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ABSTRACT
We report a theoretical discussion of the impact the composition on the maximum energy product (\((BH)_{\text{max}}\)) of core@shell FePt@CoFe$_2$ and FePt@Fe nanocylinders. We have found that the best composition is determined by the competing trends imposed by a strong ferromagnetic core@shell interface exchange energy, and the core@shell dipolar interaction energy. The dipolar interaction has a negative impact on the nanocylinder \((BH)_{\text{max}}\) value, for shell thickness above a shell material dependent threshold value. We have also found that Fe is the best shell material owing to its much larger exchange stiffness.

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I. INTRODUCTION

Systems composed of spherical bimagnetic core-shell nanoparticles have been considered for several applications of current interest. Combining different functionalities of two magnetic materials, into the effective magnetic properties of a single nanoparticle, one may optimize systems for key applications such as permanent magnets, recording media, and magnetic hyperthermia.

Furthermore, nanomagnets are currently being considered for designing arrays to produce artificial spin-orbit systems using one-dimensional quantum wires. These applications require small size magnets with controllable stray field strengths. This may turn to be a novel application of cylindrical hard-soft core@shell nanoparticles.

Recent reports on circular and rectangular cylindrical core@shell nanoparticles reveal that new magnetic phases emerge from the dipolar interaction coupling core and shell magnetic moments.

The interplay between the core@shell interface exchange energy and the core@shell dipolar interaction energy, is a key issue for defining the structure of the magnetic phases of ferrite core@shell nanoparticles and hard-soft SmCo$_5@$Fe spherical core@shell nanoparticles.

The shell reversal process of spherical SmCo$_5@$Fe core@shell nanoparticles is tunable by the values of the core diameter and shell thickness, and energy product optimization requires small core diameter values, allowing energy product enhancement of more than 370% for small core diameters SmCo$_5@$Fe nanoparticles.

We presently report a theoretical discussion of the impact core-shell composition on the maximum energy product of FePt@CoFe$_2$ and FePt@Fe nanocylinders, with the magnetization along the cylindrical axis. We have considered 30 nm high FePt(D)@Fe(\(\delta\)) and FePt(D)@CoFe$_2$(\(\delta\)) nanocylinders, for core diameter (D) values in the 7 nm - 21 nm range, and shell thicknesses from \(\delta = 1\) nm to \(\delta = 6\) nm.

We have found that the best enhancement of the energy product requires small FePt core diameter values. Furthermore, Fe is the best choice for the shell material, due to its much larger exchange stiffness value, as compared to that of CoFe$_2$. 
The small value of the exchange stiffness favors the formation of twisted states in the CoFe$_2$ shell, reducing the core@shell magnetization. It also favors switching at low external field values in the demagnetization quadrant and dropping the maximum energy product value.

For instance, a 30 nm high FePt(7 nm)@CoFe$_2$(5 nm) nanocylinder, has a small value of the maximum energy product, at an external field value of $H = -1$ kOe. At this point, as shown in Fig. 1, the CoFe$_2$(5 nm) shell displays a $\pi$-magnetization twist, with 60% of the shell magnetization switched to the direction opposite to the FePt(7 nm) core magnetization, leading to a small value of the energy product.

As seen in Fig. 2, the maximum energy product of the 30 nm high FePt(7 nm)@CoFe$_2$(5 nm) nanocylinder is 1.18 MGOe, representing 2.32% of the maximum energy product of the FePt core (51.12 MGOe).

The maximum energy product of the 30 nm high FePt(7 nm)@Fe(5 nm) core@shell nanocylinder is much larger, 78.39 MGOe, as shown Fig. 2. As we shall discuss below, due to the larger Fe exchange stiffness, at the maximum energy product point the external field strength is larger ($H = -6$ kOe) and the magnetization is rather close to the saturation value, as shown in Fig. 3.

