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Influence of Au segregation on the magnetic anisotropy of $Fe/Cu_3Au(0\,0\,1)$

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Abstract

We present a first-principles study of the magnetic anisotropy of ultrathin Fe films on Cu_3Au (0 0 1), to investigate the origin of the magnetic reorientation transition observed experimentally. Our results indicate a crucial role of the segregation of Au to the topmost surface at very low Fe thicknesses.
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The controlled deposition of ultrathin Fe films on different substrates allows the stabilization of phases distinct from the ferromagnetic BCC bulk. A high spin-state ferromagnetic FCC Fe phase has been stabilized at lattice constants exceeding a critical value close to the Cu lattice parameter [1–3]. In particular, such a phase can be formed through the deposition of few monolayers (MLs) of Fe on a $Cu_3Au(0\,0\,1)$ substrate. The $Fe/Cu_3Au(0\,0\,1)$ system features a complex evolution of the magnetic and structural properties as a function of the thickness of the Fe slab [4,5]. The ferromagnetic Fe phase is obtained for coverages over 1 ML. Initially, the magnetization aligns perpendicular to the surface and a magnetic reorientation transition (MRO) to the in-plane direction occurs at coverages between 2.5 and 3.5 MLs. A structural transformation from a pseudomorphic FCC towards a BCT phase exists at coverages of 4–5 MLs [4–6]. The magnetic phase transition of $Fe/Cu(0\,0\,1)$ has been correlated to the structural transformation from a FCT to a FCC lattice [1]. However, this kind of correlation does not seem to apply here, due to the different critical thicknesses of the corresponding phase transitions. As has already been reported for surface alloys [7], chemical disorder may have a direct influence on the preferred orientation of the magnetization. Indeed, in $Fe/Cu_3Au(0\,0\,1)$ it has been found evidence of the presence of limited amounts of Au (less than 0.1 ML) at the topmost layer, and lower concentrations at the underlying layers [6]. This trend has also been reported for $Fe/Au(0\,0\,1)$ [2].

In this paper, we address the dependence of the magnetic anisotropy of $Fe/Cu_3Au(0\,0\,1)$ on the chemical composition of the topmost layers, through the evaluation of the magnetic anisotropy energy (MAE). Fully relativistic ab-initio calculations within the screened Korringa–Kohn–Rostoker (SKKR) formalism were performed. Details can be found elsewhere [8]. First, the self-consistent electronic potentials are obtained, and then the MAE is determined as the sum of two contributions on the basis of the magnetic force theorem: the band energy (ΔE_b) and the magnetic dipole–dipole energy (ΔE_{dd}). Convergence of ΔE_b was achieved using 900 $k_{\|}$ points in the irreducible Brillouin zone. The MAE is defined as the energy difference between a uniform in-plane and a uniform perpendicular

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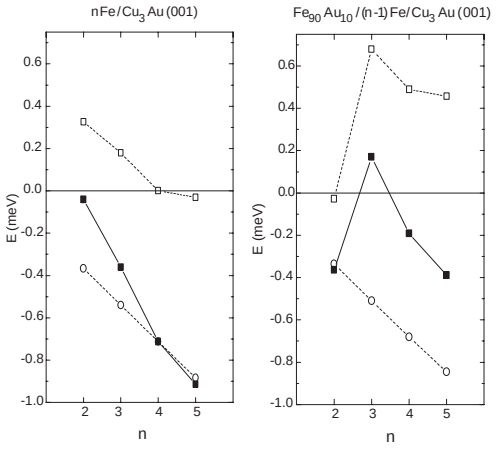

Fig. 1. Dependence of the MAE (full symbols) on the number n of Fe layers for the systems nFe/Cu_3Au(0 0 1) and $Fe_{90}Au_{10}/(n-1)$Fe/Cu_3Au(0 0 1). The ΔE_b (empty squares) and ΔE_{dd} (empty circles) contributions to the MAE are also shown. The lines connecting symbols are a guide to the eye.

orientation of the magnetization: $MAE = E(\|) - E(\perp)$, so that a positive MAE indicates a preferred magnetization direction along the normal to the surface.

The system Fe/Cu_3Au(0 0 1) was studied for Fe thicknesses ranging from 2 to 7 layers. The Cu_3Au(0 0 1) substrate was modelled within the coherent potential approximation (CPA) [9]. The ideal Cu_3Au(0 0 1) lattice was assumed for the whole slab. For all systems considered, the resulting layer-resolved charges and moments were very similar. There is almost no charge transfer from Fe to the substrate, although a significant spill-over of the electrons at the topmost Fe layer towards the vacuum was obtained. Fe shows a high spin moment around 2.65 μ_B, slightly enhanced at the surface (2.90 μ_B) and interface (2.70 μ_B) planes. Also the Cu and Au atoms adjacent to the Fe film are slightly polarized, with spin-moments of about 0.05 μ_B. The orbital moments remain almost quenched, the largest values of 0.08 μ_B correspond to the Fe atoms. In Fig. 1 (left panel) we present the MAE and its decomposition into ΔE_{dd} and ΔE_b. The MAE of the system is governed by ΔE_{dd}, which decreases almost linearly with the Fe thickness. Fe coverages higher than 5 ML (not shown in the figure) clearly remained magnetized in-plane. Only for very thin Fe films of 2–3 MLs the value of ΔE_b becomes positive and of the same order of magnitude of ΔE_{dd}. This trend is in agreement with the measured MRO, though the calculated ΔE_b cannot overcome ΔE_{dd} so as to lead to a positive MAE.

The right panel of Fig. 1 shows the MAE when we allow a limited segregation of 10% Au at the topmost layer. Except for the case $n = 2, \Delta E_b$ is extremely enhanced. The large negative value of ΔE_{dd} inhibits the change of sign of the MAE for $n \geqslant 4$, leading to a MRO at Fe coverages between 3 and 4 MLs, close to the experimental observation. The failure of the case $n = 2$ to follow this trend requires further considerations, which will be attempted in a forthcoming publication. However, for this extremely low thickness, both the influence of the interlayer spacing and the non-coalescence of Fe islands have to be taken into account.

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