



11.1 Exchange coupling in 3d metals

The Curie temperature of bulk elemental ferromagnets is

Fe: 1043 K

Co: 1388 K

Ni: 627 K

Fe has bcc structure with lattice constant $a = 0.287$ nm;

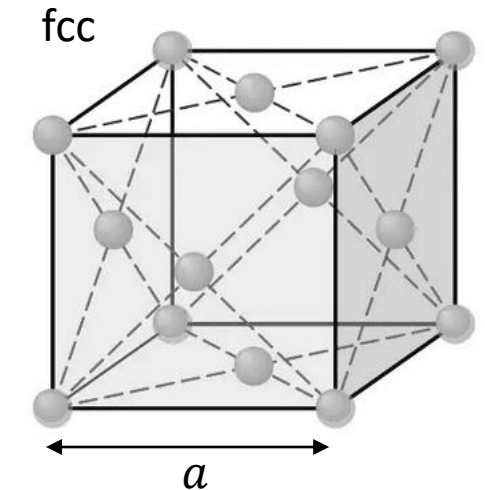
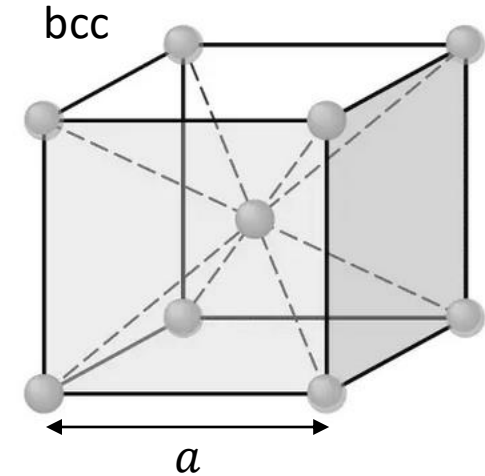
Co has fcc structure with $a = 0.25$ nm (for simplicity, in reality Co has an hcp structure);

Ni has fcc structure with $a = 0.35$ nm.

- 1) Calculate J_{ex} , the exchange coupling energy between a pair of atoms in each of the mentioned systems.

$$k_B = 8.617 \cdot 10^{-2} \text{meV K}^{-1}$$

- 2) You want to grow a single atomic layer (monolayer) with the highest Curie temperature; assuming the film grows with a (100) orientation, which element among Fe, Co, and Ni do you choose?





11.1 Exchange coupling in 3d metals - Solution

1) We know that
$$T_c = \frac{2 S(S + 1) N J_{ex}}{3 k_B}$$

Fe has a bcc structure; thus, each atom has $N = 8$ nearest neighbors.

Fe has a $4s^2 3d^6$ electronic configuration; thus, $S = 2$ and $L = 0$ due to orbital moment quenching in bulk.

$$J_{ex} = \frac{3k_B T_c}{2 S(S+1)N} = 2.8 \text{ meV}$$

Co has a hcp structure; thus, each atom has $N = 12$ nearest neighbors.

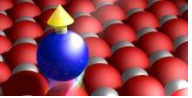
Co has a $4s^2 3d^7$ electronic configuration; thus, $S = 3/2$ and $L = 0$ due to orbital moment quenching in bulk.

$$J_{ex} = \frac{3k_B T_c}{2 S(S+1)N} = 4 \text{ meV}$$

Ni has a fcc structure; thus, each atom has $N = 12$ nearest neighbors.

Ni has a $4s^2 3d^8$ electronic configuration; thus, $S = 1$ and $L = 0$ due to orbital moment quenching in bulk.

$$J_{ex} = \frac{3k_B T_c}{2 S(S+1)N} = 3.4 \text{ meV}$$

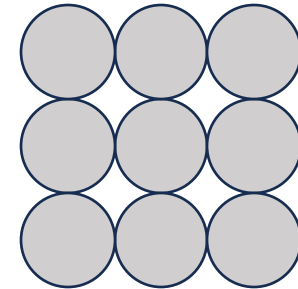


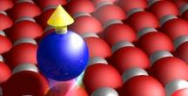
11.1 Exchange coupling in 3d metals - Solution

2) In a monolayer with (100) orientation, all materials have $N = 4$; then we can use the previously calculated value for J_{ex} to calculate T_c for each of the three materials

We have $T_c(\text{Fe}) = 521 \text{ K}$; $T_c(\text{Co}) = 463 \text{ K}$; $T_c(\text{Ni}) = 209 \text{ K}$.

Then in the monolayer regime Fe is the element with the highest Curie temperature





11.2 Intra-atomic exchange in rare earth atoms

The excerpt of the periodic table show the rare earth electronic configuration for free atoms, [Xe] 4f^N 6s² (except for Gd). Consider now Sm, Eu, Dy, Ho, and Tm in the [Xe] 4f^N 6s¹ electronic configuration.

Evaluate the intra-atomic exchange coupling energy knowing that the 4f-6s exchange constant is $J_{ex} \approx 40$ meV for all rare earths.

