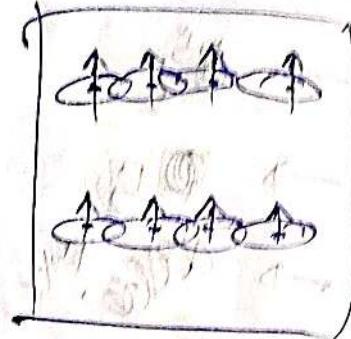
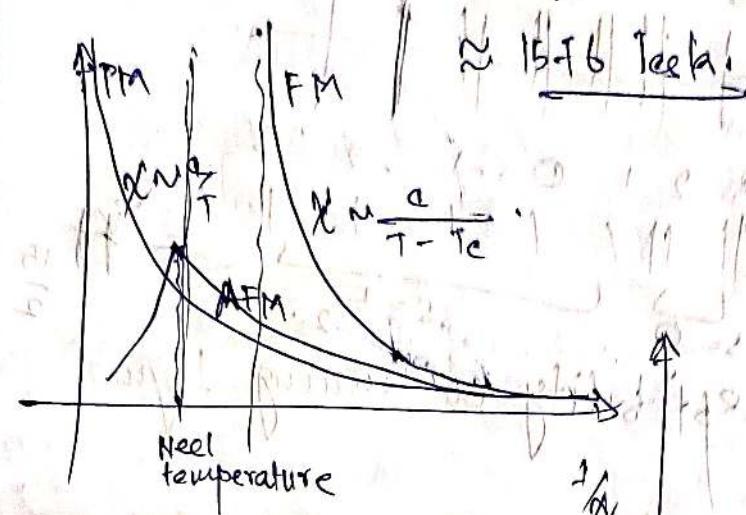


FERROMAGNETISM

$$\cancel{B_{\text{mag}}} \rightarrow B_{\text{mag}} = \delta M_s \rightarrow \frac{3k_B T_c}{J \mu_B} (\text{J.I})$$



$$\text{PM: } \chi_N \propto T \rightarrow 0$$

$$\text{FM: } \chi_N \propto T - T_c$$

$$\text{AFM: } \chi_N \propto T \rightarrow T_N$$

$$\frac{M}{M_S} = B_f(x) \approx B_f \left(\frac{g \mu_B S}{k_B T} M \right)$$

$$\frac{g \mu_B S}{k_B} = \frac{3T_c}{(J+1)M_S} = B_f \left(\frac{3J}{J+1} \frac{M}{M_S} \frac{T_c}{T} \right)$$

when $T \rightarrow T_c$, $M \rightarrow M_S$

critical exponents

$$M \propto (T_c - T)^{\beta}$$

$$\chi \propto (T - T_c)^{-\gamma}$$

$$C \propto (T - T_c)^{-\delta}$$

$$M \propto H^{\delta}$$

2nd Order phase transition.
why?

$$\chi = \frac{\partial M}{\partial H}$$

$$J \alpha (T_c - T)^{\gamma}$$

$$\frac{\partial M}{\partial H} \propto (T_c - T)^{\gamma/2}$$

$$(T_c - T)^{\gamma/2}$$

$$\delta = 1 + \frac{\gamma}{\beta}$$

→ Peltier free energy

Class of phase transitions
2nd order

$$M = \frac{\partial \chi}{\partial H}$$

$$\chi = \frac{\partial^2 M}{\partial H^2}$$

→ magnetic induction

	M	mean field
μ	$1/2$	Heisenberg.
γ	1	
δ	2	
α	0	
ν	$1/2$	

when $T \rightarrow 0$,

$$\frac{M}{M_s} = 1 - \left(\frac{1}{3}\right)^{\frac{-3}{J+1}} \frac{T_c}{T} \cdot \frac{M}{M_s}$$

magnetization
will (zero)
keep?

without external
source? field.

Nature of Weiss Molecular
field (internal) [WMF],

internal molecular field.

1907 → Weiss proposal,

In order to describe the
ferromagnetism, we have assumed
that spontaneity occurs due
to internal molecular forces.

1930 → Heisenberg

For dipolar interactions : energy of two magnetic dipoles.

$$U = \frac{\mu_0}{4\pi r^2} \left[\vec{\mu}_1 \cdot \vec{\mu}_2 - 3 (\vec{\mu}_1 \cdot \hat{r}) (\vec{\mu}_2 \cdot \hat{r}) \right]$$

+ dipole moment

depends on separation distances & degree of mutual alignment.

PM: Noninteracting dipole

FM: interacting dipole.

For each 1 Bohr magneton separated by 1 Å.

$$\sim \frac{\mu_0^2}{4\pi r^2} M^2 \sim 10^{-28} J$$

$$M \sim 10^{-19} A \cdot m^2 \quad 10^{-4} J = 10^{-4} \text{ eV.}$$

$$10^{-4} \text{ eV} \sim 1 \text{ K.}$$

pure magnetic dipole interaction in metals cannot justify WMF.

1. EM energy Δ
(static) $\propto \epsilon_0$, shells $\sim 0.1 - 1 \text{ eV.}$

2. Magnetic dipole energy $\sim 10^{-4} \text{ eV.}$

3. Typical transition of FM materials $\sim 10^3 - 1 \text{ eV.}$

Is it dipole-dipole?

Is it spin-orbit? No.

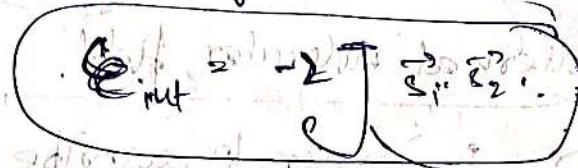
Heisenberg exchange interaction.

$$H = H_{\text{ext}} + H_{\text{ex}}$$

Ng (P) J BG) Heisenberg exchange

- Heisenberg showed that the large $W_M F$ was experienced in terms of exchange interaction b/w electrons.

Heisenberg stated/knows that the energy of interaction of atoms i & j having spin σ_i & σ_j .



$$J$$

exchange integral

related to overlap

$J = \text{pos. for FM}$ if $\sigma_i \cdot \sigma_j = 1$ if the charge dist.

$J = \text{neg. for AFM}$ if $\sigma_i \cdot \sigma_j = -1$ if atoms i & j,

Exchange interaction are nothing more than electrostatic interaction, arising due to electrons of same signs, i.e. energy when they are close & same energy when they are far apart.

Heisenberg exchange interaction

Quantum mechanical picture of two e^- system forming covalent bonding. Two ~~H-~~ "like" atom A & B whose e^- are described by wave function

$$\Psi_{A(1)}$$

$$\Psi_{B(2)}$$

such that probability of finding $|\Psi_{A(1)}|^2$ & $|\Psi_{B(2)}|^2$ when 2 atoms are brought together & are separated by a distance r_{AB} their wavefunction combine either (a) bonding or antibonding.

consider two electrons having coordinates r_1 & r_2 .
 The "wavefunction" for the combined joint state can be written as a product of single electron states.

They act like fermions:

$$1^{\text{st}} e^- \longrightarrow \Psi_a(r_1) \\ 2^{\text{nd}} e^- \longrightarrow \Psi_b(r_2).$$

Joint func: $\Psi_a(r_1)\Psi_b(r_2)$

$$\text{In case of exchange} \equiv \Psi_a(r_2)\Psi_b(r_1).$$

which is not a multiple of what we started with,

the product $\Psi_a(r_1)\Psi_b(r_2)$. So $\Psi_a(r_2)\Psi_b(r_1)$ does not obey exchange symmetry.

But, e^- are indistinguishable. But it is necessary that

$$|\Psi(r_1, r_2)|^2 dr_1 dr_2 = |\Psi(r_2, r_1)|^2 dr_2 dr_1$$

$\Psi(r_1, r_2) = \pm \Psi(r_2, r_1)$.

symmetry \rightarrow NOT happening,
antisymmetry

$\therefore \Psi_a(r_1)\Psi_b(r_2) \sim \Psi_a(r_2)\Psi_b(r_1)$ has these properties.

& NOT acceptable solution, but linear combination of them $[c_1\Psi_a(r_1)\Psi_b(r_2), c_2\Psi_b(r_1)\Psi_a(r_2)]$ is acceptable.

$$\Psi = \phi(s), g$$

$\Psi_{\text{spatial}} = \frac{1}{\sqrt{2}} [\Psi_{\text{up}} + \Psi_{\text{down}}]$ \rightarrow singlet
 $\Psi_{\text{spin}} = \frac{1}{\sqrt{2}} [\Psi_{\text{up}} - \Psi_{\text{down}}]$ \rightarrow antisym.

$s = \frac{1}{2}, -\frac{1}{2}$ \rightarrow triplet.

Singlet = 0, \rightarrow [symm].

Triplet = 1, 0, 1

spin config:

$$\chi_A = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \chi_B = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

↑

↓

$$\chi_{\text{F}} = \chi_A(1) \chi_B(2) + \chi_A(2) \chi_B(1)$$

$\frac{1}{2}(\uparrow\downarrow - \downarrow\uparrow) \rightarrow$ spin antisymmetric
spatial symmetric

$$\chi_{\text{G}} = \begin{bmatrix} \uparrow\uparrow \\ \downarrow\downarrow \end{bmatrix}$$

$\frac{1}{2}(\uparrow\downarrow + \downarrow\uparrow) \rightarrow$ spin symmetric
spatial antisymmetric

↓↓

energies / energy integrals

electrode coulombic Hamiltonian

$$H = \frac{1}{r_{AB}} - \frac{1}{r_{A1}} - \frac{1}{r_{B1}} + \frac{1}{r_1} + \frac{1}{r_2}$$

$$E_A = \int \psi_A^* H \psi_A d\tau_1 d\tau_2$$

$$E_B = \int \psi_B^* H \psi_B d\tau_1 d\tau_2$$

$$E_F = \int \psi_F^* H \psi_F d\tau_1 d\tau_2$$

The orbital symmetries

spin aligned are correlated. Therefore 2 e⁻ composite system is coupled via their spins. This coupling is proportional to the eigenvalues of $\vec{\sigma}_1 \cdot \vec{\sigma}_2$

$$\psi_S = (\psi_A(1) \psi_B(2) + \psi_A(2) \psi_B(1))$$

$$+ (\psi_A(1) \psi_B(2) + \psi_A(2) \psi_B(1))$$

$$\psi_F = (\psi_A(1) \psi_B(2) - \psi_A(2) \psi_B(1))$$

$$- (\psi_A(1) \psi_B(2) - \psi_A(2) \psi_B(1))$$

The combined spin hamiltonian for spin- $\frac{1}{2}$ system:

$$H = \omega S_1 + S_2$$

where S_1 & S_2 \rightarrow spin- $\frac{1}{2}$ systems [composite, coupled]

$$\vec{S}_{\text{tot}} = \vec{S}_1 + \vec{S}_2$$

$$\vec{S}_{\text{tot}}^2 = \vec{S}_1^2 + \vec{S}_2^2 + 2 \vec{S}_1 \cdot \vec{S}_2.$$

$$= S_1(S_1+1) + S_2(S_2+1) + 2S_1 \cdot S_2.$$

$$S_{\text{tot}}(S_{\text{tot}}+1) = \frac{3}{2} + 2S_1 \cdot S_2.$$

Singlet : $S_{\text{tot}}^2 = 0 \Rightarrow S_1 + S_2 = 0$

$$S_1 \cdot S_2 = -\frac{3}{4}$$

triplet : $S_{\text{tot}}^2 = 1 \Rightarrow S_1 + S_2 = 1$

State

$$(S_1 = m_1, S_2 = m_2)$$

singlet.

$$\frac{1}{2}(1r - 1l)$$

triplet

$$\frac{1}{2}(1l + 1r)$$

III

Quadrized values.

