PHYSICAL REVIEW B, VOLUME 64, 180407(R)

Induced V and reduced Fe moments at the interface of Fe/V(001) superlattices

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(Received 20 July 2001; published 22 October 2001)

Fe_n/V_m superlattices with $n=2,4$ and $m=2,4,5$ are studied by vibrating sample magnetometry and x-ray magnetic circular dichroism measurements. The combination of both techniques allows us to determine absolutely the induced V magnetic moment per atom. The samples with the thinnest V or Fe layers, respectively, reveal the largest induced moment of $m_V=-1.1\mu_B$/atom (Fe_4/V_2) and the strongest reduction of the Fe moment down to $m_{Fe}=1.34\mu_B$/atom (Fe_2/V_5). In addition, we probe the orbital magnetism of Fe and discuss it with respect to previous results by ferromagnetic resonance and *first principles* calculations.

DOI: 10.1103/PhysRevB.64.180407 PACS number(s): 75.70.Cn, 78.70.Dm

The evolution of film-preparation methods has, nowadays, made it possible to grow high quality single-crystalline epitaxial metallic superlattices (SL's). A characteristic example is the Fe/V SL's on MgO(001): The exceptional structural[1] and magnetic homogeneity[2] have been recently demonstrated for this system. Such SL's are used as prototype systems to investigate the rich variety of phenomena in multilayer magnetism: The reversible tuning of magnetic exchange coupling using hydrogen[3] and the optical constants of Fe via resonant magnetic scattering[4] were probed for Fe/V SL's. The separation of spin and orbital magnetism via the investigation of the spectroscopic splitting *g*-tensor[5,6] was achieved. Moreover, layer-dependent distribution of large induced V moments extending up to 4 monolayers (ML) away from the interface were reported.[7] However, the latter subject appeared to be controversial: Theoretical works[8–10] found much smaller V magnetic moments, by a factor 2–4 depending on the crystallographic direction, localized directly at the interface. In addition, experimental works revealed either no reduction of the Fe interface magnetic moment[11,12] or even a sizable reduction[13] at and beyond the interface, the latter in fair agreement with theory.[8–10] The knowledge of the magnetic and structural properties at the interface are of particular interest since the spin-dependent electron scattering at the interface contributes to the properties of oscillatory interlayer exchange, giant magnetoresistance and spin injection.[11,14] Therefore, it is crucial to know the moments of the ferromagnet as well as the induced moments of the nonmagnetic layers in the vicinity of the interface.

In this paper, we deal with the interface magnetism in Fe/V(001) SL's having two main targets: (i) To quantify the Fe and V magnetic moments at the interface and investigate their dependence on the SL's composition. For this reason, we select (Fe_n/V_m) SL's with very thin layers $n,m=2-5$ ML. This choice enables interface effects to be more pronounced. The Fe magnetic moments are determined element-specifically via the x-ray magnetic circular dichroism (XMCD) by application of the so-called "sum rules."[15,16] On the other hand, the application of the sum rules to the V XMCD has drawbacks discussed in Ref. 17. To tackle this problem we measured the total magnetization of the samples by a conventional magnetometry, namely vibrating sample magnetometry (VSM), and subtract the Fe magnetization. Thus, unlike previous works we were able to determine the V magnetic moment absolutely, i.e., no experimental standard for V is needed in the present work. The outcome is a Fe magnetic moment, which is strongly reduced at the interface *and* a V magnetic moment, which could be as high as $1.1\mu_B$/atom at the interface. Both moments depend on the SL composition. (ii) The second target is to compare results for the orbital magnetism of Fe from the only two techniques that can measure it in thin films, namely the XMCD and ferromagnetic resonance (FMR). The results are discussed with respect to *first principles* calculations.[18] Both experiments and theory deduce the same trends, i.e., enhanced orbital contributions as the Fe film thickness decreases to the ultimate limit of 2 ML.

The single-crystalline SL's of Fe/V(001) on MgO(001) have been prepared at 600 K in a three-source ultra-high-vacuum-based sputtering equipment.[1] Before magnetic measurements to be carried out our samples were structurally characterized by x-ray diffraction (XRD) experiments. In Fig. 1 we see the small-angle XRD spectrum for the Fe_2/V_5 sample. Two Bragg peaks which are indicated by numbers and the small oscillations marked by an arrow (Kiesig fringes) reveal excellent reproduction in the repeat length and a well-defined total film thickness. The high SL quality is also supported by the presence of satellite diffractions $(+1,-1)$ around the average interplanar spacing diffraction (0) in the high-angle XRD spectrum which is shown as an inset in Fig. 1.

