MAGNETISM : INTRODUCTION

Magnetism of atoms

- basic concepts
- moment in a field

Magnetism within matter

- exchange
- in a system of local moments
- itinerant electron systems
- spin waves
- magnetocrystalline anisotropy

Dipolar interactions

- domain and walls
- coercivity

Magnetic moment

An electrical current, I, is the source of a magnetic field B



Magnetic field generated by a single-turn coil



m is by definition the magnetic moment of the coil

Magnetism of matter Angular momentum vs magnetic moment

An electrical current is made of electrons in motion The motion of electrons within matter is the source of

magnetism of matter

angular momentum $\mathcal{L} = r \times p$ $\mathcal{L} = mr^2 \omega = I\omega$ Number of turns per second $\mu = iS$ $i = e \omega / 2\pi \implies \mu = -\frac{e}{2m} \mathcal{L}$ $\frac{e}{2m} = \text{gyromagnetic factor}$

Orbital magnetic moment $\vec{\mu}_{\ell} = -g_{\ell} \frac{e}{2m} \vec{L}$ with $g_{\rm l} = 1$

Magnetism in quantum mechanics

 $\vec{L}_{op} = -i\hbar \ \vec{r} \times \nabla$ Angular momentum operator

Electronic orbitals are eigenstates of L_{Zop} and L_{an}^2

$$\begin{split} L^2_{op} \Psi_{n\ell m_{\ell}} &= \hbar^2 \ \ell(\ell+1) \ \Psi_{n\ell m_{\ell}} \\ L_{z_{op}} \Psi_{n\ell m_{\ell}} &= \hbar \ m_{\ell} \ \Psi_{n\ell m_{\ell}} \end{split}$$
 /= orbital angular momentum quantum number m_{ℓ} = magnetic quantum number

The wavefunction $\Psi_{n\ell m}$, is characterized by 3 quantum numbers :

$$n, \ell, m_\ell$$

 $n:$ electronic shell
 $0 < / < n-1$
 $-/ < m_l < +/$

symbol	spdfgh					
l	012345					

quantum number

Spin versus orbital moments

S, spin angular momentum of pure quantum origin

$$S^2 \Psi_s = \hbar^2 s (s+1) \Psi_s$$
$$S_{z_{ov}} \Psi = \hbar m_s \Psi_s$$



Classical picture for *S*: rotation of the electron about itself

 $s = 1/2, m_s = +1/2, -1/2$

Conclusion : 2 contributions to the magnetic moment :

Spin :
$$\vec{\mu}_s = -g_s \frac{e}{2m} \vec{S}$$
 $g_s = 2$ cannot be explained
within classical mechanicsOrbital : $\vec{\mu}_\ell = -g_\ell \frac{e}{2m} \vec{L}$ $g_\ell = 1$

Atomic magnetic moments

Distribution of electrons on orbitals which minimizes energy : leads to orbital and spin atomic moments

Hund's rules :

1) $S = \sum m_s$, maximum, in agreement with Pauli principle 2) $L = \sum m_\ell$, maximum, in agreement with 1) 3) J = |L + S| or J = |L - S| (Spin-orbit)

Physical meaning of Hund's rules :



Spin-orbit coupling



 $\vec{J}_{op} = \vec{L}_{op} + \vec{S}_{op}$ J_{op} total angular momentum operator

Atom states defined by 4 quantum numbers : *L*, *S*, *J* and *M_J* $J = /L+S / or /L-S / -J < M_J < +J$

An example : Dy³⁺

m_{1}	1/2	1/2	1/2	1/2	1/2	1/2	1/2	-1/2	-1/2	-1/2	-1/2	-1/2	-1/2	-1/2
m_1	3	2	1	0	-1	-2	-3	3	2	1	0	-1	-2	-3

Dy³⁺ : 9 electrons L = 5, S = 5/2, J = 15/2, M_J (-15/2 < M_J < 15/2)

the ground state is 16-fold degenerated

Total magnetic moment :

$$\mu_{J} = -g_{J}\mu_{B}J$$

$$\mu_{J} = g\mu_{B}\{J(J+1)\}^{1/2}$$
where $g = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$



Figure 2.2 Vector atom model.

magnetism is a property of unfilled electronic shells

Magnetic moments in a field : Precession





 $d\mathbf{\pounds} / dt = \mathbf{\Gamma} = \mathbf{m} \times \mathbf{B}_0$ $\omega_0 = |\gamma \mathbf{B}_0|$

