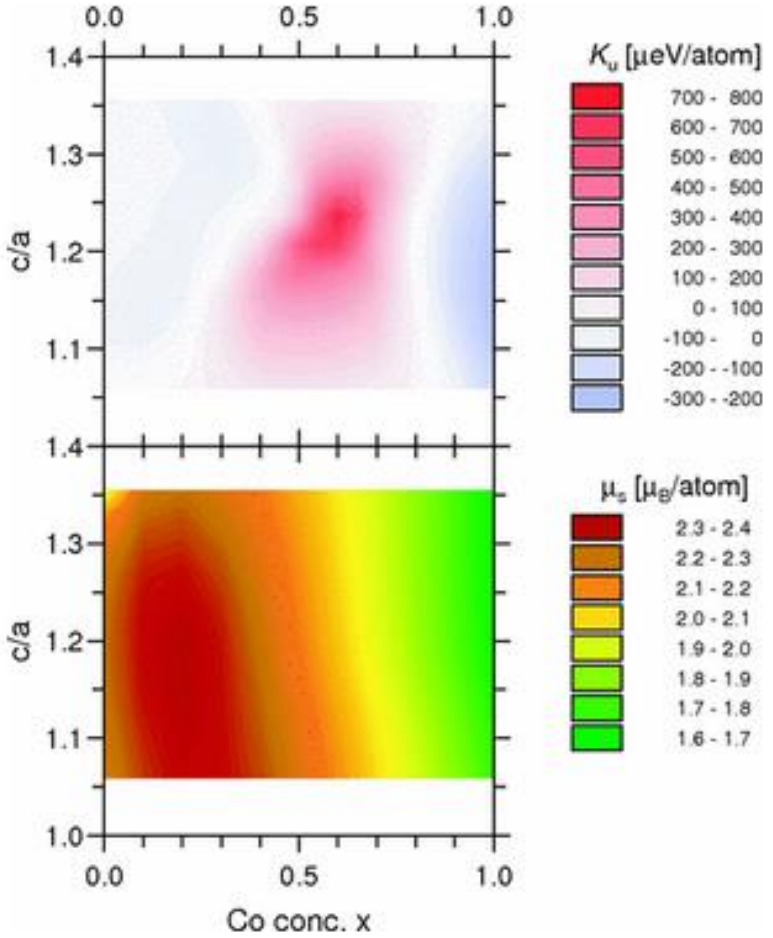
FeCo bct -> K_{MCA}= 0.8 meV/atom

Enhanced K_{MCA} for composition and *c/a* distortion giving degenerate d_{x2-y2} and d_{xy} states.



Spin orbit split these two degenerate states: maximum K_{mca} for

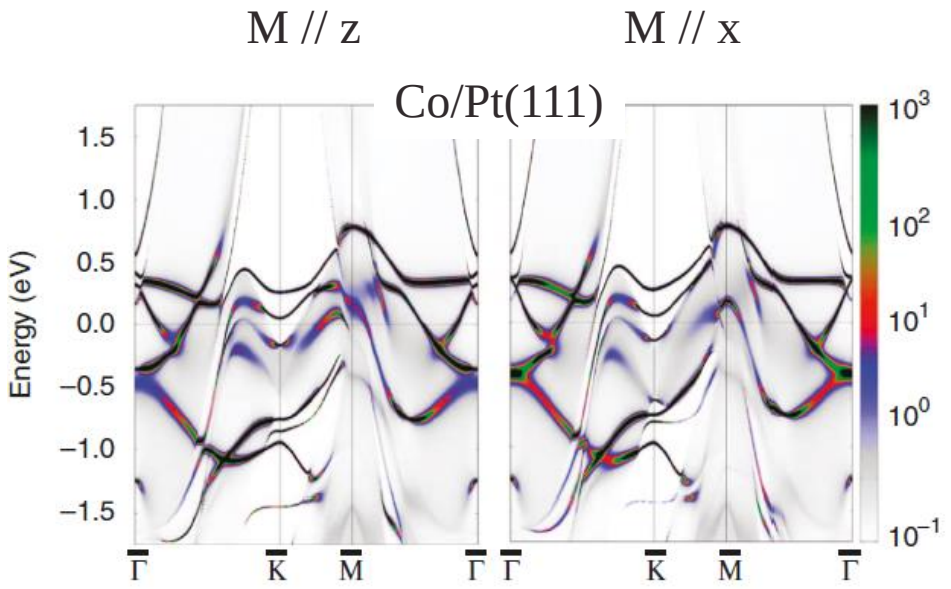
***c/a* = 1.2 and $Fe_{0.5}Co_{0.5}$**

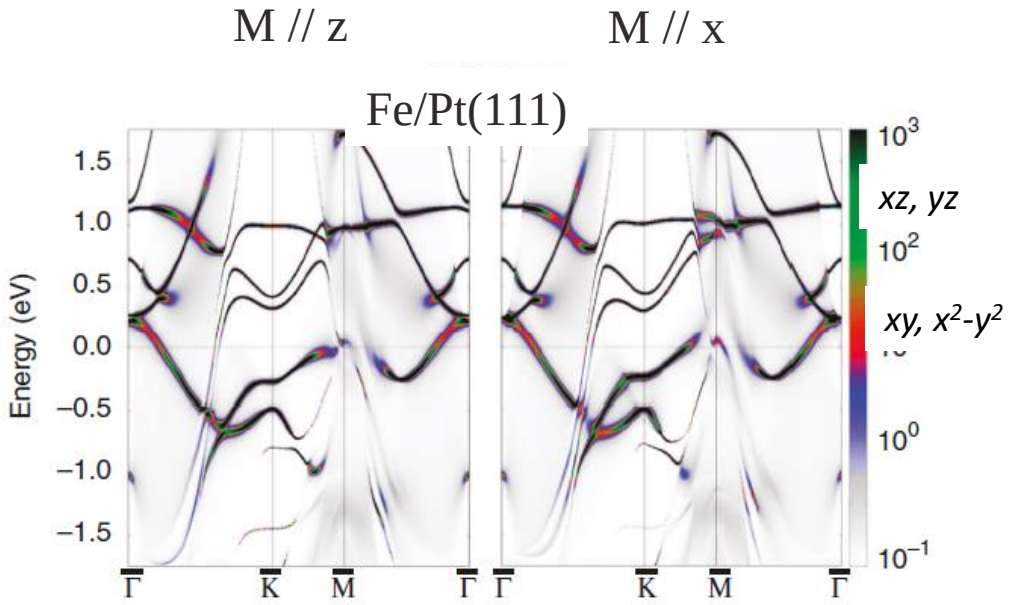


Calculated minority d-orbitals eigenvalues at the Γ point as a function of *c/a* ratio.
The Fermi energies of Fe, Co, and $Fe_{0.5}Co_{0.5}$ are indicated by dashed lines

