

Nanomagnetism and Spintronics



POLITECNICO
MILANO 1863

Lecture 3

Magnetic free energy terms

Prof. Riccardo Bertacco

Department of Physics – Politecnico di Milano

E-mail: riccardo.bertacco@polimi.it

Tel: 02 23999663

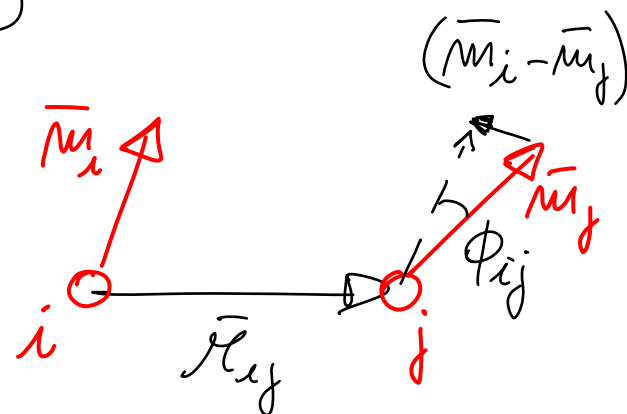
Exchange interaction

$$(E_S - E_t = 2J)$$

$$\hat{H} = - \sum_{\langle i,j \rangle} J \vec{S}_i \cdot \vec{S}_j \quad (1)$$

Hp: consider classical spins

$$\phi_{ij} \ll 1$$



$$E = -JS^2 \sum_{\langle i,j \rangle} \cos \phi_{ij} = \cos t + \frac{JS^2}{2} \sum_{\langle i,j \rangle} \phi_{ij}^2 \quad \left\{ \cos \phi_{ij} \approx 1 - \frac{\phi_{ij}^2}{2} \right\}$$

Define the REDUCED MOMENT $\bar{m} = \vec{m} / m_{\text{sat}}$

$$|\phi_{ij}| \approx |\bar{m}_i - \bar{m}_j| \approx |(\vec{r}_{ij} \cdot \vec{\nabla}) \bar{m}|$$

$\left. \begin{matrix} m_x \\ m_y \\ m_z \end{matrix} \right\} \text{ DIRECTION COSINES}$

$$E = \frac{JS^2}{2} \sum_{\vec{r}} [(\vec{r}_{ij} \cdot \vec{\nabla}) m]^2 =$$

$r_{ij} = a$ LATTICE PARAMETER

$$= \frac{A}{2} \int_V [(\nabla m_x)^2 + (\nabla m_y)^2 + (\nabla m_z)^2] d^3r$$

with $A = 2JS^2 \frac{z}{a}$

z : number of sites in the unit cell for cubic lattice

$A = 4\sqrt{2} \frac{JS^2}{a}$ for hexagonal close packed

exercise Find the expression for exchange energy in a simple cubic lattice

$$|\phi_{xy}|^2 = |\bar{u}_i - \bar{u}_j|^2 = |\Delta m_x \bar{i} + \Delta m_y \bar{j} + \Delta m_z \bar{k}|^2$$

$$= (\bar{i}_{xy} \cdot \bar{\nabla} m_x)^2 + (\bar{i}_{xy} \cdot \bar{\nabla} m_y)^2 + (\bar{i}_{xy} \cdot \bar{\nabla} m_z)^2 = [(\bar{i}_{xy} \cdot \bar{\nabla}) \bar{m}]^2$$

$$E = \frac{J S^2}{2} \sum_i \sum_j \left\{ (\bar{i}_{xy} \cdot \bar{\nabla} m_x)^2 + (\bar{i}_{xy} \cdot \bar{\nabla} m_y)^2 + (\bar{i}_{xy} \cdot \bar{\nabla} m_z)^2 \right\} =$$