For effective Hamiltonian with interactions

$$\text{Hspin} = \frac{1}{4}(E_S + 3E_I) - (E_S - E_I)\hat{s}_1 \cdot \hat{s}_2$$

= constant term + spin dependent term

\rightarrow singlet.

$$\text{Hspin } \Psi_S = \left\{ \frac{E_S}{4} + \frac{3E_I}{4} - (E_S - E_I)\left(-\frac{3}{4}\right) \right\} \Psi_S$$

$$\text{Hspin } \Psi_T = \cancel{E_S} \Psi_T, \quad \begin{array}{c} +1 \\ 0 \\ -1 \end{array} \quad \begin{array}{c} \text{singlet} \\ \text{triplet} \\ \text{singlet} \end{array}$$

\rightarrow triplet

$$\text{Hspin } \Psi_T = \left\{ \frac{E_I}{4} + \frac{3E_I}{4} - (E_S - E_I)\left(\frac{1}{4}\right) \right\} \Psi_T$$

$$\text{Hspin } \Psi_T = E_I \Psi_T, \quad \boxed{\text{H} = \sum_{i,j} J_{ij} \hat{s}_i \cdot \hat{s}_j} \quad \begin{array}{l} (\text{spin only interaction}) \\ (\text{in absence of ext mag field}) \end{array}$$

$$\text{Hspin} = -2J \hat{s}_1 \cdot \hat{s}_2$$

a) If $J > 0$, $(E_S > E_T)$,

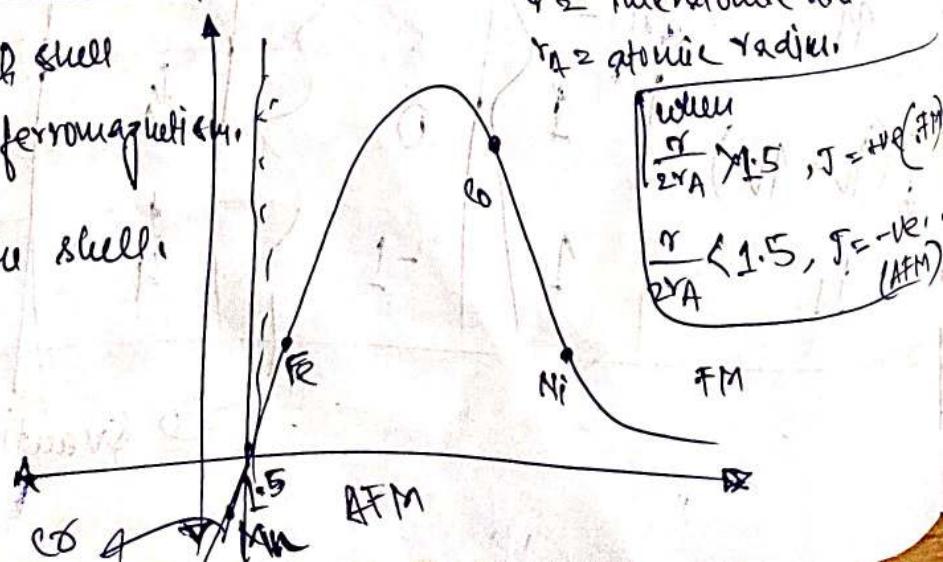
$\boxed{\text{FM}}$ $\hat{s}_1 \cdot \hat{s}_2 = +ve$ & spin triplet is favoured. ($S=1$)

b) If $J < 0$, $\boxed{\text{AFM}}$ $\hat{s}_1 \cdot \hat{s}_2 = -ve$ & spin singlet ($S=0$) is favoured

SLATER'S criterion

Importance of the 3D shell in the origin of ferromagnetism.

& the radius of the shell.



r_2 = interatomic dist
 r_A = atomic radius

$$\text{when } \frac{r}{2r_A} > 1.5, J = +ve \quad (\text{FM})$$

$$\frac{r}{2r_A} < 1.5, J = -ve \quad (\text{AFM})$$

FM

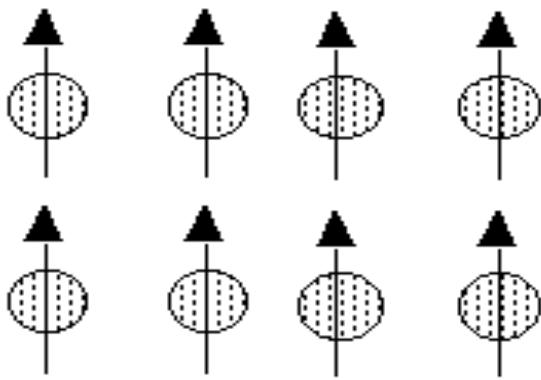
Ferromagnetism $\xrightarrow{\text{only}}$ MAINLY occurs in first row of 3d transition metal. The effects of FM reduces in 4d & 5d shell elements. Almost negligible ferromagnetism, [WEAK].

Relation b/w δ , J_{exch} & T_c .

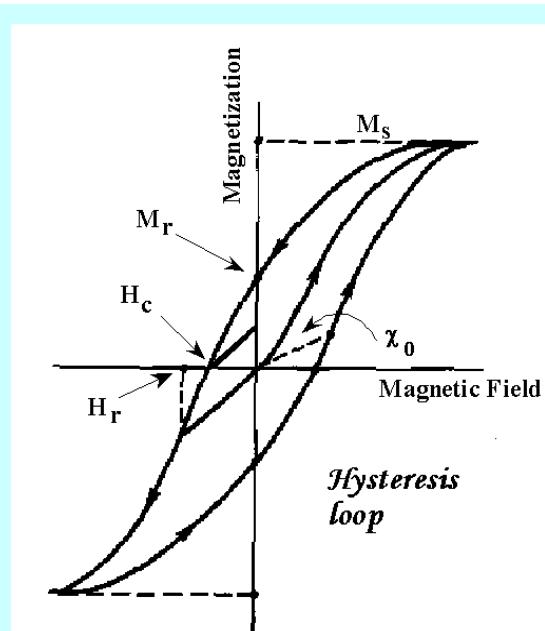
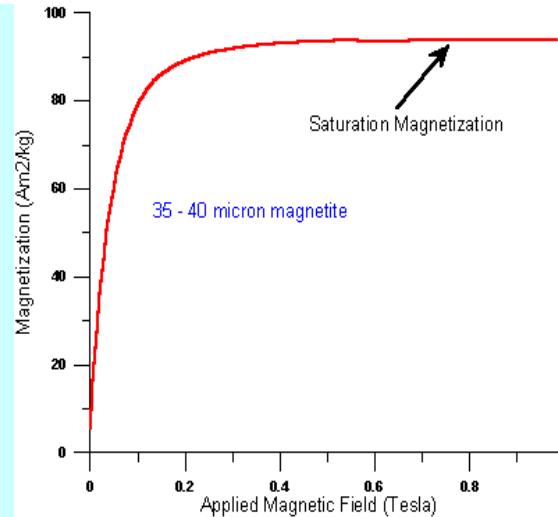
$$14 \boxed{2} 25.$$

ANY ferromagnetic system

parallel alignment



Ferromagnetism

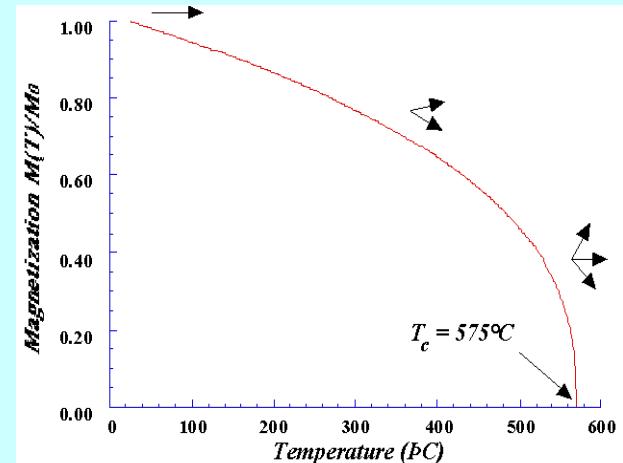


The elements Fe, Ni, and Co and many of their alloys are typical ferromagnetic materials.

Two distinct characteristics of ferromagnetic materials are their

(1) spontaneous magnetization (M_{SP})

(2) the existence of magnetic ordering temperature (T_C)



origin of exchange :

consider two electrons

having coordinates r_1 & r_2

The wave fn. for the A^2AB molecule

Joint state can be written as a product of single electron states, so that

1st electron is in state $\psi_a(r_1)$

2nd r is in state $\psi_b(r_2)$

then the joint wave fn.

Wave function $\rightarrow \psi_a(r_1) \psi_b(r_2)$

In the case of particle interchange (each of spin up does not obey exchange symmetry) we get $\psi_a(r_2) \psi_b(r_1)$ which is not multiplying what we stated with

(Pauli's exclusion principle) The over all wave fn. of electron must be anti symmetric. So the spin be either anti symmetric singlet state χ_s ($S=0$) in the case of symmetric spatial state

or

the spin up symmetric triplet state χ_T ($S=1$) in the case of anti symmetric spatial state.

for Singlet case wave fn.

$$\rightarrow \psi_S = \frac{1}{\sqrt{2}} [\psi_a(r_1) \psi_b(r_2) + \psi_a(r_2) \psi_b(r_1)] \chi_S$$

for triplet case wave fn:

$$\psi_T = \frac{1}{\sqrt{2}} [\underbrace{\psi_a(r_1) \psi_b(r_2)}_{\text{Spatial part (anti)}} - \underbrace{\psi_a(r_2) \psi_b(r_1)}_{\text{Spatial part (sym)}}] \chi_T$$

(1) ψ_S

PIONEER

(2) ψ_T

(3) χ_S

(4) χ_T

(5) ψ_S

(6) ψ_T

The energies of two possible states are

$$E_S = \int \alpha_S^* \hat{H} \psi_S dr_1 dr_2$$

$$E_T = \int \psi_T^* \hat{H} \psi_T dr_1 dr_2$$

assuming the spin part of wavefn.
 ψ_S & ψ_T are normalized.

the difference between two

$$E_S - E_T = 2 \int \alpha_A^*(r_1) \psi_B^*(r_2) \hat{H} \alpha_A(r_1) \alpha_B(r_2)$$

$$\hat{H} = \left[\frac{e^2}{r_1 - r_2} + \frac{e^2}{R_A - R_B} - \frac{e^2}{r_1 - R_A} - \frac{e^2}{r_2 - R_B} \right] dr_1 dr_2$$

~~exchange integral~~

Heitler-London theory of

$$\text{full Hamiltonian}, \hat{H} = \frac{1}{2}(E_S - E_T) = \int \psi_A^* \psi_B^* \hat{H} \psi_A \psi_B dr_1 dr_2$$

