Driving forces in the nano-magnetism world

Intra-atomic exchange, electron correlation effects:

LOCAL (ATOMIC) MAGNETIC MOMENTS

\[ \mathbf{m} \]

d or f electrons

Hund’s rules

Inter-atomic exchange:

MAGNETIC ORDER

\[ H_{exc} = -\sum_{i \neq j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \]

Spin-Orbit Coupling:

MAGNETOCRYSTALLINE ANISOTROPY:

\[ K \]

\[ H_{s.o.} = \lambda L \cdot S = \sum \xi s_i \cdot l_i \]

Dipolar Interaction:

SHAPE ANISOTROPY

\[ H_{dip} = \frac{m_1 \cdot m_2}{r^3} - 3 \frac{(m_1 \cdot r)(m_2 \cdot r)}{r^5} \]
The He atom

Ground state -> the two electrons occupy the 1s orbital
-> the spatial part of the wavefunction is symmetric (electrons have identical quantum numbers $nlm=100$)
-> the spin part must be antisymmetric (electrons are fermions)

$$\Psi_{\text{ground}} = \Psi_{\text{sym}}(r_1, r_2) \chi_{\text{antisym}}(s_1, s_2) = \frac{1}{2} [\Psi_{100}(r_1) \Psi_{100}(r_2) + \Psi_{100}(r_1) \Psi_{100}(r_2)][\alpha\beta - \beta\alpha]$$

From the previous Hamiltonian we can calculate the energy of the ground state. Because $H_{\text{He}}$ does not contain spin terms, the spin part of the wavefunction only needs to satisfy the antisymmetric condition.

Excited state -> one electron occupies the 1s orbital ($nlm=100$); the second electron is in an excited state $nlm$
1) the spatial part of the wavefunction is symmetric and the spin part is antisymmetric

$$\Psi^{S}_{\text{exci}} = \Psi_{\text{sym}}(r_1, r_2) \chi_{\text{antisym}}(s_1, s_2) = \frac{1}{2} [\Psi_{100}(r_1) \Psi_{nlm}(r_2) + \Psi_{nlm}(r_1) \Psi_{100}(r_2)][\alpha\beta - \beta\alpha] \quad \text{Singlet } S=0$$

2) the spatial part of the wavefunction is symmetric and the spin part is antisymmetric

$$\Psi^{T}_{\text{exci}} = \Psi_{\text{antisym}}(r_1, r_2) \chi_{\text{sym}}(s_1, s_2) = \frac{1}{2} [\Psi_{100}(r_1) \Psi_{nlm}(r_2) - \Psi_{nlm}(r_1) \Psi_{100}(r_2)] \chi_{\text{sym}}(s_1, s_2) \quad \text{Triplet } S=1$$

$$\alpha = \frac{1}{2}; \beta = -\frac{1}{2}$$

$$\chi_{\text{sym}}(s_1, s_2) = \alpha\alpha; \beta\beta; \frac{1}{\sqrt{2}} (\alpha\beta + \beta\alpha)$$
The exchange interaction

The singlet and triplet wavefunctions applied to $H_0$ give the same energy; the $H_{e-e}$ contribution can be calculated with the perturbation theory

\[ I = \int \int |\Psi_{100}(r_1)|^2 \frac{e^2}{4\pi\varepsilon_0 |r_1 - r_2|} |\Psi_{n l m}(r_2)|^2 \, dr_1 dr_2 \]

\[ J = \int \int \Psi_{100}(r_1) \Psi_{n l m}(r_2) \frac{e^2}{4\pi\varepsilon_0 |r_1 - r_2|} \Psi^*_{100}(r_2) \Psi^*_{n l m}(r_1) \, dr_1 dr_2 \]

$I$ is the Coulomb integral -> electrostatic repulsion between the electrons ($\Psi(r)^2$ -> $\rho$ electron density

$J$ is the exchange integral -> energy associated with a change of quantum states between the electrons

$E^S_{e-e} = I + J$

$E^T_{e-e} = I - J$

Exchange interaction: -> Coulomb repulsion between electrons

-> total anti-symmetric wave function (Pauli exclusion principle)

J is positive -> triplet ground state $S=1$ -> parallel spins

J is negative -> singlet ground state $S=0$ -> antiparallel spins

Note: we get the exchange energy from an Hamiltonian not including spin terms !!!!!
The H$_2$ molecule

