Volume contribution to perpendicular anisotropy in $Fe_{0.5}Co_{0.5}$ alloy films on Pd(001), Ir(001), and Rh(001)

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In tetragonally distorted $Fe_{0.5}Co_{0.5}$ alloy films grown epitaxially on Pd(001), Ir(001), and Rh(001) substrates the crystal field locates the electronic states near the Fermi level (E_F) with one being below E_F and the other above E_F with an energy separation smaller than in bulk nondistorted material. This results in a strong uniaxial anisotropy and an easy magnetization axis perpendicular to the film plane up to the thickness up to which the films remain tetragonally distorted. The strongest perpendicular anisotropy is achieved when the $Fe_{0.5}Co_{0.5}$ films are grown on Rh(001) ($c/a=1.24$); it systematically decreases for Ir(001) ($c/a=1.18$) and Pd(001) ($c/a=1.13$) substrates. The phenomenon can be understood as a result of an increasing uniaxial anisotropy with an increasing c/a ratio up to the maximum at $c/a=1.24$ for which the maximum uniaxial magnetic anisotropy has been theoretically predicted. © *2009 American Institute of Physics*.
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I. INTRODUCTION

The magnetic properties of ultrathin magnetic films and multilayers have received much attention for decades. One of the most attractive features, both for fundamental physics and potential applications, is the existence of magnetic anisotropy induced by symmetry breaking. A dramatic manifestation of the varying anisotropy in thin films and multilayers is the change of the preferential direction of magnetization from the commonly observed in-plane orientation to the perpendicular direction (e.g., Ref. 1).

It has been shown that a proper symmetry breaking causes the orbital moment to be less quenched than in the cubic sample. Consequently, the spin-orbit interaction becomes significant leading to large uniaxial volume magnetocrystalline anisotropy.[2–4] Such a scenario has been predicted theoretically, e.g., for bulk $Fe_{1-x}Co_x$ alloys with a tetragonally distorted structure.[5] Since the anisotropy is of volume character and does not scale with the interface contribution, it could result in a perpendicular easy magnetization axis in relatively thick films. For $Fe_{1-x}Co_x$ concentrations, where the uniaxial magnetocrystalline anisotropy is expected to be large, the magnetic moments are of the order of $2.1\mu_B$, which results in a 50% larger saturation magnetization than that of the FePt compound used for perpendicular recording.[6]

The issue is how to distort the structure tetragonally. The growth of the layers with strained or expanded atomic distances is possible by epitaxy, thus providing the necessary basis to study such new phases of materials, which do not exist as three dimensional solids under normal conditions [e.g., 7].

The aim of this study is to show experimentally how uniaxial anisotropy depends on tetragonal distortion by growing $Fe_{1-x}Co_x$ films on suitable substrates. The distortion is varied by varying the lattice constant of the single crystalline substrate on top of which the ferromagnetic layer is grown. The anisotropy is probed by measuring Kerr effect from the films vs the applied magnetic field.

II. EXPERIMENTAL ASPECTS

The $Fe_{1-x}Co_x$ alloy films were grown at room temperature (RT) by molecular beam epitaxy (MBE) in a multichamber ultrahigh vacuum system with a base pressure below 5×10^{-11} mbar and below 2×10^{-10} mbar during deposition. The Pd(001) and Rh(001) substrates were prepared using sputter-anneal cycles, plus annealing in oxygen and hydrogen atmospheres in the case of the Ir(001) crystal.[8] The quality of the sample was checked by Auger electron spectroscopy and by scanning tunneling microscopy until a clean surface with monoatomic steps was obtained. The $Fe_{1-x}Co_x$ films were grown using two effusion cells as described previously.[9]

Low energy electron diffraction (LEED) and diffracted intensities vs incident electron energy analysis [I(V)–LEED] were used to assess quantitatively the pseudomorphic growth and the tetragonal distortion, respectively. Magnetic properties were probed by utilizing the *in situ* magneto-optical Kerr effect for 1.85 eV photon energy of *s*-polarized light, mostly in polar geometry (incidence angle of 69° to the sample normal) at varying temperature (down to 5 K) and the external magnetic field up to 0.7 T.