To construct spin Hamiltonian for two
electron system (two \rightarrow spin $\frac{1}{2}$ particles)

Coupled by an interaction Hamiltonian

$$\hat{H} = \mu \vec{S}_1 \cdot \vec{S}_2$$

where \vec{S}_1 & \vec{S}_2 are the operators for the spins for the
two particles ($\frac{1}{2}$)

$$\hat{S}_{\text{tot}}^2 = \hat{S}_1^2 + \hat{S}_2^2$$

$$\hat{S}_{\text{tot}}^2 = (\hat{S}_1 + \hat{S}_2)^2 = (\hat{S}_1)^2 + (\hat{S}_2)^2 + 2\hat{S}_1 \cdot \hat{S}_2$$

Eigen values of $(\hat{S}_1)^2$ & $(\hat{S}_2)^2$ are

$$S_1(S_1+1) = \frac{1}{2}(\frac{1}{2}+1) = \frac{3}{4}$$

$$(\hat{S}_{\text{tot}})^2 = S(S+1) = (\hat{S}_1)^2 + (\hat{S}_2)^2 + 2\hat{S}_1 \cdot \hat{S}_2 = \frac{3}{4} + \frac{3}{4} + 2 \cdot \frac{1}{2} \cdot \frac{1}{2}$$

Singlet State

$$S=0$$

Triplet State

$$S=1$$

$$\uparrow \quad \uparrow \quad \uparrow \quad \uparrow$$

$$\hat{S}_1(S_1+1) + \hat{S}_2(S_2+1) + 2 \cdot \frac{1}{2} \cdot \frac{1}{2}$$

State

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$0$$

$$S_2 = m_S$$

$$\hat{S}_1 \cdot \hat{S}_2 = \frac{3}{4}$$

$$\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle)$$

$$1$$

$$0$$

$$\frac{1}{4}$$

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

$$1$$

$$0$$

$$\frac{1}{4}$$

$$|\downarrow\downarrow\rangle$$

$$1$$

$$-1$$

$$\frac{1}{2}$$

$$(\hat{S}_{\text{tot}})^2 = \frac{3}{2} + 2 \cdot \frac{1}{2} \cdot \frac{1}{2} = S(S+1)$$

for $S=0$, Singlet

$$\hat{S}_1 \cdot \hat{S}_2 = -\frac{3}{4}$$

for $S=1$, Triplet

$$\hat{S}_1 \cdot \hat{S}_2 = \frac{1}{2}(2 - \frac{3}{2})$$

$$S^2 = S_1(S_1+1) + S_2(S_2+1) + 2 \cdot \hat{S}_1 \cdot \hat{S}_2 = \frac{1}{4}$$

$$S(S+1) = \frac{3}{4} + \frac{3}{4} + 2 \cdot \frac{1}{2} \cdot \frac{1}{2}$$

$$0 = \frac{3}{2} + 2 \cdot \frac{1}{2} \cdot \frac{1}{2} - \frac{3}{4}$$

$$0 = \frac{3}{2} + \frac{1}{2} - \frac{3}{4}$$

$$2 = \frac{3}{2} + \frac{1}{2} - \frac{3}{4}$$

$$\Downarrow \hat{S}_1 \cdot \hat{S}_2 = \frac{1}{2}(2 - \frac{3}{2}) = \frac{1}{4}$$

So the effective Hamiltonian can
be written as.

$$\hat{H}_{\text{spin}} = \frac{1}{2} (E_S + 3E_T) - (E_S - E_T) \hat{S}_1 \cdot \hat{S}_2$$

E_S = eigen value for the Singlet State.

E_T = " " , the Triplet State.

for $\hat{S}_1 \cdot \hat{S}_2 = -\frac{3}{4}$, Singlet.

$$\hat{H}_{\text{spin}} = \frac{1}{2} E_S + \frac{3}{4} E_T + \frac{3}{4} E_S - \frac{5}{4} E_T$$

$$= E_S + 0 = \underline{\underline{E_S}} \text{ (eigen value)}$$

for $\hat{S}_1 \cdot \hat{S}_2 = \frac{1}{4}$, triplet.

$$\hat{H}_{\text{spin}} = \frac{E_S}{2} + \frac{3}{4} E_T - \frac{E_S}{2} + \frac{E_T}{4}$$

$$\hat{H}_{\text{spin}} = (E_T) \Psi$$

Desired Spin Hamiltonian

$$\hat{H}_{\text{spin}} = \text{constant term} + \text{spin dependent term}$$

can be absorbed in
other constant energy
term.

$$\hat{H}_{\text{spin}} = -2J \hat{S}_1 \cdot \hat{S}_2$$

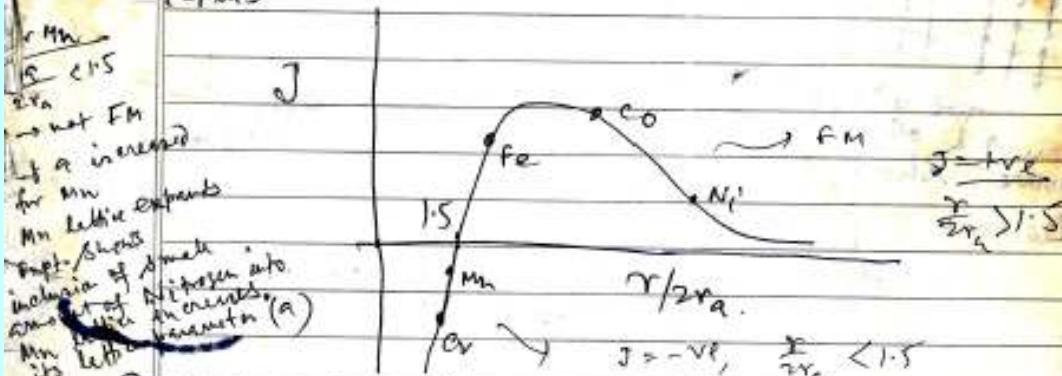
if $J > 0$, $E_S > E_T$, (triplet state $S=1$)
is favoured. ($\beta_1, \beta_2 = +ve$)

If $J < 0$, $E_S < E_T$ & the singlet state $S=0$
is favoured. ($\beta_1, \beta_2 = -ve$)

So total hamiltonian in Heisenberg model for many electron system.

$$H = - \sum_{ij} J_{ij} S_i \cdot S_j$$

J_{ij} = exchange int. between i & j k
spins



Slater's criteria for ferromagnetism.

For FM: r/a int. atomic distance. a lattice constant
of FM.

Mn: $r/a =$ atomic radius, $2r_a$ = diameter of outermost 3d shell

When $\frac{r}{2r_a} > 1.5$, always $J \rightarrow +ve$. { Fe
Co } \rightarrow FM. { Ni }

When $\frac{r}{2r_a} < 1.5$, $J \rightarrow -ve$

For Mn, $\frac{r}{2r_a} < 1.5$, $J \rightarrow -ve$

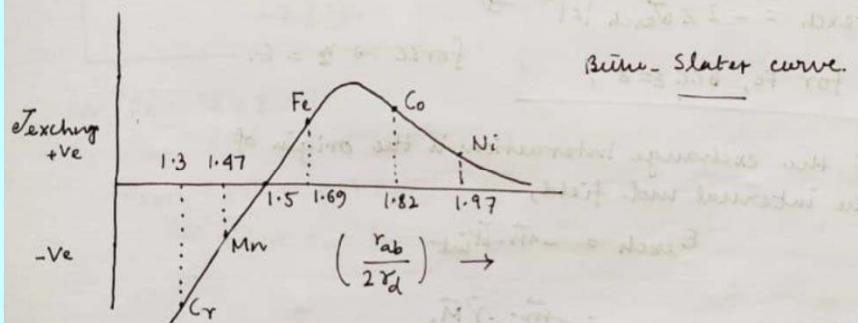
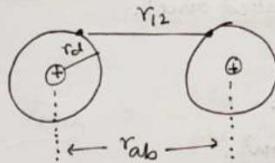
Fe, Co, Ni, Mn, Cr, etc. \rightarrow FM phenomena.

importance of the 3d shell in the origin of FM phenomena.

Exchange Interaction in FM & Bethe-Slater curve

$$H_{\text{in}} = -2 \sum_{i>j} \hat{\mathbf{s}}_i \cdot \hat{\mathbf{s}}_j J_{ij} \quad J_{ij} = +Ve, \text{ FM} \\ = -Ve, \text{ AFM.}$$

Exchange integral for different interatomic spacing of d-orbitals



The importance of the degree of overlap of the d shells, and it shows that as the degree of overlap decreases from a large to a small value δ_{exch} changes from a -ve to a +ve value.

This explains why ferromagnetism does not occur in the 2nd and 3rd row transition metal elements where the ratio of internuclear separation to the radius of the d-orbital is much smaller than from the first row.

Fe Ni Co. 3d
— 4d
— 5d.
2020/6/5 09

$$\begin{aligned}
 E_{\text{exch}} &= -2 \sum J_{ij} \hat{s}_i \cdot \hat{s}_j \\
 &= -2 \sum_{k=1}^n \sum J_k \sum_{(i,j) \neq k} \hat{s}_i \cdot \hat{s}_j \\
 &\quad \text{sum over } k \text{ th neighbours} \\
 &\quad \text{sum over all pairs of} \\
 &\quad \text{--- } k \text{ th neighbour.} \\
 &\quad (\text{provided that each pair is counted once).}
 \end{aligned}$$

J_{xx} decreases rapidly with distance.
 (Nearest neighbour interaction).

$$\boxed{
 \begin{aligned}
 E_{\text{exch}} &= -2 Z J_{\text{exch}} |s|^2 \quad \text{--- ①} \\
 \text{for Fe, BCC, } Z &= 8, \quad \text{force} \rightarrow N = 6.
 \end{aligned}
 }$$

If the exchange interaction is the origin of the internal mag. field,

$$E_{\text{exch}} = -\vec{m} \cdot \vec{H}_{\text{int}}$$

$$= -\vec{m}_i \cdot \vec{\chi} \vec{M}_s$$

$$\begin{aligned}
 |\vec{M}_s| &= N |\vec{m}|, \quad E_{\text{exch}} = -\gamma N |\vec{m}|^2 = -\gamma N g^2 \mu_B^2 s^2 \\
 T &= S, \quad L = 0, \quad m_j = T g \mu_B.
 \end{aligned} \quad \text{--- ②}$$

$$E_{\text{exch}} = -\gamma N g^2 \mu_B^2 |s|^2 = -2 Z J_{\text{exch}} |s|^2$$

Due to $\uparrow\downarrow M_s = \frac{1}{2} N g \mu_B J$ for $M = M_s$
 $J = S$
 $L = 0.$

$$\frac{2}{g \mu_B} \cdot 2JS = 2N g \mu_B S$$

$$J = \frac{2JS}{N g \mu_B}$$

$$\underline{\underline{g_x = g_S = 2}}$$

$$T_c = \frac{NN' \tilde{M_{eff}}}{3k_B}, \quad \tilde{M_{eff}} = g \mu_B \sqrt{J(J+1)}$$

$$= \frac{m^2 g^2 \mu_B^2 J(J+1)}{3k}$$

$$T_c = \frac{2N g^2 \mu_B^2 J(J+1) Z \delta}{3k N g^2 \mu_B^2}$$

$$T_c = J \left[\frac{2ZJ(J+1)}{3k} \right]$$

T_c scales with the strength of the exchange interact.