For a simple cubic there are 6 nearest neighbours

$$\sum_j \{ \} = 2 \left[\left(a \frac{\partial m_x}{\partial x} \right)^2 + \left(a \frac{\partial m_y}{\partial x} \right)^2 + \left(a \frac{\partial m_z}{\partial x} \right)^2 \right] + \quad \bar{i}_{xy} = \pm a \bar{i}$$

$$+ 2 \left[\left(a \frac{\partial m_x}{\partial y} \right)^2 + \left(a \frac{\partial m_y}{\partial y} \right)^2 + \left(a \frac{\partial m_z}{\partial y} \right)^2 \right] + \quad \bar{i}_{xy} = \pm a \bar{j}$$

$$+ 2 \left[\left(a \frac{\partial m_x}{\partial z} \right)^2 + \left(a \frac{\partial m_y}{\partial z} \right)^2 + \left(a \frac{\partial m_z}{\partial z} \right)^2 \right] \quad \bar{i}_{xy} = \pm a \bar{k}$$

$$\sum_i \{ \dots \} = 2a^2 [(\nabla m_x)^2 + (\nabla m_y)^2 + (\nabla m_z)^2]$$

$$E = \frac{1}{2} \sum_i 2a^2 [\dots] = \frac{1}{2} \int_V [\dots] d\tau$$

$$E = \frac{A}{2} \int_V [(\nabla m_x)^2 + (\nabla m_y)^2 + (\nabla m_z)^2] d\tau$$

with $A = \frac{2JS^2}{a}$ EXCHANGE STIFFNESS

in general for a cubic lattice $A = \frac{2JS^2}{a} z$

$z = \begin{cases} 1 & \text{simple cubic} \\ 2 & \text{bcc} \\ 4 & \text{fcc} \end{cases}$

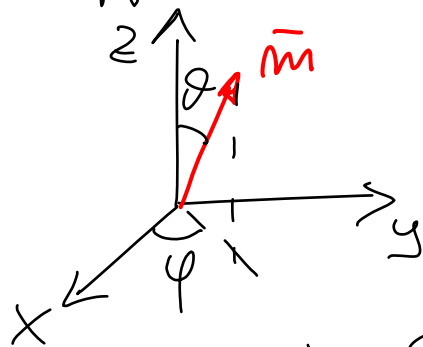
$$A_{Co} = 31 \text{ pJ/m}$$

$$A_{Fe} = 10 \text{ pJ/m}$$

Anisotropy

We are looking for the dependence of Helmholtz free en. on the orientation of \bar{M}

Consider a volume ΔV with \bar{M} uniform inside and suppose $|\bar{M}| = M_{\text{sat}}$

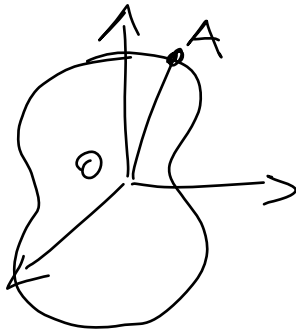


$$\bar{m} = \frac{\bar{M}}{M_{\text{sat}}}$$

$$\begin{cases} m_x = \sin\theta \cos\varphi \\ m_y = \sin\theta \sin\varphi \\ m_z = \cos\theta \end{cases}$$

$$F_{AN}(\bar{m}) = ? \quad \text{or} \quad f_{AN}(\bar{m}) = \frac{F_{AN}}{\Delta V} = ?$$

ANISOTROPY ENERGY SURFACES



$\bar{OA} \sim f_{AN}$ when \bar{m} is directed along \bar{OA}

EASY AXES : local minimum

HARD AXIS : " maximum

Uniaxial anisotropy

$f_{AN}(\vec{m})$ must be unchanged upon rotation around the anisotropy axis (z)

