Induced magnetization in thin epitaxial V films on Fe (100)

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Using spin-polarized secondary and Auger electron spectroscopy we find an induced magnetization in epitaxially grown V adlayers on Fe (100). Spin-dependent attenuation of the secondary electrons is quantitatively treated, following a model by Siegmann, to determine the adlayer magnetization. The first monolayer of V has a negative magnetic moment of $-0.3\pm0.08\mu_B$ per atom and thus couples antiferromagnetically to the Fe substrate. Subsequent V layers exhibit a positive magnetization. The reduction of the magnetization of Fe at the interface is found to be small. We determine an upper bound $(M_{\text{bulk}}-M_{\text{interface}})/M_{\text{bulk}}<0.2$ of the relative demagnetization of Fe upon V adsorption.

Induced magnetic ordering in ''nonmagnetic'' thin films deposited on the surface of a ferromagnet has attracted considerable interest. A series of recent studies include Cr, Mn, V, as well as Ru, epitaxially grown on Fe (100). An induced magnetic moment unambiguously is found which in the coverage range of the first monolayer (ML) is oriented antiparallel to the magnetization of the substrate for the $3d$-metal adlayers[1–5] and parallel for Ru.[6] For thicker adlayers an antiferromagnetic arrangement of adjacent ferromagnetic (100) sheets of about one monolayer thickness has been reported to occur in Cr (Ref. 2) and Mn,[3] whereas for V (Ref. 5) and Ru (Ref. 6) the moments basically are confined to the layers at the interface. Comparison of these experimental observations with computational predictions is a real challenge, however, if quantitative measurements of the induced magnetic moments are available. The only one in these systems to our knowledge is on Cr/Fe (100) by Turtur and Bayreuther[4] using alternating gradient magnetometry. It is the purpose of the present study to provide a further quantitative analysis of an induced magnetization in an adlayer on a surface of a ferromagnet. As a test system we choose V/Fe (100). Among the $3d$ metals V points towards less filled d bands and thus is an interesting candidate for studying effects of proximity to a ferromagnetic surface and altered atomic coordination.

V at V/Fe interfaces of slabs and multilayers is predicted to carry an induced magnetic moment antiparallel to the Fe magnetization,[7–9] accompanied by a sizeable demagnetization of the Fe atoms at the interface. Computations of induced magnetizations in further V layers away from the interface also exist[7,8] and yield decreasing magnetic moments with increasing distance from the Fe interface. An induced moment in V antiparallel to the Fe magnetization is inferred from NMR measurements on (110) oriented multilayers.[10] Recently Walker *et al.* have found antiferromagnetic coupling of the first V monolayer to the Fe substrate and parallel alignment of the second one.[5] A number of Mössbauer studies on (110) oriented multilayers are claimed to confirm the calculated reduction of the Fe magnetization at the interface.[11]

In this paper we present a quantitative study of thin V layers deposited on a bulk Fe (100) substrate. We use the combination of spin-polarized secondary-electron emission (SPSEE) and spin-polarized Auger-electron spectroscopy (SPAES) which enables us to determine the magnetic moment in V on Fe (100) and also to estimate an upper bound of the demagnetization of the Fe interface atoms upon V adsorption. We apply a model of spin-dependent attenuation lengths in transition metals first proposed by Siegmann[12] to extract quantitative magnetic moments from SPSEE data. We find that at room temperature the first ML of V on Fe (100) has a negative magnetic moment of $-0.3\pm0.08\ \mu_B$ and thus couples antiferromagnetically to the Fe magnetization. Subsequent V layers exhibit a positive magnetization. A sizeable demagnetization of the Fe interface layer can be ruled out. We note that the predicted commensurate antiferromagnetic structure in V is likely to be smeared out in the present case because of imperfect growth of adlayers thicker than one ML.

