Simulations of electron holographic observations of magnetic microstructure in exsolved titanomagnetites

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1) Introduction

Titanomagnetite inclusions in slowly-cooled rocks can contain exsolution microstructures that consist of closely-spaced ferrimagnetic magnetite (Fe_3O_4) prisms separated by paramagnetic ulvöspinel (Fe_2TiO_4) lamellae. Electron holography was used to image the magnetic remanent states of such inclusions showing that the prisms are mostly magnetostatically-interacting single domains. Figure 1 shows a set of magnetized prisms, with the orientation of their magnetic field revealed by the projected flux lines in colors (within and outside each element).

Figure 1: Magnetic microstructure measured by electron holography. Image was acquired with the sample in field-free conditions. The outlines of the magnetite-rich regions are marked in white, while the direction of the measured magnetic induction is indicated both using arrows and according to the color wheel shown at the bottom. The spacing of the black contours provides a measure of the strength of the magnetic field in the plane of the sample. Figure taken from Ref. [1].

The magnetic microstructure depends sensitively on the shapes, spacings and orientations of the prisms, as well as on magnetic history. To understand the observed magnetic microstructures, we have carried out simulations of linear arrays of uniformly-magnetized magnetite prisms by making use of known expressions for demagnetization factors.

By varying the size and spacing of the prisms it is possible to chart the magnetic microstructures of such mineral assemblages in the form of a "magnetic microstructure phase diagram".

Whereas shape anisotropy suggests that the long dimension of each prism should be its easy axis, if more elements are considered interactions change the energy balance of the combined magnetic state.

We analyze the energetics of two competing collective states of magnetization in a linear array of identical prisms: the overall anti-ferromagnetic state, where prisms are magnetized along their easy axes with alternating sign (antiparallel to each other), and the overall ferromagnetic state where prisms are magnetized along their *hard* axes.

We arrive at a multi-dimensional phase diagram illustrating the expected magnetic ground state as a function of several parameters: the prisms aspect ratio, their separation, the magnetocrystalline anisotropy, and the number of prisms in the chain.

In the simplest case of two 200-nm-wide prisms that are separated by 10 nm in a specimen of thickness 20 nm with no magnetocrystalline anisotropy, the simulations suggest that the transition between the two states occurs at a prism height of 158 nm. Visual inspection of the experimental images reveals that these theoretical estimates are consistent with observations.

2) The basics

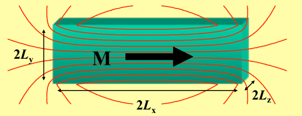
The magnetostatic energy associated to a uniformly magnetized prism of voulme V is given by:

$$E_m = \frac{1}{2}\mu_0 M_0^2 V \left(N_x m_x^2 + N_y m_y^2 + N_z m_z^2 \right)$$

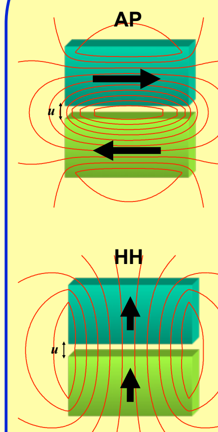
where M_0 is the saturation magnetization, $m_{x,y,z}$ are the magnetization components, and $N_{x,y,z}$ are the demagnetization factors for prisms [2] along the three symmetry axes.

The demagnetization factors, quantities varying in [0,1], always sum up to 1, and are a measure of the shape anisotropy present. The larger a demagnetization factor is, the larger it is the demagnetization field, the more difficult it is to magnetize an element along that particular direction. Hence, when the factor along an axis is close to 1, it is difficult to magnetize along that specific axis, which becomes an *hard* axis of magnetization. On the contrary, when a factor is close to zero, the axis is *easy*.

A single domain element will magnetize spontaneously in the direction with the lowest demagnetization factor. Since the factors are generally inversely related to the length of the element along a given direction, we expect a prism to magnetize along its *longer* side.



3) The competing states

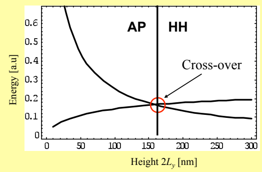


Neighboring elements are magnetostatically coupled. Anti-ferromagnetic alignment of stacked elements is intuitively expected to be favored, because the stray fields are minimized (**AP**). When the stack reaches a critical size, it becomes a single elongated magnet that is expected to magnetize along the stacking direction (hard axis of each element, **HH**).

