Solution to Exercise 4.3-2

- 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 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 $\rho_A(Co) = 2/[\frac{1}{2} \cdot c \cdot a^2 \cdot 3^{\frac{1}{2}}]$ 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_{Sat}(Fe) = 17 · 10⁵ A/m
 - $m_{Sat}(Fe) = 5 \cdot 10^5 \text{ A/m}$
 - $m_{Sat}(Fe) = 14 \cdot 10^5 \text{ A/m}$
 - 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, mBohr, we have

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

- Obviously, the unit we need is Am^2 . We obtain that by multiplying the A/m by m^3 , which makes clear that the m_{Sat} numbers given are per m^3 as they should be!
- The magnetic moments m_A per atom are thus

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

What we obtain is

$$m_{A}(Fe) = \frac{17 \cdot 10^{5} \text{ A/m}}{85.5 \text{ atoms/nm}^{3}} = \frac{17 \cdot 10^{5} \text{ A} \cdot 10^{-27} \text{ m}^{3}}{85.5} = 1.98 \cdot 10^{-23} \text{ A/m}^{2} = 2.14 \text{ m}_{B}$$

$$m_{A}(Ni) = 5.45 \cdot 10^{-24} \text{ A/m}^{2} = 0.588 \text{ m}_{B}$$

$$m_{A}(Co) = 1.55 \cdot 10^{-23} \text{ A/m}^{2} = 1.67 \text{ m}_{B}$$

- 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 $m_A(Dy) = 10.2m_B$.