T. Burkert *et al.* Phys. Rev. Lett. **93**, 027203 (2004);

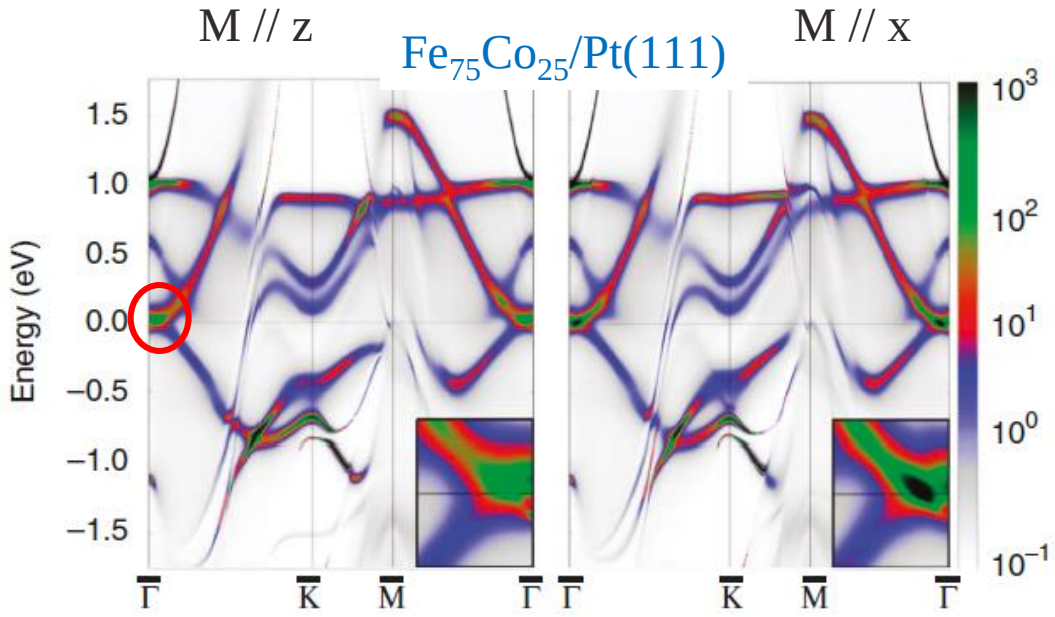
Ex.: FeCo monolayer on Pt(111)





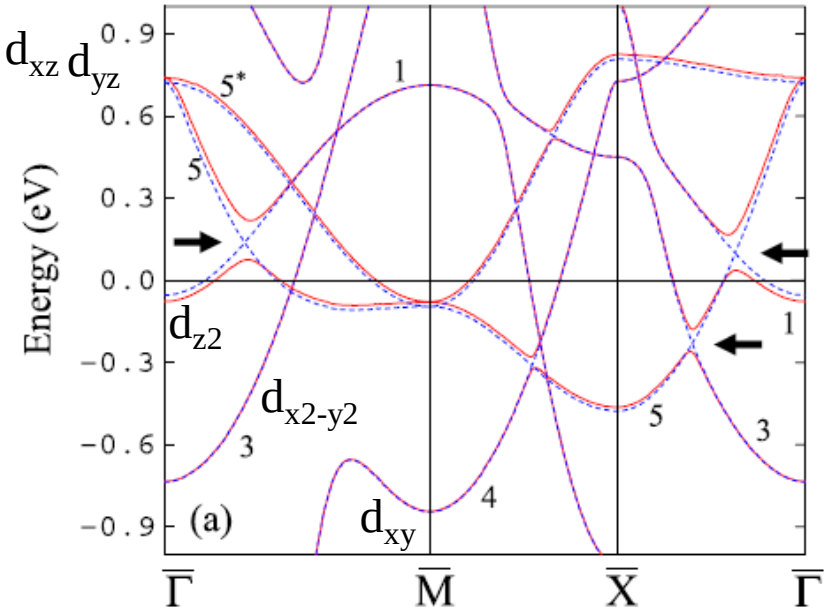
1) Degenerate d_{xy} and d_{x2-y2} orbitals at Fermi level for $Fe_{75}Co_{25}$

2) Splitting of the d_{xy} and d_{x2-y2} orbitals
-> gain in energy when M // z
-> z is the easy axis with large K_{mca}

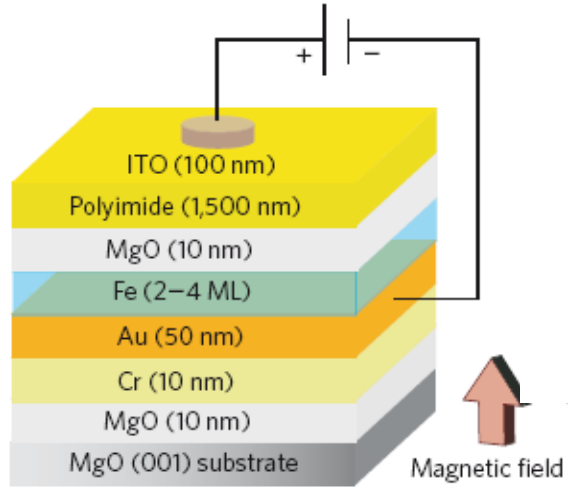


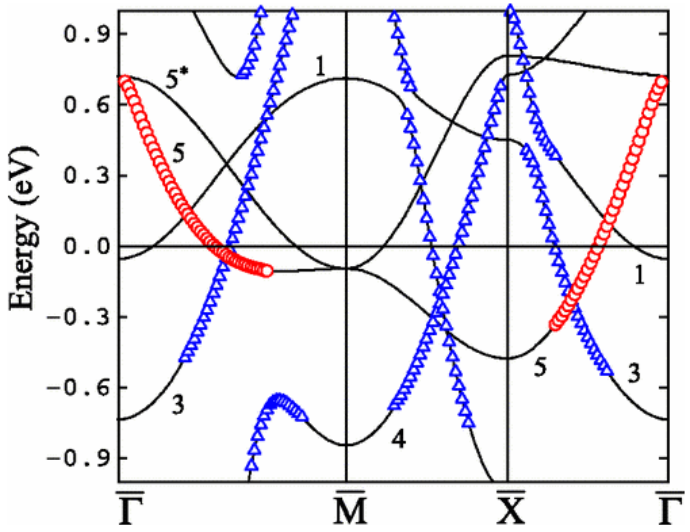
S. Ouazi *et al.* Nat. Commun. **3**, 1313 (2012); G. Moulas et al. Phys. Rev. B, **78**, 214424 (2008)

Electric field control of K_{MCA}



minority-spin band for an Fe(001) monolayer in an external electric field $\boldsymbol{E_z}$:
$\boldsymbol{E_z}$ = 0 (dotted lines)
$\boldsymbol{E_z}$ = 1 eV/Å (solid lines).
Arrows indicate band gaps induced by the electric field.





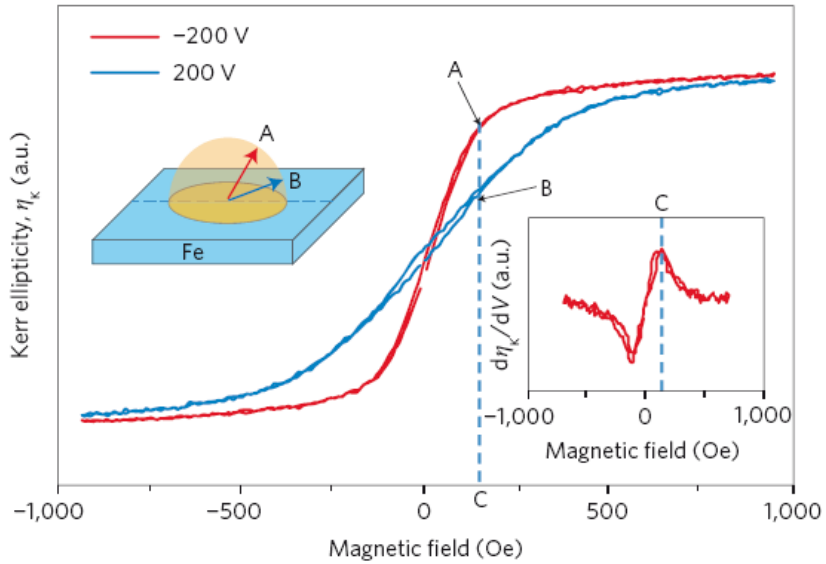
Electric field -> Y_1^0 symmetry

$$\langle l'm'|Y_1^0|lm\rangle \neq 0$$

when $l' = l+1$ and $m' = m$

small components of the p orbitals:
circles (p_z) and triangles ($p_{x,y}$)