III. RESULTS AND DISCUSSION

Tetragonal distortion is realized by growing the $Fe_{1-x}Co_x$ films on mismatching substrates such as Pd(001), Ir(001), and Rh(001). In all three cases the crystals are of a fcc structure with gradually decreasing lattice constant from 2.75 Å

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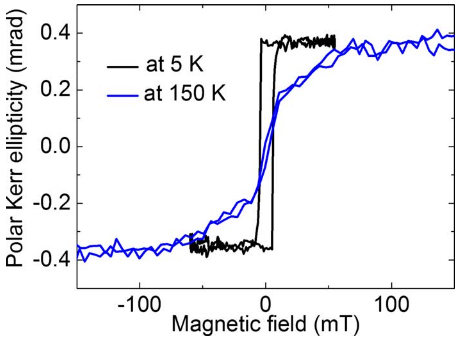

FIG. 1. (Color online) Polar hysteresis loops for 6 ML of $Fe_{0.5}Co_{0.5}$ on Pd(001) at 5 and 150 K. The rectangular easy-axis-like loop measured at 5 K evolves to a hard-axis-like loop when measured above 100 K.

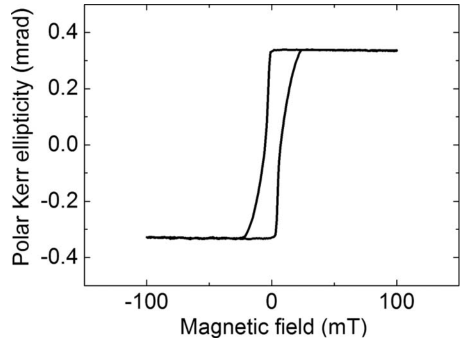

FIG. 2. Polar hysteresis loop measured at RT for 8 ML thick $Fe_{0.5}Co_{0.5}$ on Ir(001). The loop is rectangular, showing 100% saturation magnetization in remanence, and thus confirming the easy magnetization axis to be oriented perpendicular to the film plane.

for Pd to 2.72 Å for Ir, and finally 2.69 Å for Rh(001). As their in-plane lattice constants are larger than that of Co (and Fe), the $Fe_{1-x}Co_x$ overlayer lattice has to expand in plane for pseudomorphic growth. To keep the atomic volume constant, the fcc film contracts in the direction of the c axis, which leads to a c/a ratio less than $\sqrt{2}$. The c/a values obtained for $Fe_{0.5}Co_{0.5}$ films 8 ML thick grown at RT on Pd(001), Ir(001), and Rh(001) were found to be equal to 1.13, 1.18, and 1.24, respectively. For the magnetic analysis we grew $Fe_{1-x}Co_x$ alloy films at RT varying film composition and thickness.

For $Fe_{1-x}Co_x$ films grown on Pd(001) only the nominal equiatomic alloy $x=0.5$ shows a clear out-of-plane easy axis of magnetization and only at low temperature (as concluded from the disappearing longitudinal hysteresis loop and appearing rectangular loop when measured in polar geometry). The increase of the perpendicular anisotropy proceeded smoothly with composition. At the chemical compositions between $Fe_{0.6}Co_{0.4}$ and $Fe_{0.4}Co_{0.6}$ it was possible to saturate the samples perpendicular to the sample plane with a magnetic field of less than 0.2 T.[9] The volume magnetocrystalline anisotropy for $Fe_{0.5}Co_{0.5}/Pd(001)$ was found to be highly temperature dependent. As shown in Fig. 1, the polar Kerr ellipticity loop measured at 5 K is rectangular showing 100% saturation magnetization in remanence. The loops measured at 150 K and above show a hard-axis-like shape and zero magnetization in remanence. It clearly means that a temperature driven spin reorientation transition (SRT) occurs. Moreover, it also means that the volume perpendicular magnetocrystalline anisotropy is only a little larger than the shape anisotropy and thus can be easily overridden by the increasing temperature.