The spin-polarized electron spectrometer for SPSEE and SPAES has been described earlier.[13] The single-crystal Fe (100) substrate is magnetized by a small horseshoe electromagnet along an easy direction and exhibits a full remanence at which all the measurements are performed. A secondary electron cascade is excited near its surface by an unpolarized primary-electron beam of 2000 eV. The surface-normal emission of secondary and Auger electrons is resolved in energy in a cylindrical-mirror energy analyzer and subsequently submitted to spin-polarization analysis in a 100 keV Mott detector. The spin polarization is defined as $P=(N\uparrow-N\downarrow)/(N\uparrow+N\downarrow)$, where $N\uparrow(\downarrow)$ is the number of electrons with magnetic moment parallel (antiparallel) to the quantization axis of the detector, which is chosen to lie parallel to the Fe magnetization direction. The measured secondary-electron polarization at low energies is proportional to the sample magnetization in a surface region of about 4–5 Å (Ref. 14) thickness, while the extracted Auger-electron polarization gives element specific magnetic information within a probing depth of typically 10 Å (Ref. 15) for transition metals.

The V films are deposited on a well prepared Fe (100) single-crystal surface at room temperature by electron-beam evaporation. During evaporation the pressure is kept below 10^{-9} Torr. The cleanliness of the substrate and of the adlayers is checked with Auger-electron analysis. The film thicknesses are determined by the relative changes of the Fe $L_3M_{45}M_{45}$ and V $L_3M_{23}M_{45}$ Auger-electron intensities upon evaporation. They exactly follow exponential attenuation

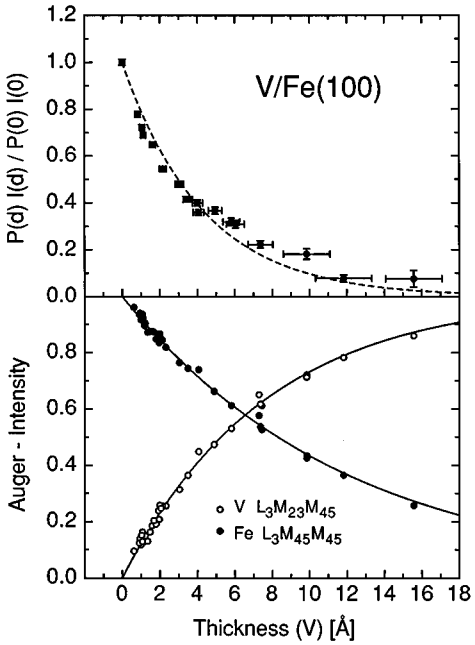

FIG. 1. Secondary-electron spin polarization times intensity *PI* (upper panel) and Auger-electron intensities (lower panel) of V/Fe (100) versus V film thickness. The dashed line in the upper panel represents an exponential background with an attenuation length of 4.3 Å.

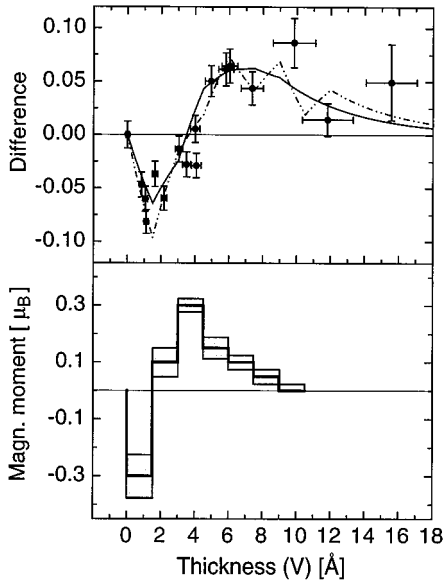

FIG. 2. Upper panel: Secondary-electron spin polarization times intensity *PI* of V/Fe (100) versus V film thickness as shown in Fig. 1, upper panel, after subtraction of an exponential background with an attenuation length of 4.3 Å (dashed line in the upper panel of Fig. 1). Lower panel: Magnetization depth profile obtained from best fit (shown as solid line in the upper panel).

