ESRF	**Experiment title:** Growth mode and correlation between structural and magnetic properties of ultra-thin Fe layers on Ag(001)	**Experiment number**: 32-03-705
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Report: EXPERIMENTAL REPORT ON PROPOSAL CRG 32-03-705

1/ Scope and expected results:

Our aim was to investigate the correlation between structural and morphological properties and magnetic behaviours of ultra-thin Fe films deposited on Ag(001) single-crystals. The most interesting property of the Fe/Ag(001) system is the spin reorientation transition (SRT) as function of the thickness and temperature. This system might be an interesting candidate in spintronic studies, for instance when coupled with antiferromagnets in an exchange-biased CoO/Fe/Ag(001) bilayer or by being controlled with an external electric field.

We want to solve the question concerning the first steps of the growth mode (Frank – van der Merwe (layer-by-layer), Welmer – Weber (3D) or Stranski – Krastanov (layer-by-layer followed by 3D)) of Fe/Ag(001) and get quantitative information on structural and morphological aspects in the 0 – 3 ML range. The epitaxial conditions and interlayer spacing (c/a ratio) will be precisely determined in a wide range of coverage, in particular within the spin reorientation transition (SRT). This will teach us which parameters are the more relevant for the perpendicular magnetic anisotropy. We expect to verify the limit of the pseudomorphic growth and the relaxation of the structure for high coverage and to see if there is any correlation with the magnetic properties. It is known that for constant thickness (4 to 6 ML) the SRT takes place by moderate heating above room temperature. We will check if there is any counterpart in the structural aspects. Surfactant effects, even if incipient, is an aspect that could come out from such diffraction experiments and could be eventually an important piece in the knowledge of the properties.

2/ Experimental results:

The first steps of Fe growth on Ag(001) was studied in situ by GIXRD at BM32 beamline. A beam energy of 22 keV was used. The films were grown at room temperature, to minimize intermixing, then moderate annealing, up to 470 K, was done to improve the quality of the surface and modify morphological aspects. The growth was followed in real time along the (1 -1)CTR - to track the perpendicular lattice parameter c - and in the plane (h,k) at the (1 -1 2.7) and (1 -1 2.83) positions in reciprocal space - to confirm (or infirm) the pseudomorphic behavior. Complete sets of CTRs were measured for some particular coverages. This allows to solve the structure and get accurate lattice parameters. We present here some remarkable outcomes. A complete quantitative analysis has not been done, yet.

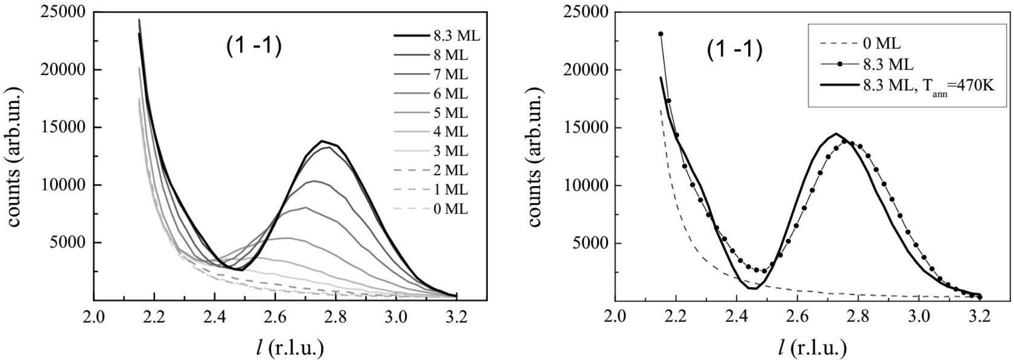

Figure 1 (a) Real time evolution of the (1 -1)CTR during the Fe deposition. (b) (1 -1)CTR before and after annealing the 8.3 ML Fe film on Ag(001).