The largest anisotropy obtained for the $x=0.5$ film composition does not come as a surprise. The alloy composition determines the number of valence electrons and thus adjusts the value of E_F to result in minimum separation energy between occupied and unoccupied states. It is predicted theoretically that the maximum uniaxial anisotropy occurs for $Fe_{1-x}Co_x$ alloys just around $x=0.5$ composition.[5] Varying the composition slightly (both to lower and higher contents of Co) results in a decrease of the uniaxial anisotropy which becomes smaller than the shape anisotropy. Consequently, the magnetization rotates into the film plane.

The experiment with $Fe_{1-x}Co_x$ films grown on Ir(001) is more complicated since the preparation of an Ir(001) single crystal is complex. Nevertheless, the effective anisotropy for the $Fe_{0.5}Co_{0.5}$ film is larger (more positive) than the one of the film of the same composition grown on Pd(001). The polar Kerr ellipticity loop measured at RT for 8 ML thick film of $Fe_{0.5}Co_{0.5}$ on Ir(001) (Fig. 2) clearly proves these findings. The loop is rectangular and shows a 100% magnetization in remanence even at RT, which confirms that the easy magnetization axis is oriented perpendicular to the film plane.

The strongest perpendicular anisotropy is obtained for $Fe_{1-x}Co_x$ films grown on Rh(001). The $Fe_{1-x}Co_x/Rh(001)$ system shows a distortion of $c/a=1.24$ which is close to the c/a value of 1.22 for which a maximum uniaxial magnetic anisotropy energy of the order of 700–800 μeV per atom is theoretically predicted.[5] The easy magnetization axis perpendicular to the sample plane is detected not only at low temperature, but also at RT and in a broad composition range $(0.3<x<0.7)$.[10,11] This simply means that even for a composition significantly different from $x=0.5$, the uniaxial anisotropy is sufficiently strong to override the shape effects of dipolar interaction. The easy axis of magnetization changes from perpendicular to in plane within a thickness of a few monolayers. In this transition thickness range the polar remanence decreases (and the polar loops become hard-axis like) whereas the longitudinal remanence increases (and the longitudinal loops become rectangular).

All these reported phenomena can be understood as a result of increasing the uniaxial anisotropy with increasing the c/a ratio up to the maximum of $c/a=1.24$ for $Fe_{1-x}Co_x$ films grown on Rh(001). This is schematically shown in Fig. 3. For reasons of simplicity only Pd and Rh substrates are included. It is common to separate the volumelike contributions to the effective anisotropy constants, K_v, from the surface/interface term, K_s, which contributes to the anisotropy energy as $1/d$ (d is film thickness). When $K_{\text{eff}}d$ is plotted, K_s is given by the intersection with the ordinate, whereas K_v determines the slope of the curve. Here it is assumed that the volume term does not depend on the thickness, which is not necessarily true because the crystallographic distortion responsible for the magnetocrystalline anisotropy is thickness dependent. For $Fe_{0.5}Co_{0.5}$ films grown on Rh(001), the slope of the curve is large since the effective volume anisotropy is large. Increasing the temperature re-

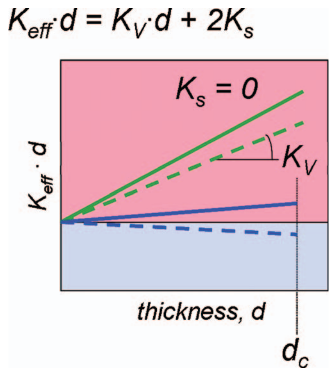

FIG. 3. (Color) Schematic representation of the effective anisotropy ($K_{\mathrm{eff}}d = K_v d + 2K_s$) referred to the volume anisotropy K_v for $Fe_{0.5}Co_{0.5}$ films grown on Pd(001) and Rh(001). The figure explains why the temperature increase has almost no effect on the easy magnetization axis for $Fe_{0.5}Co_{0.5}$ films grown on Rh(001) (green lines), whereas it results in a SRT for the $Fe_{0.5}Co_{0.5}$ film grown on Pd(001) (blue lines). Solid and dotted lines correspond to the anisotropy at low and increased temperatures, respectively. For simplicity K_s is chosen as equal zero.

