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# Magnetic properties of ferromagnetic FeCu 'superlattices' on Cu(100)

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## ABSTRACT

With respect to the parent lattice of fcc Cu the magnetic anisotropy energy of Cu(100)/(FeCu)$_n$ with $n$ varying between 2 and 15 is investigated using the spin-polarized relativistic screened Korringa–Kohn–Rostoker method. It is found that the anisotropy energy per repetition rapidly converges to a constant value of about 0.46 meV, indicating that for a system of this kind, even for a much larger number of repetitions, the orientation of the magnetization remains perpendicular-to-plane (out-of-plane). For reasonably thick films discrete Fourier transformations of the layer-resolved magnetic moments and of the layer-resolved band energies with respect to atomic layers show a period of two, namely the number of atomic layers in each repeated unit.

## §1. INTRODUCTION

Recently the electronic and magnetic properties of artificially ordered FeCu alloy 'superlattices' on Cu(100) were studied quite extensively by Kuch *et al.* (1998), using spin-resolved valence band photoemission and soft X-ray circular dichroism. Such systems consist of alternating Fe and Cu layers on Cu(100), which in the experimental study were prepared epitaxially by pulsed laser deposition. In the present communication typical magnetic properties of a repetition of a double layer consisting of one Fe and one Cu layer on Cu(100), i.e. of systems of the type Cu(100)/(FeCu)$_n$, are investigated theoretically using an *ab initio* approach for $n \leq 15$.

## §2. RESULTS AND DISCUSSION

All calculations were performed using the spin-polarized (fully) relativistic screened Korringa–Kohn–Rostoker (KKR) method. Selfconsistency for the (effective) scattering potentials and (effective) exchange fields was achieved using 45 $k_{\|}$ vectors per irreducible part of the surface Brillouin zone (ISBZ), the calculation of the band part of the anisotropy energy was based on a grid of 990 $k_{\|}$ vectors per IBSZ. For further computational details, see e.g. Szunyogh *et al.* (1995, 1996). In all cases three layers of Cu were used as 'buffer' to the semi-infinite substrate and all films terminated with a Cu layer. Only ferromagnetic coupling of the Fe layers was investigated, whereby for the selfconsistent calculations the orientation of the magnetization was chosen to be perpendicular-to-plane. For one particular system, namely Cu(100)/$(FeCu)_8$, it was checked that all single 'spin-flip' energies, see e.g. Szunyogh *et al.* (1998), are positive, a fact that strongly suggests that in these artificially ordered FeCu alloy 'superlattices' the Fe layers indeed couple ferromagnetically. All calculations refer to a parent fcc lattice corresponding to the experimental lattice spacing of fcc Cu, i.e. no layer relaxation was taken into account.

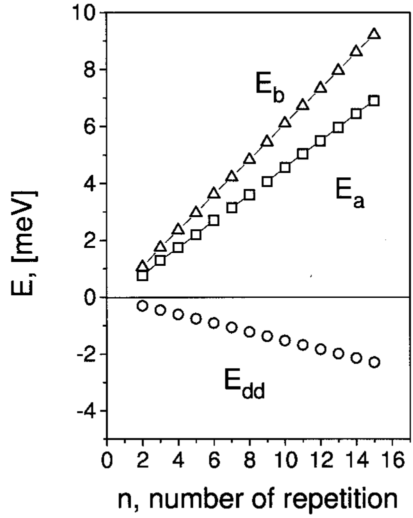

Figure 1. Magnetic anisotropy energy ($E_a$) together with its band energy ($E_b$) and magnetic dipole–dipole ($E_{dd}$) contribution as a function of the repetition $n$ in Cu(100)/$(FeCu)_n$.

