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Micromagnetics for the coercivity of nanocomposite permanent magnets

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Abstract: *Exchange spring permanent magnets may be a route towards high energy product permanent magnets with low rare-earth content. In composite magnets soft magnetic phases act as nucleation sites for magnetization reversal. We use micromagnetic simulations in order to understand the role of the size and shape of the soft inclusions on the magnetization reversal. We compare the switching field of magnetically soft spheroids, cuboids and cylinders embedded in a hard magnetic matrix. Whereas there is only little difference in the switching field for enclosed spherical or cubical soft shapes, prolate inclusions enhance the stability of the magnet.*

Keywords: *two phase nanocomposite magnets, micromagnetics simulations*

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Introduction

Micromagnetics is a continuum theory that describes magnetization processes on a length scale ranging from about a nanometer to micrometers. Using the finite element method in order to discretize the micromagnetic equations we can compute the coercive field of a permanent magnet depending on its physical and chemical structure. Especially simple geometrical models are useful, in order to understand and quantify the different factors that determine the coercive field of a composite magnet. The theory of exchange spring permanent magnets was discussed by Kneller [1], Skomski [2], and Schrefl [3]. Skomski and co-workers [4] compared the nucleation field of different hard-soft geometries. Spheres were reported to show a higher nucleation field as compared to cylinders or layered structures. In this work we apply numerical micromagnetics, in order to evaluate hard-soft shapes and their influence on magnetization reversal. In particular we are interested in the effect of shape and size of a single soft inclusion in a hard magnetic matrix. The influence of magnetostatic interactions between several soft inclusions in a hard matrix is discussed in [5].

Method

We use a finite element micromagnetic software for the solution of the Landau-Lifshitz Gilbert equation [6]. First the external field H_e is kept zero for 10 ns, in order to obtain a remanent magnetic state. Then H_e is applied at a rate of -80 mT/ns up to -8 T. The field is applied at an angle of 0.5 degrees with respect to the easy axis of the hard magnetic material. The Gilbert damping constant is one. We use a soft phase (α-Fe) with a magnetic polarization $J_s = 2.15$ T and an exchange constant $A = 21$ pJ/m. As magnetically hard phase we use $Nd_2Fe_{14}B$ with uniaxial anisotropy constant $K_1 = 4.9$ MJ/m³, $J_s = 1.61$ T and $A = 8$ pJ/m. A single α-Fe spheroid, cuboid or cylinder is embedded into a $Nd_2Fe_{14}B$ spherical or ellipsoidal shell. The demagnetizing field of a uniformly magnetized sphere or ellipsoid is uniform. Therefore we avoid any reduction of the coercive field by strong demagnetizing fields near corners or edges of the macroscopic sample [7]. Still the macroscopic demagnetizing field of the shell creates an additional field that acts on the soft inclusions. Thus when comparing the switching field of different soft shapes we add the macroscopic demagnetizing field $-NM$ of the sample to correct the loop. N is the demagnetizing factor of the macroscopic shape and M the magnetization. We define the switching field, H_{sw}, as the critical field when the hard phase switches irreversibly. For fair comparison, the volume of the differently shaped inclusions is kept the same and placed inside the same shell. For samples varying in size the volume ratio between α-Fe and $Nd_2Fe_{14}B$ is kept constant.

Results

We start with investigating the influence of the particle shape on the magnetization of an isolated $Nd_2Fe_{14}B$ particle. Fig. 1 shows that the non-uniform demagnetizing fields reduce the coercive field of a cube with respect to the coercive field of a sphere. But embedded into a hard

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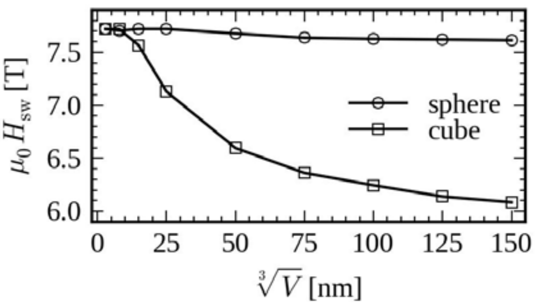

Fig. 1. Switching field of $Nd_2Fe_{14}B$ cubes and spheres with volume V.

magnetic matrix, soft spheres and soft cubes with equal volume, V_s, yield almost the same switching field. Increasing the share of magnetically hard material increases the switching field only for small inclusions with an edge length or diameter less than 10 nm to 12 nm, respectively (Fig. 2). Even for a small 4x4x4 nm³ inclusion, H_{sw} is reduced by 2 T compared to H_{sw} of a pure $Nd_2Fe_{14}B$ sphere.