For the determination of the saturation magnetization hysteresis loops were recorded along the easy axis of magnetization in the film plane at 10 K by VSM. XMCD experiments have been performed at the European Synchrotron Radiation Facility (ESRF) in Grenoble on the ID12B beamline.[19] Element-specific spectra at the $L_{2,3}$ edges of Fe and V were carried out at 10 K using the total electron yield

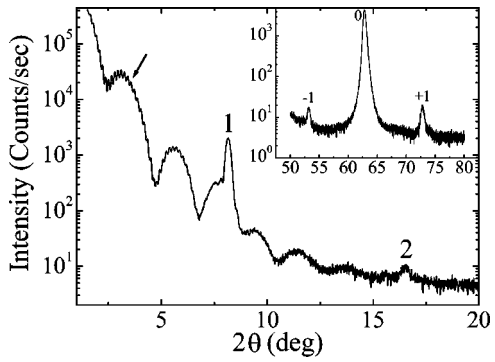

FIG. 1. The small-angle XRD spectrum and the high-angle XRD spectrum (inset) for a Fe_2/V_5 SL. Both spectra reveal the high SL quality of our samples.

(TEY) detection mode. The recorded spectra were taken along the hard axis of magnetization, i.e., normal to the surface plane. In this geometry saturation effects[20] in the TEY can be ruled out. Large magnetic fields up to 6 T were applied for complete magnetic saturation of the samples. The *k* vector of incident circular light was parallel to the applied field. The degree of circular polarization was 85%. The XMCD was measured in two ways by inverting the helicity of the light and by reversing the direction of the magnetic field. No artificial magnetic background in the dichroic spectra using the TEY in applied fields was found by this cross-check.

The normalized XMCD spectra at the Fe and V $L_{2,3}$ edges of the Fe_4/V_2 SL's are displayed in Fig. 2. The V spectrum indicates an induced magnetic moment. Although the V dichroism effect is small as the enlargement factor ''×15'' reveals, the spectrum is free of noise and of higher quality with respect to previous ones.[11] This enables a detailed analysis of the V XMCD and will be published elsewhere. However, the V dichroism reveals a complicated shape due to the small spin-orbit splitting of the initial $2p$ core levels of 7.7 eV only. This leads to a remixing of spin components of the $2p_{3/2}$ and $2p_{1/2}$ states. Consequently the application of the sum rules is more complicated for the V case. The dichroism of V and Fe reveal opposite onsets in sign (marked by the arrows in Fig. 2) indicating an antiparallel alignment between Fe and V moments in agreement with theory and previous experiments.[9–11]

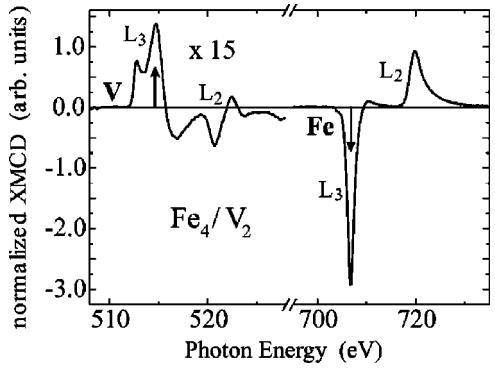

FIG. 2. Normalized XMCD spectra at the $L_{2,3}$ edges of V and Fe for a Fe_4/V_2 superlattice. For better illustration the V dichroism has been multiplied by 15. The directions of the Fe and V magnetization are indicated by the arrows.

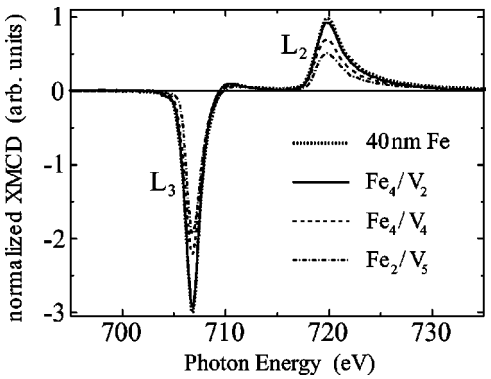

FIG. 3. Normalized XMCD spectra at the $L_{2,3}$ edges of Fe for four samples as indicated at $T=10$ K and $H=6$ T.

