

Solution to Exercise 4.3-2

Illustration

Given the type of lattice, the lattice constants of **Fe**, **Ni**, **Co** ([look it up!](#)), and the magnetization curves in [chapter 4.3-2](#): How large are the magnetic moments of these atoms in terms of a Bohr magneton?

Simple - but still a bit tricky.

First we get the basic data:

- Lattice **Fe**: **bcc**; lattice constant $a = 2.86 \text{ \AA}$; atomic density $\rho_A(\text{Fe}) = 2/0.286^3 \text{ atoms/nm}^3 = 85.5 \text{ atoms/nm}^3$
- Lattice **Ni**: **fcc**; lattice constant $a = 3.52 \text{ \AA}$; atomic density $\rho_A(\text{Ni}) = 4/0.352^3 \text{ atoms/nm}^3 = 91.7 \text{ atoms/nm}^3$
- Lattice **Co**: **bcc**; lattice constant $a = 2.51 \text{ \AA}$, $c = 4.07 \text{ \AA}$; atomic density $\rho_A(\text{Co}) = 2/[1/2 \cdot c \cdot a^2 \cdot 3^{1/2}] \text{ atoms/nm}^3 = 90.1 \text{ atoms/nm}^3$

Then we realize that the curves in [chapter 4.3-2](#) give the maximum magnetization, i.e. the magnetization state for all magnetic moments perfectly aligned. From the figure we can deduce the following numerical values for the saturation magnetization m_{Sat} :

- $m_{\text{Sat}}(\text{Fe}) = 17 \cdot 10^5 \text{ A/m}$
- $m_{\text{Sat}}(\text{Ni}) = 5 \cdot 10^5 \text{ A/m}$
- $m_{\text{Sat}}(\text{Co}) = 14 \cdot 10^5 \text{ A/m}$

However, the units shown are **A/m**, which are not what we would expect. Obviously we must convert this to - well, what exactly?

If we look at a Bohr magneton, m_{Bohr} , we have

$$m_{\text{Bohr}} = 9.27 \cdot 10^{-24} \text{ Am}^2$$

Obviously, the unit we need is **Am²**. We obtain that by multiplying the **A/m** by **m³**, which makes clear that the m_{Sat} numbers given are per **m³** - as they should be!

The magnetic moments m_A per atom are thus

$$m_A = \frac{m_{\text{Sat}}}{\rho_A}$$

What we obtain is

$$\begin{aligned} m_A(\text{Fe}) &= \frac{17 \cdot 10^5 \text{ A/m}}{85.5 \text{ atoms/nm}^3} = \frac{17 \cdot 10^5 \text{ A} \cdot 10^{-27} \text{ m}^3}{85.5 \text{ m}} = 1.98 \cdot 10^{-23} \text{ A/m}^2 = 2.14 m_B \\ m_A(\text{Ni}) &= 5.45 \cdot 10^{-24} \text{ A/m}^2 = 0.588 m_B \\ m_A(\text{Co}) &= 1.55 \cdot 10^{-23} \text{ A/m}^2 = 1.67 m_B \end{aligned}$$

Now that is an interesting result! It's satisfying because we actually get sensible numbers close to a Bohr magneton, and it's challenging because those numbers are not very close to 1, 2, or possibly 3.

For example, how can a **Ni** atom have a magnetic moment of **0.588 m_B**, and a **Fe** atom one of **2.14 m_B**, considering that the spins of the electrons carry exactly **1 m_B**?

There are two possibilities for this apparent discrepancy:

- Our calculation is somehow a bit wrong
- There are some effects not yet discussed that change the magnetic moment an atom in a crystal lattice carries around with itself somewhat.

The first possibility can be ruled out, because in standard textbooks, e.g. in the "*Kittel*" we find the following values for m_A

- $m_A(\text{Fe}) = 2.22 m_B$
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- $m_A(\text{Ni}) = 0.606 \text{ m}_B$
- $m_A(\text{Co}) = 1.72 \text{ m}_B$

Not identical, but close enough. In fact, looking more closely, the Kittel values are for $T = 0 \text{ K}$, whereas our values are for room temperature $T = 300 \text{ K}$ and thus should be a bit smaller.

- Obviously, this leaves us with some effects not yet discussed. What these effects could be, we can only guess at. Here is a short list:
 - There might be some interaction between the spins of the electrons and the "orbits" of the electrons that modifies the magnetic moment
 - The free electrons of the electron gas in our metal also "feel" the ordered spins of the atoms and react to some extent by adjusting their spins.
- This can lead to quite sizable effects. Dysprosium (**Dy**), for example, a rare earth metal, is a ferromagnet below its Curie temperature of **88 K** and its atoms than carry an $m_A(\text{Dy}) = 10.2m_B$.