Structural characterization at the atomic level of the Fe/NiO(001) interface

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The study of metal-oxide interfaces is stimulated by application in new magneto-electronic devices based on giant magnetoresistance. The magnetic phenomena, which come into play in these devices, have been shown to depend critically on the nature and quality of the interfaces involved [1]. This happens when the layers of the system become thinner and the multilayer is in practice characterized only by its surface. In order to describe the properties of these systems, a better understanding of the interfacial reactions and structural modification is fundamental. Within this context we focussed on the epitaxial Fe/NiO(001) system with the aim of obtaining an atomic level structural characterization. The experiments have been performed by means of XPS, LEED and XPD and compared with multiple scattering simulations.

NiO has been grown in the form of epitaxial films on Ag(001) substrate. As a consequence of Fe deposition an oxidation-reduction reaction occurs at the interface. The analysis of XPS data indicates that about 2 ML of NiO are reduced and 2 ML of Fe become oxidized [2].

By means of XPD we have obtained information concerning the structure of the oxidized-reduced interface. The intensity angular distributions (IADs) of Fe 2p, oxidized and metallic components of Ni 2p, and O 1s for a 5 ML Fe/10 ML NiO bilayer are shown in Fig.1. The Fe 2p IAD shows a typical bcc structure, with Fe(001)//NiO(001) and Fe[110]//NiO[100], due to a small lattice mismatch between overlayer and substrate (-3%). While Ni^{2+} 2p IAD is similar to the rock-salt structure of the substrate preceding Fe deposition, the Ni^0 IAD shows the same symmetry as Fe, giving evidence of a bcc environment surrounding Ni^0 atoms. The comparison between Ni^0 and Fe 2p data and multiple scattering simulations (Fig.1) assuming as a model for the interface a bcc FeNi alloy (Fig.2) confirms this hypothesis.

From LEED patterns the in-plane lattice parameter has been estimated for both substrate and Fe overlayer, showing that they are in registry. Then, using this information, a best fit on the out-of-plane parameter has been obtained by XPD multiple scattering simulations on a bcc FeNi alloy. This structural characterization provides previously unavailable information on the atomic scale structure of a ferromagnetic-antiferromagnetic interface.

References

[1] A.E. Berkowitz and K.Takano, *J. Magn. Magn. Mater.* **200** (1999) 552

[2] P. Luches, M. Liberati, S. Valeri, *Surf. Sci.* **532** (2003) 409

Figures

Fig.1

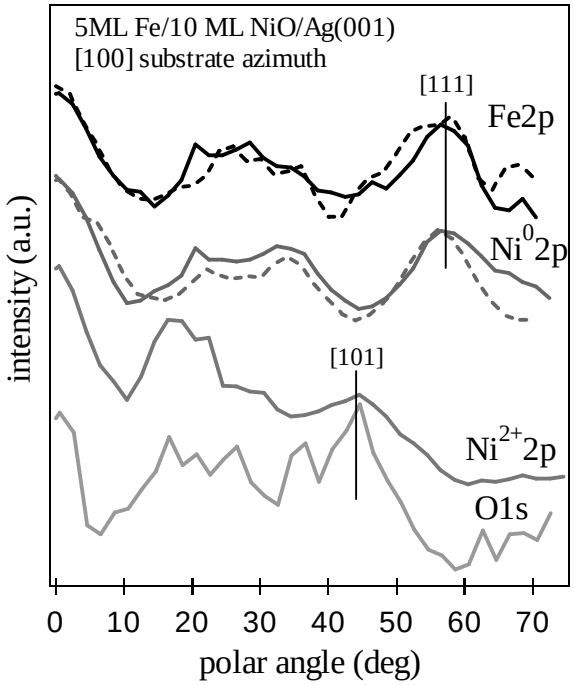

Fig.2

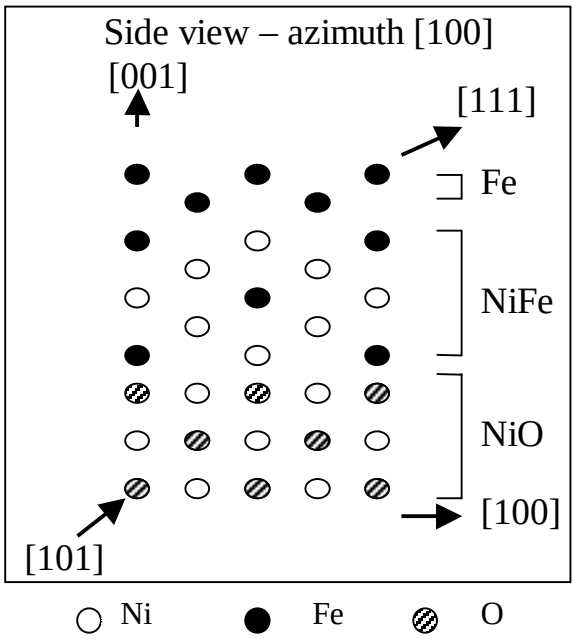

Fig.1 : Intensity angular distributions of measured (continuous) Fe 2p, Ni 2p, deconvoluted in metallic and oxidized components, and O 1s as a function of the take-off angle with respect to the surface normal, compared with calculated ones (dashed) assuming as a model a bcc FeNi alloy.

Fig.2 : Model used for XPD simulations of the Fe/NiO(001) bilayer crystal structure along the [100] azimuth.