Hamiltonian $H = H_1 + H_2 + H_{12}$, where

\[
H_1 = -\frac{\hbar^2}{2m} \Delta_1 - \frac{Ze^2}{r_1}
\]

\[
H_2 = -\frac{\hbar^2}{2m} \Delta_2 - \frac{Ze^2}{r_2}
\]

\[
H_{12} = +\frac{e^2}{r_{12}}
\]
The $\text{H}_2$ molecule

\[ \psi_1 = \frac{1}{\sqrt{2 - 2l^2}} (\phi_a(r_1)\phi_b(r_2) - \phi_b(r_1)\phi_a(r_2))(\alpha(r_1)\alpha(r_2)) \text{ triplet} \]

\[ \psi_2 = \frac{1}{\sqrt{2 - 2l^2}} (\phi_a(r_1)\phi_b(r_2) - \phi_b(r_1)\phi_a(r_2))(\beta(r_1)\beta(r_2)) \text{ triplet} \]

\[ \psi_3 = \frac{1}{\sqrt{2 - 2l^2}} (\phi_a(r_1)\phi_b(r_2) - \phi_b(r_1)\phi_a(r_2))\frac{1}{\sqrt{2}} (\beta(r_1)\alpha(r_2) + \alpha(r_1)\beta(r_2)) \text{ triplet} \]

\[ \psi_4 = \frac{1}{\sqrt{2 + 2l^2}} (\phi_a(r_1)\phi_b(r_2) + \phi_b(r_1)\phi_a(r_2))\frac{1}{\sqrt{2}} (\beta(r_1)\alpha(r_2) - \alpha(r_1)\beta(r_2)) \text{ singlet} \]

\[ E = \left\langle \psi_i \middle| H \middle| \psi_i \right\rangle = \left\langle \psi_i \middle| H_1 + H_2 + H_{12} \middle| \psi_i \right\rangle \quad \text{N.B.} \quad \left\langle \psi_i \middle| \psi_i \right\rangle = 1 \]

\[ = \frac{1}{2 \pm 2l^2} \int \int (\phi_a(r_1)\phi_b(r_2) \pm \phi_b(r_1)\phi_a(r_2))^* (H_1 + H_2 + H_{12})(\phi_a(r_1)\phi_b(r_2) \pm \phi_b(r_1)\phi_a(r_2)) d\mathbf{r}_1 d\mathbf{r}_2 \]

\[ = \frac{1}{2 \pm 2l^2} (I_1 + I_2 + K_{12} \pm J_{12}) \]
Inter-atomic exchange

\[ E = \frac{\langle \psi_i | H | \psi_i \rangle}{\langle \psi_i | \psi_i \rangle} = \langle \psi_i | H_1 + H_2 + H_{12} | \psi_i \rangle \quad \text{N.B.} \quad \langle \psi_i | \psi_i \rangle = 1 \]

\[ = \frac{1}{2 \pm 2l^2} \int \int (\phi_a (r_1) \phi_b (r_2) \pm \phi_b (r_1) \phi_a (r_2))^* (H_1 + H_2 + H_{12})(\phi_a (r_1) \phi_b (r_2) \pm \phi_b (r_1) \phi_a (r_2)) \, dr_1 \, dr_2 \]

\[ = \frac{1}{2 \pm 2l^2} (I_1 + I_2 + K_{12} \pm J_{12}) \]

\[ I_1 = \int \phi_a^*(r_1)H_1\phi_a (r_1) \, dr_1 + \int \phi_a^*(r_2)H_2\phi_a (r_2) \, dr_2 \]

\[ e_1 \text{ on atom } a \]

\[ e_2 \text{ on atom } a \]

\[ I_2 = \int \phi_b^*(r_2)H_2\phi_b (r_2) \, dr_2 + \int \phi_b^*(r_1)H_1\phi_b (r_1) \, dr_1 \]

\[ e_2 \text{ on atom } b \]

\[ e_1 \text{ on atom } b \]

\[ K_{12} = \int \int \phi_a^*(r_1)\phi_b^*(r_2)H_{12}\phi_a (r_1)\phi_b (r_2) \, dr_1 \, dr_2 + \int \int \phi_a^*(r_2)\phi_b^*(r_1)H_{12}\phi_a (r_2)\phi_b (r_1) \, dr_1 \, dr_2 \]

\[ e_1-e_2 \text{ interaction, } e_1,e_2 \text{ on different atoms} \]