Mixing of *p* and *d* states opens the gaps



K. Nakamura *et al.* Phys. Rev. Lett. **102**, 187201 (2009); T. Maruyama *et al.*, Nature Nanotech.. **4**, 158 (2009)

K_{mca} *vs.* ΔL in multi-element system

$$\Delta E_{\mathrm{so}} = \sum_{qss'} \Delta E_q^{ss'} = \sum_{qss'} \{E_q^{ss'}(\hat{n}_1) - E_q^{ss'}(\hat{n}_2)\}$$

The MAE is written as a sum over atomic species *q*, and as a double sum over the spin indices, *s* (occupied), and *s'* (unoccupied)

$$E_q^{ss'}(\hat{n}) = -\sum_{\mathbf{k}ij} \sum_{q'} \sum_{\{m\}} n_{\mathbf{k}is,qm,q'm'} n_{\mathbf{k}js',q'm'',qm'''} \frac{\langle qms|\mathcal{H}_{\mathrm{so}}(\hat{n})|qm'''s'\rangle\langle q'm''s'|\mathcal{H}_{\mathrm{so}}(\hat{n})|q'm's\rangle}{\varepsilon_{\mathbf{k}j} - \varepsilon_{\mathbf{k}i}}$$

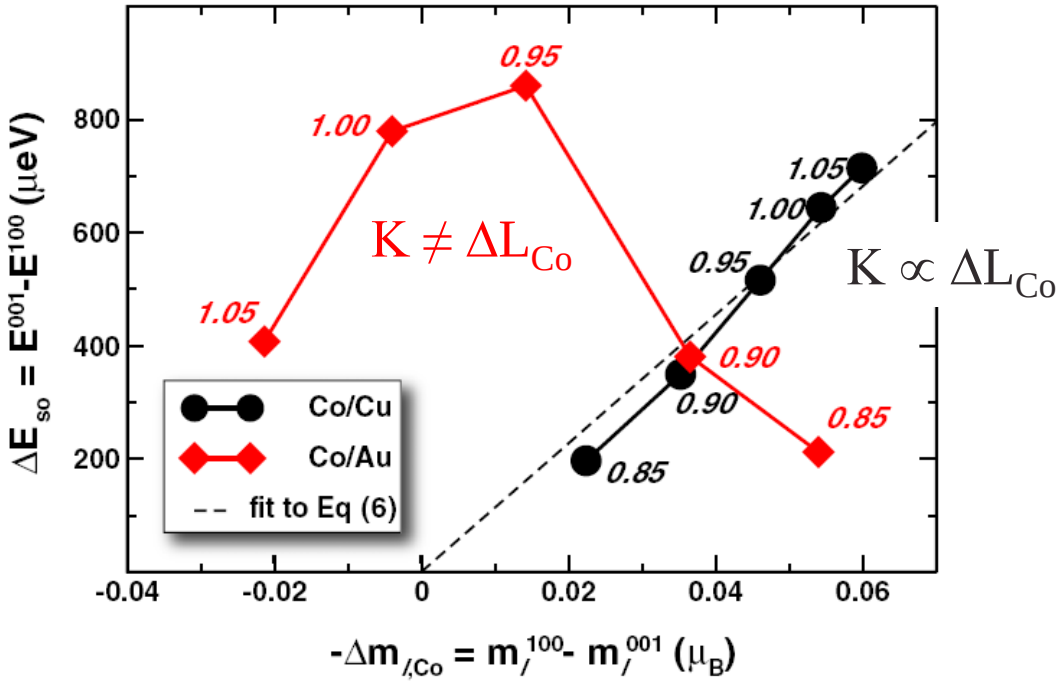
sum over all **k** points in the Brillouin zone, all occupied states *i*, all unoccupied states *j*, all species *q'* and magnetic quantum numbers *m*

sum over all sites gives off-site contributions ($q \neq q'$) through the spin-orbit scattering (or coupling) at other sites.

Au is $5d^{10}\ 6s^1$ -> negligible *S* and *L* ->
a) *S* and *L* can be not zero due to orbital hybridization
b) very high spin-orbit constant $\zeta \cong 600$ meV

The magnetization easy axis does not always coincide with the largest orbital moment

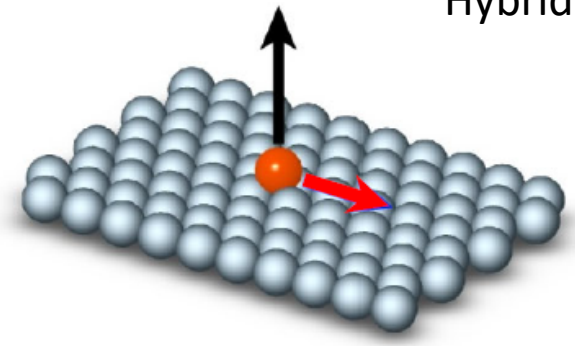
Calculation as a function of the deformation parameter $\chi = (c/a)/\mathrm{sqrt}(8/3)$



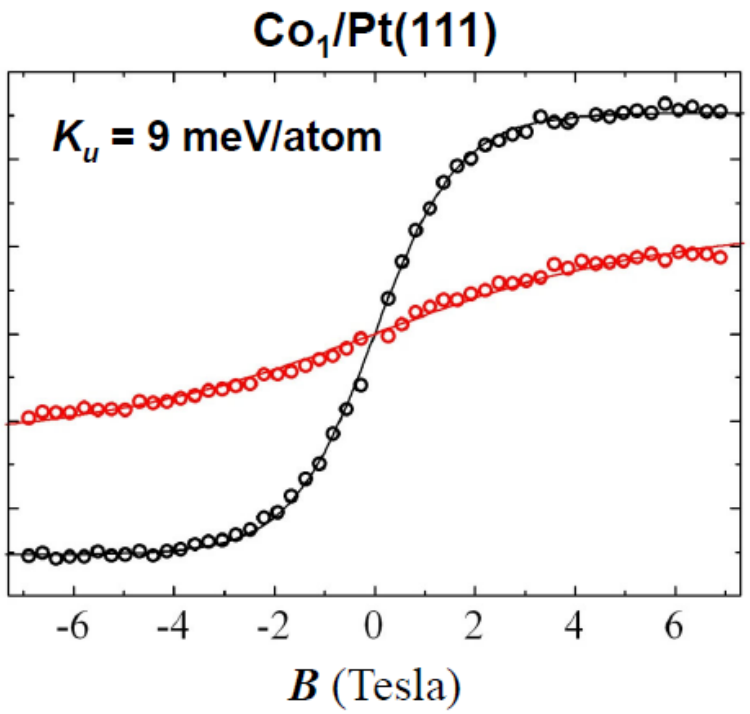
C. Andersson *et al.* Phys. Rev. Lett. **99**, 177207 (2007)