In general for a FM

$$\hat{H} = \underbrace{-\sum J_{ij} \vec{s}_i \cdot \vec{s}_j}_{\text{exchange energy.}} + g\mu_B \sum \vec{s}_j \cdot \vec{B}$$

zeeman energy.

Heisenberg exchange model -

$$H = -\sum_j J_j \vec{s}_i \cdot \vec{s}_j$$

exchange integral.

$J_{ij} = +ve$ for FM.

$= -ve$ for A.F.M.

Explain
9th Feb:
2:4

The total exchange interaction b/w i-th and its neighbouring spins i.e.,

$$-2 \sum J_{ij} \vec{s}_i \cdot \vec{s}_j$$

$$= -g\mu_B \vec{s}_i \cdot \vec{B}_{mf}$$

$$\boxed{B_{mf} = \frac{2}{g\mu_B} \sum_j J_{ij} s_j}$$

$$B_{mf} = \frac{2}{g\mu_B} \cdot \sum_j J_{ij} s_j$$

$$\boxed{B_{mf} = \frac{2}{g\mu_B} \sum J_i s_i}$$

We assume that the exchange interaction only occurs b/w \approx nearest neighbours with the constant strength J .

Spontaneous magnetization: mean-field theory



Lecture 15: GMR, spin model and mean-field theory, Ising mod...

Heisenberg model with a magnetic field



Watch later

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$$\hat{\mathcal{H}} = - \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + g\mu_B \sum_j \mathbf{S}_j \cdot \mathbf{B}$$

Zeeman energy

we assume as before $L=0$ and $J=S$

Typically such models are hard to solve exactly, so one does a 'mean-field' (also called molecular field) or Weiss theory

Define a mean (molecular) field: $\mathbf{B}_{mf} = -\frac{2}{g\mu_B} \sum_j J_{ij} \mathbf{S}_j$ This can be thought of as the field due to all spins (except i^{th} site spin) on the i^{th} site spin

The total exchange interaction between the i^{th} spin and its neighbours is $-2 \sum_j J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$. (factor 2 represents double counting)

Approximation: $-2 \sum_j J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \longrightarrow -2 \mathbf{S}_i \cdot \sum_j J_{ij} \mathbf{S}_j = -g\mu_B \mathbf{S}_i \cdot \mathbf{B}_{mf}$ from the definition of \mathbf{B}_{mf} above

Therefore $\hat{\mathcal{H}} = g\mu_B \sum_i \mathbf{S}_i \cdot (\mathbf{B} + \mathbf{B}_{mf})$ approximation to the original $\hat{\mathcal{H}}$
all spins experience the same field $\mathbf{B} + \mathbf{B}_{mf}$

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paramagnet in an effective magnetic field $\mathbf{B} + \mathbf{B}_{mf}$



Lecture 15 : GMR, spin model and mean-field theory, Ising mod...

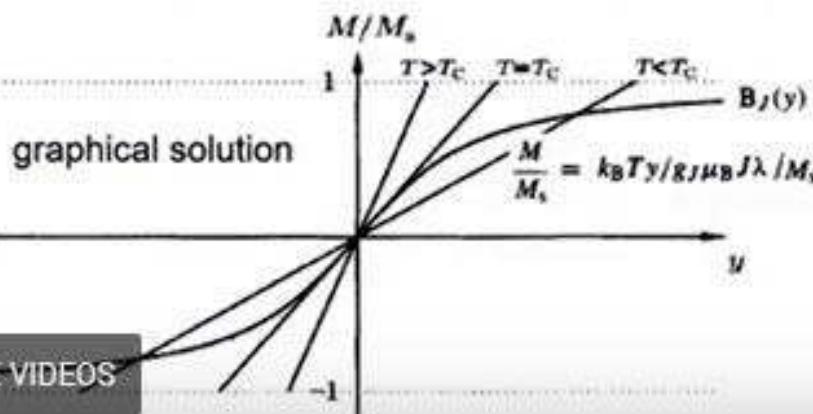
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Since $\sum_i S_i = M$ then $B_{mf} = \lambda M$ For a ferromagnet, $\lambda > 0$.

Note that B_{mf} is an aligning "internal" molecular field and at low T will align all moments into FM (even if $B=0$)
As T rises, the thermal fluctuation destroys this order at a critical $T=T_c$

To find M , we remember our calculations for the paramagnet

$$\frac{M}{M_s} = B_J(y) \quad y = \frac{g_J \mu_B J (B + \lambda M)}{k_B T}$$



take $B = 0$, so that $M = k_B T y / g_J \mu_B J \lambda$

Spontaneous magnetization ($B=0$) at T_c

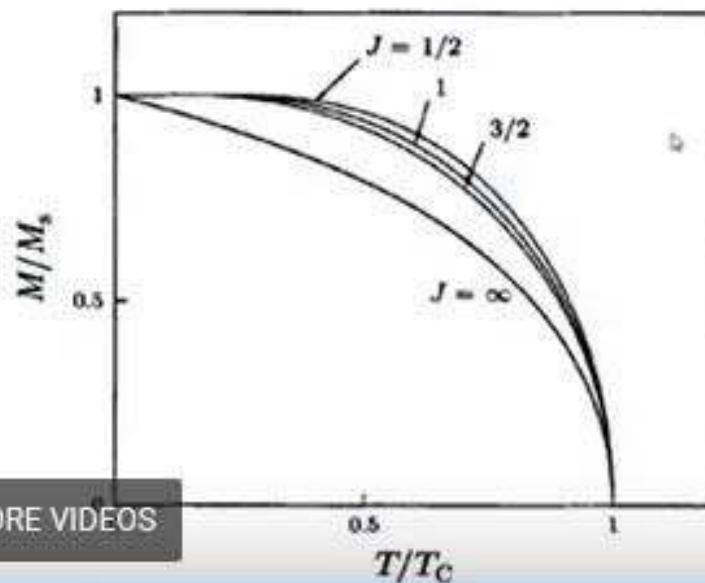


Lecture 15 : GMR, spin model and mean-field theory, Ising mod...

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For small y , $B_J(y) = (J+1)y/3J + O(y^3)$

Curie temperature $T_C = \frac{g_J\mu_B(J+1)\lambda M_s}{3k_B} = \frac{n\lambda\mu_{\text{eff}}^2}{3k_B}$

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The molecular field $B_{\text{mf}} = \lambda M_s$ is thus $3k_B T_C / g_J \mu_B (J+1)$ and so for a ferromagnet with $J = \frac{1}{2}$ and $T_C \sim 10^3$ K, $B_{\text{mf}} = k_B T_C / \mu_B \sim 1500$ T. This is an enormous effective magnetic field and reflects the strength of the exchange interaction.

The magnetization is continuous at $T = T_C$, but its gradient is not. This classifies the phase transition between the non-magnetic and ferromagnetic phases in this molecular field model as a **second-order phase transition**. The order of a phase transition is the order of the lowest differential of the free energy which shows a discontinuity at the transition.

A second-order phase transition has a discontinuity in the second derivative of the free energy, i.e. in quantities like the compressibility or the heat capacity. In the present case the discontinuity is in the gradient of the magnetization, i.e. in the second derivative of the free energy, so the transition is second order.

Blundell, op. cit.

Due to $\lambda M = \lambda n g_J \mu_B J$ for $M = M_S$ and $J = S$ because of the assumption $L = 0$ we obtain:

$$\frac{2}{g_J \mu_B} zJS = \lambda n g_J \mu_B S \quad (5.47)$$

and thus:

$$\lambda = \frac{2zJ}{ng_J^2 \mu_B^2} \quad (5.48)$$

The critical temperature was expressed as (see (5.15)):

$$T_C = \frac{n\lambda\mu_{\text{eff}}^2}{3k} \quad (5.49)$$

with $\mu_{\text{eff}} = g_J \mu_B \sqrt{J(J+1)}$. Thus, we get:

$$T_C = \frac{n\lambda g_J^2 \mu_B^2 J(J+1)}{3k} \quad (5.50)$$

Using (5.48) results in:

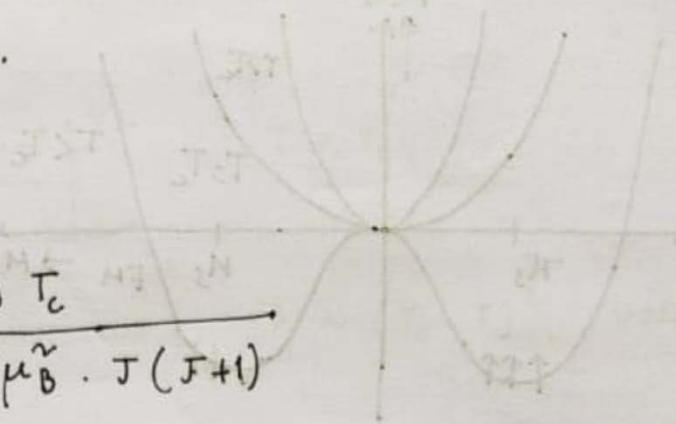
$$T_C = \frac{2ng_J^2 \mu_B^2 J(J+1)zJ}{3kn g_J^2 \mu_B^2} \quad (5.51)$$

$$= J \cdot \frac{2zJ(J+1)}{3k} \quad (5.52)$$

i.e. T_C scales with the strength of the exchange interaction.

$$J_{\text{exch}} = \frac{g^* N \mu_B^2}{2Z}.$$

$$\begin{aligned} \gamma &= \frac{T_c}{C} \\ &= \frac{3k_B T_c}{N g^* \mu_B^2 \cdot J(J+1)} \end{aligned}$$



$\Rightarrow J_{\text{exch}} = \frac{3k_B T_c}{N g^* \mu_B^2 J(J+1)} \cdot N g^* \mu_B^2 \cdot \frac{1}{2Z}$

$$J_{\text{exch}} = \frac{3k_B T_c}{2ZJ(J+1)}$$

$$J_{\text{exch}} = \boxed{\frac{3k_B T_c}{2Zg(J+1)}}$$

$$J \rightarrow S_+ = ? + \vec{S} = (M)$$

simple Z: 6.

For Fe: $Z = 8$
 $J = S = 1$.

$$J_{\text{exch}}(\text{Fe}) \approx 0.1 k_B T_c$$

Find out for Ni?

Homework

Exercises

1 The Curie temperature of nickel, $T_C = 628.3$ K, and the saturation magnetization is $0.6\mu_B$ per atom. Calculate the molecular field according to the Weiss theory. Your answer should be very large!