\[ J_{12} = \int \int \phi_a^*(r_1)\phi_b^*(r_2)H_{12}\phi_b (r_1)\phi_a (r_2) \, dr_1 \, dr_2 + \int \int \phi_a^*(r_2)\phi_b^*(r_1)H_{12}\phi_b (r_2)\phi_a (r_1) \, dr_1 \, dr_2 \]

\[ \text{exchange interaction: } e_1,e_2 \text{ swap from } b \text{ to } a \text{ and } a \text{ to } b, \text{ respectively, due to the action of } H_{12} \]

\[ \text{exchange interaction: } e_1,e_2 \text{ swap from } a \text{ to } b \text{ and } b \text{ to } a, \text{ respectively, due to the action of } H_{12} \]
The $\text{H}_2$ molecule

The magnetic ground state depends on the interaction between electrons belonging to two different atoms.

\[
\begin{align*}
E_s &= \frac{1}{2+2l^2} \left( I_1 + I_2 + K_{12} + J_{12} \right) \\
E_t &= \frac{1}{2-2l^2} \left( I_1 + I_2 + K_{12} - J_{12} \right)
\end{align*}
\]

\[
\Rightarrow E_s - E_t = \frac{1}{4-4l^4} \left[ -4l^2 \left( I_1 + I_2 + K_{12} \right) + 4J_{12} \right]
\]

Ground state depends on the relative strength of $J_{12}$ (always $> 0$) in respect to $-4l^2(I_1+I_2+K_{12})$.

- $J_{12} > 4l^2(I_1+I_2+K_{12}) \Rightarrow$ ground state is magnetic (triplet)
- $J_{12} < 4l^2(I_1+I_2+K_{12}) \Rightarrow$ ground state is non magnetic (singlet)

Ex: $\text{H}_2$ molecule $\Rightarrow$ singlet ground state

The molecule magnetic ground state depends on the interaction between electrons belonging to two different atoms.
The Heisenberg Hamiltonian is an effective Hamiltonian extending to larger atoms the electron-electron interaction seen in the He atom.

\[ H_{\text{Heisenberg}} = H_0 + H_{\text{Coulomb}} + H_{\text{exchange}} \]

\[ H_{\text{exchange}} = -2 \sum_{i<j}^N J_{ij} s_i \cdot s_j; \]

\[ J_{ij} = \int \int \psi_i^*(r_i) \psi_j^*(r_j) \frac{e^2}{4\pi\varepsilon_0 |r_i - r_j|} \psi_i(r_j) \psi_j(r_i) dr_i dr_j \]

The Heisenberg Hamiltonian is used to describe:
- coupling of individual spins located on the same atom (intra-atomic exchange)
- coupling of atomic spin moments on different atoms (inter-atomic exchange)

[Stö06]
Magnetic coupling between atoms: inter-atomic exchange

Generalization to N-atoms system:

• **Coulomb interaction + Pauli’s principle** → The spins of the electrons are correlated
  i.e., there is a magnetic splitting in the energy spectrum of electrons in systems of atoms with open el. shells,
  true for systems of any size, doesn’t tell what type of magnetic coupling

• The energy spectrum is represented by a model system of pairwise interacting spins

\[
H = - \sum_{i \neq j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \quad \text{Heisenberg model}
\]

≈ correct to 2nd order in the overlap orbitals, cannot be proven rigorously

• There are many possible exchange-interaction Hamiltonians…

\[
H = -J_z \sum_{i \neq j} S_i^z S_j^z - J_\perp \sum_{i \neq j} \left(S_i^x S_j^x + S_i^y S_j^y\right) \quad \text{Anisotropic Heisenberg model and XY model (} J_z=0)\]

\[
H = -J_z \sum_{i \neq j} S_i^z S_j^z \quad \text{Ising model}\]
Magnetic coupling between atoms: FM and AFM coupling

\[ H = - \sum_{i \neq j} J_{ij} S_i \cdot S_j \]

\[ \begin{cases} J > 0 & \text{ferromagnetic coupling} \quad (10-50 \text{ meV in Fe, Co, Ni}) \\ J < 0 & \text{antiferromagnetic coupling} \quad (30-100 \text{ meV in Mn, Cr;} \\ & 20 \text{ meV in NiO superexchange}) \end{cases} \]

\( J < 0 \), depending on formula unit, system dimensions, topology:

- fully compensated AFM
- ferrimagnetism (uncompensated AFM)
- frustrated AFM

Cr(100) surface

G-type
C-type
A-type
All spins in the grain must be ferromagnetically aligned

exchange energy $J$ coupling spins

$$H_{exc} = -\sum_{i \neq j} J_{ij} S_i \cdot S_j$$

$H_{exc} \ll kT$

Coupling is destroyed and the net magnetic moment is zero

Domain formation -> magnetic moment is strongly reduced

Gain in the magnetostatic energy at the expenses of the exchange energy
Which is the origin of the aligned atomic spin moments in a ferromagnetic domain (spontaneous magnetization)?