At room temperature, the magnetic easy axis of Fe/Ag(001) changes from out-of-plane to in-plane around 6 MLs. By tracking the in-plane lattice parameter of the deposited layer up to 8, 11 and 14 ML, in three different depositions, and even after annealing at 470 K, we could eliminate a possible relaxation of the Fe film as an explanation for the SRT: the Fe films grow pseudomorphically taking the in-plane lattice parameter of Ag, which is larger than the bulk bcc Fe by 0.8%. Interestingly, however, the c/a does not become smaller than one, as it would be expected after pseudomorphic growth at constant volume.

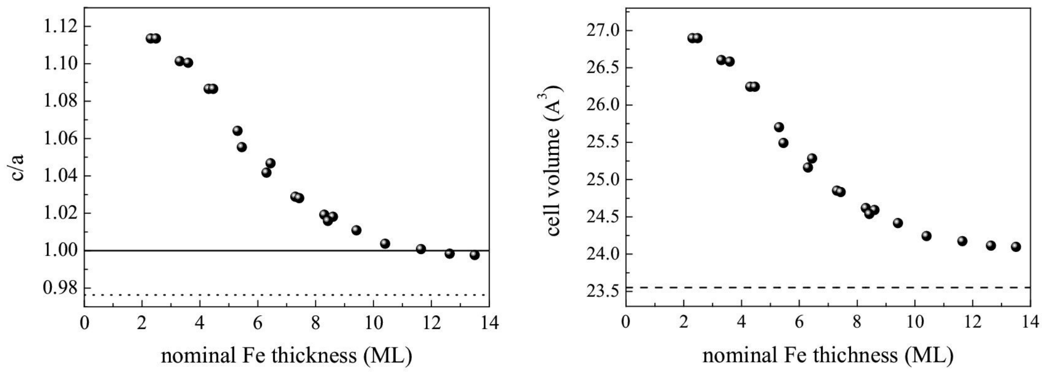

Figure 2 : (a) Tetragonal distortion as function of coverage; the solid line gives the limit of no distortion; the dotted line gives the situation where the volume of the unit cell would be the same as bulk bcc Fe. (b) volume of the unit cell for the Fe film as function of the coverage. The dash lines gives the volume of the bulk Fe bcc.

The real time evolution of the (1 -1) CTR during Fe on Ag(001) deposition for a up-to-8.3 ML film is presented in figure 1-a. Tracking the peak position yields a good average estimation of the c/a value. In figure 2-a, we present the estimation of the tetragonal distortion for two different experiments, namely for the up-to-8 and up-to-14 ML depositions. One clearly see that the distortion is larger than one up to about 10 ML. Nevertheless, we must emphasize that the in-plane parameter is that of Ag(001) and, even above 10 MLs where c/a is close to one, the volume of the Fe layer unit cell is still larger than for bulk Fe. In figure 2-b one can observe the evolution of the cell volume at different coverages. For very low coverages, the average cell volume of Fe films is larger by about 14%.

One additional comment concerns the annealing at 470 K that is often mentioned in the literature. This is normally done to improve the morphology by reducing the surface roughness. Fe and Ag have a high degree of immiscibility and this would help to separate a possible presence of Ag on the Fe layer. In figure 1-b we show the effect of the annealing on the (1 -1)CTR for the 8.3 ML film. The annealing reduce the roughness, as seen from Kiessig oscillations (not shown), and has the effect of increasing the c lattice parameter, while keeping the pseudomorphism (no changes in plane lattice parameter). In addition, from

Kiessig oscillations (not shown) we observe that the initial rough surface is thicker than the nominal value but decreases after annealing. Auger electron spectroscopy showed an increased amount of Ag compared to Fe after the annealing.

To summarize, we verified the limit of the pseudomorphic growth and demonstrated that there is no relaxation of the Fe films up to coverages of 14 MLs, and even after mild annealing at 470 K. We obtained the variation of the tetragonal distortion as function of the Fe coverage and observed that the unit cell volume is always larger than bulk. It is known that for constant thickness (4 to 6 ML) the SRT takes place by moderate heating above room temperature. We have shown that the structural counterpart is an increase of the tetragonal distortion and the appearance of a surfactant layer of Ag.

3/ References:

[1] Marcio M. Soares, PhD thesis 2011.
http://tel.archives-ouvertes.fr/docs/00/60/37/54/PDF/Soares_Marcio_2011_archivage_1_.pdf