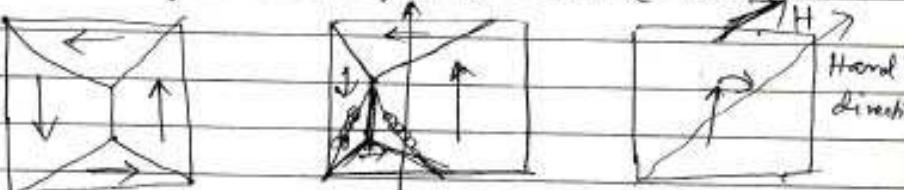
(b) Use Hund's rules to determine the values of S , L , and J for an isolated Ni atom with electronic structure $(4s)^2(3d)^8$. What are the allowed values of the magnetic moment along the field axis for a Ni atom?

Calculate the room-temperature paramagnetic susceptibility of an ideal gas, in which each atom has $J = 1$ and $g = 2$. (Remember the ideal gas law: $PV = nRT$.) These are in fact the values of J and g for molecular oxygen. Note that your answer is small and positive.

Domains & Domain Wall

PAGE NO. _____

In order to explain the ferromagnetism Weiss first postulated that the materials contain a large no. of small regions, called domains.



(a) no-magnetized (b) Wall motion (Domain wall movement) (c) Domain rotate

The size of the domains vary from 10^{-2} to 10^{-6} m and the material within each domain is fully magnetized. The boundary between two domain is generally called domain wall. The direction magnetisation varies from domain to domain resulting zero net magnetisation of the sample.

The no. of domain and domain structure will depend on the size and shape of the crystal.

A simple structure is shown in fig. (a)

Fig. (a) \rightarrow there is no net magnetisation in zero applied field.

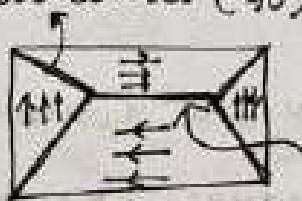
Fig. (b) \rightarrow When mag. field is applied & fig.(c) then magnetisation occurs either by growth of one domain by the expense of other shown in fig. (b)

Ferromagnet has magnetic domains.

- Ferromagnetic domains: Domain walls (Bloch walls),
(domain wall dynamics).

Ferromagnets have a large no. of domains.
domain walls (90°)

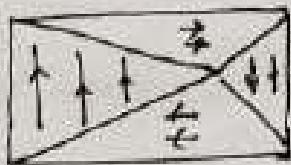
$$\text{size} \sim 10^{-6} - 10^{-4} \text{ m}$$



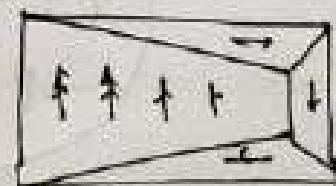
→ ① Magnetic Force microscopy (MFM).
② Lorentz Force microscopy (

- Weiss postulated a large no. of domains in FM.
- To minimize the energy there are multi-domains.

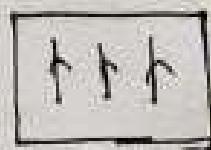
$$\vec{H} \uparrow$$



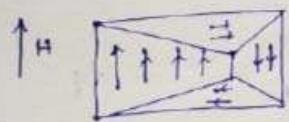
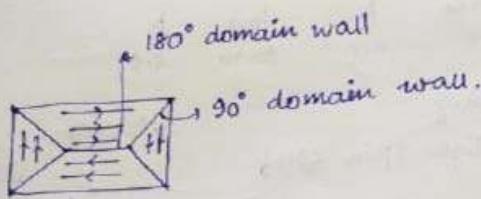
increase \vec{H}



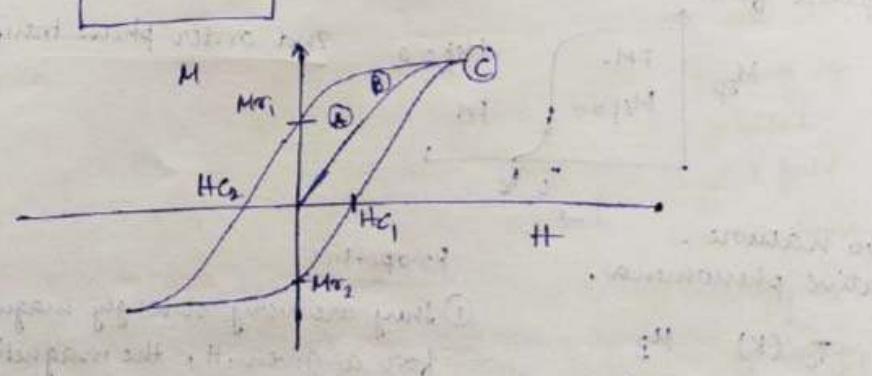
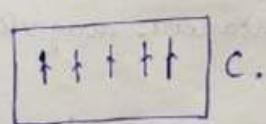
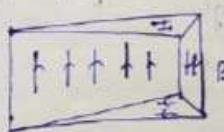
increase \vec{H}



Domain wall motion - domain rotation



A. Domain wall moves due to external magnetic field.



Q: Why do we see multi-domain in a ferromagnet?
 ⇒ Due to minimize the magnetostatic energy.

Super paramagnets (single domain).

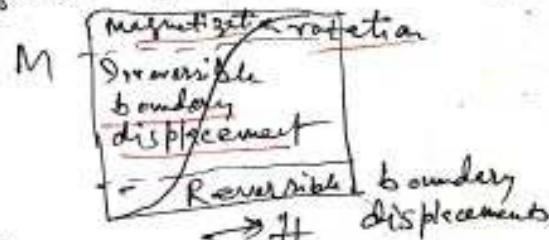
or by domain rotation shown in fig. (c)

Figure No.

weak field \rightarrow reversible magnetization
Strong field \rightarrow irreversible beam
crystal imperfection prevent
the domain wall to return
in original configuration when the field
removed \Rightarrow Hysteresis.

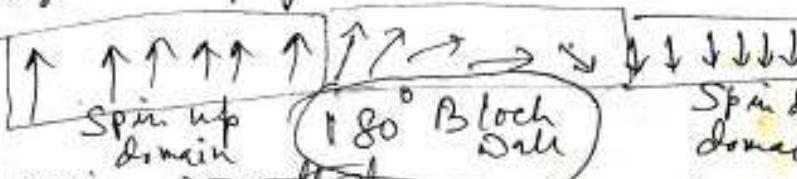
Domain structure occurs in order to minimize
the total energy of ferrimagnetic substance.

$$\begin{array}{l} B \\ \text{or} \\ \cancel{B} \\ H_c + H \\ B = \mu_0(H + M_s) \end{array}$$

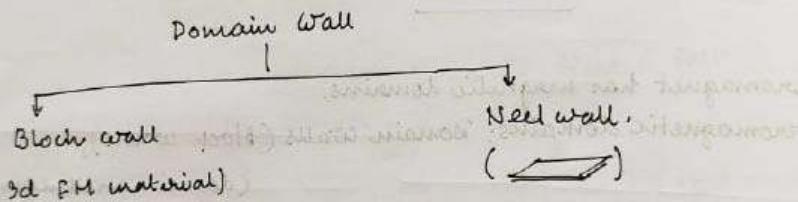
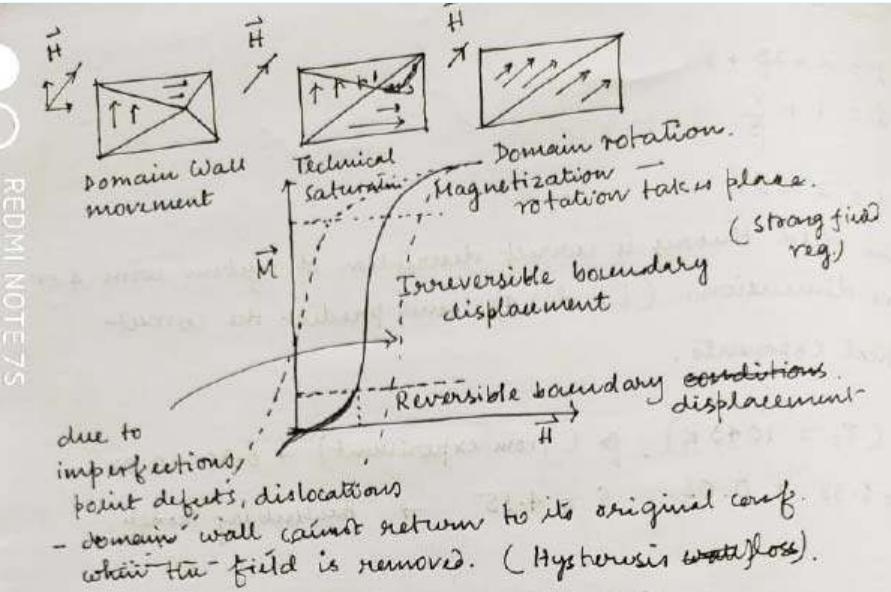


Block Wall : (domain wall) :

According to Bloch, in going from one domain to another domain, the spin direction does not change abruptly but it changes gradually

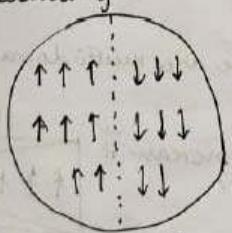


transition region is oscillated
between two oppositely magnetized domain is called
Bloch Wall.
No Sharp boundary wall



- Block wall:

According to Bloch in going from one domain to another the spin directions does not change abruptly but it changes gradually

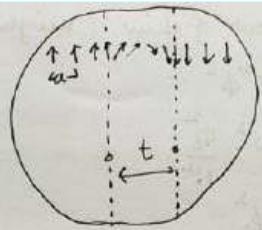


An abrupt domain boundary.
(more costly exchange energy)

NOT POSSIBLE.



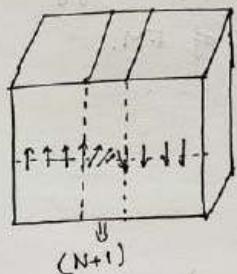
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$t = \text{Na}$.
Thickness of the domain wall.

A boundary with a finite width over which a gradual change in spin direction takes place. \rightarrow More realistic picture observed in real crystal.

Block wall!



Consider two nearest atoms i and j , having spin s_i and s_j - with parallel spins.

$$\text{Exch. Energy: } E_{\text{exch}} \sim -2 J_{\text{ex}} s^2$$

when two spins make an angle ϕ ,

$$E_{\text{exch}2} \sim -2 J_{\text{ex}} s^2 \cos\phi.$$

$$\text{For small } \phi: \cos\phi = (1 - \frac{\phi^2}{2!} + \dots)$$

$$\Rightarrow E_{\text{exch}2} \sim -2 J_{\text{exch}} s^2 (1 - \frac{\phi^2}{2}).$$

Thus in the process of changing the angle b/w the spins from 0 to ϕ , the energy is increased $= E_{\text{exch}2} - E_{\text{exch}1}$

$$= J_{\text{exch}} s^2 \phi^2.$$

Let us consider now, a row of $N+1$ spins within the block wall separating two domains of which magnetization direction make an angle θ_0 w/ the angle b/w two successive spins $\phi = \frac{\theta_0}{N}$.