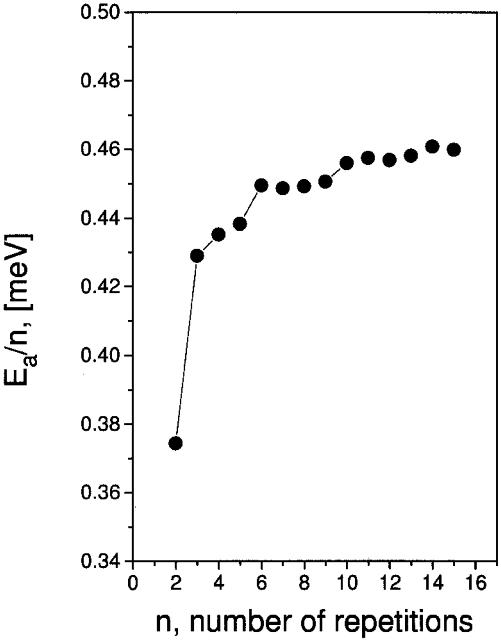

Figure 2. Magnetic anisotropy energy per repetition in Cu(100)/$(FeCu)_n$.

In figures 1 and 2 the main results of this communication are shown, namely in figure 1 the magnetic anisotropy energy together with its contributions, the band energy and the magnetic dipole–dipole part, as a function of the number of repetitions, while in figure 2 the magnetic anisotropy energy per repetition is displayed versus the number of repetitions. As can be easily seen from figure 1, in all cases the magnetic anisotropy energy is positive, indicating that in these films the orientation of the magnetization remains out-of-plane (perpendicular-to-plane). Both the band energy part as well as the magnetic dipole–dipole contribution vary almost linearly with the number of repetitions. However, since the band energy part grows much faster than the shape anisotropy (magnetic dipole–dipole contribution) decreases, no reorientation transition is observed. Figure 2 shows quite convincingly that by repeating units of (FeCu) layers beyond 15 repetitions the magnetic anisotropy energy per repetition remains constant. This kind of 'superlattice' behaviour for the magnetic anisotropy energy was previously observed by Zabloudil *et al.* (1998), for free and capped surfaces of $Cu(100)/(Cu_3Ni_3)_n$.

This behaviour is also addressed in figures 3 and 4, showing the layer-resolved band energy parts of the anisotropy energy and the layer-resolved magnetic

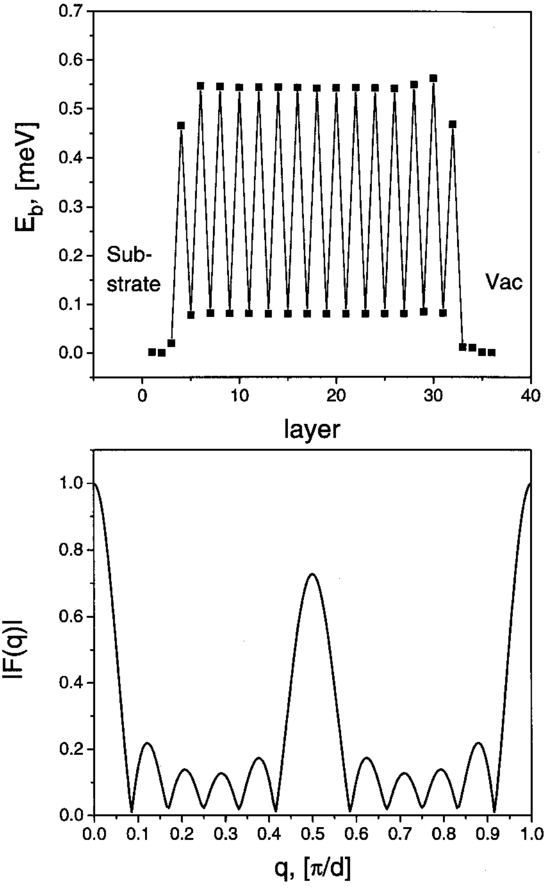

Figure 3. Layer-resolved band energy contributions to the magnetic anisotropy energy in $Cu(100)/(FeCu)_{15}$ (top) and corresponding discrete Fourier transformation (bottom).