Magnetization easy axis and MAE value depend on supporting substrate

Hybridization with the substrate defines the MAE

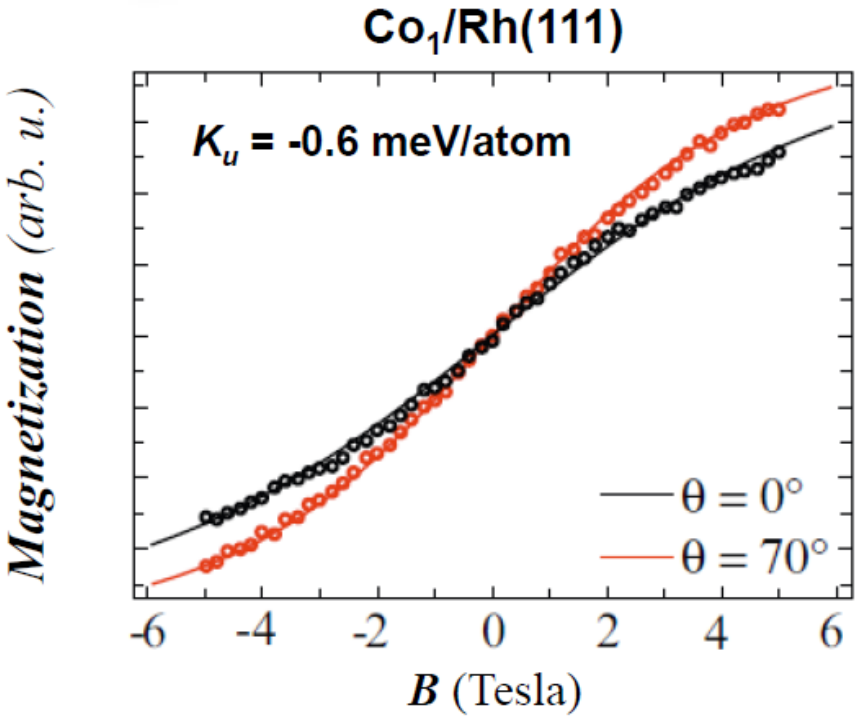


Out-of-plane easy axis



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

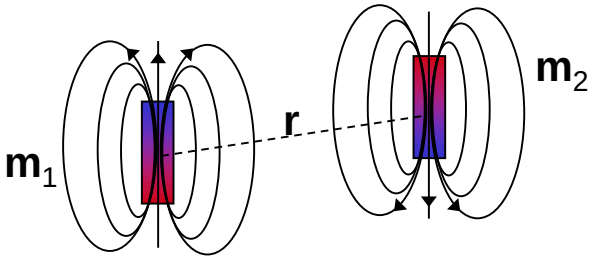
in-plane easy axis



A. Lehnert et al., *Phys. Rev. B* **82**, 094409 (2010)

Dipolar interaction

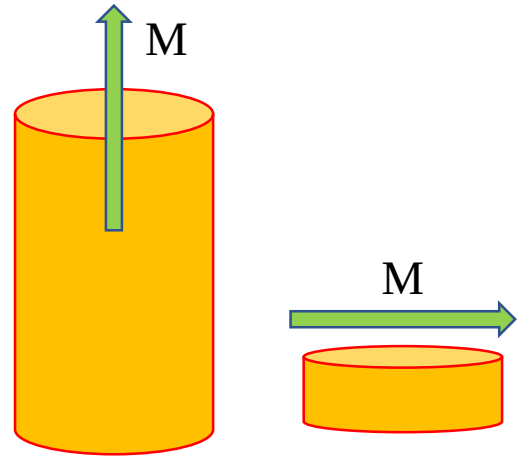
Long range interaction between magnetic moments



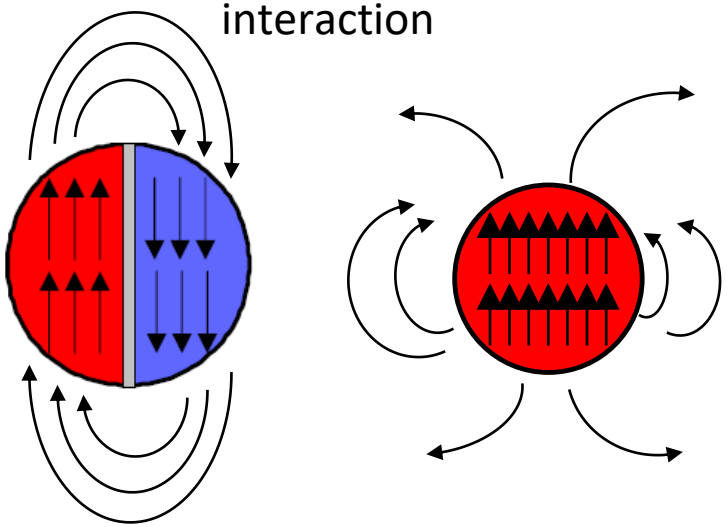
$$H_{dip} = \frac{\mathbf{m}_1 \cdot \mathbf{m}_2}{r^3} - 3\frac{(\mathbf{m}_1 \cdot \mathbf{r})(\mathbf{m}_2 \cdot \mathbf{r})}{r^5}$$

$\mathbf{m}_1$ and **$\mathbf{m}_2$** : magnetic moments of two atoms in a particle or moments of two particles

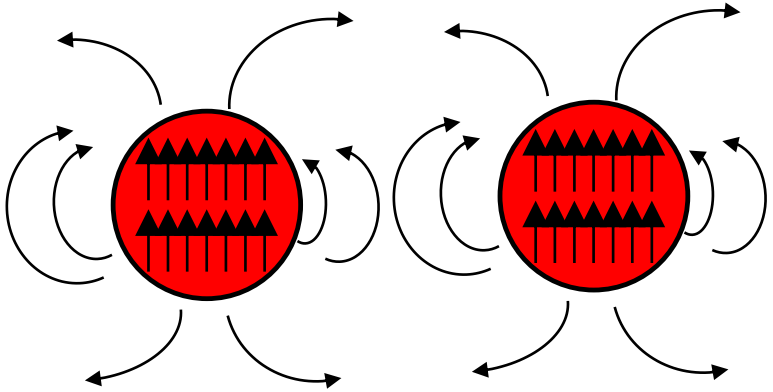
Magnetization orientation



Domain formation:
competition between exchange and dipolar interaction



Interaction between close particles

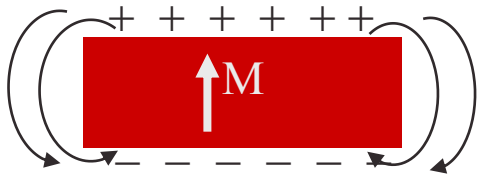


Demagnetizing field: shape anisotropy

Infinite plate

poles only at very far ends ->
no magnetic field outside the plate $H_{dem} \approx 0$

finite plate



poles at the two faces -> $\boldsymbol{H}_{dem} \neq 0$

$\boldsymbol{H}_{dem}$ is the demagnetizing field

$$E_{dip} = -\frac{\mu_0}{2}\int \mathbf{M}\cdot\mathbf{H}_{dem}\,dV$$

$$\mathbf{H}_{dem} = -\mathbf{D}\,\mathbf{M}$$

Sphere:

$$D = \begin{bmatrix} \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{3} \end{bmatrix}$$

$$E_{x,y,z} = \frac{\mu_0}{6}M^2$$

∞-Cylinder:

$$D = \begin{bmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$E_{x,y} = \frac{\mu_0}{4}M^2 \quad E_z = 0$$

∞-Plane (thin film):

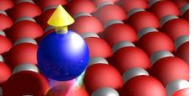
$$D = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$E_{x,y} = 0 \quad E_z = \frac{\mu_0}{2}M^2$$

Shape anisotropy:
the shape determines
the magnetization easy axis.
It is proportional to the volume

$\boldsymbol{H}_{dem}$ forces $\boldsymbol{M}$ along the
longer side of the nanostructure:

Sphere → $\boldsymbol{M}$ isotropic
Cylinder → $\boldsymbol{M}$ // cylinder axis
Disk → $\boldsymbol{M}$ // disk surface