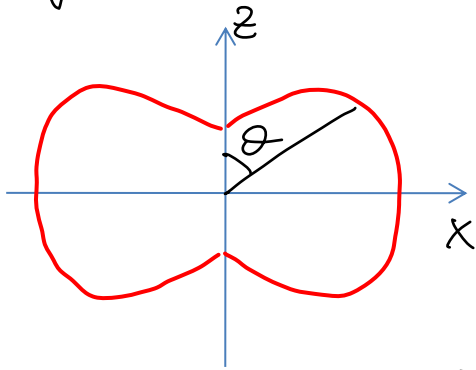
must be an even function of $m_z = \cos\vartheta$

$m_x^2 + m_y^2 = 1 - m_z^2 = 1 - \cos^2\vartheta = \sin^2\vartheta$ is the good variable for the expansion of f_{AN}

$$f_{AN} = K_0 + K_1 \sin^2\vartheta + K_2 \sin^4\vartheta + K_3 \sin^6\vartheta + \dots \quad K: \frac{\text{energy}}{\text{volume}}$$

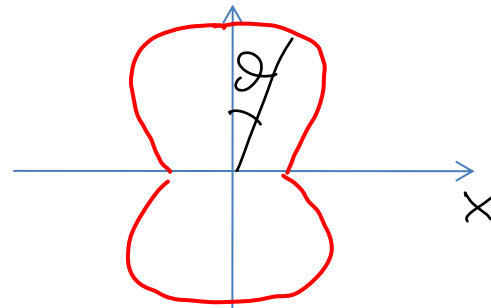
Usually $f_{AN} = K_0 + K_1 \sin^2\vartheta$

a) if $K_1 > 0$



EASY AXIS ANISOTROPY
(MINIMA FOR $\vartheta = 0, \pi$)

b) if $K_1 < 0$



EASY PLANE ANISOTROPY
(MINIMA FOR $\vartheta = \frac{\pi}{2}, \frac{3\pi}{2}$)

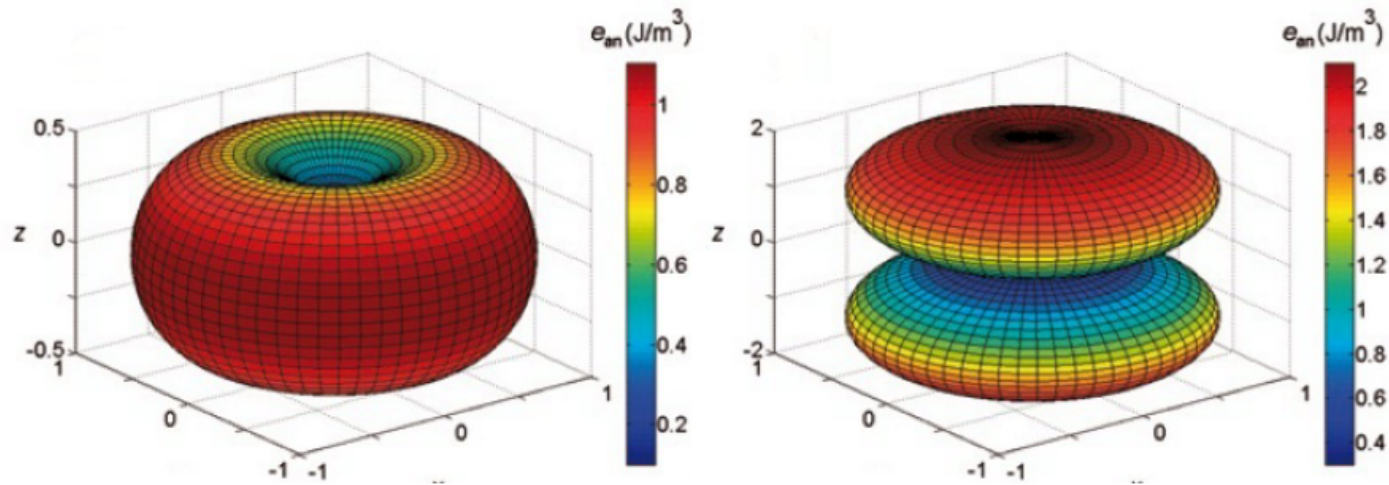


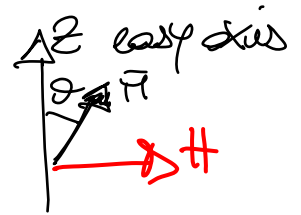
Figure 2.1: Uniaxial anisotropies represented by energy surfaces. The length of the plotted radial coordinate is proportional to the energy density for that direction. The anisotropy constants are chosen to illustrate different cases at similar energy scales. (left) Easy perpendicular direction (right) Easy plane