Now we turn to the investigation of the magnetic moments of Fe by means of XMCD. To calculate magnetic moments of Fe [m_{Fe} (Ref. 21)] in our samples we applied the sum rules.[15,16] The detailed procedure of the analysis of experimental spectra for the transition elements with the help of the sum rules is well established (see, e.g., Chen *et al.*,[22] Srivastava *et al.*[23] and references therein). The analysis of the Fe reference sample, i.e., 40 nm Fe/MgO(001), leads to a total moment which is within 6% the literature value [$2.22\mu_B$ for bulk Fe (Ref. 24)] using a value of $n_h=3.4$ *d* holes per atom.[22] In Fig. 3 we show the dichroic spectra of Fe in Fe_n/V_m with $n/m=4/2,4/4$, and 2/5. The spectra for Fe/V SL's are compared to the one of the reference sample. The XMCD amplitude is approximately proportional to the Fe average magnetic moment in our samples. The XMCD signal of the Fe_4/V_2 sample reveals only slightly smaller intensities compared to the bulk Fe reference sample. In contrast, the signal of Fe_2/V_5 is reduced strongly at the L_3 and the L_2 edges by about 35% and 45%, respectively. This indicates a reduction of the Fe magnetic moment and an enhanced ratio of the orbital to spin moment as will be discussed below. Our results show that the average magnetic moment per Fe atom m_{Fe} (see Table I) is strongly influenced by the numbers *n* and *m* of Fe_n and V_m layers in two ways: (i) By decreasing *n* and keeping *m* constant, the moment of Fe reduces. (ii) By increasing *m* and keeping *n* constant, a sizable reduction larger than 20% of the Fe moment is deduced. Both trends were also observed in Ni/Pt multilayers.[25] The Fe moment reduction supports theoretical calcula-

TABLE I. Total magnetic moment m_{tot} measured by VSM and normalized to the number of Fe atoms only, Fe moment m_{Fe} by XMCD and V moment m_V obtained as explained in the text. Typical error bars by the VSM and XMCD technique are in the range of 5–10%.

Sample	m_{tot} (μ_B/atom)	m_{Fe} (μ_B/atom)	m_V (μ_B/atom)
40 nm Fe		2.22	
$(Fe_4/V_2)_{60}$	1.59	2.12	−1.06
$(Fe_4/V_4)_{45}$	1.28	1.70	−0.42
$(Fe_2/V_5)_{50}$	0.67	1.34	−0.27

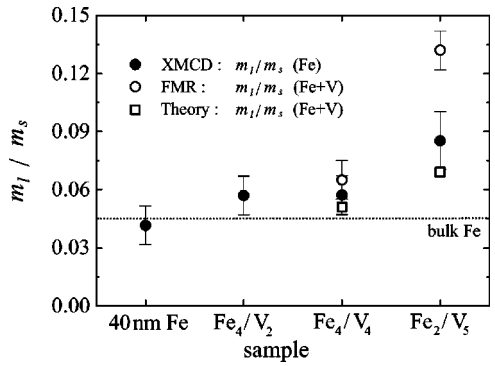

FIG. 4. The ratio m_l^{Fe}/m_s^{Fe} for Fe (full circles) in three superlattices and the bulk reference sample as indicated. The ratios m_l^{Fe+V}/m_s^{Fe+V} for those samples (open circles) are deduced by FMR (Ref. 6). Note that the FMR data were recorded on a "Fe_2/V_5" which was in reality a $Fe_{1.6}/V_5$ sample and therefore showed a larger orbital contribution. Theoretical calculations are given as open squares (Ref. 18).

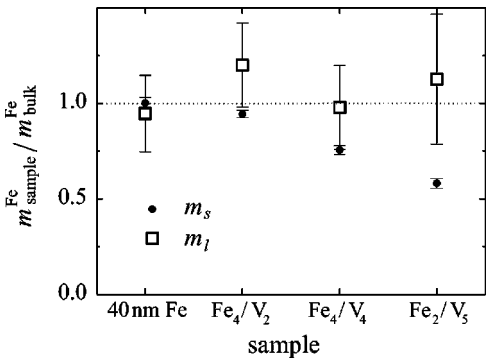

FIG. 5. The orbital and the spin moment for three superlattices and the bulk reference sample as indicated.

tions[8–10] and a previous experiment for Fe_{10}/V_m SL's with $m=5-10$ ML.[13] Moreover, here we demonstrate a clear influence of the sample composition on the Fe magnetic moment.