Magneti anisotropy energy (MAE)

The magnetic anisotropy energy (MAE) is the sum of MCA and shape

Magnetic anisotropy energy (MAE)

$$K_{MAE} = K_{MCA} + K_{shape}$$

$$K_{MAE}(\theta) = Ksin^2\theta = -Kcos^2\theta$$

Empirical relationship with $\theta = 0$ giving the easy axis direction of magnetization

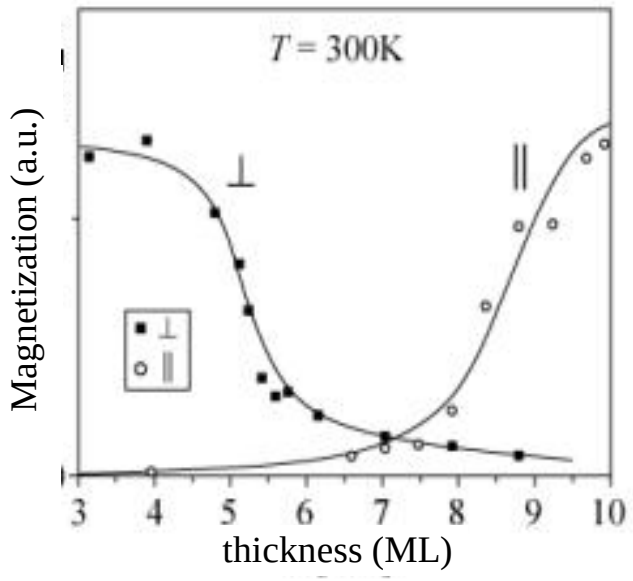
Note that MCA can have more than one source:

- film crystal structure,
- interaction with a supporting substrate,
- interaction with a cupping layer,
- strain
- ….

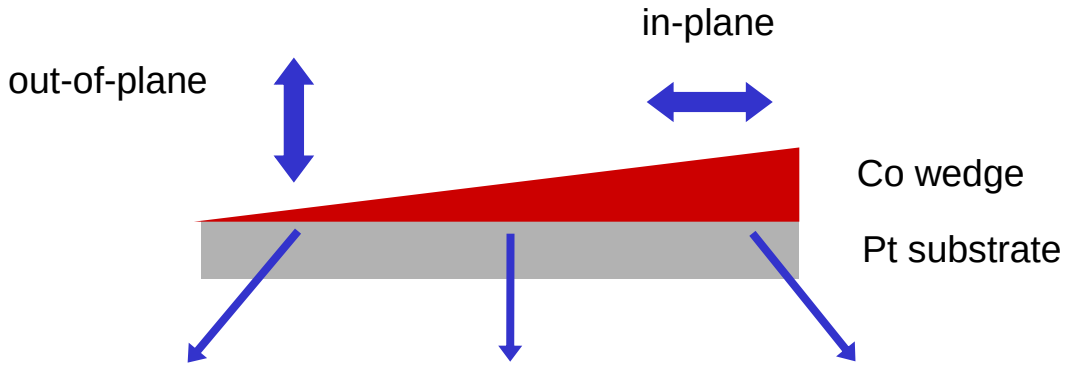
Spin re-orientation transition in thin films

See exercise: 4.3

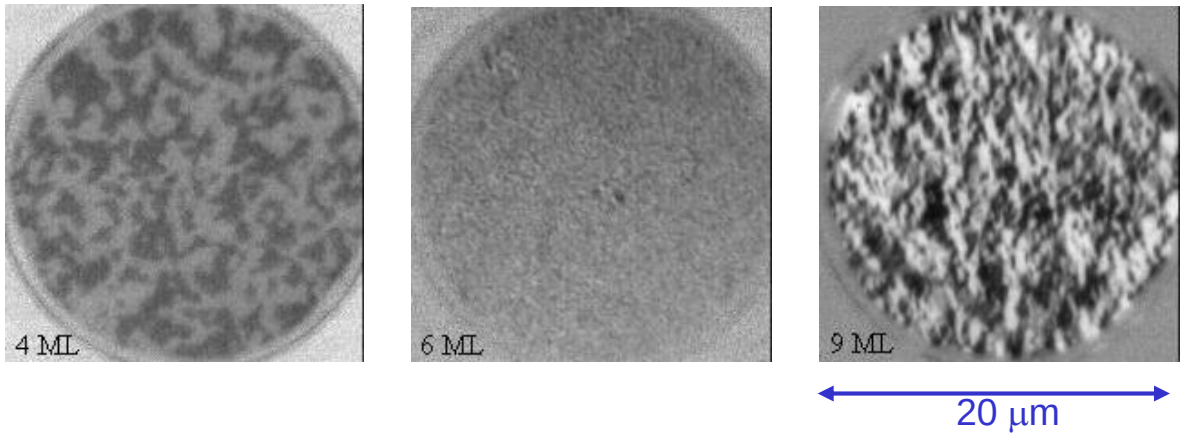
Co/Pt(111)



Easy axis defined by the competition between MCA (hybridization with substrate) and shape anisotropy



Orientation and shape of Co magnetic domains



S. Rusponi, P. Gambardella et al.: X-ray photoemission electron microscopy, SIM beamline @ Swiss Light Source

Magnetic domains

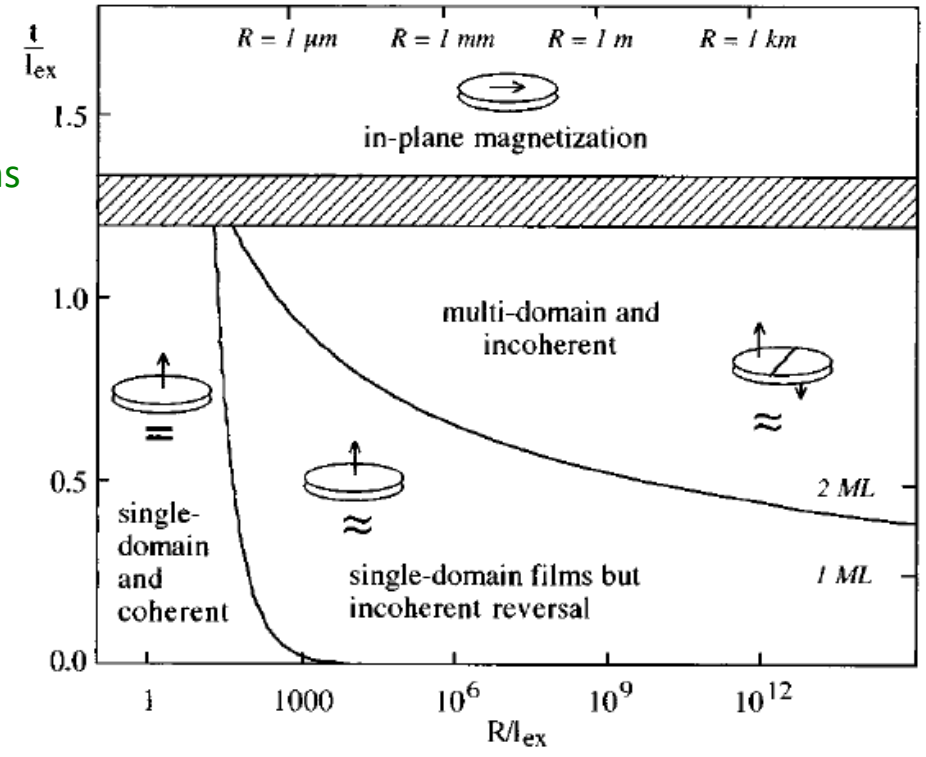
The magnetic configurations are determined by the competition, at a local scale, of four different energies: Zeeman, exchange, magnetocrystalline anisotropy, and dipolar coupling.

