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LETTER TO THE EDITOR

Induced V moments in Fe/V(100), (211), and (110) superlattices studied using x-ray magnetic circular dichroism

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Abstract. Element-specific magnetic moments in Fe/V superlattices are studied using x-ray magnetic circular dichroism (XMCD). Superlattices are simultaneously deposited with the epitaxial orientations (100), (211), and (110), to explore the orientation dependence of these moments. The layer-averaged vanadium moments are antiparallel to those of the Fe and are larger than those observed in alloys with similar composition. The V moments decay monotonically and relatively slowly with distance from the Fe interface (exponential decay length: $\approx$3.0 Å) in qualitative agreement with recent calculations. In contrast to calculations, the magnitudes of the V moments fall on a universal curve for the three orientations.

Only a handful of elements are ferromagnetic (FM) at room temperature, and the applications of FM elements are limited. One way to tailor the properties of these elements is to alloy them with 'nonmagnetic' (NM) elements, whereupon the NM elements sometimes acquire a magnetic moment. Vapour deposition provides another way to mix elements, through the fabrication of multilayers. In multilayers, the NM element is segregated, and makes contact with the FM element only at the layer interface. Thus, multilayers allow control of the degree of contact between FM and NM elements, by varying the number and thickness of the layers.

Faced with mixtures like FM/NM superlattices, element-specific techniques such as x-ray magnetic circular dichroism [1] (XMCD) are required to independently measure the moments of the FM and NM atoms. Here we study Fe/V superlattices using XMCD to characterize both the Fe and induced V magnetic moments. We do this both as a function of V thickness and as a function of epitaxial orientation. Since both Fe and V possess bcc crystal structures (lattice mismatch of 6%) it is possible to prepare superlattices with a unique crystallographic orientation.

Calculations [2–4] of magnetic moments in Fe (3–5 ML)/V superlattices predict that the interface Fe moments are suppressed while interior Fe moments are enhanced, but little net change on average. The average V moments are antiparallel to the Fe layers and decay quickly with increasing V thickness. One tight-binding study of reference [3] found that this decay was due to moment cancellation caused by layer antiferromagnetism in V(100). More recent first-principles self-consistent calculations [4] find a *monotonic* moment decrease toward the V layer interior for the (100), (211), and (110) orientations. Calculations also predict [2, 4] that both the Fe and V moments depend on epitaxial orientation. Here we present an experimental exploration of the behaviour of the V moments.

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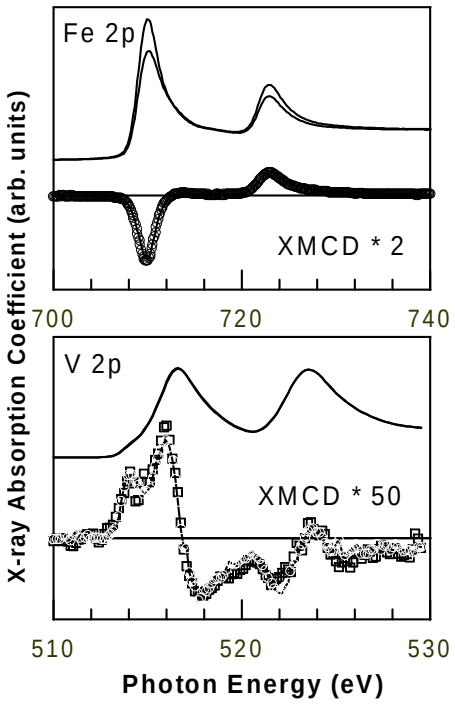

Figure 1. X-ray absorption (solid lines) and XMCD (symbols) at the Fe and V edge of an Fe 7.5 Å/V 9 Å (100) oriented superlattice. Superimposed on each XMCD spectrum is a scaled 'standard' spectrum, from which we deduce the average moment on atoms of each element.

In previous experimental studies, Walker and Hopster [5] used spin-polarized electron energy-loss spectroscopy to study thin V films on Fe(100). They found that only the first and second V monolayers had magnetic moments greater than 0.4 μ_B, aligned antiparallel and parallel to the Fe, respectively. For the same system Fuchs *et al* [6] used spin-polarized secondary-electron and Auger electron spectroscopies to find a first V layer with -0.3 ± 0.08 μ_B (i.e. aligned antiparallel to Fe) while the second and third layers had $+0.1$ and $+0.3$ μ_B (i.e. aligned parallel to Fe).