**Weiss** -> molecular field $H_W$ (or mean field theory) of unknown origin

**Heisenberg** -> molecular field originating from the interaction of the atomic spin moment with the spin sea of all the other atoms

$$E_i = -2s_i \sum_j J_{ij} s_j = -m_i H_W; \quad H_W = -\frac{2}{g \mu_B} \sum_j J_{ij} s_j$$

Two energy levels: +/- $\mu_B H$ with an occupation probability given by $\exp(+/\mu_B H/kT)$

**Example:**

single spin $s=1/2$

$$M(H,T) = M\uparrow - M\downarrow = N \mu_B (\frac{e^x}{e^x + e^{-x}} - \frac{e^{-x}}{e^x + e^{-x}}) = N \mu_B \tanh(x); \quad x = \frac{\mu_B H}{k_B T}$$

Sea of spin $s=1/2$

$$x = \frac{\mu_B (H + \beta M(T))}{k_B T}$$

$\beta M(T)$ -> molecular field

**Curie temperature:** temperature at which the spontaneous magnetization ($H=0$) goes to zero

$M(T) \rightarrow 0$ when $\tanh(x) \rightarrow 0$

when $x \rightarrow 0$ i.e. $\tanh(x) = x$

$$M(T_c) \approx N \mu_B x = N \mu_B \frac{\mu_B (\beta M(T_c))}{k_B T_c} \Rightarrow T_c = \frac{N \mu_B^2 \beta}{k_B} = \mu_B \frac{\beta M(0)}{k_B}$$

The magnetization goes to zero when the thermal energy equals the energy of a single spin in the molecular field ($H_W=g s \mu_B \beta M(0)$)
Curie and Neel temperatures

For a general spin value $s$ and moment $m = -g \mu_B s$ 

$$T_C = \frac{2 \langle s \rangle^2 J_0}{3k_B} ; \quad J_0 = \sum_j J_{ij} = NJ_{01}$$

$$H_W = \frac{2 \langle s \rangle^2 J_0}{m}$$

<table>
<thead>
<tr>
<th>element</th>
<th>$\langle s \rangle^2 J_{01}$ [meV]</th>
<th>$N$</th>
<th>$N \langle s \rangle^2 J_{01}$ [meV]</th>
<th>$\langle s \rangle^2 J_0$ [meV]</th>
<th>$T_C$ [K]</th>
<th>$B_W$ [$10^3$ T]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe (bcc)</td>
<td>19.5</td>
<td>8</td>
<td>156</td>
<td>183</td>
<td>1414</td>
<td>2.9</td>
</tr>
<tr>
<td>Co (fcc)</td>
<td>14.8</td>
<td>12</td>
<td>178</td>
<td>212</td>
<td>1645</td>
<td>4.3</td>
</tr>
<tr>
<td>Ni (fcc)</td>
<td>2.8</td>
<td>12</td>
<td>34</td>
<td>51</td>
<td>397</td>
<td>2.9</td>
</tr>
</tbody>
</table>

Neel temperature: is the equivalent to the Curie temperature for an antiferromagnet

A few Neel temperatures

NiO $T_N = 525$ K
CoO $T_N = 290$ K
FeO $T_N = 298$ K
Curie temperature size dependence

\[ T_C = \frac{2\langle s \rangle^2 J_0}{3k_B} \]

\[ J_0 = \sum_j J_{ij} = NJ_{01} \]

The number of magnetic neighbours (\(N\)) is reduced in a thin film

\[ N = \frac{t_b N_b + t_i N_i}{t_b + t_i} = z_b - 2 \frac{N_b - N_i}{t} \]

The phase transition temperature \(T_C\) depends on the atomic coordination.

