Experimental report

Correlation between structural properties and magnetic behaviors of
Fe1-xCox thin films grown on the Ir(001) surface

1/ Background:

Our aim was to correlate the structural properties and magnetic behavior of tetragonally distorted Fe1-xCox alloys grown on Rh(001) and Ir(001) surfaces. This work builds upon the ESRF-SI2092 proposal where we have obtained structure-property correlation for these alloys grown on the Rh(001) surface. Both Rh and Ir(001) surfaces induce tetragonal distortion in pseudomorphically grown Fe1-xCox layers [1,2]. This tetragonal distortion modifies the symmetry of the orbitals and the electronic structure around the Fermi level such that the spins are forced to align perpendicular to the film plane [3]. Thus structural distortion of the lattice induces perpendicular magnetic anisotropy (PMA). As the film thickness is increased structural relaxation can be expected leading to weakening of the PMA and at a critical thickness tc the spins reorient to lie within the film plane. A direct correlation of the spin reorientation transition (SRT) to the structural relaxation of the film is yet to be reported.

Our results on the Rh(001) surface show that the SRT does not coincide with any abrupt structural relaxation: the film remains pseudomorphic well above tc, with a simultaneous c/a ratio and unit cell volume monotonous decrease.

Conversely, qualitative results on the Ir(001) surface show that the structural relaxation commences several monolayers (ML) below tc. This is counter-intuitive since magnetic measurements show that for a given composition the tc is larger for Ir(001) than for Rh(001) suggesting that the Ir(001) surface is better suited for pseudomorphic growth of Fe1-xCox. Comparison of the relaxation mechanisms and magnetic properties of Fe1-xCox alloys on Rh and Ir(001) will help explaining this contradiction and provide fundamental insight into the mechanism of PMA.

2/ Experimental results:

We have used the surface preparation and electron beam deposition techniques at the UHV X-ray diffractometer at BM32 beamline to gather information on the growth of Fe1-xCox (0 < x < 0.5) alloys. Grazing incidence X-ray diffraction (GIXRD) using 22 keV photons has been employed to optimize the growth route and to measure the crystallographic structure (in-plane and out-of-plane lattice parameters) as function of the coverage and composition on Rh(001) and Ir(001).

In the case of the Rh(001) substrate, we were able to study three different compositions (x=0, 0.25, 0.5). A short experiment was done, in addition, on the Ir(001) crystal for the composition x=0.5.

The deposition rate was calibrated for both Fe and Co using a quartz balance. For the x=0.5 sample the calibration was at about 1ML/18min. At each stage of the growth the c/a ratio was determined. At the end of each thin layer preparation, the composition was checked by Auger spectroscopy. A summary of the main results that has been found up to now (further analysis is required) are given below (see figure).

For the deposition of Fe1-xCox alloys on **Rh(001)**, we have obtained:

x=0.5 (figure, red squares):
There is no in plane layer relaxation at all, i.e., the in-plane parameter of the Fe50Co50 alloy is strictly the same as that of Rh crystal up to 19 ML. The interlayer spacing decreases with increasing thickness and reaches the nearly saturated value of c=3.181A above 12-14 ML. This gives a c/a=1.18A and a cell volume of 11.50A^3. The analysis has been based on a model where the d-spacing – or c/2 – is the same for the whole thin layer, except for the d-spacing between the Rh surface and the first alloy layer. The blue point (figure) at 1 ML represents that value, which is almost independent on the layer thickness.

x=0.25 (green circles):
The thin layer displays a similar behavior at that composition. However, the layer starts to relax around 8-10 ML, where the (c/a) is about 1.20. One can observe that the (c/a) (green circles) is larger for all

unrelaxed (up to 10 ML) thickness compared to x=0.5 (red squares) which is expected because there is more Fe in the composition.