$$E = -\mu_0\mu\mathbf{H}\sum_i \mathbf{m}_i - J\sum_{\langle i,j\rangle} \mathbf{m}_i\cdot\mathbf{m}_j - \sum_i k_i(\mathbf{m}_i\cdot\mathbf{e}_i)^2 - \frac{\mu_0\mu^2}{8\pi}\sum_{i,j\neq i}\left[\frac{3(\mathbf{m}_i\cdot\mathbf{r}_{ij})(\mathbf{m}_j\cdot\mathbf{r}_{ij})}{r_{ij}^5} - \frac{\mathbf{m}_i\mathbf{m}_j}{r_{ij}^3}\right],$$

exchange, magnetocrystalline energy -> short range

dipolar energy -> long range

Ex.: Magnetic phase diagram for ultrathin films with perpendicular anisotropy (l_{ex} = 2nm)



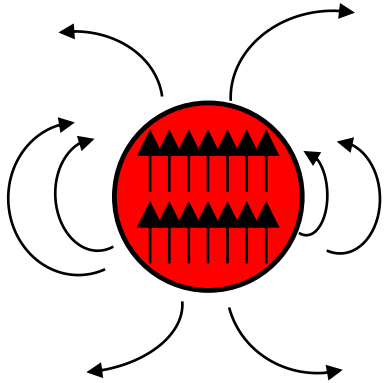
$$l_{ex} = \pi\sqrt{\frac{2A}{\mu_0 M^2}}$$

$A = 2JS^2/a$ is the stiffness

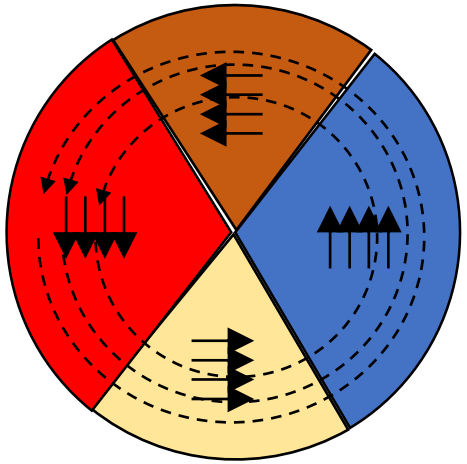
M. Bode, Rep. Progr. Phys. **66**, 523 (2003); R. Skomski et al. Phys.Rev. B **58**, 3223 (1998)

In-plane magnetized particles

Increasing the particle size, domain formation minimizes the magneto-static energy due to the dipolar field

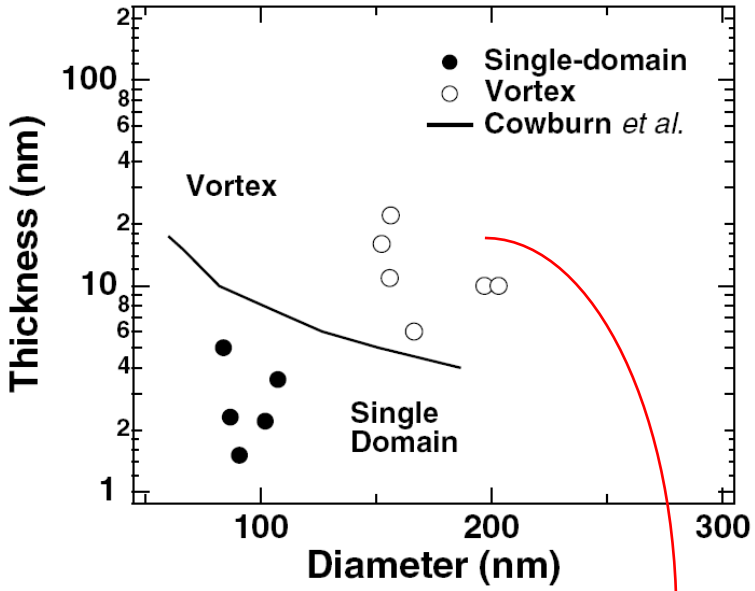


Flux lines extend outside the particle



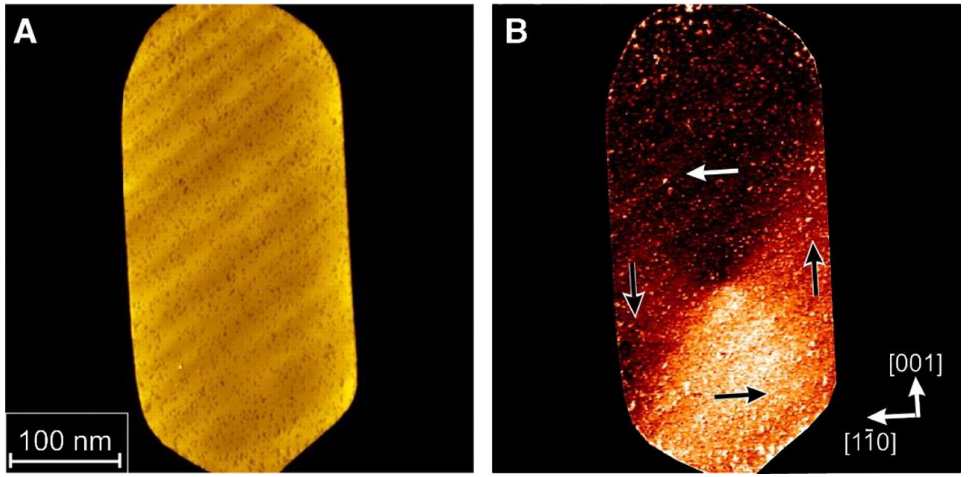
Flux lines are confined inside the particle

Magnetic phase diagram for ultrathin particles with in-plane anisotropy (Fe/W(001))



Topography

SP- STM

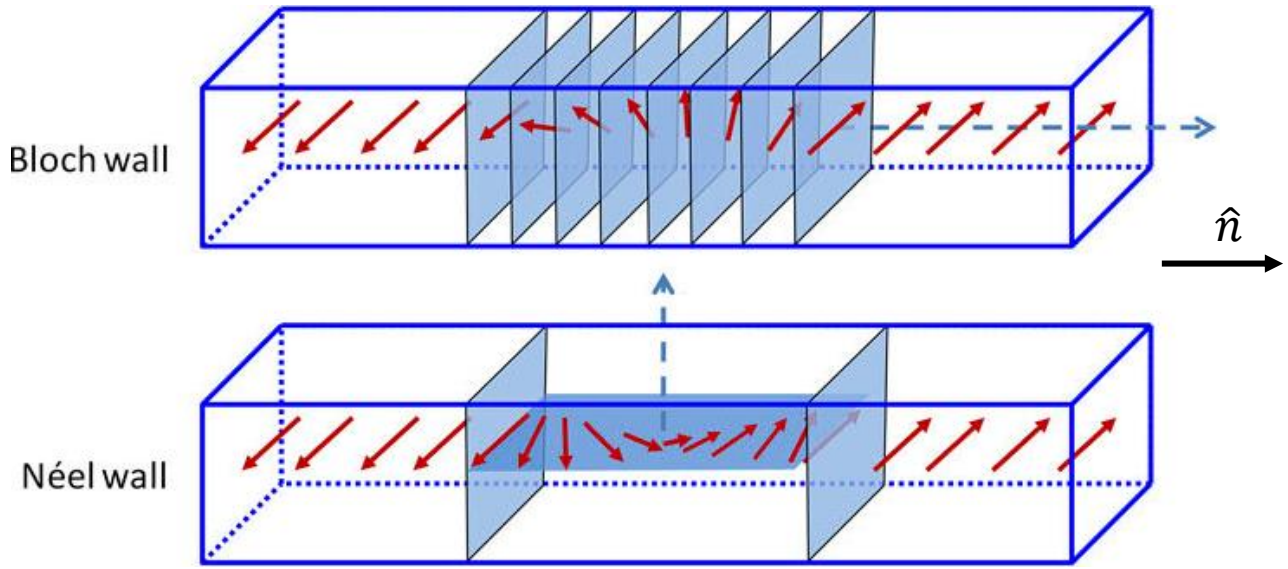


magnetic domain pattern of a 8 nm high Fe particle grown on W(110)