Nanostructures \(< T_C\) bulk
Curie temperature size dependence

Critical Temperatures of Ising Lattice Films

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\[ T_C(\infty) - T_C(t) = t^{-\lambda}, \quad \lambda = 1 \]

Experiments and finite-size scaling model:

\[ \frac{T_C(\infty) - T_C(t)}{T_C(\infty)} = \left( \frac{t}{t_0} \right)^{-\lambda'}, \quad \lambda' = 1 - 1.6 \]


This model accounts for the decrease of \( T_C \) with \( t \) down to a critical thickness \( t_0 \approx 4 \) monolayers.

\( t \) is a continuous parameter \( \rightarrow \) in the ultra thin limit \( t \) becomes discrete (number of atomic layers)

Ultra thin limit:

linear decrease

\[ \frac{T_C(\infty) - T_C(t)}{T_C(\infty)} = A - (n - 1) / 2N_0 \]


\( N_0 \) is the spin-spin coupling range (typically a few atomic sites)

A takes into account the observation that for \( n=1 \) ferromagnetism can exist
Curie temperature and band structure

**Paramagnet**
the magnetic moments are randomly oriented due to thermal fluctuations

**T>T_C**

**Ferromagnet**
unlike the moments in a paramagnet, these moments will remain parallel even when a magnetic field is not applied

**T<T_C**

**Antiferromagnet**
Adjacent magnetic moments from the magnetic ions align antiparallel to each other without an applied field.

Spin resolved inverse photoemission spectroscopy for 3d bands as a function of temperature for Ni(110)

T=T_C -> spin transition from minority and majority states are equal -> \(\Delta=0\)

[Stö06]
Spin resolved inverse photoemission

- Monochromatic low-energy spin polarized electron beam is incident on a single crystal surface.
- Upon entering the crystal the electron momentum in vacuum $k'$ and inside the crystal $k$ need to match.
- The incident electron (with $E > E_V$) occupies excited states and then decays in lower unoccupied bands with the emission of a photon (dipolar transition conserves momentum $k$ and spin $s$)

[Stö06]

Energy conservation (assuming free electron like electrons)

$$\Phi = E_V - E_F \rightarrow \text{work function}$$

Momentum conservation (assuming free electron like electrons)

$$p_e = (2mE)^{1/2} \rightarrow \sim 4 \times 10^{-25} \text{ for } 1 \text{ eV electron}$$

$$p_{hv} = E/c \rightarrow \sim 3 \times 10^{-28} \text{ for } 1 \text{ eV photon}$$

$$\frac{\hbar^2 k'^2}{2m} = E_V + \frac{\hbar^2 k'_{\perp}^2}{2m}$$

$$\bar{k}_{\parallel} = \bar{k}'_{\parallel} + \bar{G}$$

$$k_{\perp} = \sqrt{(k'_{\perp})^2 + \frac{2mE_V}{\hbar^2}}$$

First Brillouin zone $G = 0$
Angle resolved photoemission spectroscopy (ARPES)

Surface states in metals: free like electrons

Energy Conservation

\[ E_{kin} = h\nu - \phi - |E_B| \]

Momentum Conservation

\[ p_\parallel = \hbar k_\parallel = \sqrt{2mE_{kin}} \cdot \sin \vartheta \]

\[ k = \sqrt{k_{\parallel}^2 + k_\perp^2} = \frac{\sqrt{2mE}}{\hbar} \]
Electrons that are photoemitted from a sample by ultraviolet radiation are energy and angle selected by an electrostatic analyzer and detected in two orthogonal Mott polarimeters.

In an electrostatic beam deflection system the spin direction is conserved and polarimeter I measures the polarization components $P_y$ and $P_z$, while polarimeter II measures $P_x$ and $P_z$.

The beam is switched between the two in order to allow quasi-simultaneous data collection. In the figure, the polarimeter system is shown rotated by 90° for graphical clarity, i.e. in reality the z axis is directed straight to the left and parallel to the electron lens of the spectrometer.
Mott spin detector

Electron scattering from a thin film of atoms with large Z (typically Au). In the rest system of the electron the atomic core is moving and then generating an inhomogeneous magnetic field. A force $F = m \ \text{grad}(H)$ deflects the electron depending on the electron spin.

Exchange-scattering spin detector

The unoccupied bands above the vacuum level are the relevant bands for the incident polarized electrons. Asymmetry peak at 10 eV where the majority spins have available states at the upper edge of the gap. Majority spins are less reflected compared to the minority ones.