2020/6/1 09:



An abrupt domain boundary

More costly
in exchange
energy
(not possible)



A boundary with a finite width over which a gradual change in spin direction takes place.

more real picture
observed in real crystal

nearest neighbor spins (s_i & s_j)

consider two electrons with parallel spins. The exchange energy $\propto -2 J_{ex} s^2$
when two spin make angle ϕ
the exchange energy $\approx -2 J_{ex} s^2 \cos \phi$
 $\approx -2 J_{ex} s^2 \left(1 - \frac{\phi^2}{2}\right)$

This is the process of changing the angle between the spins from 0 to ϕ ,
the energy is increased $\propto 2 J_{ex} s^2 \phi^2$

Let us consider now a row of N_{11} spins
within a Bloch Wall separating two domains
of which magnetization direction makes an angle ϕ_0 .

Let the angle between successive spins be $\phi = \phi_0$.

The exchange energy of the row of spins (taking into account only nearest neighbor interaction)

$$(E_{ex})_{\text{row}} = N J_{ex} s^2 \phi^2 = N J_{ex} s^2 \frac{\phi_0^2}{N} = J_{ex} s^2 \frac{\phi_0^2}{N}$$

BORDEK

PAGE NO.



BLOCH WALL

Hence energy decreases if N increases
 why does not the wall become infinity thick?
 Figure No. Influence of anisotropy energy must be considered.

Spins within the wall are nearly all directed away from easy axes
 anisotropy energy \propto thickness of the wall.
 \Rightarrow This limits thickness of the wall.

Let us consider wall of 1 cm^2 area
 the thickness = Nq , where q = lattice constant

The total wall energy per cm^2 may be written as

$$\Omega = \Omega_{\text{ex}} + \Omega_{\text{an}} \quad \text{for exchange energy through wall}$$

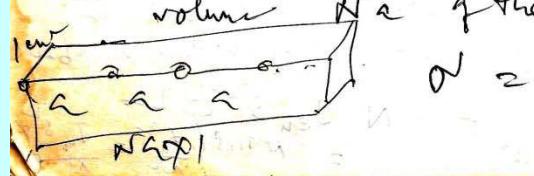
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exchange energy anisotropy energy

Exchange energy per cm^2 is obtained

$$\Omega_{\text{ex}} = \frac{(E_{\text{ex}})_{\text{vol}}}{a^2} = \frac{\text{Ten}^{5^2} \phi^2}{Nq^2}$$

$\Omega_{\text{an}} = \text{anisotropy energy per } \text{cm}^2$
 \approx anisotropy constant (K) times the volume a^2 of the wall $\approx KNq$.



$$\Omega = \frac{\text{Ten}^{5^2} \phi^2}{Nq^2} + KNq \quad (1)$$

The exchange energy of the rows of spins (in units of intensity)

$$(E_{\text{ex}})_{\text{row}} = N \sigma_{\text{exch}} S^2 \phi^2$$

$$= N \sigma_{\text{exch}} S^2 \frac{\phi_0^2}{N^2}$$

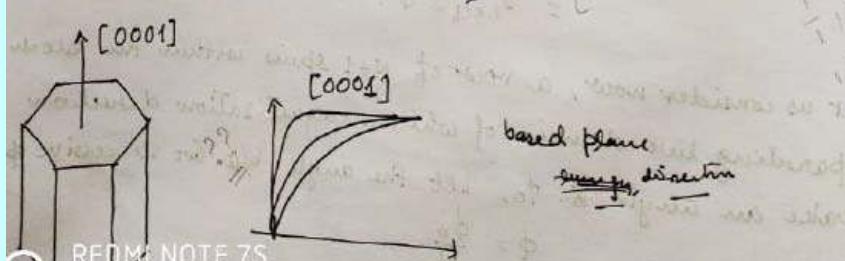
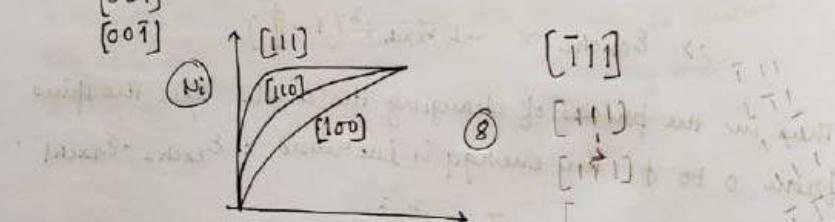
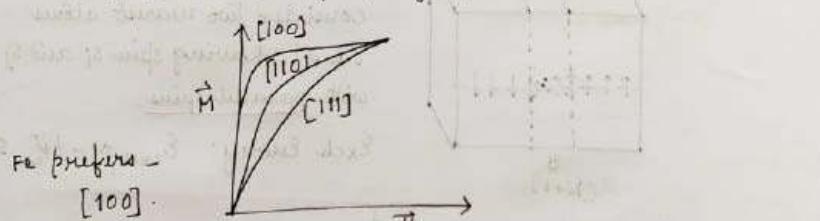
$$= \frac{\sigma_{\text{exch}} S^2 \phi_0^2}{N}$$

Larger the N , lower the E_{ex} .

- why does not the domain wall become infinitely thick?

- Magnetocrystalline anisotropy energy - (MAE)

MAE is inherent property of FM.



The equilibrium value of N may be obtained minimizing or with respect to N putting $\frac{d\sigma}{dN} = 0$

$$\sigma = \frac{d\omega}{dN} = k_a \cancel{\frac{J_e S^2 \phi_0^2}{c^2 N^2}}$$

$$N = \left[\frac{J_e S^2 \phi_0^2}{k_a^3} \right]^{\frac{1}{2}} \quad (1)$$

(Wall thickness a) In the case of f_0 , $J_e = \frac{k_a \phi_0}{T_e}$

$$\phi_0 = \pi (180^\circ \text{ domain wall})^{\frac{3}{2}}$$

$$K = 10^5 \text{ erg/cm}^3, S = \frac{1}{2} \frac{k_B T_c}{225}, J_e = \frac{\pi}{225}, z = 6$$

$$N = \left[\frac{K \phi_0^2}{3} \left(\frac{1}{2} + \frac{1}{z} \right) \right]^{\frac{1}{2}} \quad (2)$$

$$\approx 300 \quad \text{at } T_c \approx 1000 \text{ K}$$

t_2 thickness of the wall

The total energy per unit of ϕ_0

Bloch wall may be estimated by putting N in (2) in σ in (1)

$$\sigma = 2S \phi_0 \left(\frac{J_e K}{k_a} \right)^{\frac{1}{2}}$$

For iron, it is of the order of $\approx 1 \text{ erg/cm}^2$ $K = 10^5 \text{ erg/cm}^3$

$$\delta = N\lambda$$

Figure No.

$$N_{\text{Well}} = \frac{\tan^2 \pi^2}{\delta a} + K_1 \delta^{-1/2}$$

$$\frac{\delta \theta}{\delta \delta} = 0 \Rightarrow \delta = \left(\frac{\tan^2 \pi^2}{K_1 a} \right)^{1/2}$$

$$N = \left(\frac{\tan^2 \pi^2}{K_1 a^3} \right)^{1/2}$$

$$\theta = \frac{\tan^2 \pi^2 (k_1 a)^{-1/2}}{\left(\frac{\tan^2 \pi^2}{K_1 a^3} \right)^{1/2}} + K_1 \left(\frac{\tan^2 \pi^2}{K_1 a} \right)^{1/2}$$

$$= \left(\frac{\tan^2 \pi^2}{K_1 a^3} \right)^{1/2} + K_1 \left(\frac{\tan^2 \pi^2}{K_1 a} \right)^{1/2}$$

$$= \left(\frac{\tan^2 \pi^2 K_1}{a} \right)^{1/2} + \pi \left(\frac{\tan^2 K_1}{a} \right)^{1/2}$$

$$\theta = 2\pi \left(\frac{\tan^2 K_1}{a} \right)^{1/2}$$

$$\theta = 2\pi \left(\frac{\tan^2 K_1}{a} \right)^{1/2}$$

$$K_1 = 10^5 \text{ erg/cm}^2, \quad J_{2u} = \frac{K T_e}{3}, \quad S = \frac{1}{2}$$

$$11^{\circ} 30' \quad t \approx 100 \text{ K}$$

$$\theta \approx \text{erg/cm}^2$$

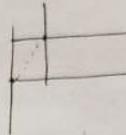
Spins within the wall are nearly all directed away from axis.

Anisotropy energy \propto thickness of the wall.

This limits thickness of the wall.

Let us consider, wall of 1 cm^2 area.

The thickness = Na , where a : Lattice const.



The total energy/cm² may be

written as $\sigma = \sigma_{\text{exch}} + \sigma_{\text{anisotropy}}$

$$\Rightarrow \sigma_{\text{exch.}} = \frac{(\text{Exch})_{\text{per unit area}}}{a^2} = \frac{\sigma_{\text{ex}} s^2 \phi^2}{Na^2}$$

$\sigma_{\text{an}} = \text{anisotropy energy}/\text{cm}^2$ is -

$$\begin{aligned} &\sim \text{anisotropy const}(k) \times Na \\ &= kNa. \end{aligned}$$

a^2 area \rightarrow 1 line - per unit area $\rightarrow \frac{1}{a^2}$ line.

$$\sigma = \sigma_{\text{exch}} + \sigma_{\text{an}} = \frac{\sigma_{\text{ex}} s^2 \phi^2}{Na^2} + kNa.$$

$$\Rightarrow \frac{d\sigma}{dN} = 0 \Rightarrow \sigma_{\text{ex}} \frac{s^2 \phi^2}{a^2} \left[-\frac{1}{N^2} \right] + ka = 0.$$

$$\Rightarrow N = \frac{ka}{\sigma_{\text{ex}} s^2 \phi^2 \cdot ka} \left[\frac{\sigma_{\text{ex}} s^2 \phi^2}{ka^3} \right]^{\frac{1}{2}} \quad \boxed{I}$$

$$\Rightarrow \sigma_{\text{exch}} =$$

$$t = Na. \quad t = \left[\frac{\sigma_{\text{ex}} s^2 \phi^2}{ka^3} \right]^{\frac{1}{2}} \rightarrow \boxed{II} \quad \begin{aligned} \sigma &: \text{domain wall energy} \\ &\text{per cm}^2. \end{aligned}$$

$$\text{or for Fe: } \sigma = 2\phi_0 \left[\frac{\sigma_{\text{ex}} s^2 k}{a} \right]^{\frac{1}{2}} \quad - \boxed{III}$$

In case of Fe, $\phi_0 = \pi$ (180° domain wall)

$$K = 10^5 \text{ erg/cc.}$$

$$J = S = \frac{1}{2}$$

$$S = \frac{1}{2}, \quad \sigma_{\text{ex}} = \frac{3k_B T_c}{2zJ(J+1)} \rightarrow \frac{1}{3} k_B T_c$$

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$$N = \frac{\frac{k_B T_c}{3} \cdot \left(\frac{1}{2}\right)^2 \pi^2}{10^5 a^3} \cdot \sim 300. \quad a \sim 2.85 \text{ \AA}$$

$$t \sim 1000 \text{ \AA} \quad T_c \sim 1094 \text{ K.}$$

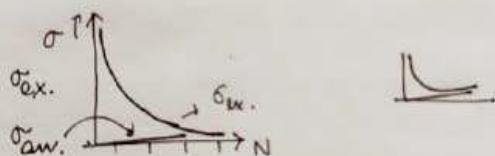
$$\sigma = 2s\phi_0 \left[\frac{J_{ex} k}{a} \right]^{\frac{1}{2}}$$

$$\sigma = 1 \text{ erg/cm}^2.$$

a: Domain wall σ_{ex} σ_{an}
 ↓
 $k N a$ $\rightarrow (\sigma_{ex})$

- (a) Plot the form of exch. energy cost, the anisotropy energy cost σ_{an} and the sum of these two energy cost for Fe for which $k = 0.5 \times 10^5 \text{ J/m}^3$.

$$a = 0.3 \text{ nm}, T_c = 770^\circ\text{C}.$$



- (b) Assuming that the exchange and anisotropy energy are the principal contributions to the domain-wall energy, derive an expression for the no. of atomic layers in a domain wall as a fct. of T_c, k, a .

