



Experiment title: Fe local atomic environment and oxidation state in Fe/NiO layer structures

Experiment number:
SI941

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Report:

The aim of this experiment was to obtain a quantitative description of the Fe local atomic environment at the Fe/NiO(001) interface. The motivation for this study is that the chemical and structural modifications at ferromagnetic/antiferromagnetic interfaces, widely employed in magnetoelectronic devices, can strongly influence the magnetic couplings. At the Fe/NiO interface we have already shown, by means of x-ray photoelectron spectroscopy (XPS) and X-ray photoelectron diffraction (XPD), that some reduction of the interfacial NiO layer is induced by absorption of Fe [1]. While XPS and XPD allowed to have an accurate description of the atomic environment of Ni, XPS was not sensitive enough to distinguish the Fe oxidation state in the ultrathin layers. For this reason we applied for and obtained beamtime on the GILDA beamline to address the problem by means X-ray absorption spectroscopy (XAS) at the Fe K-edge.

The samples measured were three Fe films of different thickness, 2, 5 and 10 ML, grown on a 10 ML thick NiO film, in turn grown on Ag(001). They have been prepared in ultra-high vacuum in S3 laboratories in Modena, capped by a 10 nm Au film, which proved to be effective in preventing Fe oxidation, and carried to the site in a non reactive atmosphere. Polarization dependent XAS spectra of the films were measured at different angles between the electric field of the photon beam and the surface plane. XAS spectra of metallic Fe and of Fe₃O₄, Fe₂O₃ and FeO powders were also measured for comparison. The films were measured in the fluorescence mode, whereas for the standards the transmission mode was used.

From the x-ray absorption near edge spectra (XANES), shown in Fig.1, we obtained some qualitative information on the system. The XANES of the Fe films, in fact, show significant deviations compared to the metallic Fe one. In particular, the white line is shifted towards lower photon energies, i.e. towards the FeO white line position. The spectra of the films also show a larger relative intensity of the white line compared to the higher energy structures, which is characteristic of the FeO and of the other Fe oxide XANES. This is a clear indication of the presence of a fraction of Fe atoms coordinated with O in the films. The grazing incidence 2 ML Fe XANES (blue curve in Fig.1) shows a stronger metallic character, indicating that the oxidized phase is confined at the interface.

This qualitative evidence is confirmed by inspection of the $\chi(k)$ spectra in the extended energy region shown in Fig. 2 (a). The structures of the 10 ML spectrum resemble the ones of metallic Fe. For the 2 ML film the

deviations are small when it is measured at grazing incidence. The 2 ML $\chi(k)$ measured at 75° , instead, deviates significantly from the metallic Fe one and shows some oscillations also found in the FeO sample.

A quantitative analysis of the XAS spectra in the extended energy region has been performed by the multiple scattering FEFF code and allowed to obtain an accurate description of the Fe atomic environment. The k^3 -weighted Fourier transforms of the $\chi(k)$ spectra, together with the relative fits, are shown in Fig.2. The fit of the 10 ML Fe sample spectrum shows that the film has a body centered tetragonal structure, in which the pseudomorphic strain is starting to relax. A satisfactory fit of the 2 ML Fe film was obtained using a model which consists of a FeO layer at the interface and body centered tetragonal Fe on top. The in plane Fe-O interatomic distance has been found to be 2.07 Å, corresponding to pseudomorphism with the NiO substrate, and some buckling between Fe and O atoms in the plane was assumed. The further layers instead do not include oxygen atoms and are in a strained bcc structure. The necessity to include in the model more than 2 Fe atomic layers is an indication that the metal forms islands on the oxide surface. The oxide-metal interfacial distance was found to be significantly expanded to 2.39 Å. A comparably expanded interface distance was found by XAS and electron diffraction at other metal/oxide systems such as NiO/Ag(001) [2], MgO/Ag(001) [3] and Ag/MgO(001) [4].

The presence of a FeO layer, antiferromagnetic in its bulk form, and the expanded value of the interface distance are expected to strongly influence the exchange bias effect at the Fe/NiO interface.

The results from the experiments have been presented at national and international conferences and the preparation of a scientific publication is in progress.

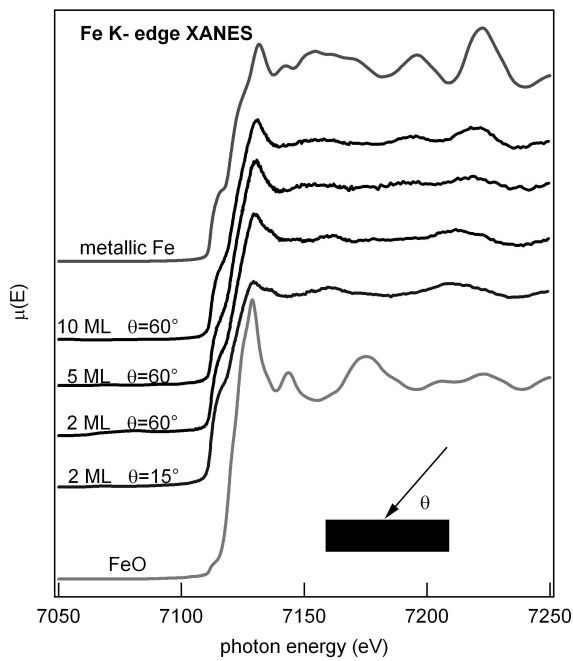


Figure 1. Fe K- edge XANES for 2, 5 and 10 ML Fe films. Reference spectra of bulk metallic Fe and FeO are also shown for comparison.

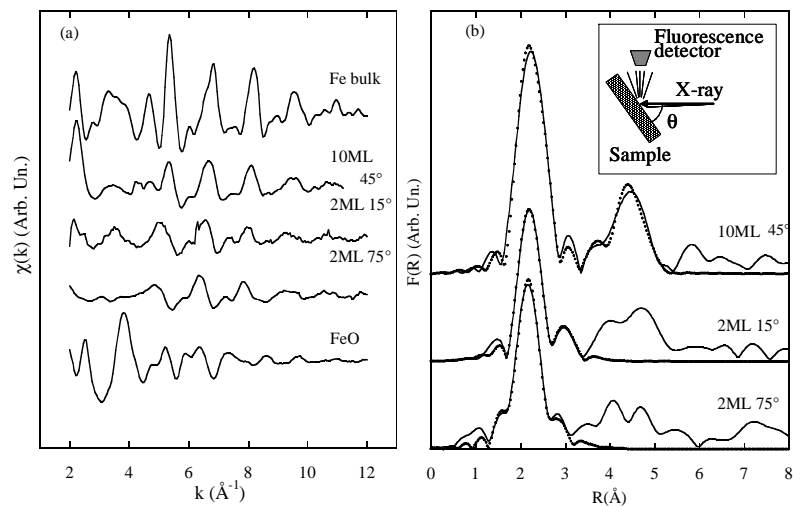


Figure 2. (a) $\chi(k)$ spectra for the metallic Fe, FeO, 2 ML and 10 ML Fe samples; (b) k^3 -weighted Fourier transform of $\chi(k)$ (solid line) for the 2 ML and 10 ML Fe samples and relative fits (dotted line).

References

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