To quantify the trade-off size of this "spin-reorientation" transition we calculate and compare the energies of the two competing states searching for the global minimum as a function of the various parameters involved (distance u, number N, thickness t, etc.).

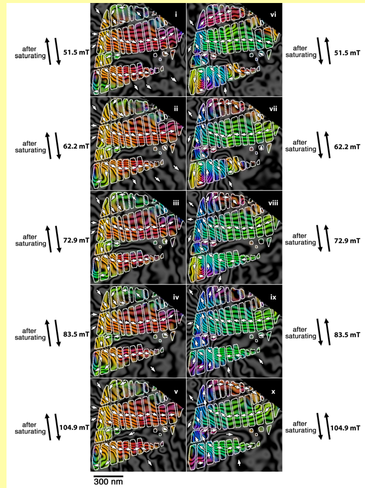
$$E_{AP} = 2E_{self}^{\rightarrow} + E_{int}^{\rightleftarrows} \qquad E_{HH} = 2E_{self}^{\uparrow} + E_{int}^{\uparrow\uparrow}$$

Due to the favorable alignment of the elements, the interaction energy terms may be expressed as a combination of demagnetization factors for prisms [3].

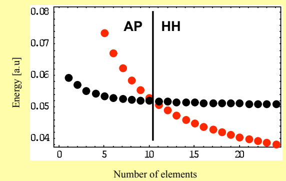


Plotting the energies we find a *Cross-over* point, where the state of minimum energy changes. The simplest "phase diagram" is shown above, revealing a critical point at a height of 158 nm for two 200 nm wide prisms of 20 nm thickness separated by 10 nm.

4) Stacks of elements

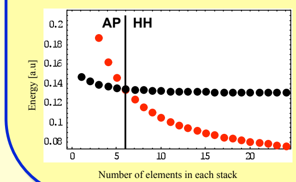


The number of elements in a stack is a relevant parameter in establishing the cross-over critical point. In the figure above (from Ref. [4]), elements are highly anisotropic if considered alone (the aspect ratio of most elements is between 2 and 4), but we still observe **HH**-type configurations. Fixing the aspect ratio of each element to 3, we can re-calculate the cross-over point as a function of number of elements in the stack, finding that at least 10 elements are needed to establish the **HH** state.

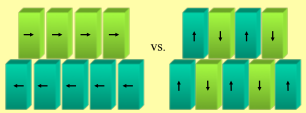


5) Collective behavior

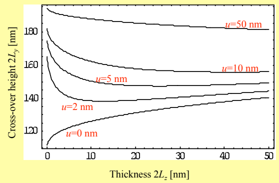
Figure 2. Above: portion of the experimental image in section 4 (51.5 mT reversal field) showing the reciprocal stabilizing effect of adjacent stacks when they are slightly misaligned and anti-parallel to each other. Below: the phase diagram associated to these collective states.



A closer look at the experimental images reveals that **HH**-type states are more frequent than we may expect on the basis of the simple theory we just introduced. For instance, the stack of 7 elements with aspect ratio 4 in Fig. 2 (top) is not supposed to be **HH** according to theory. However, in the same image we note the presence of the top stack of 6 smaller elements with aspect ratios closer to 2 or 3, that is also in **HH** state, but with the magnetization pointing in the opposite direction (and with a lateral misalignment). It is reasonable to assume that the presence of this second stack makes it possible for the lower stack to maintain an **HH** state. To confirm this, we have re-calculated the plot showing the cross-over dependence on the number of elements for a double-stack system. The new phase diagram shows that, indeed, for a system that resembles the one observed experimentally, a dual **HH** state with slightly misaligned anti-parallel stacks is the ground state.



6) Thickness and distance



The cross-over point depends on the thickness of the elements $2L_z$, a quantity that is not easy to estimate experimentally. It also depends, and to a larger extent, on the separation distance u between the elements. This is shown in the plot above, where critical curves (phase boundaries) are drawn as a function of thickness for several values of the separation u. The **HH** state is expected above the phase boundary, while the **AP** state is expected below it. The curves refer to prisms of lateral size $2L_x$=200 nm.

References

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