- (c) Calculate the thickness of the domain wall in Fe. How much energy is stored in 1 m area

REDMI NOTE 7S
of a DUALGAMMA cell?

2020/6/1 09:27

Magnetic anisotropy

① Crystal anisotropy

② Shape anisotropy

③ Stress anisotropy

④ Anisotropy induced by:

① Magnetic anisotropy annealing

② Magnetic deformation.

③ Irradiation

⑤ Exchange anisotropy.

Magneto crystalline anisotropy

Intrinsic property, (origin: $S-O$ coupling).

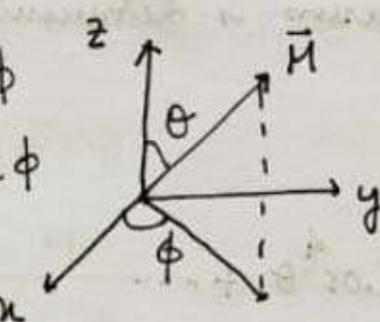
Extrinsic

Direction
cosines

$$\alpha_1 = \cos a = \sin \theta \cos \phi$$

$$\alpha_2 = \cos b = \sin \theta \sin \phi$$

$$\alpha_3 = \cos c = \cos \theta.$$



Magneto crystalline anisotropy energy →

$$E = K_0 + K_1 [\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_3^2 \alpha_1^2] + K_2 [\alpha_1^2 \alpha_2^2 \alpha_3^2].$$

K_0, K_1, K_2 : anisotropy const. (erg/cc).

The value of E when \vec{M}_s lies in the particular direction.

$[u \ v \ w]$	a	b	c	α_1	α_2	α_3	E .
---------------	-----	-----	-----	------------	------------	------------	-------

$$[1 \ 0 \ 0] \quad 0^\circ \quad 90^\circ \quad 90^\circ \quad 1 \quad 0 \quad 0 \quad K_0.$$

$$[1 \ 1 \ 0] \quad 45^\circ \quad 45^\circ \quad 90^\circ \quad \frac{1}{\sqrt{2}} \quad \frac{1}{\sqrt{2}} \quad 0 \quad K_0 + \frac{K_1}{4}.$$

$$[1 \ 1 \ 1] \rightarrow 54.7^\circ \quad 54.7^\circ \quad 54.7^\circ \quad \frac{1}{\sqrt{3}} \quad \frac{1}{\sqrt{3}} \quad \frac{1}{\sqrt{3}} \quad K_0 + \frac{K_1}{3} + \frac{K_2}{27}.$$

- Magneto-crystalline anisotropy energy - (MAE)

MAE is inherent property of FM.

surface tension due to surface

→ Due to surface tension

surface tension due to surface

→ Due to surface tension

surface tension due to surface

→ Due to surface tension

Fe prefers -

[100]

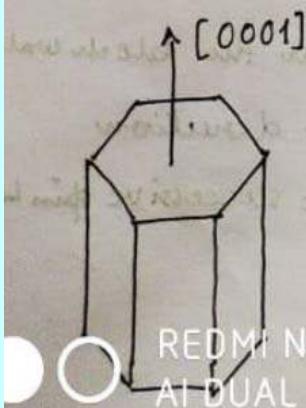
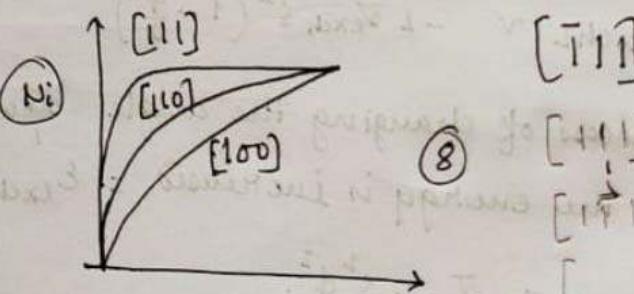
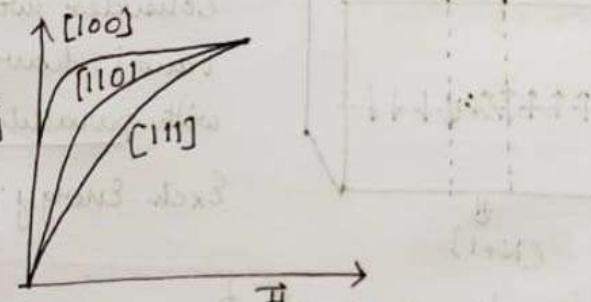
[-100]

[010] ⑥

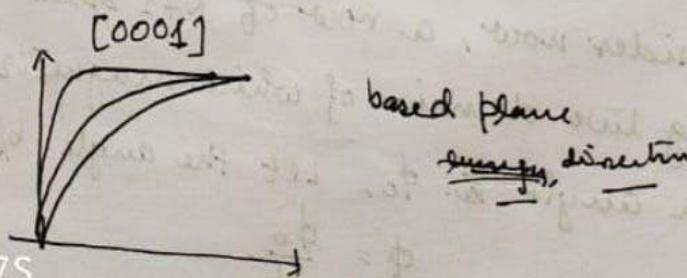
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Table 7.1 Crystal Anisotropy Energies for Various Directions in a Cubic Crystal

$[uvw]$	a	b	c	α_1	α_2	α_3	E
[100]	0	90°	90°	1	0	0	K_0
[110]	45°	45°	90°	$1/\sqrt{2}$	$1/\sqrt{2}$	0	$K_0 + K_1/4$
[111]	54.7°	54.7°	54.7°	$1/\sqrt{3}$	$1/\sqrt{3}$	$1/\sqrt{3}$	$K_0 + K_1/3 + K_2/27$

Table 7.2 Directions of Easy, Medium, and Hard Magnetization in a Cubic Crystal
(from Bozorth [G.4])

K_1	+	+	+	-	-	-
K_2	+ ∞ to - $9K_1/4$	- $9K_1/4$ to - $9K_1$	- $9K_1$ to - ∞	- ∞ to 9 K_1 /4	9 K_1 /4 to 9 K_1	9 K_1 to + ∞
Easy	$\langle 100 \rangle$	$\langle 100 \rangle$	$\langle 111 \rangle$	$\langle 111 \rangle$	$\langle 110 \rangle$	$\langle 110 \rangle$
Medium	$\langle 110 \rangle$	$\langle 111 \rangle$	$\langle 100 \rangle$	$\langle 110 \rangle$	$\langle 111 \rangle$	$\langle 100 \rangle$
Hard	$\langle 111 \rangle$	$\langle 110 \rangle$	$\langle 110 \rangle$	$\langle 100 \rangle$	$\langle 100 \rangle$	$\langle 111 \rangle$

when $K_2 = 0$, then the direction of easy magnetization
is determined by K_1 ,

If $K_1 = +ve$, $E_{100} < E_{110} < E_{111}$.

Easy magnetization axis [100]. / e.g. Fe, Ferrites.

If $K_1 = -ve$, $K_2 = 0$,
 $E_{111} < E_{110} < E_{100}$.

Ni [111] is easy magnetization direction.

If $K_2 \neq 0$; the easy axis is determined by K_1, K_2

H.C.P.

$$E = K_0' + K_1' \cos^2 \theta + K_2' \cos^4 \theta + \dots$$

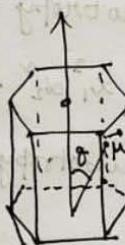
θ : angle b/w \vec{M}_s and c axis.

$$E = K_0 + K_1 \sin^2 \theta + K_2 \sin^4 \theta + \dots$$

$K_1 = +ve$, $K_2 > -K_1$

then the energy E is
minimum for $\theta = 0$.

c axis is the easy axis.



② $K_1 = -ve$, $K_2 < K_1$

E is minimum, $\theta = 90^\circ$

one direction to another. Table 7.1 gives the value of E when the M_s vector lies in a particular direction $[u\ v\ w]$.

When K_2 is zero, the direction of easy magnetization is determined by the sign of K_1 . If K_1 is positive, then $E_{100} < E_{110} < E_{111}$, and $\langle 100 \rangle$ is the easy direction, because E is a minimum when M_s is in that direction. Thus iron and the cubic ferrites containing cobalt have positive values of K_1 . If K_1 is negative, $E_{111} < E_{110} < E_{100}$, and $\langle 111 \rangle$ is the easy direction. K_1 is negative for nickel and all the cubic ferrites that contain no cobalt.

When K_2 is not zero, the easy direction is determined by the values of both K_1 and K_2 . The way in which the values of these two constants determine the directions of easy, medium, and hard magnetization is shown in Table 7.2.

7.3 ANISOTROPY IN HEXAGONAL CRYSTALS

Magnetization curves of cobalt, which has a hexagonal close-packed structure, are shown in Fig. 7.5. The hexagonal c axis is the direction of easy magnetization, and, within the accuracy of the measurements, any direction in the basal plane is found to be equally hard. Under these circumstances the anisotropy energy E depends on only a single angle, the angle θ between the M_s vector and the c axis. Therefore,

$$E = K'_0 + K'_1 \cos^2 \theta + K'_2 \cos^4 \theta + \dots \quad (7.2)$$

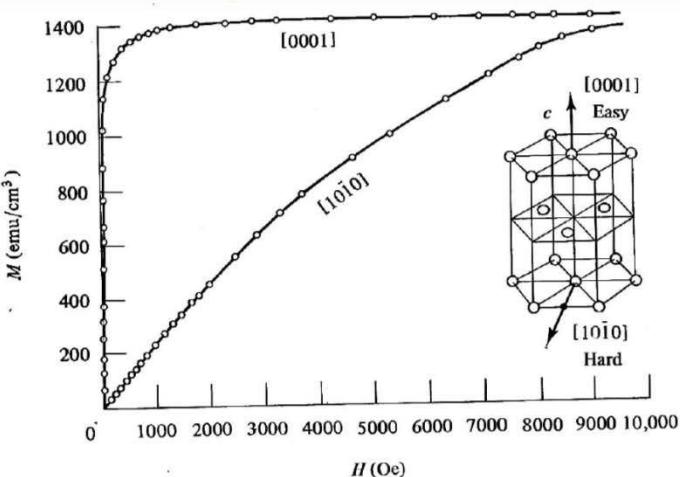


Fig. 7.5 Magnetization curves for a single crystal of cobalt (by Kaya [7.3]).