ANISOTROPY FIELD (H_a) (FOR EASY AXIS ANISOTROPY)
 H_a is defined as the field needed to rotate \vec{M} along the hard axis.

If the uniaxial anisotropy is the only energy term to be considered in F

$$g_L \hat{=} K_1 \sin^2 \theta - \mu_0 M_s H \cos\left(\frac{\pi}{2} - \theta\right)$$

$$= K_1 \sin^2 \theta - \mu_0 M_s H \sin \theta$$



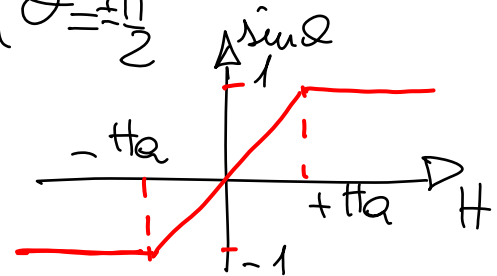
$$\frac{\partial g_L}{\partial \theta} = (2K_1 \sin \theta - \mu_0 M_s H) \cos \theta$$

$$\frac{\partial^2 g_L}{\partial \theta^2} = +2K_1 \cos 2\theta + \mu_0 M_s H \sin \theta$$

$$\frac{\partial^2 g_L}{\partial \theta^2} \left(\theta = \frac{\pi}{2} \right) = -2K_1 - \mu_0 M_s H > 0$$