In order to study the influence of reduced exchange coupling between the magnetically hard matrix and the soft magnetic inclusion, we introduce a 1 nm thick interlayer. The volume of the shell plus interlayer is seven times the volume of the soft body, V_s. The material constants of the interlayer are adjusted according to $A_i = fA_{hard}$, $J_{s,i} = J_{s,hard}(A_i/A_{hard})^{1/2}$, and $K_{1,i} = K_{1,hard}(J_{s,i}/J_{s,hard})^3$, whereby the subscript 'hard' refers to the $Nd_2Fe_{14}B$ constants. Fig. 3 shows the soft phase reversal field (open markers) and the hard phase switching field (filled markers). Here we define the soft phase reversal field as the critical field at which the magnetic polarization reaches $0.9J_s$.

With full coupling (square markers) we observe

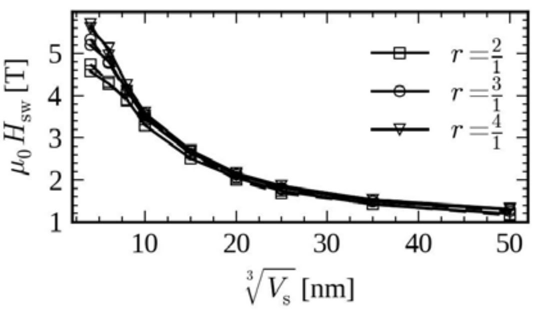

Fig. 2. Switching field of α-Fe cubes (solid line) and spheres (dashed line) with equal volume V_s in a $Nd_2Fe_{14}B$ spherical shell. r denotes the ratio of hard to soft magnetic volume.

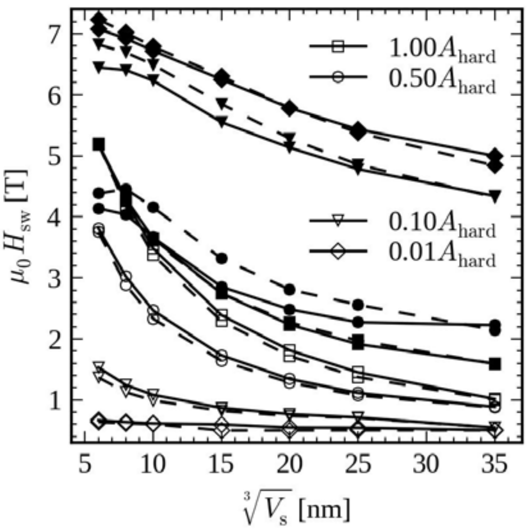

Fig. 3. α-Fe cubes (solid line) and spheres (dashed line) enclosed by a 1 nm interlayer in a $Nd_2Fe_{14}B$ spherical matrix. The interlayer exchange constant $A_i=fA_{hard}$ is reduced to decouple inclusion and shell. Open markers refer to the soft phase reversal field and filled markers to the hard phase switching field.

the transition from a one-step magnetization reversal for small inclusions (V_s < 10x10x10 nm³) to a two-step reversal for larger embeddings. The difference between the soft phase reversal field and the hard phase switching field is less than 0.6 T shrinking with the size of the soft body. With reduced exchange coupling the switching fields of the two phases are clearly distinct. The difference in H_{sw} increases to about 1.5 T when the coupling is reduced by $f = 0.5$. For $f = 0.01$ the soft phase reversal field approaches for the macroscopic demagnetizing field *NM* whereas the hard phase reverses at switching fields between 5 T and 7.2 T depending on the size of the inclusion. The shape of the inclusion has only little influence on the reversal of the soft phase. But samples with a spherical inclusion show a more stable hard phase when coupling is reduced.

