ESRF	**Experiment title:** The $Fe_{30}Co_{70}$/NiO(111) interface during its formation - Structure and morphology by Grazing Incidence X-Ray Diffraction (GIXD)	**Experiment number**: 32-3-48
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Report:

This experiment aimed at studying in detail the growth of a CoFe film on NiO(111) single crystals and the interface formation. This study was performed within a larger project of investigation of ferromagnetic (F) films (Co, NiFe and CoFe) on polar oxide surfaces like NiO(111) which we can prepare with a high cristalline quality (see experimental reports **SI-398**, **SI-536**).

Depending on the composition, CoFe alloys show an FCC or BCC structure. While for the relaxed FCC structure in (111)//(111) epitaxy on the substrate an homothetical reciprocal space is observed due to the smaller lattice parameter (~18%), the BCC structure is expected mainly to chose a (110)//(111) epitaxy. From the lattice parameters and peak positions of the (110)$_{BCC}$ phase compared to the NiO ones it is possible to determine the preferential epiatxy. In the following, the expected cubic structures will be denoted by:

(a) $[110]_{BCC}//[100]_{hex\_NiO}$

(b) $[110]_{BCC}//[110]_{hex\_NiO}$

Several samples were prepared, varying the substrate temperature during the deposition: 250, 330 and 350°C. In all cases, the CoFe layer was prepared by co-deposition from two Omicron Co and Fe sources, at a typical deposition rate of 1 Å/min. All situations were investigated in detail by Grazing Incidence X-ray Diffraction (GIXD): for each thickness starting from fractions of monolayer (ML) up to 100 Å, in-plane and out-of plane scans were performed.

At the lower deposition temperature, signal is found only for relatively high thicknesses of CoFe. No particular epitaxial relationship is found. The CoFe seems to adopt mainly the BCC structure, with a (110) texture, as seen by almost constant intensity diffraction rings in the surface plane. This situation is not well suited for GIXD. At higher temperatures, the film adopts both the FCC and the BCC structures (figure 1). The structures develop during the deposition process, as shown by the intensity increase of the peaks in figure 1 with increasing the deposited CoFe. An in-plane large rocking scan at corresponding $q_{//}$ transfer moment (1.26 r.l.u. of NiO(111)) shows the presence of the (a) and (b) epitaxy, with twins (figure 2). Only traces (<10%) of the (b) structure are found. The relatively large width of the peaks (about 15° compared to ~1-2°

for the Co and NiFe films) may be the consequence of the different symmetry (4) of the layer crystalline structure with respect to the hexagonal one of the substrate.

Like in the case of the permalloy on NiO, high temperature deposition leads to formation of a spinel interface due to some Fe diffusion into the NiO substrate. This is evidenced by the occurrence of peaks having half spacing in the reciprocal space (double unit cell with respect to NiO, in the real space). In figure 3 is shown the integrated intensity of a p(2×2) NiO reconstruction peak (the $(1/2,1/2,0)_{NiO}$). At the beginning, the deconstruction of the surface by metallization leads the signal in this peak to vanish. Then, the signal increases more than its initial value, due to the spinel formation. This spinel layer was also evidenced by later high resolution and energy filtered Transmission Electron Microscopy (HR- and EF-TEM).

The decay of the reconstruction signal is much faster than for the case of the Co/NiO(111) and similar to the NiFe/NiO(111) case, showing the benefic effect of the Fe (in Fe-rich layers) in wetting the NiO(111) single crystalline substrate.

Although the cristaline quality of the CoFe film remains well poorer than the one of the Co or NiFe films, mainly due to the formation of the cubic structure, it also show the general feature of such films on NiO(111): the exchange coupling manifested through an increase of the coercivity of the F layer. The poor crystalline quality is manifested by a smaller coupling, evidencing the important role of the structure in the exchange phenomenon.

