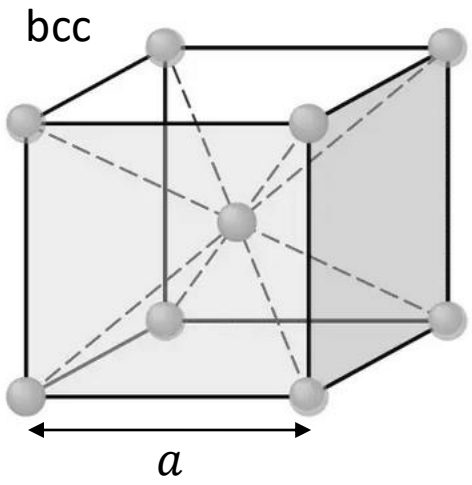
11.1 Exchange coupling in 3d metals

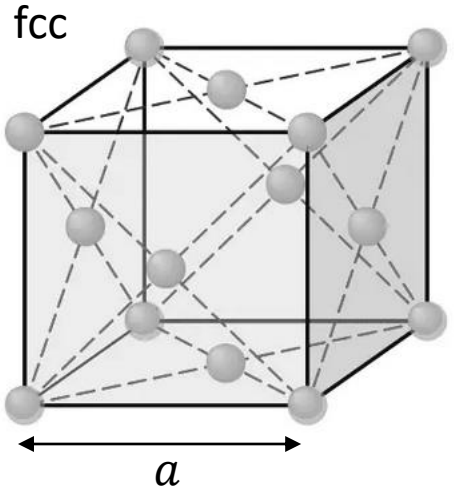
The Curie temperature of bulk elemental ferromagnets is
Fe: 1043 K
Co: 1388 K
Ni: 627 K

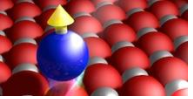
Fe has bcc structure with lattice constant $a = 0.287$ nm;
Co has fcc structure with $a = 0.25$ nm (for simplicity, in reality Co has an hcp structure);
Ni has fcc structure with $a = 0.35$ nm.

1) Calculate J_{ex} , the exchange coupling energy between a pair of atoms in each of the mentioned systems.
$k_B = 8.617 \cdot 10^{-2}$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.

$J_{ex} = \frac{3k_BT_C}{2\,S(S+1)N}$ = 2.8 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.

$J_{ex} = \frac{3k_BT_C}{2\,S(S+1)N}$ = 4 meV

Ni has a fcc structure; thus, each atom has $N = 12$ nearer neighbors.
Ni has a $4s^2\ 3d^8$ electronic configuration; thus, $S = 1$ and $L = 0$ due to orbital moment quenching in bulk.

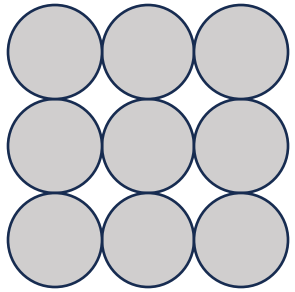
$J_{ex} = \frac{3k_BT_C}{2\,S(S+1)N}$ = 3.4 meV

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 $T_C(\mathrm{Fe}) = 521\ \mathrm{K}$; $T_C(\mathrm{Co}) = 463\ \mathrm{K}$; $T_C(\mathrm{Ni}) = 209\ \mathrm{K}$.

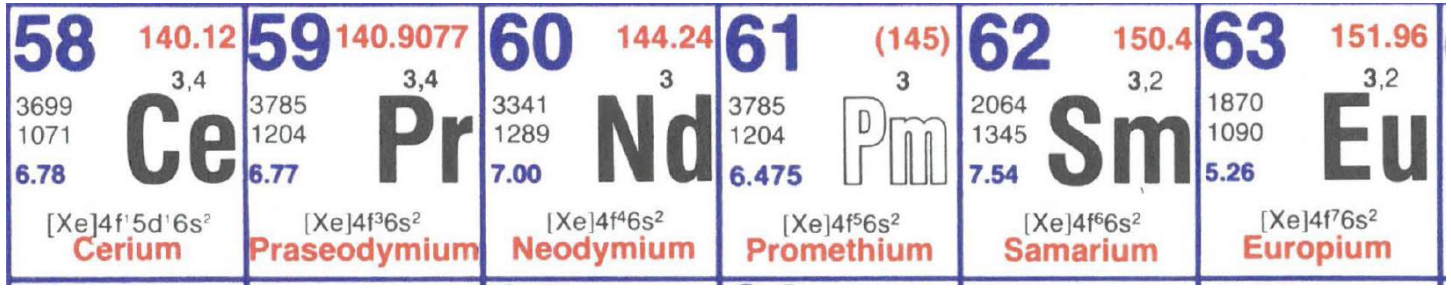
Then in the monolayer regime Fe is the element with the highest Curie temperature