A recent investigation of a polycrystalline Fe/V multilayer [7] demonstrated the feasibility of using XMCD to characterize V. Here we present the first element-specific moment measurements on Fe/V superlattices. Three simultaneously prepared epitaxial orientations are studied: (100), (211), and (110). We find that the average Fe moment is close to that of bulk Fe, and that the V moments are aligned antiparallel to those of the Fe, with magnitudes comparable to those predicted by theory. The average V moment decays monotonically with increasing V layer thickness, but this decay is slower than $1/t_V$. Employing a simple model for the moment decay, we deduce that even the fourth layer from the V interface possesses a significant moment. In contrast to calculational results, the induced V moment does not depend on the epitaxial orientation, but only the V layer thickness.

The superlattices were prepared in a magnetron sputtering system at Ohio University with a base pressure of 1×10^{-9} Torr. MgO(100), MgO(110), and $Al_2O_3(11\bar{2}0)$ substrates were inserted together and initially heated to >550 °C for 20 min; this was followed by growth of the buffer layer (Cr, 25 Å). The substrates were allowed to cool to 100 °C ($\approx$4 h) at which time a superlattice with structure Fe 7.5 Å/[V t_V Å/Fe 7.5 Å]$_{40}$ was deposited, followed by a protective Al 20 Å capping layer. Here $t_V = 1.5, 4.5, 9, 15$ Å. It was found that with an Al 20 Å capping layer, no detectable oxidation of the Fe or V was evident in

any of the films.

Following deposition, the samples were characterized by specular x-ray diffraction (XRD). The diffraction scans indicated a single vertical orientation of (100), (211), or (110) for films deposited on MgO(100), MgO(110), and $Al_2O_3(11\bar{2}0)$, respectively. Rocking curves through the principal superlattice features ((200), (211), and (110), respectively) show full width at half-maxima of $\approx 1^\circ$ for (200), (211) and $\approx 2^\circ$ for (110).

The samples were characterized using MOKE loops along various in-plane azimuthal orientations. From these loops, the easy and hard axes of each sample were determined. All of the samples had in-plane magnetic anisotropies consistent with their epitaxial orientation.

XMCD studies were performed at the Synchrotron Radiation Center on the 10M toroidal grating monochromator which allows the selection of 85% circularly polarized radiation (used in all of the experiments here). The photon beam was incident at an angle of 45°, and the projection of the photon beam direction into the sample plane was either parallel or antiparallel to the sample magnetization, which was switched at each photon energy. Two absorption spectra, $\alpha_r(\hbar\omega)$ and $\alpha_l(\hbar\omega)$, were thereby obtained using a total-electron-yield technique, which were then normalized to the incident photon flux. The XMCD was measured in remanence where possible, or in saturating magnetic fields of up to 1.5 kOe.

Examples of absorption spectra from an Fe 7.5 Å/V 9 Å superlattice are shown in figure 1. At both the Fe and V 2p edges, $\alpha_r(\hbar\omega)$ and $\alpha_l(\hbar\omega)$ are different, indicating net Fe and V magnetic moments. The XMCD spectra ($\alpha_r(\hbar\omega) - \alpha_l(\hbar\omega)$) are also plotted for each element on an expanded scale (symbols). As in a previous study [7], the V XMCD shows a rather complicated structure as compared with the Fe. At the L_3 edge, the V XMCD is mainly positive, while the Fe is negative. This indicates that the induced V moment is aligned antiparallel with that of the Fe.

Using these XMCD spectra, we deduce the Fe or V moments in an unknown sample by comparison to 'standard' samples where the moments are known, as follows. First, the absorption spectra of both the standard and unknown are normalized to a per atom basis. The standard XMCD spectrum is then scaled by a constant factor, M, which minimizes the least-squares difference between the known and unknown XMCD spectra. M then represents the element-specific moment in the unknown in terms of that in the standard. From the quality of this fit, we are also able to estimate the statistical error of M. This procedure is described in more detail in reference [8]. The best fits of the standard spectra are shown as solid curves overlaying the XMCD data in figure 1. Note that XMCD has an inherent systematic error of at most 20% caused mainly by the magnetic dipole contribution to the XMCD [9, 8].

Figure 2 displays the saturated Fe and V magnetic moments in all of the superlattices. The Fe spectra were compared to a standard spectrum from a 250 Å Fe(211) thin film (with the usual Al capping layer), for which we assumed the bulk Fe moment ($2.18\mu_B$). There is a trend where the overall Fe moment decays slightly with increasing t_V, but for the most part the Fe moments are bulk-like.