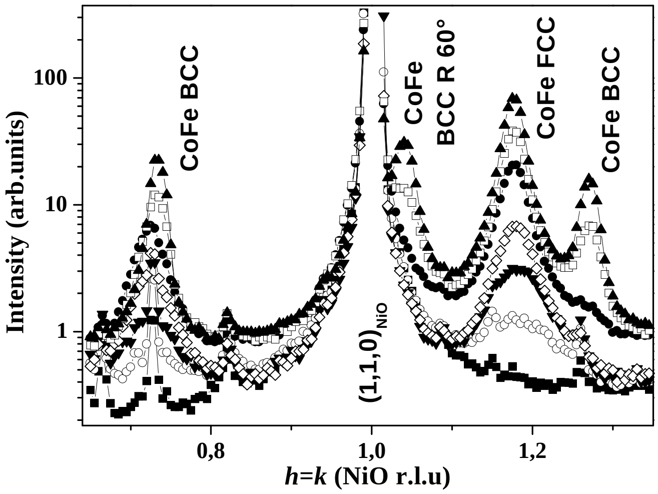

Figure 1: In-plane scan along the $[h,h,0]_{NiO}$ direction for different thicknesses (from 0 to 100 Å) of the CoFe film. This direction crosses the Bragg peak common to the FCC and twinned-FCC structure (h=1.18) and the one characteristic of the (b) BCC variant (h=1.26).

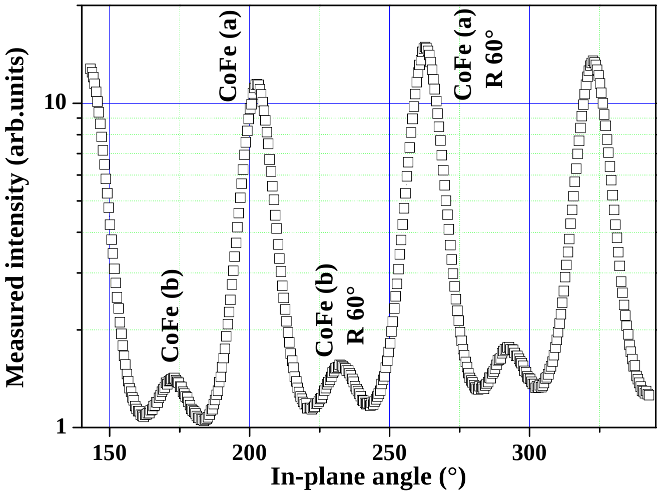

Figure 2: In-plane rocking scan at $q_{//}$=1.26 NiO r.l.u. The (a) and (b) CoFe BCC structure are evidenced.

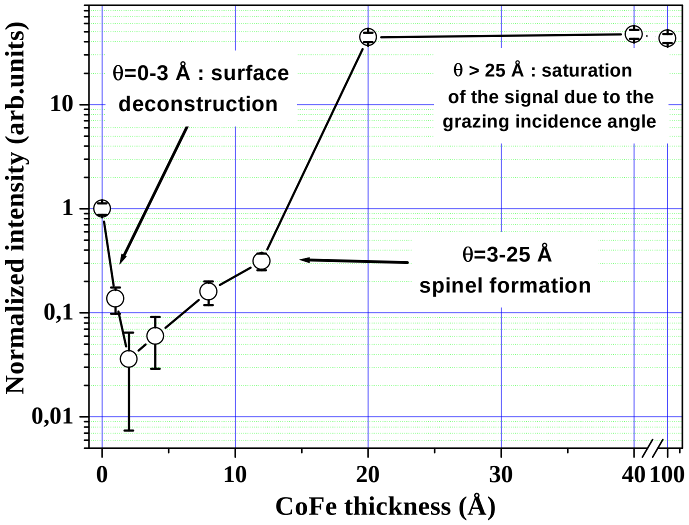

Figure 3: The intensity of the $(1/2,1/2,0)_{NiO}$ measured for different deposited CoFe thicknesses. The thickness domains corresponding to the different regimes of intensity evolution are marked on the figure.