x=0.00 : Qualitatively, we observed a similar behavior with a decreasing (c/a) as thickness increases. In addition, a clear relaxation process starts around 6 to 8 ML. As for x=0.25, the relaxation process is gradual. A quantitative fitting involving both relaxed and unrelaxed phases has to be done.
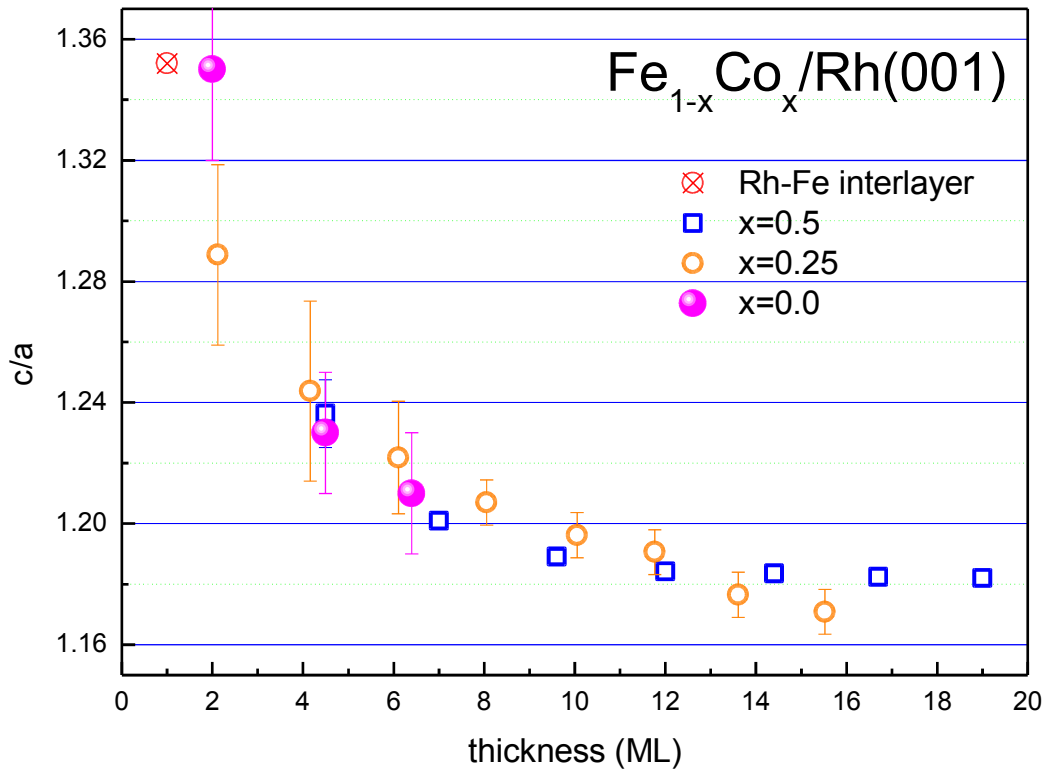

Figure 1: c/a variation as function of the layer thickness for different Fe/Co compositions on Rh(001).

For the Fe1-xCox/**Ir(001)**, the crystal quality was not so good and we had some problems with sources stability. We have obtained some preliminary qualitative results:

First of all, we checked that the Ir reconstruction is washed out after 0.4 to 0.5 ML deposit.

x=0
Pure Fe grows pseudomorph up to 8 ML and starts to relax around 9-10 ML;
in-plane parameter relaxes to 2.745A (a_Ir=2.715A) and the out-plane parameter to 3.16A,
giving (c/a)=1.15 after relaxation around 8ML.
in-plane parameter relaxes to 2.770 A (a_Ir=2.715A) and the out-plane parameter to 3.074A,
giving (c/a)=1.11 after relaxation around 13MLs.

X=0.5
During the deposition of the x=0.5 alloy, the Co deposition rate was extremely stable. However, the Fe source decreased slowly, giving a composition with an excess in Co.

x=0.5 (first experiment)
The film started to relax around 12-13 ML. The final sample with about 18 ML gave an in-plane parameter of 2.753A (a_Ir=2.715A) and an out-plane of 3.012A, giving a (c/a)=1.09.

x=0.55 (second experiment)
relaxation around 10 to 12 ML, but in both sources deposition rates decreased, with probably the largest variation in the Fe source. Up to 8 ML, Fe source flux decreased from 5.4 nA to 2.2 nA and Co source decreased from 31% to 27% of 30nA. Probably, we have got an excess in Co larger than 55%. (c/a) relaxed to 1.15 at 12 ML

x=0.50 (third experiment)
during this deposition, the Co source was extremely stable. Nevertheless, the Fe source decreased slowly: starting flux 3.7 nA; flux at about 8-9 ML 2.9 nA (20% less). The film started to relax again around 12-13 ML (nominal). After reajusting Fe source conditions, we deposited up to about 18 ML and measured the relaxed film: in-plane parameter relaxes to 2.753A (a_Ir=2.715A) and the out-plane parameter to 3.012A, giving (c/a)=1.09

At the end we checked the source: Co gave the same figures as from the beginning; Fe showed a deposition rate close to half the initial value. So, we probably have less Fe then Co.
We checked the Fe/Co composition by X-ray fluorescence spectroscopy in this final sample, covered by 10 ML of Ir, and found that the composition was close to 50/50 within an error bar of 10%.

6/ References:

[1] "Giant magnetic anisotropy in tetragonal FeCo alloys", T. Burkert, L. Nordstrom, O. Eriksson, and O. Heinonen, Phys. Rev. Lett. **93**, 027203 (2004).
[2] "Tight-binding approach to the orbital magnetic moment and magnetocrystalline anisotropy of transition-metal monolayers", P. Bruno, Phys. Rev. B **39**, 865 (1989)
[3] "Strongly enhanced orbital moment by reduced lattice symmetry and varying composition of Fe1-xCox alloy films", F. Yildiz, F. Luo, C. Tieg, R.Abrudan, X. L. Lu, A.Winkelmann, M. Przybylski, J.Kirschner, Phys. Rev. Lett. **100**, 037205 (2008)
[4] "Volume contribution to perpendicular anisotropy in Fe0.5Co0.5 alloy films on Pd(001, Ir(001), and Rh(001)", F. Yildiz, M. Przybylski, J. Kirschner, Journal of Applied Physics **105**, (7), pp 07E129/1-3 (2009)