Turning now to the V moments, we find that the largest average V moments are induced for the thinnest V layers. This was expected, since the V atoms at the Fe interface should acquire the largest moment. The ordinate scale for the V moment of figure 2 was fixed using a standard spectrum from an $Fe_{94}V_6$ alloy film (capped with Al) for which previous studies indicate a V moment of $\approx -0.6\ \mu_B$. Note that reference [10] also found an Fe moment of 2.2 μ_B which is confirmed by the present measurement. Starburst symbols for the alloy are placed on figure 2 at the horizontal position of a superlattice with the same composition.

Only dilute alloys such as $Fe_{94}V_6$ show significant V moments, as both the V and Fe

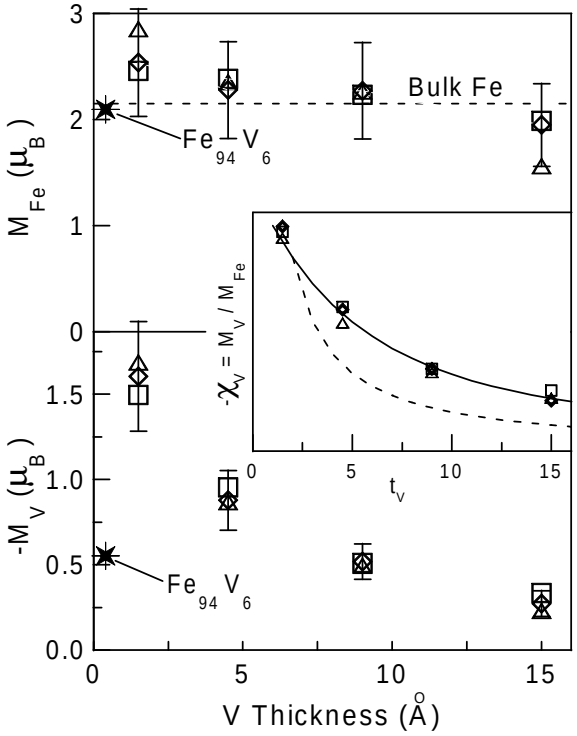

Figure 2. The Fe and V magnetic moments as deduced from XMCD. Squares, diamonds, and triangles correspond to superlattices grown on the (100), (211), and (110) orientations, respectively. The error bars are dominated by systematic errors (see the text), and the data are experimentally reproducible to within $\approx 0.1\ \mu_B$ in all cases. It is observed that neither the Fe nor the V moments depend significantly on the epitaxial orientation, but only on the V layer thickness. In the inset, we plot the V layer susceptibility ($\chi_V = M_V/M_{Fe}$), and two fits (dashed and solid lines) to this quantity described in the text.

moments decrease rapidly with increasing V concentration. Thus it is interesting to note that Fe/V superlattices with an average composition of $Fe_{84}V_{16}$ ($t_V = 1.5$ Å) show more than twice the V moment seen in the $Fe_{94}V_6$ alloy. Moreover, the superlattices have more than ten times the V moment observed in a true $Fe_{84}V_{16}$ alloy [10]. We stress that this result is independent of the exact ordinate scale since we have made a *direct* comparison of the alloy and superlattice XMCD spectra. This 'enhancement' of the V moment in superlattices over alloys was predicted in recent calculations [4].

One striking result is that the induced V moments are quite insensitive to the epitaxial orientation. This is in contrast with what is predicted by calculations [2–4], and might be related to interface roughness (discussed below).

To deduce more quantitative conclusions from this data, we employ the following model. Suppose that any V atom at position z in the layer is exchange coupled to the adjacent Fe layers with a strength that decays exponentially with distance from the Fe layer:

$$\boldsymbol{M}_V \propto [\boldsymbol{M}^0_{Fe} \exp(-z/\lambda_V) + \boldsymbol{M}^{t_V}_{Fe} \exp(-(t_V - z)/\lambda_V)] \tag{1}$$

where $\boldsymbol{M}^0_{Fe}$ and $\boldsymbol{M}^{t_V}_{Fe}$ are the magnetizations of the adjacent Fe layers located at $z = 0$ and $z = t_V$, respectively. To obtain the average V moment, we integrate $\boldsymbol{M}_V$ over the layer

thickness and divide by t_V, to obtain

$$\chi_V \equiv \frac{M_V^{Ave}}{M_{Fe}^{Ave}} = A\ \frac{[1 - \exp(t_V/\lambda_V)]}{t_V} \tag{2}$$

where we have defined the V layer susceptibility, χ_V, which is the average V moment divided by the average Fe moment, λ_V is the exchange coupling decay parameter [8], and A is an arbitrary constant. We choose this model mainly for its simplicity, and because it has the correct asymptotics: M_V^{Ave} is finite as $t_V \to 0$, and falls as $1/t_V$ for $t_V \to \infty$ [11].