duces the anisotropy (the slope becomes smaller), but it has almost no influence on the easy magnetization axis. For $Fe_{0.5}Co_{0.5}$ films grown on Pd(001) the slope is very small (because the effective volume anisotropy is small, i.e., the uniaxial magnetocrystalline is only a little larger than the shape anisotropy) yet still positive at least at low temperature. The anisotropy is temperature dependent, thus the slope changes a little with increasing temperature, however, the change is enough to result in negative effective volume anisotropy (the magnetocrystalline anisotropy becomes smaller than the shape anisotropy). This is why at RT $Fe_{1-x}Co_x$ films on Pd(001) are magnetized in plane regardless of the film composition and thickness. Obviously, the slope changes as the thickness of the film structure relaxes and the uniaxial anisotropy disappears (above d_c).

An option for verifying the crucial role of the distortion is to keep the optimum lattice constant by covering the $Fe_{0.5}Co_{0.5}$ film with Rh and grow another $Rh/Fe_{0.5}Co_{0.5}$ sequence on top of it. In this way one can produce perpendicularly magnetized multilayers.[12] Depending on the thickness of the Rh spacer layer, the magnetizations of the $Fe_{0.5}Co_{0.5}$ films are either ferromagnetically or antiferromagnetically (AFM) coupled.[12,13] Figure 4 shows the polar Kerr ellipticity loop measured at RT after the sequence Rh(5 ML)/$Fe_{0.5}Co_{0.5}$(6 ML) is repeated $N=5$ times, with the Rh thickness (5 ML) relating to the AFM coupling. Independently of the number of the sequence repetition, the measured Kerr ellipticity minor loops (applying the magnetic field smaller than the saturation field) are rectangular. An uncompensated (nonzero) net Kerr ellipticity signal is due to varying the thickness of each $Fe_{0.5}Co_{0.5}$ layer within the multilayer structure.

In summary, it is clearly shown that $Fe_{1-x}Co_x$ films offer interesting magnetic properties when grown on substrates forcing the cubic film structure to be expanded in the film plane. In particular, the perpendicular anisotropy can be sufficiently strong to orient the easy magnetization axis perpendicular to the film plane. Combined with pseudomorphic

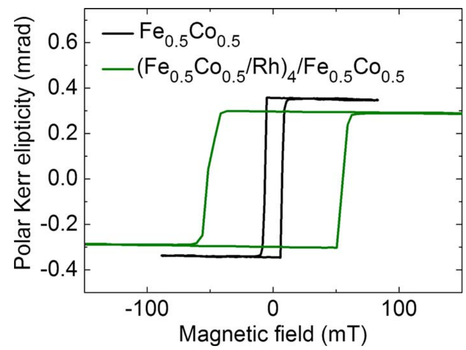

FIG. 4. (Color online) Polar Kerr ellipticity loop measured for a $(Fe_{0.5}Co_{0.5}/Rh)_4/Fe_{0.5}Co_{0.5}/Rh(001)$ multilayer at RT. The loop is rectangular showing 100% saturation signal in remanence. A nonzero net Kerr ellipticity signal is due to varying thickness of each $Fe_{0.5}Co_{0.5}$ layer within the multilayer structure. The loop of a single $Fe_{0.5}Co_{0.5}/Rh(001)$ film is shown for comparison.

growth of $Fe_{1-x}Co_x$ films, in particular on a Rh(001) substrate, it results in a perpendicular spontaneous magnetization up to a films thickness of 17–20 ML.

IV. CONCLUSIONS

It is shown that a strong perpendicular anisotropy in $Fe_{0.5}Co_{0.5}$ alloy films can be achieved by an appropriate tetragonal distortion of their cubic structure. The easy magnetization axis perpendicular to the film plane up to the thickness of 17 ML is kept due to distortion. The uniaxial magnetic anisotropy is strongest in the $Fe_{0.5}Co_{0.5}$ films grown on Rh(001) and then systematically weaker for films grown on Ir(001) ($c/a=1.18$) and Pd(001) ($c/a=1.13$). The anisotropy depends on the distortion which is determined by the lattice mismatch between the film and the substrate. Keeping the distortion by growing spacers from the same material as the substrate (Rh) results in the perpendicular easy magnetization axis in all the $Fe_{0.5}Co_{0.5}$ films forming the multilayer.

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