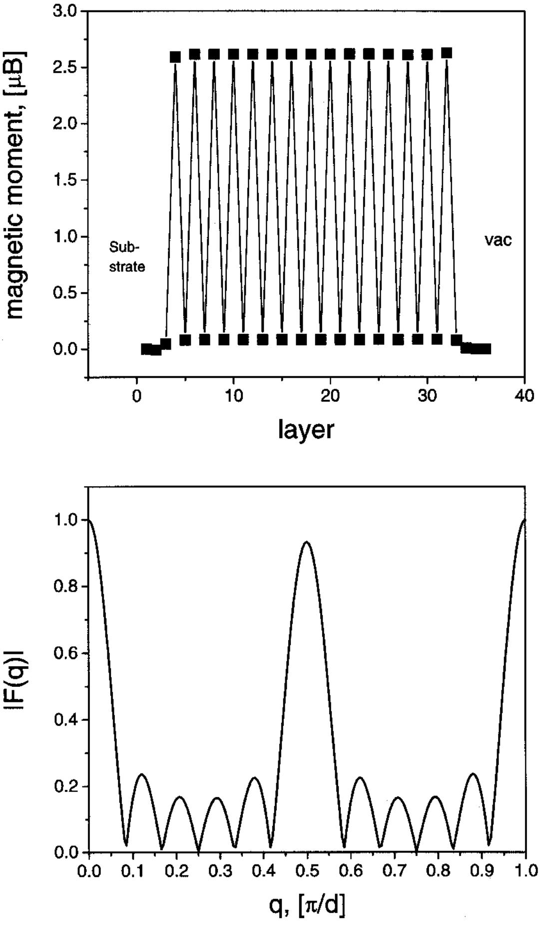

Figure 4. Layer-resolved (spin-only) magnetic moments in Cu(100)/$(FeCu)_{15}$ (top) and corresponding discrete Fourier transformation (bottom).

(spin-only) moments in the system Cu(100)/$(FeCu)_{15}$, and their corresponding discrete Fourier transformations, see also Zabloudil *et al.* (1998). Both, the layer-wise representations as well as the discrete Fourier transforms show for a sufficiently large number of repetitions, $n \geq 6$, a period of two, indicating that the unit of one layer Fe and one layer Cu also serves as a characteristic unit for the magnetic moments and the magnetic anisotropy energy, but also that the notation 'superlattice' seems to be justified. The layer-resolved orbital moments for Cu(100)/$(FeCu)_{15}$ are displayed in figure 5 and—as to be expected—also show a period of two.

## §3. COMPARISON TO EXPERIMENT

The so-called experimental magnetic moments, spin moment as well as orbital moment, are usually obtained from XMCD measurements using a sum rule analysis. The spin-only moment for 'Fe atoms' found experimentally by Kuch *et al.* (1998), is surprisingly low, about $1.8\mu_B$, while the corresponding orbital moment of about $0.21\mu_B$, seems to be quite large. In the theoretical calculations a typical Fe layer sandwiched by two Cu layers carries a spin-only magnetic moment of about $2.61\mu_B$

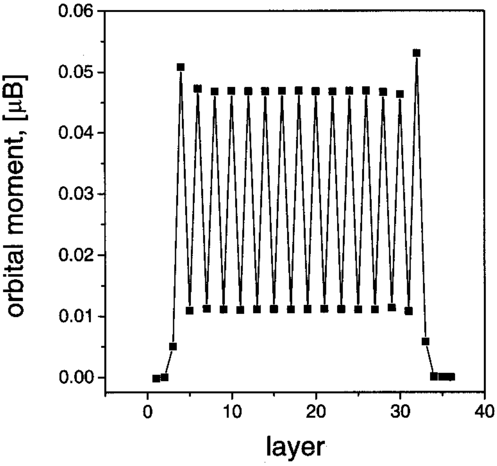

Figure 5. Layer-resolved orbital moments in Cu(100)/$(FeCu)_{15}$.

per site and an orbital moment of about $0.05\mu_B$, for a comparison to the system Cu(100)/$Fe_n$ see also Újfalussy *et al.* (1996), Lorenz and Hafner (1996) and Szunyogh *et al.* (1997). The experimental spin and orbital moments for 'Cu atoms' of 0.05 and 0.006 $\mu_B$, respectively, seem to agree much better with the corresponding values of 0.085 and $0.011\mu_B$ found theoretically for Cu layers sandwiched by Fe layers. From figures 1 and 2 it is obvious that the tentative conjecture by Kuch *et al.* (1998), that the experimentally found enhancement of the orbital moment of 'Fe atoms' indicates a strong in-plane magnetic anisotropy, which was proposed also by Sundar Manoharan *et al.* (1998), from the ferromagnetic-like hysteresis loops seen in MOKE measurements for the same system, cannot be confirmed.

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