laws as shown in Fig. 1, lower panel, with perfect consistency of the respective attenuation lengths[15] at the relevant energies. This gives evidence of a growth mode without island formation or interdiffusion. The absolute V thickness, however, is based on published attenuation lengths.[15] The crystalline structure of the V layers is examined by low-energy electron diffraction (LEED) analysis. We find that V on Fe (100) displays the same LEED pattern as clean Fe for V thicknesses up to 3 ML. The intensity maxima occur at the same electron energies as with Fe, and no diffuse background is observed. V is adopting the structure of bcc Fe, maybe with a slight out-of-plane tetragonal distortion, for small thicknesses. At larger film thicknesses, however, the LEED pattern gradually obscures and eventually vanishes. This indicates a reduced crystalline quality of the subsequent layers. All measurements are performed at room temperature with a working pressure of $(2–5)\times10^{-10}$ Torr.

Using energy-resolved SPSEE we measure the spin polarization P and intensity I below 2 eV kinetic energy versus V thickness. The observed thickness dependence of the weighted secondary-electron spin-polarization PI, which for a nonmagnetic overlayer is expected to exhibit the attenuation of the substrate polarization by virtue of the overlayer, is presented in Fig. 1, upper panel. The signal deviates from a simple exponential attenuation law in pronounced contrast to the Auger intensities depicted in the lower panel of Fig. 1. The comparison with the Auger data demonstrates that the deviations of the PI signal from an exponential are of magnetic origin and do not relate to the growth properties of the adlayer. The best possible exponential fit to the data is shown as a dashed line in Fig. 1, upper panel, with an attenuation length of $\lambda=0.43$ nm. The difference between the data and this exponential is shown in Fig. 2, upper panel. The deviations from the exponential are found to be significant. In principle they can be interpreted in the following ways: either by an induced magnetization in the V adlayer or by a considerable demagnetization of the substrate surface layer, or by a combination of the two. In order to firmly establish the existence of an induced magnetization in V and to quantify the demagnetization of the Fe surface layer we use SPAES for magnetic measurements[16] at the Fe and V sites.

Figure 3 shows the Fe $L_3M_{45}M_{45}$ and the V $L_3M_{23}M_{45}$ emissions at 700 and 470 eV, respectively. P_{Auger} of the pure Fe substrate is measured and compared to the corresponding value of Fe covered by 1 ML of V. No significant change in

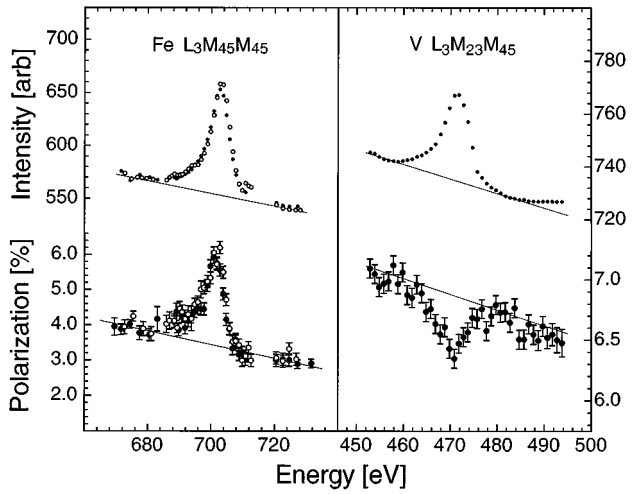

FIG. 3. Spin polarization and intensity of Auger electrons. Left panel: Fe $L_3M_{45}M_{45}$ emission of clean Fe (100) (open circles) and with 1 ML of V (dots). Right panel: V $L_3M_{23}M_{45}$ emission of 1 ML of V on Fe (100).

