Solution to Exercise 4.3-2

Given the type of lattice, the lattice constants of **Fe**, **Ni**, **Co** (<u>look it up!</u>), and the magnetization curves in <u>chapter 4.3-</u> <u>2</u>: 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 Å; atomic density ρ_A(Fe) = 2/0.286³ atoms/nm³ = 85.5 atoms/ nm³
- Lattice Nifcc; lattice constant a = 3.52 Å; atomic density ρ_A(Ni) = 4/0.352³ atoms/nm³ = 91.7 atoms/ nm³
- Lattice Co: bcc; lattice constant a = 2.51 Å, c = 4.0 7Å; atomic density ρ_A(Co) = 2/[½ · c · a² · 3^½ atoms/nm³ = 90.1 atoms/nm³

Then we realize that the curves in <u>chapter 4.3-2</u> 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}:

- $m_{\text{Sat}}(\text{Fe}) = 17 \cdot 10^5 \text{ A/m}$
- $m_{\text{Sat}}(\text{Fe}) = 5 \cdot 10^5 \text{ A/m}$
- *m*_{Sat}(Fe) = 14 · 10⁵ 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, mBohr, we have

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

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

$$m_{A} = \frac{m_{Sat}}{\rho_{A}}$$

What we obtain is

m _A (Fe) =	17 · 10 ⁵ A/m	17 · 10 ⁵ /	$\frac{17 \cdot 10^5 \text{ A} \cdot 10^{-27} \text{ m}^3}{} = 1.98 \cdot 10^{-23} \text{ A/m}^2 = 2.14 \text{ mg}^2$		
	85.5 atoms/nm ³	= 85.5	m	$= 1.96 \cdot 10^{-9} \text{ A/m}^{-} = 2.14 \text{ m}_{\text{B}}$	
m _A (Ni) =				$5.45 \cdot 10^{-24} \text{ A/m}^2 = 0.588 \text{ m}_{\text{B}}$	
m _A (Co) =				$1.55 \cdot 10^{-23} \text{ A/m}^2 = 1.67 \text{ m}_{\text{B}}$	

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:

- 1. Our calculation is somehow a bit wrong
- 2. 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(Fe) = 2.22 m_B

- m_A(Ni) = 0.606 m_B
- m_A(Co) = 1.72 m_B

Not identical, but close enough. In fact, looking more closely, the Kittel values are for T = 0 K, whereas our values are for room temperature T = 300 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 $m_A(Dy) = 10.2m_B$.