Frequency of Larmor precession

The magnetic moment precesses about the field, it does not align along it



High temperature susceptibility Curie law



Magnetic moments in a field : Quantum system





79 out of the 103 first elements are magnetic in their ground state A few of them only are magnetic in the solid state



Magnetic ordering Evidence for interactions between moments



Ferromagnetic



Antiferromagnetic





Exchange interactions

of electrostatic nature

Pauli principle :

2 electrons cannot be in the same quantum state

Many-electron wavefunctions are antisymmetric with respect to the exchange of 2 electrons



Superexchange



Most often antiferromagnetic Explains the magnetism of transition metal oxides

J. B. Goodenough, Metallic Oxides, Pergamon Press Ltd., (1971) Magnetism and the Chemical Bond, Interscience and Wiley, New York (1963)

Magnetic structure of MnO, NiO, CoO





M. Imada, A. Fujimori and Y. Tokura, Rev. Mod. Phys., 70 (1998) 1040

Crystal field splitting

Double exchange

La1-xCaxMnO3 : Metallic Ferromagnetic Mn3+ $- O - Mn4+ \Leftrightarrow Mn4+ - O - Mn3+$





Double-exchange $(E_F < E_{AF})$

Exchange interactions in rare-earth metals



Magnetic 4f electrons localised 5d, 6s itinerant 4f moments coupled via

indirect RKKY interactions

B. Coqblin, The Electronic Structure of Rare-Earth Metals and Alloys : the Magnetic Heavy Rare Earths, Academic Press, London (1977)

RKKY interactions



Magnetic structures of rare-earth metals



Diversity of structures Characteristic of RKKY interactions

Localised versus itinerant electrons 3d metals : itinerant character of 3d electrons



E.P. Wohlfarth, Iron, Cobalt and Nickel, in Ferromagnetic Materials, vol.1, E.P. Wohlfarth ed., North Holland, Amsterdam, (1988)

Pauli susceptibility





Em=Unnny $\Delta E_{M} = \widetilde{U} \left[\frac{N}{2} + n \left(\varepsilon_{F} \right) \delta \varepsilon \right] \left[\frac{N}{2} - n \left(\varepsilon_{F} \right) \delta \varepsilon \right] - \widetilde{U} \left[\frac{N}{2} \right]^{2}$ $= -\tilde{U} n(E_{F}) \delta \tilde{E}$ $\Delta E_{c} = n (E_{F}) \delta E^{2}$ $\Delta E_T = u(E_F) \delta E^2 (I - Un(E_F))$ $\Delta E_z = -2 \mu_B n(E_F) B$ Surrephibility: $m = N_B(N_P - N_J) = \frac{2N_B^2 n(E_F)}{B}$ 1-Un(Er) X= 2NB NON (EF) 1-UN(Er)

Exchange mechanism in 3d metals



Itinerant nature of 3d electrons + on-site electrostatic interactions (Hund's rules)

J. Friedel, Nuovo Cim. Suppl. 7 (1958) 287

Stoner criterion

Exchange integral U

$$\chi = \frac{2 N_B N_O n (E_F)}{1 - U n (E_F)}$$

DOS at
$$E_F$$
, $N(E_F)$

Magnetism becomes stable ^{Product}



Magnetism stable only for 3d series elements

R-M alloys



Induced 5d moment antiparallel to 3d Large R-M interactions

J.J.M. Franse and R.J. Radwanski, Magnetic Properties of Binary Rare-Earth 3d-Transition-Metal Intermetallic Compounds, in Handbook of Magnetic Materials, vol. 7, K.H.J. Buschow ed., Elsevier, Amsterdam (1995) D. Courtois and D. Givord,

J. Magn. Magn. Mater., (1999)

Thermal variation of the spontaneous magnetization





k=0

k=π/a

Allows entropy gain without loosing too much in exchange enrgy

Wave and quasi-particle which well defined spectrum of possible energies

 $E(k) = \hbar \omega_k = 2S(J(0) - J(k))$

$$J(k) = J \sum_{i} e^{-ik(r_i - r_j)}$$

Ground state S=1/2

Spin wave : linear combination of states such as



Number of excited spin-waves :

$$\sum_{k} < n_{k} > = \sum_{k} \frac{1}{e^{\frac{\hbar\omega_{k}}{k_{B}T}} - 1} = \frac{V}{8\pi^{3}} 4\pi \int_{0}^{\infty} \frac{k^{2}dk}{e^{\frac{ck^{2}}{k_{B}T}} - 1} \qquad \hbar\omega_{k} = ck^{2} \quad \text{For } k \sim 0$$