58 3699 1071 6.78 [Xe]4f ¹ 5d ¹ 6s ² Ce	59 3785 1204 6.77 [Xe]4f ³ 6s ² Pr	60 3341 1289 7.00 [Xe]4f ⁴ 6s ² Nd	61 (145) 3785 1204 6.475 [Xe]4f ⁵ 6s ² Pm	62 2064 1345 7.54 [Xe]4f ⁶ 6s ² Sm	63 1870 1090 5.26 [Xe]4f ⁷ 6s ² Eu
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64 3539 1585 7.89 [Xe]4f ⁷ 5d ¹ 6s ² Gd	65 3496 1630 8.27 [Xe]4f ⁹ 6s ² Tb	66 2835 1682 8.54 [Xe]4f ¹⁰ 6s ² Dy	67 2968 1743 8.80 [Xe]4f ¹¹ 6s ² Ho	68 3136 1795 9.05 [Xe]4f ¹² 6s ² Er	69 2220 1818 9.33 [Xe]4f ¹³ 6s ² Tm	70 1467 1097 6.98 [Xe]4f ¹⁴ 6s ² Yb
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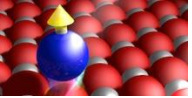
11.2 Intra-atomic exchange in rare earth atoms - Solution

RE	configuration	S_{4f}	S_{6s}	$E_{ex} = 2 \cdot 40 \cdot 1 \cdot S_{4f}$ meV
Sm	[Xe] 4f ⁶ 6s ¹	3	1/2	240
Eu	[Xe] 4f ⁷ 6s ¹	7/2	1/2	280
Dy	[Xe] 4f ¹⁰ 6s ¹	2	1/2	160
Ho	[Xe] 4f ¹¹ 6s ¹	3/2	1/2	120
Tm	[Xe] 4f ¹³ 6s ¹	1/2	1/2	40

You can compare these values with the ones shown in the lecture

58 140.12 3699 1071 6.78 3,4 Ce [Xe]4f ³ 5d ¹ 6s ² Cerium	59 140.9077 3785 1204 6.77 3,4 Pr [Xe]4f ³ 6s ² Praseodymium	60 144.24 3341 1289 7.00 3 Nd [Xe]4f ⁴ 6s ² Neodymium	61 (145) 3785 1204 6.475 3 Pm [Xe]4f ⁵ 6s ² Promethium	62 150.4 2064 1345 7.54 3,2 Sm [Xe]4f ⁶ 6s ² Samarium	63 151.96 1870 1090 5.26 3,2 Eu [Xe]4f ⁷ 6s ² Europium
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64 157.25 3539 1585 7.89 3 Gd [Xe]4f ⁷ 5d ¹ 6s ² Gadolinium	65 158.9254 3496 1630 8.27 3,4 Tb [Xe]4f ⁹ 6s ² Terbium	66 162.50 2835 1682 8.54 3 Dy [Xe]4f ¹⁰ 6s ² Dysprosium	67 164.9304 2968 1743 8.80 3 Ho [Xe]4f ¹¹ 6s ² Holmium	68 167.26 3136 1795 9.05 3 Er [Xe]4f ¹² 6s ² Erbium	69 168.9342 2220 1818 9.33 3,2 Tm [Xe]4f ¹³ 6s ² Thulium	70 173.04 1467 1097 6.98 3,2 Yb [Xe]4f ¹⁴ 6s ² Ytterbium
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Evaluate the magnetic dipolar interaction E_{dip} for the magnetic moments of two Fe atoms in Fe bulk at a distance r_0 equal to the nearest neighbor distance.

Fe: bcc structure with $a = 0.287$ nm

$$\mu_0 = 4\pi \cdot 10^{-7} \text{ T m A}^{-1}$$

$$\mu_B = 9.27 \cdot 10^{-24} \text{ J T}^{-1}$$

$$1 \text{ J} = 6.24 \cdot 10^{18} \text{ eV}$$

$$k_B = 8.617 \cdot 10^{-2} \text{ meV K}^{-1}$$

Provide E_{dip} in terms of temperature and compare it to the Curie temperature of Fe.



Nearest neighbor distance: half of the cube diagonal: $r_0 = \frac{a}{2}\sqrt{3} = 0.248 \text{ nm}$

Most favourable configuration: magnetic moments coaxial and parallel

$$E_{dip} = -\frac{\mu_0}{4\pi} \frac{2 \mu_1 \mu_2}{r_0^3}$$

With $\mu_1 = \mu_2 = 2.2 \mu_B$ (value in bulk, see lecture 10 on nano-magnetism)

$$|E_{dip}| \approx 5 \cdot 10^{-24} \text{ J} \approx 0.033 \text{ meV}$$

$$T_{dip} = E_{dip}/k_B \approx 0.4 \text{ K}$$

An alignment of the dipoles due to this interaction can only occur at extremely low temperatures. This value is not compatible with the Curie temperature of Fe (1043 K). This confirms that dipole-dipole interaction cannot be the origin of the ferromagnetic properties of materials. The interaction that gives rise to magnetic order is exchange interaction.