Reflection spin asymmetry $A$ from the surface of a Fe(100) crystal.

$$A = \frac{I^{\uparrow\downarrow} - I^{\uparrow\uparrow}}{I^{\uparrow\downarrow} + I^{\uparrow\uparrow}}$$


[Stö06]
Bias exchange

a) In an external field and above the Néel temperature $T_N$, antiferromagnetic spins located at the interface with the ferromagnet are aligned, like the ferromagnet, with the external field.

b) Once cooled below $T_N$, these interface spins keep their orientation and appear "pinned" because they are tightly locked to the spin lattice in the bulk of the antiferromagnet, which is not sensitive to external fields. Consequently these pinned spins produce a constant magnetic field at the interface that causes the hysteresis loop of the ferromagnet to shift.

c) This intuitive picture overestimates the magnitude of the loop shift by orders of magnitude.

$$\frac{H_b}{H_c} \approx \frac{W}{\xi} \approx 2 \text{ eV} / 50 \text{ meV} \approx 30$$

When $T < T_N$ you need several tens of tesla to reverse the AFM coupled spins ("pinning")

only a small fraction (5%) of interfacial spins is actually pinned, and these cause the horizontal hysteresis loop shifts.

\[ H_B = \frac{\sigma}{M_{FM} t_{FM}} = J \frac{S_{AFM} S_{FM}}{a_{AFM}^2 M_{FM} t_{FM}} \]

**TABLE I.** Effective and corrected interface energies \( \sigma \) calculated from the macroscopic loop shift and the coverage with pinned spins \( \rho \).

<table>
<thead>
<tr>
<th>Sample</th>
<th>( \rho ) (ML)</th>
<th>( \sigma_{\text{eff}} ) (mJ/m(^2))</th>
<th>( \sigma ) (mJ/m(^2))</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>3 nm Co/NiO</td>
<td>0.04 ± 0.01</td>
<td>0.052 ± 0.005</td>
</tr>
<tr>
<td>B</td>
<td>2 nm Co/IrMn</td>
<td>0.04 ± 0.01</td>
<td>0.168 ± 0.020</td>
</tr>
<tr>
<td>C</td>
<td>1 nm CoFe/PtMn</td>
<td>0.03 ± 0.01</td>
<td>0.124 ± 0.014</td>
</tr>
<tr>
<td>D</td>
<td>2 nm CoFe/PtMn</td>
<td>0.04 ± 0.01</td>
<td>0.188 ± 0.015</td>
</tr>
<tr>
<td>E</td>
<td>3 nm CoFe/PtMn</td>
<td>0.04 ± 0.01</td>
<td>0.229 ± 0.027</td>
</tr>
</tbody>
</table>
AFM order at the atomic scale

1 monolayer Mn/W(110):
Ground state

SP-STM

Sensibility limited to the sample surface

Photoemission Electron microscopy (PEEM) utilizes electron emission to generate image contrast. The excitation is produced by synchrotron radiation or X-ray sources. PEEM collects the emitted secondary electrons generated in the electron cascade that follows the creation of the primary core hole in the absorption process. PEEM is a surface sensitive technique because the emitted electrons originate from a very shallow layer.
GMR: giant magneto resistance

\[ \Delta R / R = \frac{R_{\uparrow\downarrow} - R_{\uparrow\uparrow}}{R_{\uparrow\uparrow}} \]
GMR: giant magneto resistance

Electric current

Pinned layer

Free layer

AFM ←
Pinned FM ←
Free FM ←

J. Appl. Phys. 69, 4774 (1991)
The atom spins are coupled together

In non magnetic materials \( J = 0 \)

Domain wall between two pinned ferromagnetic materials with opposite orientation of the magnetization

Without the spacer two (negative) scenarios depending on the strength of the exchange force in respect to the pinning force:

a) The free layer magnetization always aligns parallel to the magnetization of the pinned layer

b) A domain wall forms which produces the spin current depolarization

\[
H_{\text{exc}} = -\sum_{i \neq j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j
\]

J. Appl. Phys. 69, 4774 (1991)
Magnetic random access memory (MRAM)

Ferromagnetic (FM) - nonmagnetic (NM) - ferromagnetic (FM) junction

Science 282, 1660 (1998); Nat. mater. 6, 813 (2007)
Reading-writing head in HDD

Reading:
the bit stray field defines the magnetization direction of the free layer

