	Experiment title: Oxygen-induced spin reorientation and structure of epitaxial Ni-layers on Cu(001)	**Experiment number**: SI-1076
Beamline: ID-03	**Date of experiment**: from: 22. Sept. 2004 to: 28. Sept. 2004	**Date of report**: 22. Feb. 2004
Shifts: 21	**Local contact(s)**: Iona POPA	*Received at ESRF:*

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Report:

The impact of adsorbate-coverage on the magnetic anisotropy of epitaxial ferromagnetic monolayers in the thickness range of several atomic layers has gained considerable attention in both experimental [1, 2] and theoretical [3, 4] studies recently. Calculations identify the decisive role of adsorbate-driven structural relaxations for the resulting magnetic anisotropy [3, 4]. However, highly accurate structural investigations during SRTs are scarce, and we performed in this experiment a first careful structural analysis of the O-Ni-Cu(001) system.

We followed the preparation recipe as given in a recent work [5], which is based on the assumption of a surfactant-action of pre-adsorbed oxygen during subsequent deposition of Ni. Thus we use the missing-row reconstructed O-$\sqrt{2}\times 2\sqrt{2}$ Cu(001) surface as a template for the Ni growth. We used surface X-ray diffraction (SXRD) to monitor the formation of the O-induced missing row reconstruction in situ during exposure of the heated Cu crystal (500 K) to O_2 at 1.5×10^{-6} mbar. Our results indicate indeed that the pre-adsorbed oxygen flows on top of the subsequently deposited Ni stack. The structural analysis suggests that at most the equivalent of 0.1 ML oxygen is distributed within the stack, the predominant amount of oxygen is adsorbed at the Ni surface, where it gives rise to a c(2x2)-structure.

The subsequent growth of Ni at 300 K was monitored by SXRD of the (0 -1 0.1) intensity as a function of Ni deposition time. Clear oscillations with monolayer period are observed, which give a highly accurate Ni thickness calibration. The same procedure was also employed to obtain a thickness calibration for deposition

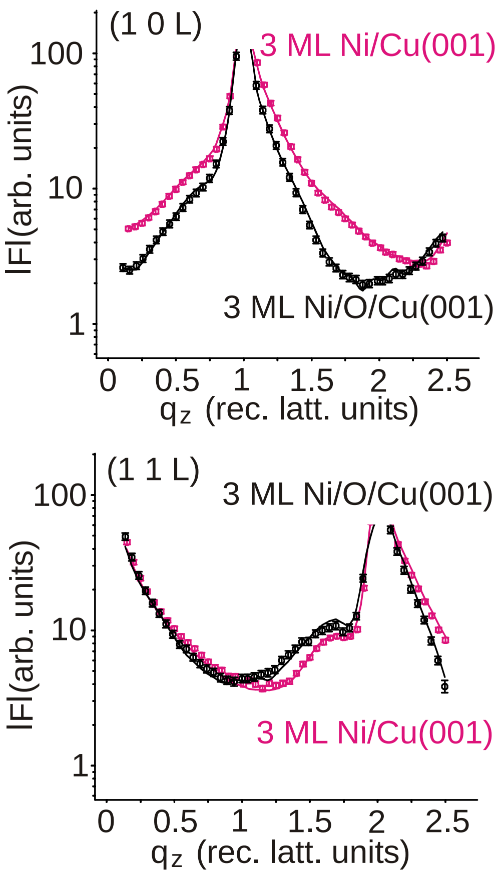

Figure 1: CTRs of 3 ML Ni deposited on clean and O-pre-covered Cu(001).

of Ni onto the clean Cu(001) surface. We performed a structural analysis based on intensity measurements of several crystal truncation rods (CTR) of 3 ML Ni and 5 ML Ni on i) the O-pre-covered and ii) on the clean Cu(001) surface. In addition, the structure of 1.25 ML and 2.25 ML on the O-covered surface was investigated.

The intensity of the diffraction measured along various CTRs differs significantly for deposition on the O-pre-covered surface as compared to the clean Cu(001) surface. We present in Figure 1 an example which shows how the structure factor amplitudes F varies in between the Bragg peaks for the (1 0 L) and (1 1 L) CTR, and it indicates how the intensity is affected by the presence / missing of oxygen. The solid line through the data points is the calculated intensity as derived from our structural models. The structural models describe the experimental data reliably, as shown by the good agreement between the data points and the solid curves.

The most important result of our structural analysis is presented in Figure 2. We analyzed the layer spacing of the Ni-Cu stack for both O-pre-covered and clean Cu(001) surfaces. The horizontal solid line gives the layer spacing in bulk Cu(001) as 1.81 Å, the dashed lined indicates the calculated layer spacing of 1.71 Å, as calculated from the tetragonal distortion due to the in-plane strain of the epitaxial Ni film of +2.5 %. The most dramatic impact of the O-pre-coverage is a significant outward relaxation of the topmost layer spacing which increases from 1.71 Å to 1.82 +/- 0.02 Å for the 5 ML Ni film (3 ML Ni: outward relaxation from 1.75 Å to 1.81 Å). This finding suggests that the O-surfactant, which is adsorbed at the surface, induces this drastic outward relaxation by 0.1 Å. We conclude that the structural relaxation is limited to the surface layer, whereas the deeper layer spacings do not differ for the O- vs. the clean system within our accuracy of +/- 0.02 Å.

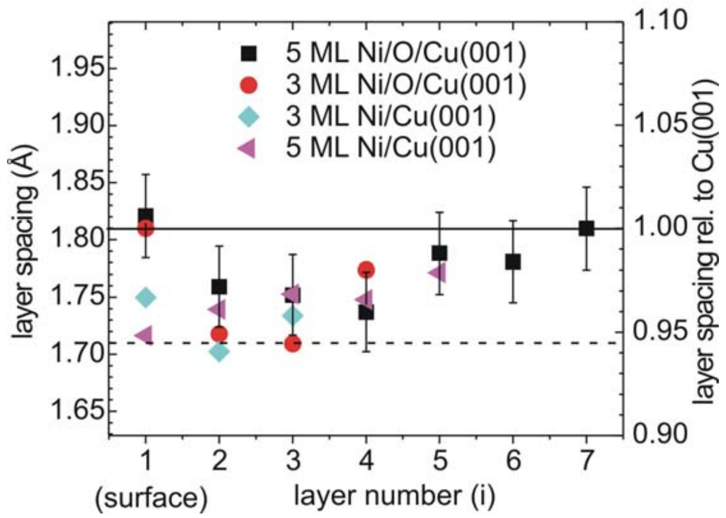

Figure 2: Calculated layer spacings within the Ni-Cu stack.

The easy magnetization direction of 5 ML Ni is in-plane, whereas it switches to out-of-plane for the O-pre-covered surface. Our combination of structural and magnetic data suggests that the outward relaxation is a key factor which determines the magnetic anisotropy. The magnetic surface anisotropy of the clean Ni film favors an in-plane magnetization. However, an outward relaxation reduces the tetragonal distortion of the surface layer and changes the crystal field near the surface to a more cubic symmetry. A quenching of the orbital moment results, and this reduces the magnetic surface anisotropy. Now the magnetoelastic anisotropy induced by the epitaxial strain wins over the surface anisotropy and this drives the SRT to the out-of-plane direction. Note that the sign of layer relaxation is opposite to what is needed to enhance the magnetoelastic anisotropy. This supports the view of a reduced magnetic surface anisotropy due to adsorbate-coverage [1,2,3].

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