R. Skomski *et al*. Phys.Rev. Lett. **91**, 127201 (2003)
A. Wachowiak *et al*.. Science **298**, 577 (2002)

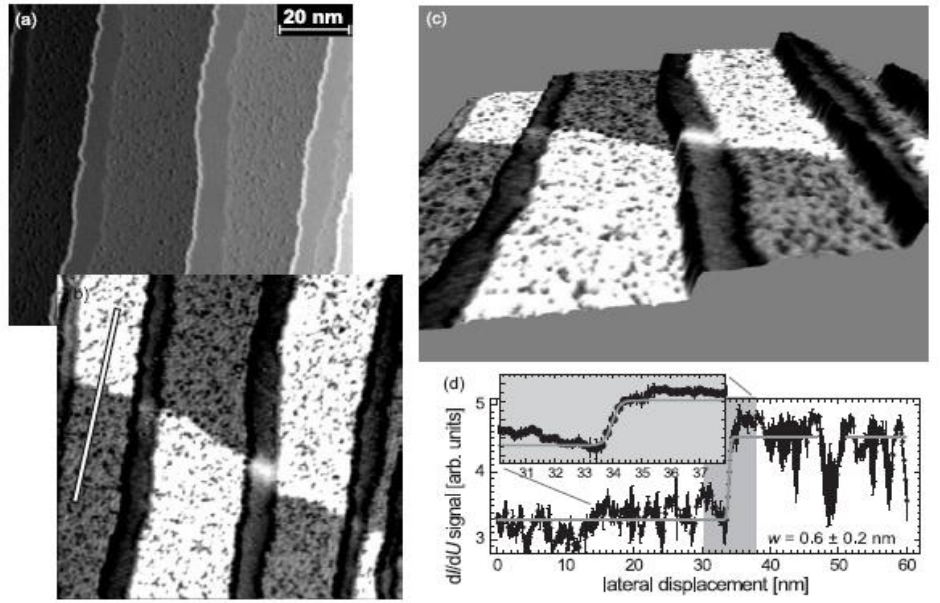
Domain wall

In a Bloch domain wall, the magnetization rotates about the normal $\hat{n}$ of the domain wall

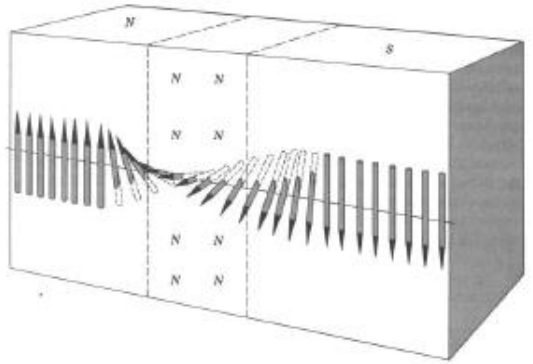


In a Néel domain wall, the magnetization rotates about a line that is orthogonal to the normal $\hat{n}$ of the domain wall.

Ex.: SP-STM of 1.3 monolayers Fe / stepped W(110)



Bloch wall



DOI:10.1063/1.5087925

M. Bode, Rep. Progr. Phys. **66**, 523 (2003)

Bloch vs Néel domain walls

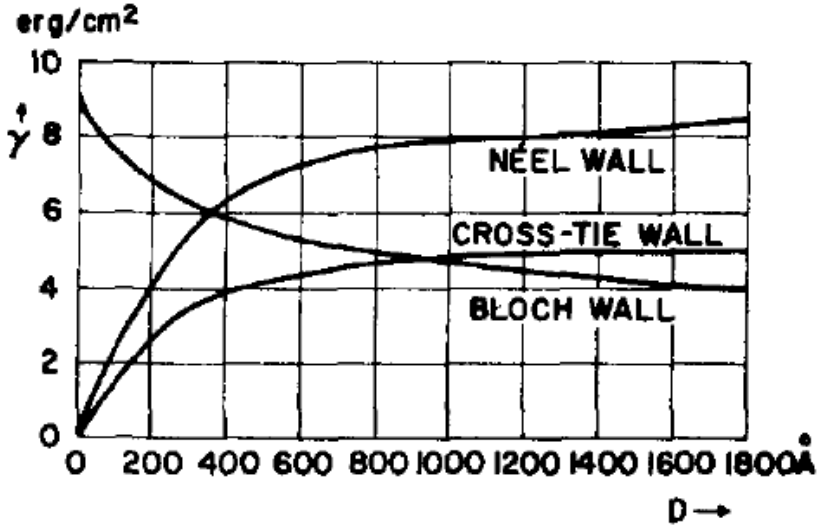


FIG. 1. Energy per unit area of a Bloch wall, a Néel wall and a cross-tie wall as a function of the film thickness [$A = 10^{-6}$ ergs/cm, $M_S = 800$ G, and $K = 1000$ ergs/cm^3].

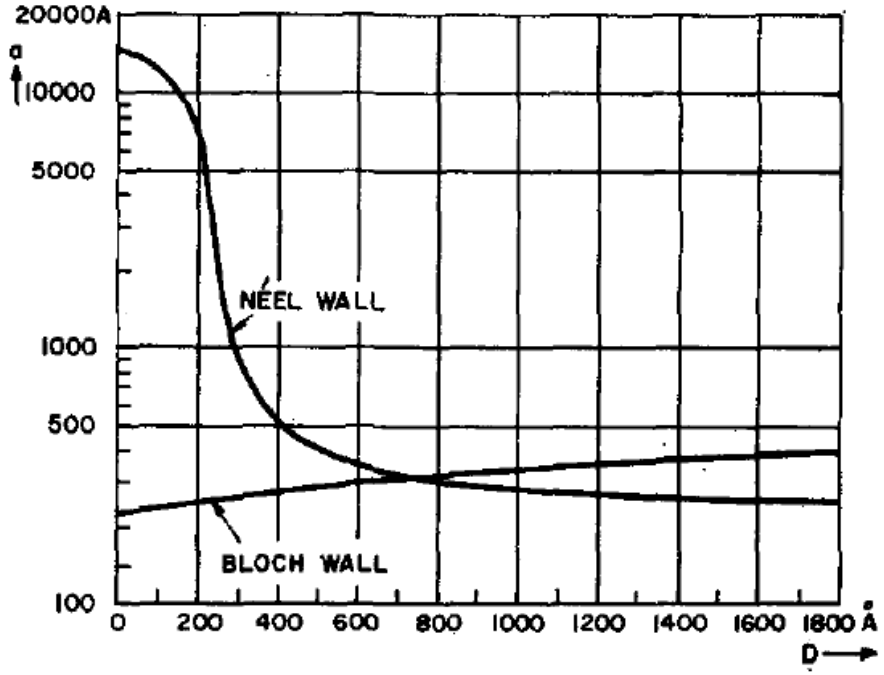


FIG. 2. Wall width of a Bloch wall and of a Néel wall as a function of the film thickness [$A = 10^{-6}$ ergs/cm, $M_S = 800$ G, and $K = 1000$ ergs/cm^3].