In [8] it has been reported that the nucleation field can be enhanced significantly by transforming a soft magnetic sphere to an elongated shape such as a cylinder or a prolate spheroid but H_c plateaus for aspect ratios larger than 5. Fig. 4 shows the switching field for such prolate soft inclusions inside a $Nd_2Fe_{14}B$ prolate spheroid. The shell's minor axis is twice the inclusion diameter. The major axis is adjusted to fit the elongated inclusions keeping the ratio of

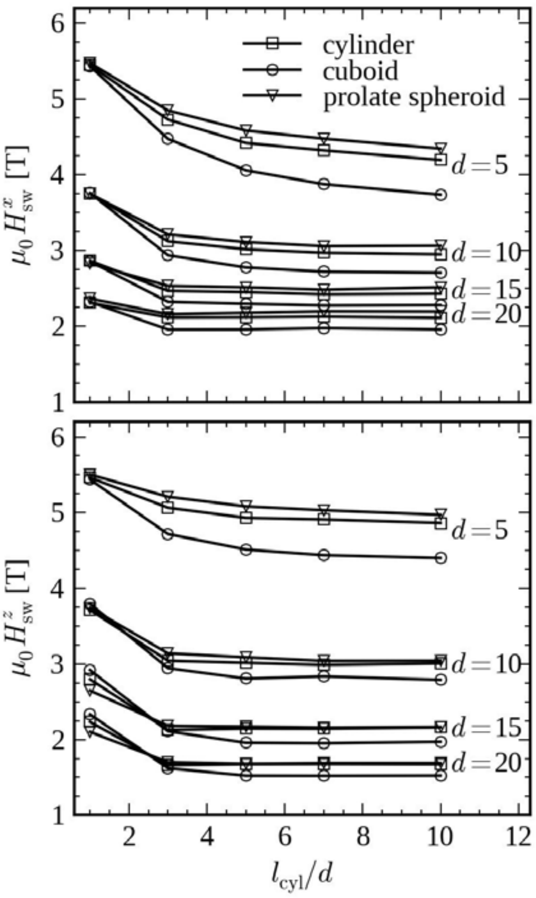

Fig. 4. Switching field of prolate α-Fe inclusions in an ellipsoidal hard magnetic shell. The volume of the soft phase is equal to the volume of a cylinder with diameter d and length l_{cyl}. The diameter d is common for all three embeddings but the length is adjusted to comply with the volume constraint. The volume ratio of shell to inclusion is 4:1. 'x' and 'z' in the axes labels refer to an orientation of the inclusions' long axis perpendicular or parallel to the easy axis of the hard phase, respectively.

magnetically hard to soft material at 4:1. We compare two orientations. In the upper figure of Fig. 4 we choose the long axis of the soft inclusion to be perpendicular to the easy axis of the hard material and the applied external field. We refer to this orientation with '*x*'. The figure below deals with a configuration with the long axis parallel to the easy axis and external field ('z'). In general, an ellipsoidal shaped inclusion stabilizes the magnet better than a cylinder or cuboid. With raising diameter the differences diminish. Unlike the single phase results, elongating the soft magnetic inclusions still decreases the switching field but it plateaus again for higher aspect ratios. For small diameters, an inclusion aligned parallel to the easy axis results in a more stable magnet than a configuration with an inclusion perpendicular to the easy axis. The difference in the switching field is 0.6 T shrinking with lower aspect ratios l_{cyl}/d. However, for diameters larger than 10 nm a soft phase in '*x*'-orientation results in a 0.2-0.5 T higher switching field. If we compare H_{sw} of similar inclusion volumes in Figures 2 and 4 we notice significantly higher switching fields for prolate inclusions than for cubes or spheres. (Cylinder: $d = 10$ nm, l_{cyl} = 100 nm; cube 20x20x20 nm^3).

Conclusions

For small soft magnetic inclusions within a hard magnetic matrix, the shape of the soft inclusions was found to contribute to the coercive field with prolate spheroids showing the highest switching field. If lateral extension of the soft inclusion was greater than 10 nm the shape effect was suppressed. For elongated soft inclusions such as cylinders or prolate spheroids it is preferable to align them parallel to the easy axis if the diameter is smaller than 10 nm. For wider soft inclusions an orientation perpendicular to the easy axis leads to better stability.

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