Equation (2) is compared (solid line) with the measured χ_V in the inset of figure 2. The parameters A and λ_V have been adjusted to obtain the best fit. The model shows excellent agreement with the data on all three orientations, and allows us to extract $\lambda_V = 3.0$ Å.

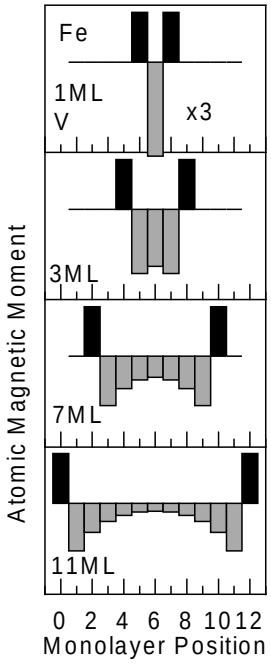

Figure 3. Using the solid-line fit of figure 2, we deduce the configuration of V moments within layers sandwiched between Fe(100) layers; see the text.

To help visualize equation (2), we present in figure 3 the model results for the V moment distribution in several Fe/V(100) superlattices. The Fe layers are all assumed to have a moment of 2.2 μ_B (shown as black bars). The V moments (cross-hatched bars) are multiplied by 3 to bring out their detail. It is seen that the largest V moment is developed for 1 ML V sandwiched between Fe. For thicker V, the average moment gradually drops, although the total moment of the V slab rises monotonically. The total V moment saturates at around 11 ML, after which additional V atoms added to the centre of the slab carry negligible moment. Above 3 ML, the magnetic moment for interface V atoms remains steady at about 0.7 μ_B. The above model is not unique, since any distribution which gives the same average V moment will also be compatible with the data. However, this is the simplest model which describes the data, and it agrees qualitatively with theoretical calculations (reference [4]), particularly with regard to the monotonic decay of the V moments.

One issue that we have neglected until now is interface roughness. Such roughness may partially explain the lack of orientation dependence to the induced V moment. Although we have no way of characterizing roughness in our films, a recent study by Duda *et al* [12]

found 2 Å interface roughness for similarly prepared films. Of contributors to interface roughness, interface alloying is probably the most relevant quantity here. Consider then how alloying might affect the V layers in the $t_V = 1.5$ Å superlattice. In general, the 'V' layers could vary in composition from 100% V (no alloying) down to 16% V (complete alloying). However, bulk alloys with V compositions $>15\%$ show only tiny V moments. Thus, in some respects, the present films behave essentially as superlattices. Conversely, one superlattice effect, the sensitivity to epitaxial orientation, appears to be extremely sensitive to interface roughness, as it is not observed here.

If we assume 2 Å of alloying at each interface, then beyond 2 Å V, one is adding approximately pure V layers to the structure. To highlight our result that these additional V atoms possess a moment, we compare in figure 2 a $1/t_V$ curve (short-dashed line) with the data. If only the interface V atoms had a moment, then beyond $t_V = 2$ Å the V moment should fall like $1/t_V$. Instead, we find that the data fall much more slowly than $1/t_V$. Specifically, the data at 4.5 Å (9 Å) are 1.6 (1.9) times higher than that predicted by $1/t_V$. This means that the *total* V moment is 60% (90%) higher at 4.5 Å (9 Å) than at 2 Å. This is strong evidence that the V atoms in the layer interior possess moments qualitatively similar to those of the diagrams in figure 3.

In conclusion, we present the first element-specific measurements of moments in Fe/V superlattices. The V moments are aligned antiparallel to the Fe, with a maximum of $\approx 1.5\ \mu_B$ for 1 ML V. For thicker V, the interface V moments are $\approx 0.7\ \mu_B$, and the V moment decays monotonically and relatively slowly toward the layer interior. One surprising result is that the Fe and V moments are nearly independent of the epitaxial orientation. The V layers do respond, however, to the 'quantum confinement' caused by the adjacent Fe layers, since the V moments are ten times larger than those observed in alloys with the same composition.

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Note that while these Fe–V alloys were measured at 6 K, their Curie temperature is much higher than room temperature, so the moment values should not change significantly.

[11] This must be the case since for very thick V layers, only a fixed number of vanadium atoms near the interface will possess a moment.

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