Transition of magnetocrystalline anisotropy and domain structure in epitaxial Fe(001) nanomagnets

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The magnetocrystalline anisotropy of epitaxially grown bcc-Fe(001) films on GaAs(001) shows a transition from a fourfold intrinsic anisotropy in thick films to an uniaxial one in ultrathin films (<3 nm) and hence can be tuned by varying the film thickness. Here we investigate the consequence of such an anisotropy tuning for the magnetization configurations of nanomagnets. The thickness was varied between 2.5 and 30 nm in steps of 2.5 nm. Disks with diameters between 200 nm and 2 μm were patterned with electron beam lithography and ion beam etching. The remanent and ac-demagnetized states as well as the switching behavior were examined by magnetic force microscopy. In addition, we employed micromagnetic simulations to compare with the measured results. © 2003 American Institute of Physics. [DOI: 10.1063/1.1558256]

The growing number of investigations on micro- and nanomagnets made of epitaxial Fe(001) and Fe(110) grown on different substrates during the last few years indicates an increasing importance of this material system. This interest is not only motivated by the special magnetic properties of single crystalline iron, but also by large magnetoresistance effects predicted for magnetic tunnel junctions using single crystal iron contacts on semiconductor barriers. The demonstration of spin injection from epitaxially grown Fe contacts into GaAs (Ref. 10) or AlGaAs (Ref. 11) illustrates the importance of epitaxial contacts. However, the understanding of the domain formation and the magnetization reversal of ferromagnetic elements is crucial for their application in magnetoelectronic devices. In this respect the thickness dependent transition of strength and symmetry of the magnetocrystalline anisotropy in bcc Fe(001) films is an interesting property. Here we present an investigation of the influence of this transition on the domain configuration in nanomagnets made of such films.

The intrinsic anisotropy of the bcc Fe(001) films on GaAs(001) consists of a superposition of an effective fourfold term with a constant $K_1$ and a uniaxial component ($K_u$), both depending on the film thickness. In films thicker than 7 ML the easy axes of the fourfold anisotropy are oriented along [100] and [010], as expected for bulk Fe. The uniaxial easy axis is oriented along [110]. While the uniaxial component, which originates from the Fe/GaAs interface, increases with decreasing film thickness, the fourfold component decreases. As a result the effective intrinsic anisotropy shows a transition from a mainly fourfold symmetry in thicker films ($K_u < K_1$) to a dominating uniaxial one in thinner films ($K_u > K_1$).

By using molecular beam epitaxy (MBE) epitaxial Fe films were grown at room temperature on a GaAs(001) substrate. During evaporation the residual pressure was kept below $4 \times 10^{-10}$ mbar. The substrate was prepared by annealing in UHV at 900 K for 1 h, Ar+ ion etching (500 eV) at 900 K for 30 min, and further annealing for 1 h at 900 K. In order to obtain Fe films on the same substrate and grown under the same conditions a sample with stepped thicknesses was prepared using a shadow mask. The thicknesses varied from 2.5 to 30 nm in steps of 2.5 nm. Finally, all Fe films were covered with a 4 nm thick Au layer to prevent oxidation.

The films were patterned into elements with different shapes and sizes between 200 nm and 2 μm. First, a Ti etch mask was prepared on the Fe films by employing electron beam lithography (EBL) and lift-off. The structures were transferred into the iron film by using 500 eV Ar+ ion beam etching (IBE). In order to reduce the interaction between the magnetic force microscopy (MFM) tip and the sample, especially during the topography scan, the elements were finally coated with a 10 nm Ti layer. This was done by rotating the tilted sample (tilt angle 60°) around its surface normal to also cover the edges of the elements.

The domain configurations of the epitaxial Fe elements are a result of the competition between the uniaxial and fourfold intrinsic anisotropies as well as of the shape anisotropy. Circular disks without any in-plane shape anisotropy but also different rectangles were used for this investigation. The effect of the transition of the intrinsic anisotropy on the domain structure will be shown by comparing samples with four different thicknesses: 2.5, 5, 7.5, and 15 nm.