Giant Magnetoresistance (GMR)

Current Perpendicular to Plane (CPP)

Current In Plane (CIP)
Magnetic order in 1D: atomic chains

Finite system ($N$ localized moments):

- **Ground state:** $E = E_0 = -J(N-1)$
  - $M_{\text{tot}} \neq 0$

- **Lowest excited state:** $E = E_0 + 2J$
  - $M_{\text{tot}} = 0$
  ( $N$-1 states)

Change in free energy: $\Delta F = \Delta(U-TS) = 2J - kT \ln(N-1)$

If $\Delta F < 0$ the excited state is more favourable than the ground state $\Rightarrow$
no ferromagnetism for $N-1 > \exp(2J/kT)$ or $T_C = 2J/(k \ln(N-1))$

Infinite chain $\Rightarrow T_C = 0$ i.e. no magnetism $(M_{\text{tot}} = 0)$ at any temperature $\neq 0$
Magnetic order in 2D

NxN localized Ising moments

exact solution (due to Onsager) : long-range magnetic order prevails for

\[ kT < \frac{2J}{\ln(1 + \sqrt{2})} \]

A 2D Ising system is less sensitive to thermal fluctuations with respect to the 1D case.

A finite Curie temperature exists, given by

\[ T_c = \frac{2J}{k \ln(1 + \sqrt{2})} \]

[Bel89]


Heisenberg model → no FM state in 1D and 2D at \( T > 0 \)

\[ H_{\text{heisen}} = -\frac{1}{2} \sum_{i,j} J_{ij} s_i \cdot s_j - \mu \sum_i s_i \cdot H \]

Ising model → no FM state in 1D at \( T > 0 \)

\[ H_{\text{ising}} = -\frac{1}{2} J \sum_{i,j} s_i^z s_j^z - \mu H \sum_i s_i^z \]

Ising, Z. Phys. 1925; Bander & Mills, PRB 1989

In general

(Infinite systems)
The 1D case: exchange+MAE

Inter-atomic exchange energy for Co -> $2J \approx 15\text{-}20$ meV

Finite chain

$T_C = \frac{2J}{k \ln(N-1)}$ -> ferromagnetism only for $N < 50$ atoms at $T = 50$ K

Ising model + anisotropy -> FM state in 1D at $T > 0$ in an infinite system

$$H_{\text{ising}} = -\frac{1}{2} J \sum_{i,j} s_i^z s_j^z - \mu H \sum_i s_i^z - \frac{1}{2} K \sum_i (s_i^{\text{easy}})^2$$

Spin blocks oriented along the easy axis by the external field needs to overcome the MAE barrier to reverse the orientation

The MAE stabilizes the direction of the spin blocks -> $M_{\text{tot}} \neq 0$ when the external field is put back to 0
Atomic chains: growth

Ni/Pt(997) 1 x 2 alloy
$T = 200$ K

Atomic chains: Ag/Pt(997)

\[ T = 340 \text{ K}, \quad \Theta_{\text{Ag}} = 0.04 \text{ ML} \]

\[ \Theta_{\text{Ag}} = 0.13 \text{ ML} \]

Preferential nucleation at the lower step edges: 1D Ag islands

Coalescence of 1D islands: continuous atomic chains

Mono-atomic chains: Co/Pt(997)

deposition template: stepped platinum surface
detail of the Pt steps
array of parallel cobalt monatomic chains

diffusion of Co atoms at the step edges results in self-assembled monatomic chains

From STM  \( N = 60-90 \) atoms/chain

\[
T_C = \frac{2J}{(k \ln(N-1))} = 50 \text{ K?}
\]
\( (N=80) \)

\[
E(\theta, \theta_0, \varphi) = -\mathbf{\mu} \cdot \mathbf{B} - K \cos^2(\text{easy} \cdot \mathbf{\mu})
\]
\[
|\mathbf{\mu}| = m_L + m_S
\]

\[
M_z = n\mu \langle \cos \theta \rangle = M_{\text{sat}} \frac{\int \int \cos \theta \exp \left[-E(\theta, \theta_0, \varphi)/kT\right] \, d\theta d\varphi}{\int \int \exp \left[-E(\theta, \theta_0, \varphi)/kT\right] \, d\theta d\varphi}
\]

\( m_s = 2.07 \ \mu_B \)
LDA calculations (S. Blügel, FZ Jülich)