1D or 2D : divergence No magnetic order in 1 or 2 dimensions

However, anisotropy must be considered



favours well-defined crystallographic directions of the moments

determined by λ LS + CEF + exchange



Mechanisms of anisotropy





Anisotropy energy

Magnetostriction



Demagnetizing field energy

 $\mathsf{B} = \mu_0(\mathsf{M} + \mathsf{H})$



$$E_{\text{dem}} = -\frac{1}{2} \int_{V} \mathbf{M}(\mathbf{r}) \cdot \mathbf{H}_{\text{dem}}(\mathbf{r}) \cdot dV$$



Domain formation



Fe-Si

Nd-FeB

Domain walls



Wall energy and width



Magnetization processes Domain wall motion

Under B

Energy terms involved :

Demagnetising field energy Zeeman energy

Exchange and Anisotropy Not involved

$$E = -\mu_0 MH + \frac{1}{2} N M^2$$

 $M = (1/N)$



Growth of domains under field









Coercivity

Main magnetic functional properties of ferromagnets



Coercivity



Coercive field for coherent rotation (Stoner-Wohlfarth)

 $E = K_1 \sin^2\theta + \mu_0 M_s H \cos\theta$ M $\partial E / \partial \theta = K_1 \sin 2\theta - \mu_0 M_s H \sin \theta$ = sin θ (2 K₁ cos θ – μ_0 M_s H) $\theta_{\rm B}$ final E_{\min} : $\sin\theta = 0$, $\theta = 0$ or π θ_{B1} θ_{B2} θ_{B0} E_{max} : $\cos\theta = \mu_0 M_s H / 2K_1$ $H_0 = H_A$ E/K' Coercive field : 0 $H_0 = 0$ E_{min} and E_{max} join together : $\mu_0 H_c = 2K_1 / \mu_0 M_s = H_A$ 30 60 90 0 120 150 180 θ , degrés

E.C. Stoner and E.P. Wohlfarth, Phil. Trans. Roy. Soc. London 240A (1948) 599

Micromagnetism

↑Ζ

$$\Phi = \int \{A_{\text{ex}}(\nabla \theta(\mathbf{r}))^2 + K_1 \sin^2 \theta(\mathbf{r}) - \frac{1}{2} \mu_0 \mathbf{H}_{\text{s}}(\mathbf{r}) \cdot \mathbf{M}_{\text{s}}(\mathbf{r}) - \mu_0 \mathbf{H}_{\text{ext}} \cdot \mathbf{M}_{\text{s}}(\mathbf{r})\} d^3 r$$

For any z (1D expression) :

$$E = A_{ex} (d\theta/dz)^{2} + K_{1} \sin^{2}\theta + \mu_{0} M_{s} H \cos\theta$$

$$2A_{ex} d^{2}\theta/dz^{2} + K_{1} \sin 2\theta - \mu_{0} M_{s} H \sin\theta = 0$$

$$\int_{exch} \int_{K} \int_{K} \int_{Z} \int_{K} \int_$$

Are there non-uniform processes which would cost less than coherent rotation ?

Dipolar interactions not equivalent to magnetocrystalline anisotropy

Anisotropy due to dipolar interactions Curling



Non uniform configuration allows dipolar energy gain at the expense of exchange

Magnetocrystalline anisotropy : Brown paradox



 $2A_{\rm ex}d^2\theta/dz^2 + K_1\sin 2\theta - \mu_0 M_sH\sin\theta = 0$

 E_{\min} : $\theta = 0$, $d\theta/dz = 0$

$$E_{\max}: \cos\theta = 1 - \frac{2A_{exch}}{\mu_0 M_s H_A} \frac{1}{\sin\phi} \, \partial^2\theta / \partial z^2 \,)$$

Reversal should occur by coherent rotation with $H_c = H_A$



Coercivity analysis : influence of defects on reversal

Schematic representation of magnetization reversal



Domain wall Activation volume

Coercive field due to pinning

Heterogeneity on K No discontinuity assumed on A

 $E(z) = \gamma(z) - 2\mu_0 MHz$

to 1st order, γ does not depend on H

 $\partial E/\partial z = \partial \gamma/\partial z - 2 \mu_0 M H$

 $\mu_0 H_c = (\delta/2M) \ \partial K/\partial z$

When $\partial K/\partial z$ is not constant, H_c is determined by $(\partial K/\partial z)_{max}$

Soft materials : homogeneous at the scale of walls Hard materials : heterogeneous at this scale