II. THEORETICAL MODEL

We consider a single cylindrical core@shell nanoparticle. We assume that both core and shell materials have a uniaxial magnetic anisotropy, with the easy axis along the nanocylinder $z$-axis. The magnetic structure is described using small cubic cells with 1 nm edge, and the energy density is given by:

$$E = -H\hat{z} \cdot \sum_j M_j \hat{S}_j - \sum_j K^j (M_j^z)^2 + \frac{1}{2} \sum_j \sum_k M_j^z M_k^z \times \frac{\hat{n}_j \cdot \hat{n}_k}{\hat{n}_j^3} - \frac{3(\hat{m}_j \cdot \hat{n}_k)(\hat{m}_j \cdot \hat{n}_j)}{\hat{n}_j^5} \hat{n}_j \times \hat{m}_j$$

The first two terms are the Zeeman and anisotropy energies. $M_j^z$ and $K^j$ are the $j$-cell saturation magnetization and uniaxial anisotropy density, and $\hat{m}_j$ is the magnetization direction. In the dipolar energy, $\hat{n}_{jk}$ is the distance between the cells $j$ and $k$ in units of cell edge. The exchange energy, couples nearest neighbor cells. $A_{jk}$ is the core or
the shell exchange stiffness, for cells $j$ and $k$ within the same material. Otherwise, it represents the effective interface exchange energy.

The effective magnetic coupling of the core and shell materials is, on one hand, one of the crucial features which allows improving the core@shell energy product. On the other hand, it is one of the many possible interesting manifestations of the magnetic proximity effects which have so far been reported when two magnetic materials are put in close contact. Interestingly, the proximity effect has been reported even for superlattices made of insulating antiferromagnetic materials, exploring measurements of the superlattice thermal expansion coefficient, and theoretical modelling of the magnetic heat capacity.

The local environment of the magnetic ions near the interface is affected by composition gradients, voids and vacancies, lattice mismatch and the lattice relaxation in both materials. Thus, the core-shell exchange interaction is likely to be site-dependent and depend on sample preparation. We make the simplifying assumption of an uniform interface, with an effective interface exchange energy equal to that of the core material.

The equilibrium configuration is found using a self-consistent algorithm. The magnetization $\mathbf{m}_j$ is adjusted to be parallel to the local magnetic field $\mathbf{H}_j^{\text{eff}} = -(1/M_j)(\partial E/\partial \mathbf{m}_j)$, so that, within a reasonable numerical precision, $\langle \mathbf{m}_j \times \mathbf{H}_j^{\text{eff}} \rangle = 0$. Convergence is checked to guarantee a maximum torque of $10^{-26}$.

For Fe we use $M_s = 1700$ emu/cm$^3$, $A = 25 \times 10^{-7}$ erg/cm$^3$, and $K = 4.8 \times 10^5$ erg/cm$^3$. For CoFe$_2$ we use $M_s = 1800$ emu/cm$^3$, $A = 1.9 \times 10^{-7}$ erg/cm$^3$, and $K = 1.7 \times 10^5$ erg/cm$^3$. For FePt we use $M_s = 1139$ emu/cm$^3$, $A = 1.0 \times 10^{-6}$ erg/cm$^3$, and $K = 6.6 \times 10^5$ erg/cm$^3$.

**III. RESULTS AND DISCUSSIONS**

In order to find an optimum core@shell composition, taking advantage of the large core anisotropy energy density and the large shell magnetization, one has to deal with two competing trends: the core-shell interface exchange energy and the core-shell dipolar energy.

A strong ferromagnetic core-shell interface exchange energy interaction contributes to keeping the core and shell magnetizations parallel, favoring large values of the energy product.

However, the interface exchange energy is a contact interaction coupling directly only the core and shell magnetic moments at the interface. The dipolar interaction, on the other hand, is long-ranged and couples all the core and shell magnetic moments and tends to align the core and shell magnetizations in opposite directions.

For both shell materials, beyond a critical value of the shell thickness ($\delta^*$), the dipolar interaction prevails, and, as shown in Fig. 2, the core@shell maximum energy product starts dropping.

In Fig. 2, we show the maximum energy product of 30 nm high FePt(7 nm)@CoFe$_2$(4 nm) and FePt(7 nm)@Fe(4 nm) nanocylinders. The energy product of the FePt(7 nm)@CoFe$_2$(4 nm) nanoparticles drops much more rapidly than that corresponding to the FePt(7 nm)@Fe(4 nm) nanoparticles. The Fe shell critical thickness, $\delta^* = 4$ nm, is larger than that of the CoFe$_2$ shell, $\delta^* = 2$ nm, leading to a more significant enhancement of the energy product of the FePt(7 nm)@Fe(4 nm) nanoparticles.

