Micromagnetic simulation of magnetization reversal in small particles with surface anisotropy

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In order to study the effect of surface anisotropy, we have developed a three-dimensional finite element micromagnetic model. The finite element mesh of the particles is split into a core region with bulk properties and a surface region (shell) of variable thickness with modified material parameters. We have studied the magnetization reversal in FePt nanoparticles. The effect of surface anisotropy strongly reduces their coercivity. An Fe–oxide shell with low anisotropy in the plane of the surface has been considered as well as surface anisotropy with high anisotropy constants and axis orientation perpendicular to the surface. © 2004 American Institute of Physics.

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I. INTRODUCTION

High density magnetic storage media require tight control of the grain size, grain size distribution, chemical composition, and microstructure to ensure the thermal stability of the bits and keep the media noise low. However, as the areal density increases, the grain size and the magnetic switching volume need to decrease and the surface to volume ratio increases. Thus, surface effects become more and more important for the properties of magnetic nanoparticles.

In order to maintain the stability materials with higher uniaxial anisotropy than the common CoCrPt alloys are required. FePt thin films1 and self assembled nanoparticles2 are promising candidates for high density magnetic storage media.3,4 Their magnetocrystalline anisotropy is 50–100 times larger than in CoCrPt media alloys which may allow areal densities in the Tbit/in² regime.

II. THE FINITE ELEMENT MODEL

The numerical computer simulations have been carried out using a three dimensional hybrid finite element/boundary element micromagnetic code5 with a magnetic scalar potential for the calculation of the demagnetizing field and a limited memory variable metric algorithm (quasi-Newton method) for minimization of the total energy.6,7 The total energy consists of the contributions from the magnetocrystalline anisotropy energy, exchange, magnetostatic, and Zeeman energy.

III. POLYCRYSTALLINE FePt NANO Particles

We have assumed a simple geometry with a hexagonal basis and a particle diameter between 15 and 120 nm with constant aspect ratio (diameter/height) of 3. The following material parameters for FePt have been assumed:4,8 K$_V$ = 7.7 MJ/m³, J$_S$ = 1.43 T, and A = 10⁻¹¹ J/m, where K$_V$ denotes the magnetocrystalline anisotropy constant, J$_S$ the saturation polarization, and A the exchange constant. The particle has been split into six different parts (according to its hexagonal shape) in which the orientation of anisotropy axes has been varied. In addition a surface shell of variable thickness surrounding the core of the particle has been defined to introduce surface anisotropy. Figure 1 shows an exploded view of the model.

The influence of the magnetostatic field has been shown to be negligible9 as compared to the anisotropy field and has been omitted in all simulations, since the nucleation field (i.e. the coercive field of these particles) is reduced by less than 5%.

IV. OXIDIZED SURFACE SHELL

The magnetic properties of the surface of FePt nanoparticles can be altered by oxidation. Fe$_3$O$_4$ and other oxidation states have been found by near edge x-ray absorption fine
FIG. 2. Coercivity (in units of the anisotropy field $H_{\text{eff}} = 2K_V/J_s$) as a function of particle diameter for a particle with a single anisotropy axis and reduced surface anisotropy ($\gamma$-Fe$_3$O$_4$ material parameters with in-plane anisotropy). The anisotropy axes in all six core parts are parallel to the $z$ axis; “SW” indicates the switching field of a Stoner–Wohlfarth particle for an external field applied at 3° from the anisotropy axis; $s2-8$ stands for the thickness of the surface shell as given in Table I.

V. SURFACE ANISOTROPY

If we assume strong surface anisotropy for FePt nanoparticles, effective anisotropy values as high as $K_{\text{eff}} = K_s/t = 46.2$ MJ/m$^3$ may arise in the surface shell, where $t$ indicates its thickness. This corresponds to a ratio $K_{\text{eff}}/K_V = 6$. As a result, we find a strongly disturbed magnetization distribution as shown in Fig. 4 for a uniaxial FePt nanoparticle with a diameter of 45 nm and a surface layer thickness of 1.5 nm.

The influence of the surface anisotropy on the coercivity of uniaxial FePt nanoparticles is shown in Fig. 5. For small particle sizes (but still large as compared to the exchange length) the coercivity approaches the nucleation field, because the thickness of the shell is on the order or below the domain wall thickness. As the particle size (and the shell thickness) increase, the coercivity is reduced by 50%. The disorder in the magnetization distribution on the surface of the particle facilitates the nucleation process and reduces the coercivity. For large particles the reduced coercivity remains

![Image](http://example.com/image.png)

**FIG. 3.** Coercivity as a function of particle diameter for different thicknesses of the surface shell ($s8$ gives the results without an oxide shell). A polycrystalline particle with 2:2:2 configuration of the magnetocrystalline anisotropy axes has been assumed (cf. Fig. 1).

**FIG. 4.** Remanent magnetization configuration of a uniaxial FePt nanoparticle with a diameter of 45 nm and effective surface anisotropy $K_{\text{eff}}/K_V = 6$ and a surface layer thickness of 1.5 nm. The arrows indicate the magnetization distribution in a cut plane parallel to the hexagonal faces through the center of the particle.

### TABLE I. Thickness $t_s$ and volume of the surface shell $V_{\text{shell}}$ in comparison with the core volume $V_{\text{core}}$ for a particle diameter of 60 nm.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>$t_s$ (nm)</th>
<th>$V_{\text{shell}}$ (nm$^3$)</th>
<th>$V_{\text{core}}$ (nm$^3$)</th>
<th>$V_{\text{shell}}/V_{\text{core}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$s2$</td>
<td>1</td>
<td>8000</td>
<td>38 000</td>
<td>0.21</td>
</tr>
<tr>
<td>$s4$</td>
<td>2</td>
<td>16 000</td>
<td>30 000</td>
<td>0.53</td>
</tr>
<tr>
<td>$s8$</td>
<td>4</td>
<td>29 000</td>
<td>17 000</td>
<td>1.71</td>
</tr>
</tbody>
</table>
constant, because the nucleation process does not depend on the particle size, when the thickness of the shell is larger than the domain wall size.

For particles with a diameter on the order of a few nanometers, Monte-Carlo simulations have shown this competition between surface and bulk anisotropy, which leads to throttled and “hedgehog” spin structures.\textsuperscript{14}

VI. CONCLUSIONS

We have studied the influence of core/shell configurations on the coercivity of FePt nanoparticles using micromagnetic simulations. Surface oxidation during the processing of FePt nanoparticles can lead to the formation of Fe–oxides with reduced magnetocrystalline anisotropy. The simulations show a reduction of the coercivity up to 75\% depending on the particle size and thickness of the oxide shell. A similar effect is observed for “pure” FePt nanoparticles due to intrinsic surface anisotropy. Strong surface anisotropy perpendicular to the surface facilitates the nucleation and magnetization reversal, which leads to a similar reduction of the coercivity.

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