For the MFM investigations we employed a Digital Instruments Multimode atomic force microscope in noncontact mode and phase detection of the magnetic force gradients. Commercial MFM tips from Nanosensors with ~40 nm CoCr coating were used. The lift-height was set to 30 nm. All MFM measurements were carried out at ambient conditions.

The results of the MFM measurements were compared to micromagnetic simulations. Therefore disks with diameters of 300 and 700 nm where modeled by using version 2.46 of the LLG Micromagnetics Simulator. This program

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K u disks with a diameter of 300 nm the C state has even a lower slightly higher than the energy of the S state. For smaller

<table>
<thead>
<tr>
<th>Thickness (nm)</th>
<th>$K_u$ (erg/cm$^3$)</th>
<th>$K_1$ (erg/cm$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>$2.25 \times 10^5$</td>
<td>$3.0 \times 10^5$</td>
</tr>
<tr>
<td>5.0</td>
<td>$3.0 \times 10^5$</td>
<td>$1.5 \times 10^5$</td>
</tr>
<tr>
<td>7.5</td>
<td>$3.25 \times 10^5$</td>
<td>$1.0 \times 10^5$</td>
</tr>
<tr>
<td>15.0</td>
<td>$3.5 \times 10^5$</td>
<td>$0.5 \times 10^5$</td>
</tr>
</tbody>
</table>

solves the time evolution of the magnetization configuration inside a ferromagnet, which is described by the Landau–Lifshitz–Gilbert (LLG) equation. The simulation volume is discretized by a uniform cubic grid. The size of the cubic cells was set to 2.5 nm for most elements and to 3.75 nm for the larger 7.5 and 15 nm thick disks. The quasistatic configurations were calculated by using a high damping parameter of $\alpha=1$. The magnetic material parameters of the simulated Fe were the saturation magnetization of $M_s=1714$ emu/cm$^3$ and the exchange stiffness of $A=2.1 \times 10^{-6}$ erg/cm. The effective anisotropy constants $K_1$ and $K_u$ were determined at room temperature by alternating gradient magnetometer (AGM) measurements on separate unpatterned Fe(001) films prepared under identical conditions as the patterned film. Table I shows the values used for the simulation.

First, the remanent states of the disks after saturation along the [110] direction will be compared. In Fig. 1 the MFM images of the remanent states of disks with a diameter of 700 nm and different thicknesses are shown with corresponding simulated magnetization configurations. The MFM image of the 2.5 nm thick disk [Fig. 1(a)] shows a clear dipole contrast which was also found for all other diameters. This indicates a single domain configuration which is stabilized by the dominating intrinsic uniaxial anisotropy. This assumption is confirmed by the simulation.

The 5 nm thick iron disks have a fourfold intrinsic anisotropy instead of a uniaxial one. Two different contrasts are found by MFM. The upper image in Fig. 1(b) indicates on the first glance a rotated dipole contrast, but with distorted poles. A corresponding simulation, shown on the right-hand side, displays an S-shaped magnetization configuration. The second MFM image of Fig. 1(b) is the result of a C-shaped magnetization configuration as shown in the corresponding simulation. It is interesting to note that the magnetization does not rotate very smoothly, but is mostly oriented along the easy axes of the intrinsic anisotropy. The images of the 7.5 nm thick disks [Fig. 1(c)] qualitatively show the same S- and C-shaped states as the 5 nm thick disks. In all cases the C-shaped magnetization occurs only if the angle between the [110] direction and the applied field is nearly zero. By rotating the external field by about $\pm 5^\circ$ it is possible to induce an S state and a mirrored S state, respectively. This behavior was confirmed by the simulations, but the C state occurred only after starting from a random configuration. This difference is possibly caused by the edge roughness of the real disks. Nevertheless, the total energy $e_{tot}$ of the C state is only slightly higher than the energy of the S state. For smaller disks with a diameter of 300 nm the C state has even a lower energy than the S state. The MFM images of 5 and 7.5 nm thick disks are shown in Fig. 2, together with the corresponding simulations. The S-shaped magnetization configuration of these small disks is less pronounced. It looks like a rotated single domain state as shown by the simulation in Fig. 2.