\( m_L = 0.68 +/- 0.05 \ \mu_B \)
XMCD measurements

From 1D atomic chains to a 2D layer: theoretical prediction

Magnetic Anisotropy of One-Dimensional Nanostructures of Transition Metals

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« One-dimensional finite and infinite chains show Magnetic Anisotropy Energies which are an order of magnitude larger than in two-dimensional thin films. … The Magnetic Anisotropy Energy of multichains oscillates as a function of chain width and depends strongly on the transversal structure »

From 1D atomic chains to a 2D layer: easy axis

$\Phi$ $\Theta$

$0^\circ$ $90^\circ$

$-90^\circ$ $0^\circ$ $90^\circ$

$+43^\circ$ $-60^\circ$ $-60^\circ$ $-6^\circ$

Remanent Magnetization (a. u.)

$\Phi$ (deg) $\Theta$ (deg)

From 1D atomic chains to a 2D layer: MAE

$K = 2.1 \text{ meV/atom}$  $m_L = 0.68 \mu_B$

$K = 0.34 \text{ meV/atom}$  $m_L = 0.37 \mu_B$

$K = 0.47 \text{ meV/atom}$  $m_L = 0.33 \mu_B$

$K = 0.13 \text{ meV/atom}$  $m_L = 0.31 \mu_B$

From 1D atomic chains to a 2D layer: orbital moment

Orbital moment decreases with increasing chain thickness
Dipolar magnetic field produced by an array of uniformly magnetized chains of length $N$ and width $w$

Dipolar magnetic energy:

$$E_{dip} = mB_{dip} \ll K$$

with $m = 3.8 \mu_B$  \[ E_{dip} = 0.2 \text{ meV/(Tesla atom)} \]

For $w = 3$  \[ B_{dip} < 0.015 \text{ meV/atom} \]

$K = 0.4 \text{ meV/atom}$

Dipolar interaction

Long range interaction between magnetic moments

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

\( m_1 \) and \( m_2 \) can be the magnetic moments of two atoms in a particle or the moments of two particles.

In out-of-plane configuration the dipolar interaction is reduced.
The magnetic configurations are determined by the competition, at a local scale, of four different energies: **Zeeman**, **exchange**, **magnetocrystalline anisotropy**, and **dipolar coupling**.

$$E = -\mu_0 \mu \sum_i m_i - J \sum_{\langle i,j \rangle} m_i \cdot m_j - \sum_i k_i (m_i \cdot e_i)^2 - \frac{\mu_0 \mu^2}{8\pi} \sum_{i,j \neq i} \left[ \frac{3(m_i \cdot r_{ij})(m_j \cdot r_{ij})}{r_{ij}^5} - \frac{m_i m_j}{r_{ij}^3} \right],$$

- exchange, magnetocrystalline energy -> short range
- dipolar energy -> long range

Structure of a domain wall between two ferromagnetic domains with opposite orientation of the local magnetization (180° wall)

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

Magnetic phase diagram for ultrathin films with perpendicular anisotropy ($l_{ex} = 2\text{nm}$)

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

Magnetic domain pattern of perpendicularly magnetized ultra-thin Fe particles grown on Cu(0 0 1)

Magnetic domain pattern of in-plane magnetized ultra-thin Fe particles grown on W(0 0 1)


Demagnetizing field: shape anisotropy

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

\[ \mathbf{H}_{dem} = -D \mathbf{M} \]

Pushes the magnetization \( \mathbf{M} \) along the longer side of the nanostructure:
- Cylinder -> \( \mathbf{M} \parallel \text{axis} \)
- Disk -> \( \mathbf{M} \parallel \text{disk surface} \)

\[
\begin{align*}
D &= \begin{bmatrix}
\frac{1}{3} & 0 & 0 \\
0 & \frac{1}{3} & 0 \\
0 & 0 & \frac{1}{3}
\end{bmatrix} \\
\infty-\text{Cylinder}: & \quad D &= \begin{bmatrix}
\frac{1}{2} & 0 & 0 \\
0 & \frac{1}{2} & 0 \\
0 & 0 & 0
\end{bmatrix} \\
\infty-\text{Plane (thin film)}: & \quad D &= \begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 1
\end{bmatrix}
\end{align*}
\]

Co/Pt(111)

Orientation and shape of Co magnetic domains

X-ray photoemission electron microscopy, SIM beamline @ Swiss Light Source