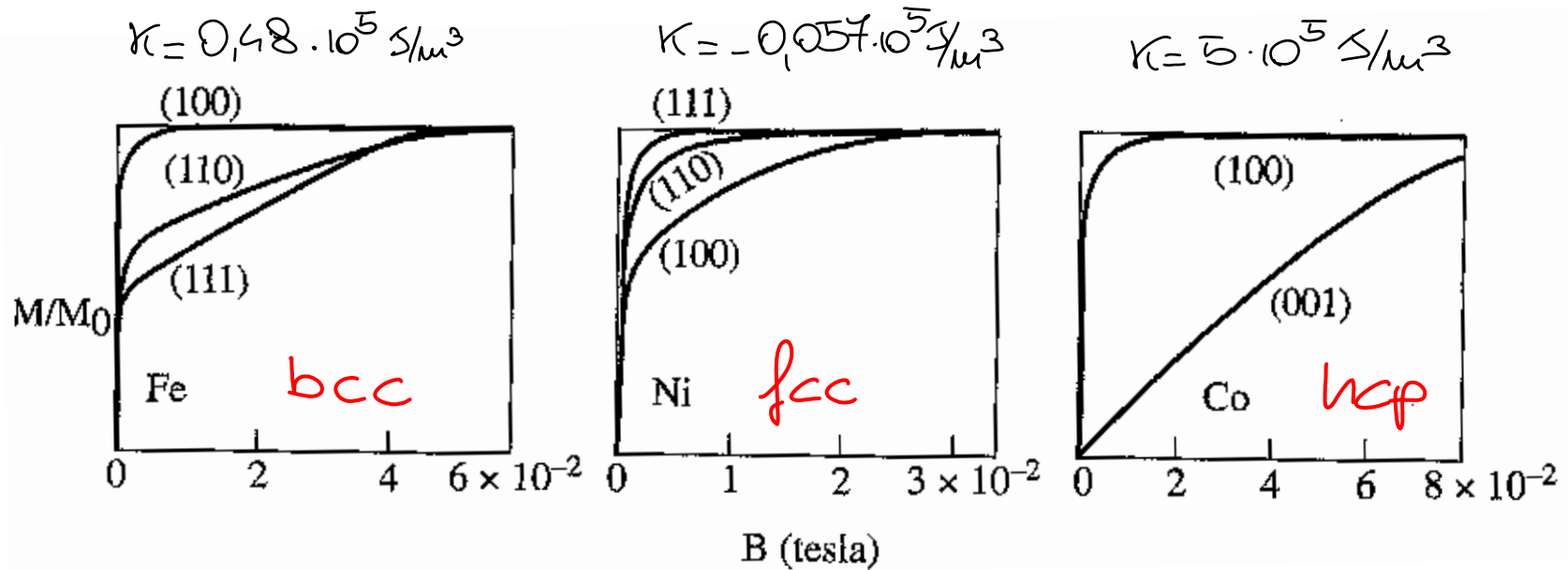
$$H < -\frac{2K_1}{\mu_0 M_s} = -H_a$$

$$\left\{ \begin{array}{l} \sin \theta = \frac{\mu_0 M_s H}{2K_1} \\ \theta = \pm \frac{\pi}{2} \end{array} \right.$$

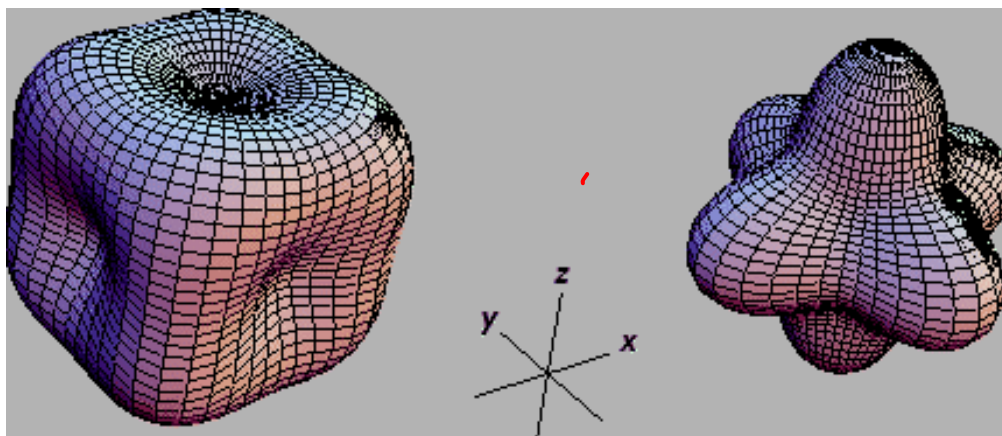


$H_a = \frac{2K_1}{\mu_0 M_s}$ indicates the strength of the anisotropy

Magnetocrystalline anisotropy

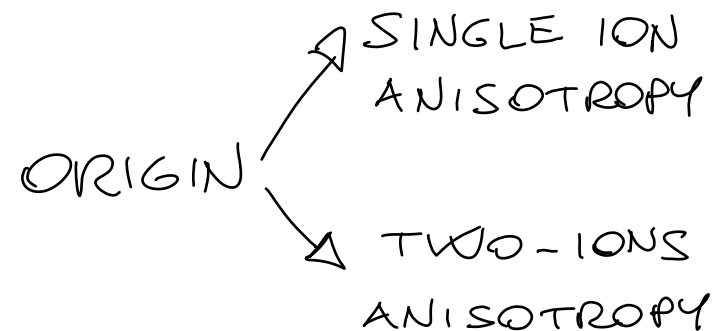


Magnetocrystalline anisotropy energy surfaces



Fe (bcc)

Ni (fcc)



Single-ion anisotropy

Due to electrostatic interaction of the orbitals containing unpaired electrons with the crystal field -

Crystal field tends to stabilize a particular orbital (e.g. t_{2g} in octahedral symmetry): L is fixed!