The material and geometry decide the type of magnetic domain

- The Neel walls are favored in thin easy-plane anisotropy films
- The Bloch walls are favored in thin perpendicular anisotropy films

S. Middelhoek; *J. Appl. Phys.* 34, 1054–1059 (1963) https://doi.org/10.1063/1.1729367

Bloch wall energy and width

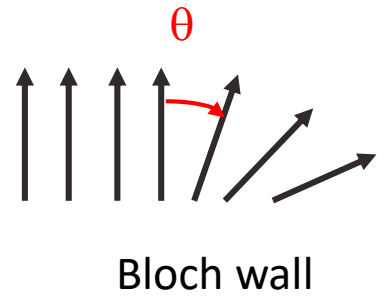
Exchange contribution for a couple of spins:

Aligned: $2J\boldsymbol{S}_i \cdot \boldsymbol{S}_j = 2JS^2$

Wall: $2J\boldsymbol{S}_i \cdot \boldsymbol{S}_j = 2JS^2 \cos\theta = 2JS^2(1-\frac{\theta^2}{2})$

$\Delta E_{exc} = 2JS^2 - 2JS^2(1-\frac{\theta^2}{2}) = JS^2\theta^2$ ➡ Variation in exchange energy for a wall of N spins

$\Delta E_{exc} = NJS^2\theta^2 = NJS^2(\frac{\pi}{N})^2 = JS^2\frac{\pi^2}{N}$



Bloch wall

Exchange contribution, per unit area, for thin film of material with lattice parameter a: $\gamma_{exc} = JS^2\frac{\pi^2}{Na^2}$

Anisotropy contribution :

Aligned: $K\sin^2\theta = 0$

Wall: $\sum_i^N K\sin^2\theta_i = \frac{NK}{\pi}\int_0^\pi \sin^2\theta\, d\theta = \frac{NK}{2}$ ➡

Anisotropy contribution, per unit area, for thin film of material with anisotropy per unit volume K: $\gamma_{ani} = \frac{NKa}{2}$

Total DW energy per unit area is:

$\gamma_{DW} = \gamma_{ani} + \gamma_{exc} = \frac{NKa}{2} + JS^2\frac{\pi^2}{Na^2}$

The width of the wall is obtained following: $\frac{d\gamma_{DW}}{dN} = 0$ ➡ $N = \pi S\sqrt{\frac{2J}{Ka^3}}$

Bloch wall energy per unit area: $\gamma_{DW} = \pi S\sqrt{\frac{2JK}{a}} = \pi\sqrt{AK}$

$A = 2JS^2/a$ is the stiffness

Bloch wall width: $\delta_{DW} = Na = \pi S\sqrt{\frac{2J}{Ka}} = \pi\sqrt{\frac{A}{K}}$

Skyrmion size

a

The skyrmion size results from a balance between:
(i) the DMI energy which favors larger skyrmions,
(ii) the cost in anisotropy and exchange energy at larger radius, which favours smaller skyrmions,
(iii) the curvature energy cost at low radius due to the exchange energy
(iv) the stray field (dipolar energy) which tends to increase the Skyrmion

Table 1. Selection of thin film multilayered materials illustrating Néel skyrmion stabilization. We indicate the material (multilayer system), the measured diameter of the skyrmion core, the magnitude of the DMI $|D|\left(\frac{mJ}{m^2}\right)$, the temperature of the skyrmion stability and the reference of the paper containing the study.

Multilayer System	Diameter of Skyrmion Core (nm)	$\lvert D\rvert\left(\frac{mJ}{m^2}\right)$	Temperature of Skyrmion Stability (K)	Reference
Pt/Co/Ta	75–200	1.3	$\leqslant 300$	[5]
Pt/Co/MgO	70–130	2.0	$\leqslant 300$	[6]
Ir/Co/Pt	25–100	N.A.	$\leqslant 300$	[7]
$[Ir/Co/Pt]_{10}$	100	2	> 300	[8]
Pt/CoFeB/MgO	<250	1.35	$\leqslant 300$	[9,10,11]
Pd/CoFeB/MgO	<200	0.78	$\leqslant 300$	[12]
W/CoFeB/MgO	250	0.3–0.7	$\leqslant 300$	[13]
Ta/CoFeB/MgO	300	0.33	$\leqslant 300$	[14]
Ta/CoFeB/Ta/MgO	1000–2000	0.33	>300	[14]

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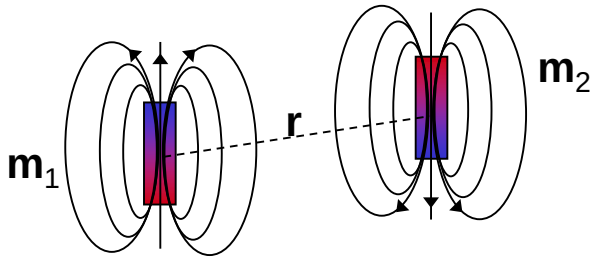
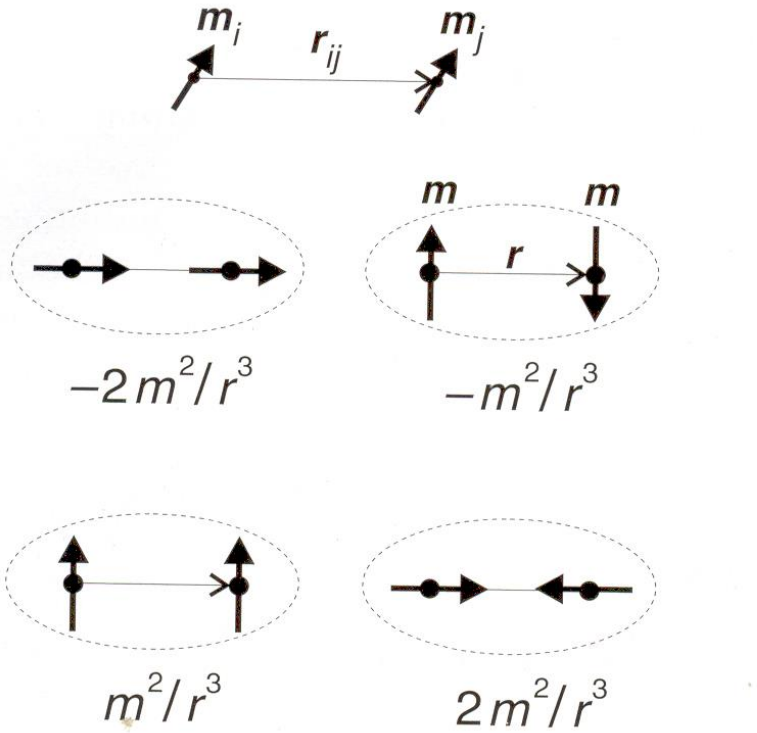
Dipolar long range interaction

Long range interaction between magnetic moments

$$H_{dip} = \frac{\mathbf{m}_1 \cdot \mathbf{m}_2}{r^3} - 3\frac{(\mathbf{m}_1 \cdot \mathbf{r})(\mathbf{m}_2 \cdot \mathbf{r})}{r^5}$$



m_1 and m_2 the magnetic moments of two particles



In the last decade, to overcome the 1Tbit/in^2 limit, the storage media has adopted perpendicular magnetized media in place of the longitudinal media (ex. the $L1_0$ phase in FePt)

The out-of-plane configuration reduces the dipolar interaction