Almost all remanent states of the 15 nm thick disks show a vortex-like magnetization configuration [see Fig. 1(d)]. This vortex is not a homogeneous circular magnetization state as found in Permalloy disks, but is more like a four domain state with the magnetization aligned along the easy axes of the fourfold intrinsic anisotropy. The rarely occurring nonvortex configurations are very unstable. It was not possible to image them completely by MFM because they al-

![FIG. 1. MFM images of Fe(001) disks with a diameter of 700 nm and different thicknesses after saturation along the [110] direction together with corresponding micromagnetic simulations. The easy axes are indicated by arrows in the plots of the magnetocrystalline anisotropy energy density.](image-url)
ways switched into a vortex state during the scan. The fact that only a few specific disks showed this behavior suggests that some imperfections stabilize the nonvortex-like configurations. In the simulation the saturated starting configuration always leads to stable S-shaped magnetization configuration in remanence, but their total energy was more than four times higher than the energy of a vortex state. This difference in remanence, but their total energy was more than four times higher than the energy of a vortex state. This difference to the experimental result could be due to finite temperature effects (simulations are done at $T = 0$ K) or small uncertainties in the determination of the anisotropy constants used. While the 15 nm thick disks seem to be close to the transition inhabitable stable and nonvortex-like magnetization configurations, in 25 nm thick disks only vortex-like configurations were observed (see also Ref. 7).

The change of the anisotropy constants and the increasing in-plane demagnetization energy with increasing film thickness leads to a change of the remanent states from single domain over C or S states to vortex-like configurations. Qualitatively the same transitions were observed after ac-demagnetization perpendicular to the [110] direction. The main difference to the previous result is that the vortex state appears at lower film thicknesses. Again all 2.5 nm thick elements remain in one of the two possible single domain states independent of the direction of the applied ac field. Most of the 5 nm thick elements display a S state, some C states and, in contrast to the remanent states, some of the smaller disks show a vortex configuration. This is confirmed by the simulations, which randomly show all three configurations after starting from a random configuration. Furthermore all disks with a thickness of 7.5 nm and above show a vortex-like configuration.

The fact that not only the disks but all other shapes like rectangles and ellipses prepared from the 2.5 nm thick Fe(001) film always remain in a single domain state is remarkable and interesting from the application point of view. Even narrow rectangles with their long side perpendicular to the easy intrinsic axis are in a single domain state aligned along the easy axis after ac-demagnetization, as shown in Fig. 3. This independence of shape and the high stability of the single domain state are interesting properties for ferromagnetic memory cells. Another point, also important for applications, concerns the switching field which is necessary to reverse the magnetization of the particle. By measuring the magnetization states of the disks at zero field after applying different in-plane fields along the [110] direction it was possible to determine the switching field of the disks without any disturbance by the MFM tip. The disks with diameters between 500 nm and 1 $\mu$m switched at a field value between 190 and 205 Oe. By simulating the switching of a disk with a diameter of 500 nm we found a value of 235 $\pm$ 5 Oe. This seems to be a reasonable value for memory applications.

While the simulated switching field fits the experiment very well, the simulation of disks with diameters of 300 and 700 nm starting from a random configuration do not perfectly agree with the experiment. The simulation resulted not only in single domain states but also in two-domain states with a vortex at the center of the wall similar to the configuration found for 35 nm thick epitaxial Fe(110) disks.7 Such configurations have never been observed in the experiment.

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**References**

13. See http://llgmicro.home.mindspring.com