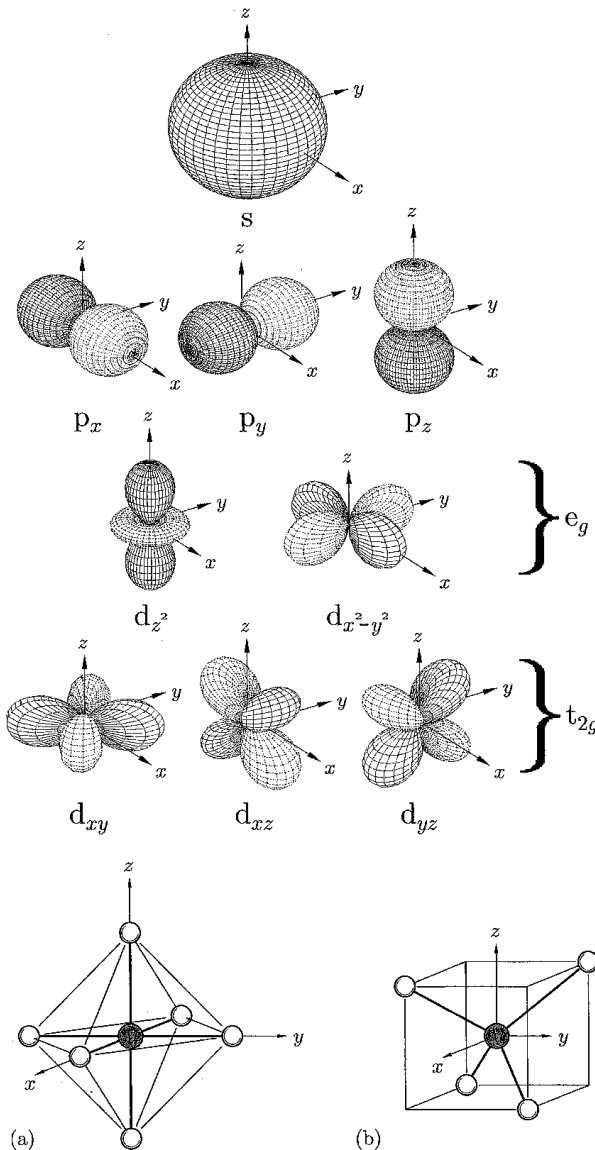
Don't forget spin orbit interaction

$$H_{so} = \alpha \bar{L} \cdot \bar{S}$$

\bar{H} is given by \bar{S} and therefore the easy axis is that along which spin-orbit energy is minimized

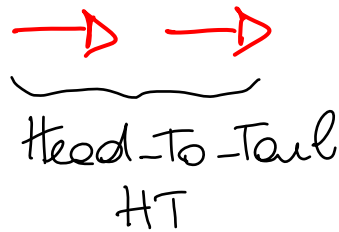
NOTE: This is the case of weak spin orbit coupling

For strong spin orbit, it induces a def. of the orbitals if \bar{S} precesses $\bar{H} \Rightarrow$ ENERGY COST!



Two-ions anisotropy

This term reflects the anisotropy of dipolar interaction between two magnetic moments



For two interacting dipoles

$$E_p - E_{HT} = \frac{3\mu_0 m^2}{4\pi r^3}$$

However the dipole-dipole interaction over the entire lattice must be considered.

For a cubic lattice we have seen that there is no net dipolar contribution to the local field \Rightarrow NO TWO-IONS ANISOTROPY

In non-cubic lattices dipolar interaction can give appreciable magnetic anisotropy.