Now we discuss the determination of the V moments. V is nonmagnetic in the bulk. Therefore, the V XMCD spectra from FeV alloys of known concentration and magnetic moment were previously used as a reference.[11] However, the determination of the V moment following this procedure is questionable. For this reason we preferred to measure the total magnetization with VSM and subtract the Fe moment yielding absolute values for the V moments. In Table I we show the average total magnetic moment $m_{tot}=m_{Fe}+m_V$ per Fe atom from the VSM data and the average magnetic moment per V atom m_V. The negative sign of m_V indicates that V couples antiparallel to Fe in agreement to the sign of our spectra, see Fig. 2. As was discussed above for Fe, the V moments also seem to depend on the SL composition. The maximum induced V moment $m_V=-1.06\mu_B$/atom is obtained by intercalating very thin V layers $(m=2)$ between thicker Fe ones $(n=4)$. Such a large induced moment cannot account for perfectly sharp Fe/V interfaces as *first principles* calculations reveal.[9] However, they are consistent with m_V values measured in similarly prepared SL's with ultrathin V layers[11] and may indicate some intermixing at the interface.[10] By increasing m the V moment decreases considerably. Moreover, by keeping m almost constant, we observe a decrease of m_V when the Fe thickness n is decreasing. The induced V magnetic moment seems to scale with the one of Fe (see the last two rows of Table I).

Our second target is the analysis of the ratio of the orbital-to-spin moment m_l/m_s.[21] Note that n_h and the degree of circularly polarized x rays do not enter into the analysis of the ratio m_l/m_s. The results for Fe determined by the use of the sum rules are denoted by full circles in Fig. 4. We find a systematic enhancement of m_l/m_s by going from the bulk towards the thinner Fe layers. For the Fe_2/V_5 sample this enhancement is about 100%. In the same figure we give m_l/m_s (open circles) determined by g-tensor measurements via FMR.[5,6] Since FMR is not element-specific, it provides an averaged m_l/m_s value for the entire sample (Fe+V). Due to the antiferromagnetic coupling between Fe and V, the spin moments of Fe and V are antiparallel but the orbital moments are aligned in parallel. This means that for FMR measurement the spin moments partially cancel out and the orbital moments add up. Hence the ratio probed by FMR is apparently larger than the one of Fe probed by XMCD as Fig. 4 reveals. The same trend for the enhancement of the total ratio is determined by *first principles* theoretical calculations (open squares).[18]

In order to understand the origin of the enhanced m_l/m_s at the ultrathin Fe limit, we separated m_l from m_s. Figure 5 reveals that within the error bar m_s reduces at the ultrathin limit by 40%, while m_l stays constant. This suggests that hybridization at the interface appears to affect stronger the spin moment than the orbital one. It is well known that at the ultrathin limit there is a significant unquenching of the orbital moment, see, e.g., Refs. 26 and 27 and references therein. Therefore, the constant orbital moment could be interpreted as the outcome of a competition between a negative (hybridization) and a positive (unquenching of m_l) contribution.

In conclusion, by combining an element-specific and a conventional magnetometry we deduce absolutely the Fe and the V magnetic moments in Fe/V(001) superlattices with very thin Fe and V layers. We can evidence an unambiguous reduction of the interface Fe moment, in agreement with *first principles* calculations. We deduce considerable V moments, coupled antiparallel to Fe. We have demonstrated that both Fe and V moments at the ultrathin limit depend on the superlattice composition. Separation into spin and orbital magnetic moment contributions is provided and the results are discussed with respect to ferromagnetic resonance experiments and recent *first principles* calculations. Enhanced orbital over spin magnetism is revealed by decreasing the Fe layer thickness.

A. Tagliaferri, P. Ohresser, and K. Larsson are acknowledged for their technical assistance and the ESRF staff for the excellent operational conditions. This work was supported by BMBF(05KS1 KEB4), DFG Sfb290, and the ESRF.

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