In Fig. 3, we show the demagnetization curves of 30 nm high FePt(7 nm)@Fe(4 nm), FePt(7 nm)@Fe(5 nm) and FePt(7 nm)@CoFe$_2$(4 nm) nanoparticles. The maximum energy product points for FePt(7 nm)@Fe(4 nm) and FePt(7 nm)@Fe(5 nm) core@shells occur with the magnetization near the saturation value, at external fields of $H = -9$ kOe and $H = -6$ kOe. Fig. 4 shows that even for a smaller field strength, near 50% of the CoFe$_2$(4 nm) shell magnetization has switched to the direction...
FIG. 6. $yz$–plane magnetization maps of a 30 nm high FePt(7 nm)@CoFe$_2$(5 nm) nanocylinder, at the maximum energy product point, corresponding to $H = -1$ kOe. The color bar code gives the $x$–component of the magnetization, in units of the $M_S$. The opposite to the core magnetization, and the nanocylinder magnetization has dropped to 40% of the saturation value, as shown in Fig. 3.

For an external field of $H = -9$ kOe, a 30 nm high FePt(7 nm)@Fe(5 nm) nanocylinder has a $\pi$ twist, from the core-shell interface to the shell surface, with 75% of the shell magnetization opposite to the core magnetization, and the core-shell magnetization switched to -36% of the saturation value.

We have found that the 30nm high FePt(7 nm)@Fe(4 nm) nanocylinder has a maximum energy product of 95.92 MGOe, which is almost 88% larger than that of the FePt core (51 MGOe). Also, using a CoFe$_2$ shell, the maximum energy product is 78.2 MGOe, for a 2 nm thick CoFe$_2$ shell.

As shown in Fig. 2, 30 nm high FePt(7 nm)@Fe(5 nm) and FePt(7 nm)@CoFe$_2$(5 nm) nanocylinders have maximum energy product values of 78.39 MGOe and 1.18 MGOe. The difference is due to the large dipolar field at the CoFe$_2$(5 nm) shell, as shown in Fig. 5, which produces a $\pi$–twist in the shell, with 60% of the shell magnetization switched to the direction opposite to the core magnetization (see Fig. 6).

Fig. 7 shows that the stray field of a 30 nm high FePt(7 nm)@Fe(4 nm) nanocylinder is larger than that of a FePt(7 nm)@CoFe$_2$(4 nm) nanocylinder. At 7nm distance from the pole, the FePt(7 nm)@Fe(4 nm) nanocylinder stray field is around 2.7 kOe, and is a hundred times larger than that of the FePt(7 nm)@CoFe$_2$(4 nm) nanocylinder at the same distance from the pole (0.023 kOe). The FePt(7 nm)@Fe(4 nm) nanocylinder magnetization is uniform and saturated at remanence. Owing to the smaller exchange stiffness energy, the CoFe$_2$ shell of the FePt(7 nm)@CoFe$_2$(4 nm) nanocylinder shows, at remanence, a large reduction of the magnetization component perpendicular to the circular faces of the nanocylinder, with a reduction of the stray field.

In addition to the results presented above, in Table I we compare FePt(D)@Fe(\(\delta\)) and FePt(D)@CoFe$_2$(\(\delta\)) nanocylinders with 11 nm and 21 nm FePt core diameter values.

### IV. CONCLUSIONS

In summary, we have found that the optimization of the energy product requires small values of the FePt core diameter and Fe shells. The Fe exchange stiffness energy (25 $\times$ 10$^{-7}$ erg/cm), is 13.16 times larger than that of CoFe$_2$ (1.9 $\times$ 10$^{-7}$ erg/cm). Therefore, the exchange energy cost for a twist in the shell magnetization, is larger in the FePt@Fe nanocylinders than in the FePt@CoFe$_2$ nanocylinders. A twist in the shell magnetization of a given magnitude requires a thicker Fe shell, as compared to the CoFe$_2$ shell thickness for the same magnitude of twist.

Thus, although having a smaller magnetization ($M_S = 1700$ emu/cm$^3$) than CoFe$_2$(\(M_S = 1800$ emu/cm$^3$), Fe is the...
choice material for the shell, because the large value of exchange stiffness energy exchange favors coherent magnetization rotation in the demagnetization quadrant, and larger maximum energy product value.

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