However, it is customary to write the equation for E in hexagonal crystals in powers of $\sin \theta$. Putting $\cos^2 \theta = 1 - \sin^2 \theta$ into Eq. (7.2), we have

$$E = K_0 + K_1 \sin^2 \theta + K_2 \sin^4 \theta + \dots \quad (7.3)$$

When K_1 is positive and $K_2 > -K_1$, the energy E is a minimum for $\theta = 0$, and the c axis is one of easy magnetization. These conditions are met for cobalt and hexagonal barium ferrite $\text{BaO} \cdot 6\text{Fe}_2\text{O}_3$. A crystal with a single easy axis, along which the magnetization can point either up or down, is referred to as a *uniaxial crystal*. Its domain structure in the demagnetized state is particularly simple (Fig. 7.6).

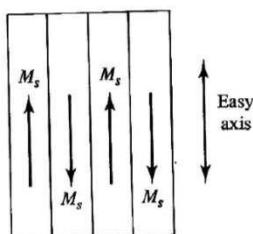


Fig. 7.6 Domain structure of a uniaxial crystal.

The energy E will have a minimum for $\theta = 90^\circ$ if K_1 is negative and $K_2 < |K_1|/2$, or if K_1 is positive and $K_2 < -K_1$. The basal plane is then an *easy plane* of magnetization. A stable intermediate value of θ can also exist: if K_1 is negative and $K_2 > |K_1|/2$, then E is a minimum for $\theta = \sin^{-1}(-K_1/2K_2)^{1/2}$. The M_s vector may then lie anywhere on the surface of a cone with a semivertex angle of θ . Both of these states (a minimum in E at $\theta = 90^\circ$ or a particular value between 0 and 90°) are unusual but have been observed in cobalt at high temperatures.

7.4 PHYSICAL ORIGIN OF CRYSTAL ANISOTROPY

Crystal anisotropy is due mainly to *spin-orbit coupling*. By coupling is meant a kind of interaction. Thus we could speak of the exchange interaction between two neighboring spins as a spin-spin coupling. This coupling is very strong and keeps neighboring spins parallel, or antiparallel, to one another. But the associated exchange energy is isotropic; it depends only on the angle between adjacent spins, as stated by Eq. (4.29), and not at all on the direction of the spin axis relative to the crystal lattice. The spin-spin coupling therefore cannot contribute to the crystal anisotropy.

The orbit-lattice coupling is also strong. This follows from the fact that orbital magnetic moments are almost entirely quenched, as discussed in Section 3.7. This means, in effect, that the orientations of the orbits are fixed very strongly to the lattice, because even large fields cannot change them.

There is also a coupling between the spin and the orbital motion of each electron. When an external field tries to reorient the spin of an electron, the orbit of that electron also tends to be reoriented. But the orbit is strongly coupled to the lattice and therefore resists the attempt to rotate the spin axis. The energy required to rotate the spin system of a domain away from the easy direction, which we call the anisotropy energy, is just the energy required to overcome the spin-orbit coupling. This coupling is relatively weak, because fields of a few hundred oersteds are usually strong enough to rotate the spins. Inasmuch as the "lattice" is really constituted by a number of atomic nuclei arranged in space, each with its surrounding cloud of orbital electrons, we can also speak of a spin-lattice coupling and conclude that it too is weak. These several relationships are summarized in Fig. 7.7.

The strength of the anisotropy in any particular crystal is measured by the magnitude of the anisotropy constants K_1 , K_2 , etc. Although there is no doubt that crystal anisotropy is due to spin-orbit coupling, the details are not clear, and it is not yet possible to calculate the value of the anisotropy constants from first principles.

Nor is there any simple relationship between the easy, or hard, direction of magnetization and the way atoms are arranged in the crystal structure. Thus in iron, which is body-centered cubic, the direction of greatest atomic density, i.e., the direction in which the atoms are most closely packed, is $\langle 111 \rangle$, and this

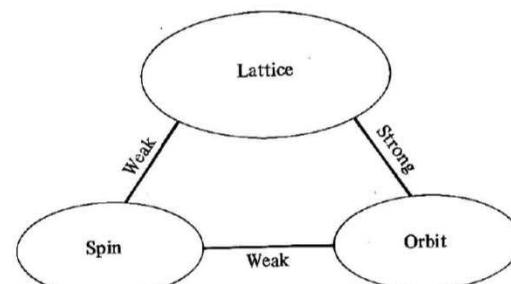


Fig. 7.7 Spin-lattice-orbit interactions.

Q) Importance of 3d Shell in the origin of FM. The radius of the shell is small plays a crucial role in FM phenomena.

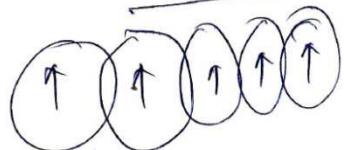
$$H_{\text{spin}} = - \sum J_{ij} \vec{S}_i \cdot \vec{S}_j \quad (\text{each})$$

1. for only products of pairs of spin operators to appear in eqn. (each), it is necessary that all magnetic ions be far enough apart that the overlap of the electric wave function is very ~~not~~ small.
 2. when the angular momentum of each ion contains an orbital as well as spin part, the coupling in the spin Hamiltonian may depend on the absolute as well as the relative spin orientation.
- The Spin Hamiltonian is known as Heisenberg Hamiltonian.

The Spin Hamiltonian is known as the exchange coupling.
& the J_{ij} are known as the exchange constants.

Direct exchange

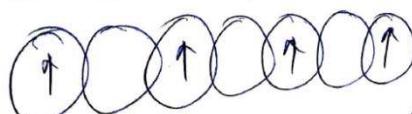
(a)



ΔE , in which magnetic ions interact because their charge distribution overlap.

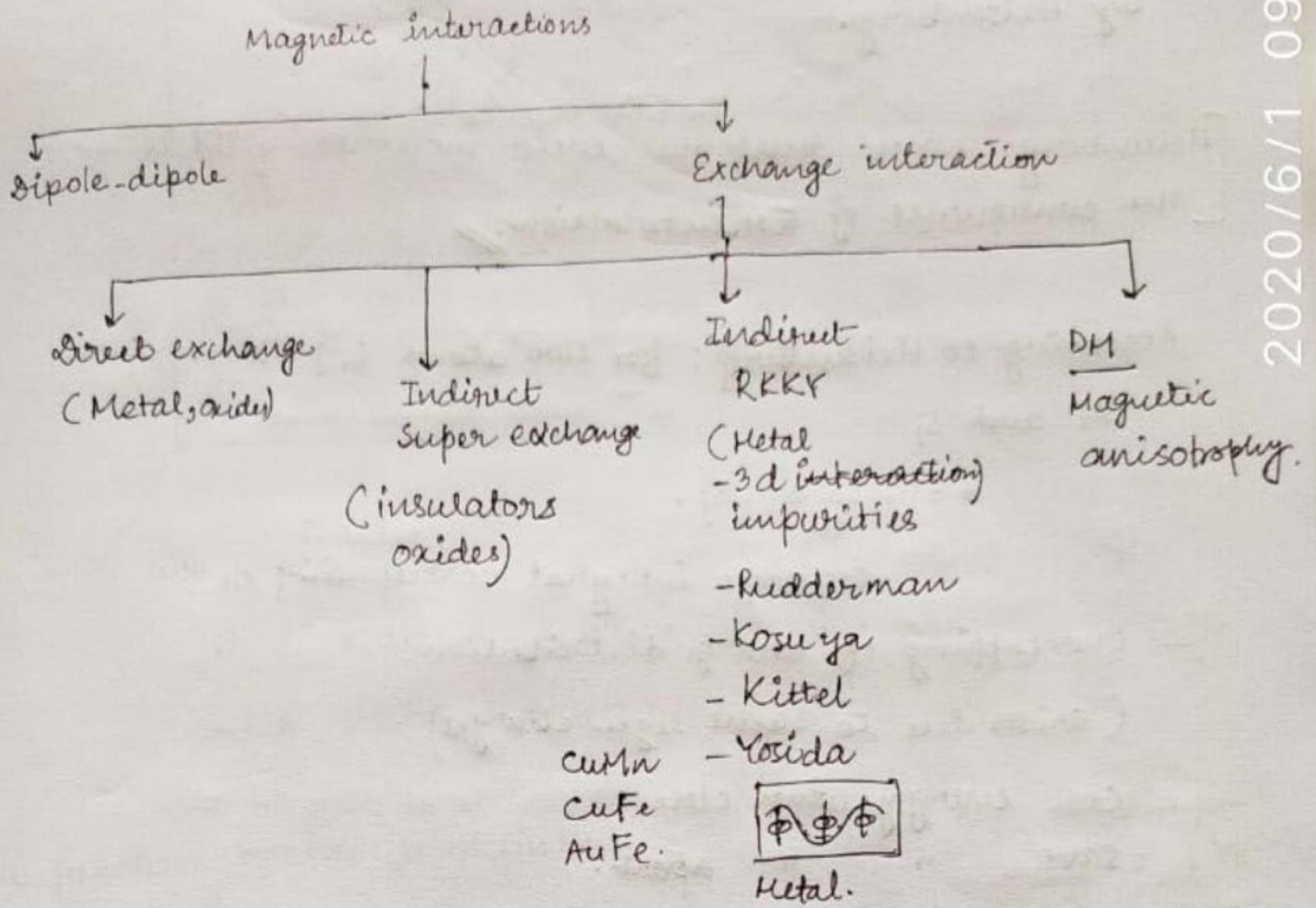
Super DE RKKY Dzyaloshinskii

(b)

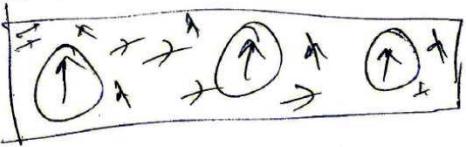


Super exchange, in which magnetic ions with no overlapping charge distribution interact because both have overlap with the same

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(c)



Indirect exchange.
in which absence of
overlap a magnetic int. is
mediated by interaction with
the conduction electron.

Ferromagnetic ground state

The Heisenberg Hamiltonian can be written.

$$\begin{aligned} H &= - \sum_{i>j} J_{ij} S_i \cdot S_j \\ &= - \sum_{i>j} J_{ij} \left(S_i^z S_j^z + \frac{1}{2} S_i^+ S_j^- + \frac{1}{2} S_i^- S_j^+ \right) \end{aligned}$$

here the raising & lowering operator S_i^+, S_i^-
are defined as $S_i^\pm = S_i^x \pm i S_i^y$
& the commutation reln. $[S_i^\pm, S_j^\pm] = \pm \delta_{ij} S_i^\pm$
 $[S_i^+, S_j^-] = 2 \delta_{ij} S_i^z$.

It is noted that spin operators for different site
commute.

$$\frac{1}{2} S_i^- S_j^+ + \frac{1}{2} S_i^+ S_j^- = i (S_i^x S_j^y - S_i^y S_j^x)$$

which is anti-symmetric so that $\sum_{i>j} (S_i^- S_j^+ - S_i^+ S_j^-) = 0$ so vanishes.

on summing, $\therefore \sum_{i>j} J_{ij} (S_i^z S_j^z + S_i^- S_j^+)$

so, $\therefore H = - \sum_{i>j} J_{ij} (S_i^z S_j^z + S_i^- S_j^+)$
if $J_{ii} = 0$ define $J_{ii} = 0$.