Cubic anisotropy

$f_{AN}(\bar{m})$ must respect the cubic symmetry \Rightarrow expansion in terms containing:

$$\left[m_x^2 m_y^2 + m_y^2 m_z^2 + m_z^2 m_x^2 \right] \left\{ \begin{array}{l} \text{unchanged upon} \\ \text{exchange of } x, y, z \end{array} \right.$$

$$\{ m_x^2 m_y^2 m_z^2 \}$$

NOTE: The other possible combination $(m_x^4 + m_y^4 + m_z^4)$ depends on the other two:

$$\{ m_x^4 + m_y^4 + m_z^4 \} + 2 [m_x^2 m_y^2 + m_y^2 m_z^2 + m_z^2 m_x^2] = (m_x^2 + m_y^2 + m_z^2)^2 = 1$$

$$f_{AN}(\bar{m}) = K_0 + K_1 [\text{...}] + K_2 \{ \text{...} \} + \dots$$

in spherical coordinates:

$$f_{AN}(\bar{m}) = K_0 + K_1 \left(\frac{\sin^2 \theta \sin^2 \phi}{4} + \cos^2 \theta \right) \sin^2 \theta + K_2 \frac{\sin^2 \phi \sin^2 2\theta}{16} + \dots$$

if $\theta = \pi/2$ (m stay in the film plane, for instance)

$$f_{AN} = K_0 + K_1 \frac{\sin^2 2\phi}{4}$$

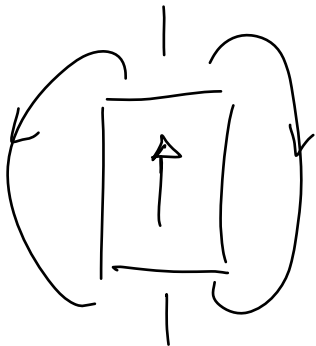
Domain formation

In any case it costs energy to make a DW; why domains form?

The reason is the minimization of

demagnetizing energy =
= magnetostatic energy =
= dipolar energy

$$E_D = -\frac{\mu_0}{2} \int_V \vec{M} \cdot \vec{H}_d d\vec{r} = \frac{\mu_0}{2} \int_{A.S.} H_d^2 d\vec{r}$$



CLOSURE DOMAIN
STRUCTURE

Domains and domain walls

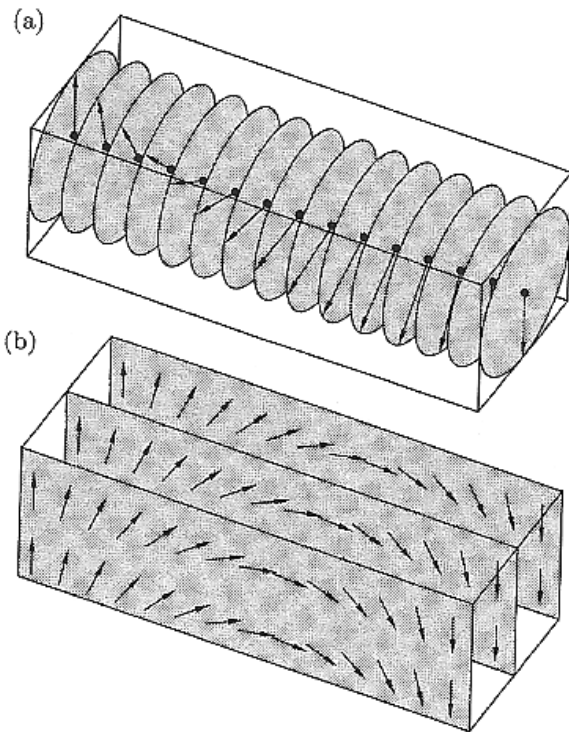
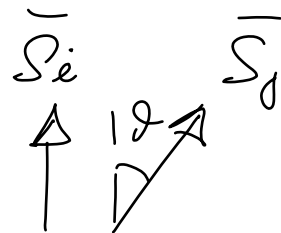


Fig. 6.20 (a) A Bloch wall. (b) A Néel wall.