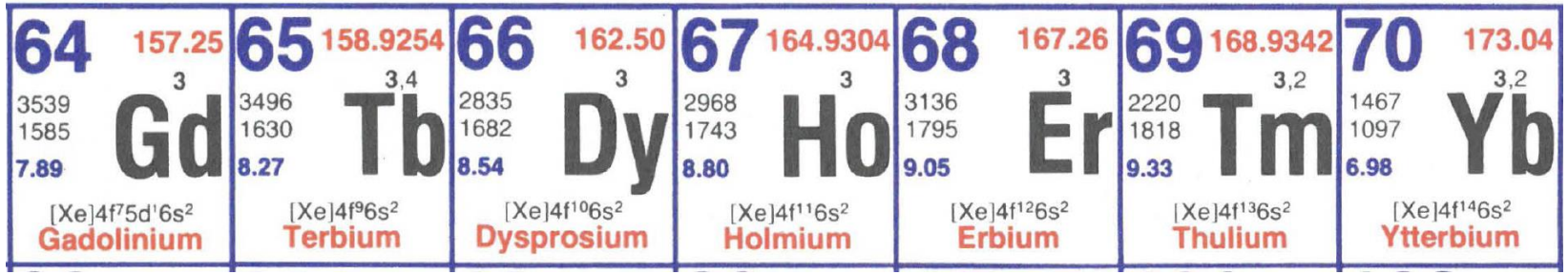


11.2 Intra-atomic exchange in rare earth atoms

The excerpt of the periodic table show the rare earth electronic configuration for free atoms, [Xe] $4f^N$ $6s^2$ (except for Gd).
Consider now Sm, Eu, Dy, Ho, and Tm in the [Xe] $4f^N$ $6s^1$ 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.

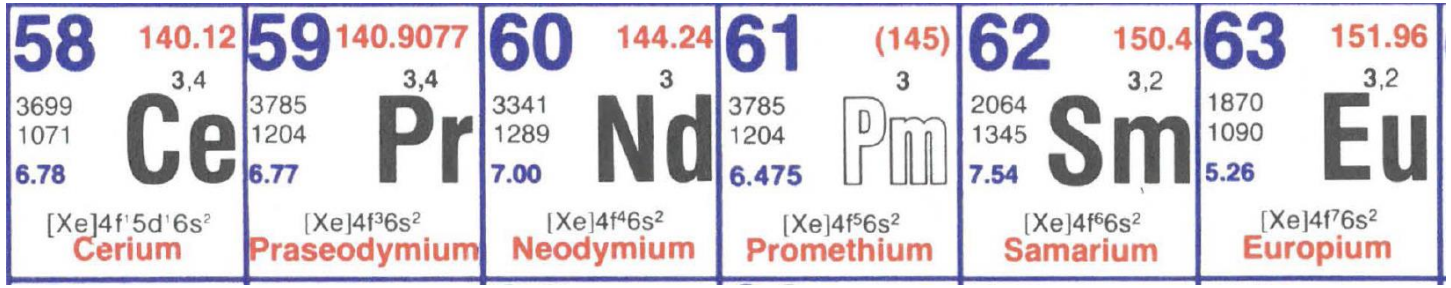


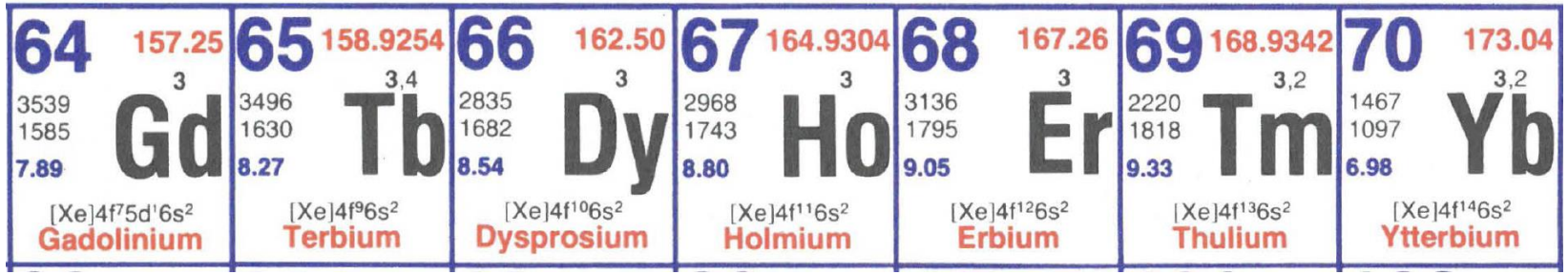


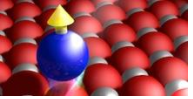
11.2 Intra-atomic exchange in rare earth atoms - Solution

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





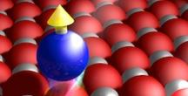


11.3 Dipolar interaction

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
$\mu_0 = 4\pi \cdot 10^{-7}$ T m A^{-1}
$\mu_B = 9.27 \cdot 10^{-24}$J T^{-1}
$1\,\text{J} = 6.24 \cdot 10^{18}$eV
$k_B = 8.617 \cdot 10^{-2}$meV K^{-1}

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



11.3 Dipolar interaction - Solution

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

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

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