$$E = -2JS\vec{S}_1 \cdot \vec{S}_2 = -2JS^2 \cos \theta$$

The energy cost for $\theta \neq 0$ is:
 $\Delta E = JS^2 \theta^2$ if $\theta \ll 1$ $\left\{ \cos \theta \approx 1 - \frac{\theta^2}{2} \right\}$

FOR A BLOCH DW the spins rotate by π over N sites

$$\Delta E = N \cdot \left(JS^2 \left(\frac{\pi}{N} \right)^2 \right) = JS^2 \frac{\pi^2}{N}$$

The energy per unit area is

$$\sigma_{BW} = \frac{\Delta E}{Q^2} = \frac{JS^2 \pi^2}{NQ^2}$$

$$\lim_{N \rightarrow \infty} \sigma_{BW} = 0$$

\Rightarrow SINGLE DOMAIN CONFIG. SHOULD BE FAVORED !!!

But we must consider also anisotropy!

Assume $E_{an} = K \sin^2 \theta$ ($K > 0$)

The anisotropy energy contribution associated to a BW:

$$\sum_{i=1}^N K \sin^2 \theta_i \approx \frac{N}{\pi} \int_0^{\pi} K \sin^2 \theta d\theta = \frac{NK}{2}$$

in terms of energy per unit area: $\frac{NK}{2} \cdot a$

The total energy cost of a BW is:

$$\sigma_{BW} = \underbrace{\frac{5S^2\pi^2}{N\alpha^2}}_{\substack{\nearrow \\ \text{BIG DOMAIN}}} + \frac{NK\alpha}{2} \searrow \text{SMALL DOMAINS}$$

Equilibrium configuration: $\frac{dE_{BW}}{dN} = 0$

$$N = \pi S \sqrt{\frac{2S}{K\alpha^3}}$$

the width of the DW is:

$$\delta = Na = \pi S \sqrt{\frac{2S}{K} a}$$

large $K \Rightarrow$ thin
large $S \Rightarrow$ thick

$$\sigma_{BW_{eq}} = \pi S \sqrt{\frac{2SK}{a}}$$

for the exchange energy we used $A = 2SS^2 \frac{z}{a}$

$$\begin{cases} \delta = \pi \sqrt{\frac{A}{K}} \\ \sigma_{BW_{eq}} = \pi \sqrt{AK} \end{cases}$$

Width and energy per unit surface of a Bloch DW

	M_s (MA m ⁻¹)	A (pJ m ⁻¹)	K_1 (kJ m ⁻³)	δ (nm)
Ni ₈₀ Fe ₂₀	0.84	10	0.15	800
Fe	1.71	21	48	64
Co	1.44	31	410	24

For Fe $\delta = \pi \sqrt{\frac{21 \cdot 10^{-12}}{48 \cdot 10^3}} \simeq 6,4 \cdot 10^{-8} \text{ m}$

$\sigma = \pi \sqrt{21 \cdot 10^{-12} \cdot 48 \cdot 10^3} = 31,4 \cdot 10^{-5} \text{ J/m}^2$

Exercise

1. Si consideri un film sottile di Co nella configurazione micro magnetica a chiusura di flusso rappresentata in figura 1, con domini prevalenti aventi bordi paralleli all'asse di anisotropia uniassiale ($K = 5 \cdot 10^5 \text{ Jm}^{-3}$) e domini triangolari, agli estremi, con magnetizzazione perpendicolare all'asse di anisotropia. L'energia per unità di superficie associata alle pareti di dominio a 180° vale $\sigma_w = 4 \times 10^{-3} \text{ Jm}^{-2}$, mentre il contributo all'energia totale delle pareti a 90° ai bordi può essere trascurato nell'ipotesi che $L \gg D$.

a) Dimostrare che in queste condizioni la larghezza dei domini D si può esprimere come:

$$D = \sqrt{\frac{2\sigma_w L}{K}}$$

b) Nell'ipotesi che L sia pari a 5 mm calcolare la larghezza dei domini