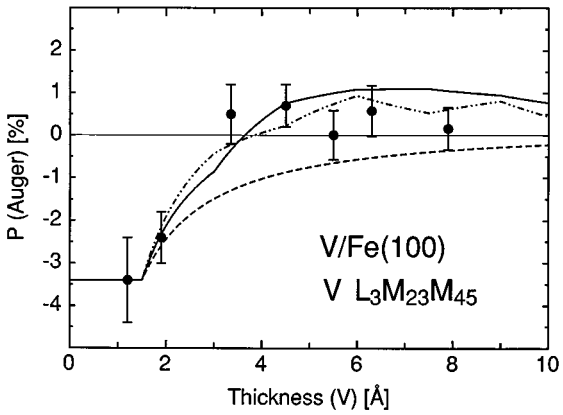

FIG. 4. Auger-electron spin polarization of V in the V/Fe (100) adlayer versus V film thickness. The lines are the integrated polarization depth profiles described in the text.

polarization and intensity can be detected (Fig. 3, left panel). After background subtraction we find for the relative change of P_{Auger} of Fe upon V adsorption $\Delta P_{\mathrm{Auger}}/P_{\mathrm{Auger}}=0\pm0.03$. Because of the large attenuation length the experimental uncertainty of P_{Auger} translates into an upper bound $(M_{\mathrm{bulk}}-M_{\mathrm{interface}})/M_{\mathrm{bulk}}<0.2$ of the relative reduction of magnetization in the outermost Fe layer. From this we conclude that a large depolarization of the Fe at the interface must be ruled out. We then focus our attention on P_{Auger} of the V emission. The spin polarization and intensity of the thinnest film of approximately 1 Å thickness are shown in Fig. 3, right panel. After background subtraction[16] we obtain a negative spin polarization of $P_{\mathrm{Auger}}=(-3.4\pm1)\%$. This gives clear evidence of an induced magnetization in V which is oriented antiparallel to the magnetization of the Fe substrate. Films of various thicknesses are deposited and the corresponding P_{Auger} is depicted in Fig. 4. By completion of the second ML we already observe a positive value of P_{Auger} indicating that the magnetization neither remains negative nor falls to zero after the first ML like in Ru/Fe (100).[6]

In the following we will attempt to extract a magnetization profile of the V adlayer on Fe (100) from the thickness dependence of PI measured by SPSEE, as shown in Figs. 1 and 2, lower and upper panels, respectively. Generally, the determination of absolute magnetic moments from secondary-electron spin-polarization measurements is fraught with difficulties. The spectrum of polarization of secondary electrons at low kinetic energies is characterized by an energy and spin dependent inelastic mean free path which determines the value of polarization near the vacuum level. Therefore, in order to extract absolute magnetic moments an energy-resolved experiment and precise knowledge of the spin dependent scattering cross section at fixed energy are required. A substrate which is covered by a homogeneous adlayer of thickness d emits a secondary-electron current for each spin, which in absence of exchange scattering is given by

$$I^{\pm}(d)=I_s^{\pm}\exp(-d\sigma^{\pm})+i^{\pm}[1-\exp(-d\sigma^{\pm})], \qquad (1)$$

where $I_s^{\pm}$ is the emission from the substrate, $\sigma^{\pm}$ is the spin dependent inelastic scattering cross section $\sigma^{\pm}=1/\lambda^{\pm}$, and $i^{\pm}$ the secondary-electron production rate in the adlayer. If the adlayer carries a magnetic moment $\mu=(n^{+}-n^{-})\mu_B$ per atom, then the valence band acquires the so called band polarization $P_0=(n^{+}-n^{-})/(n^{+}+n^{-}+n_{sp})$, where $n^{\pm}$ and n_{sp} are the numbers of d and sp electrons, respectively. For true secondary or cascade electrons we assume the production rates to be proportional to the number of valence electrons. This yields

$$i^{\pm}=(1\pm P_0)i/2, \qquad (2)$$

with $i=i^{+}+i^{-}$. Measuring the spin polarization $P(d)$ and intensity $I(d)=I^{+}+I^{-}$ of true secondary electrons versus adlayer thickness d then allows one to determine the band polarization P_0 and hence the magnetic moment μ of the adlayer. However, this requires knowledge of the spin dependent scattering cross section $\sigma^{\pm}$. As a simple but powerful rule Siegmann pointed out that the inelastic cross section in transition metals is proportional to the number of unoccupied d states.[12] We apply this model and adopt

$$\sigma^{\pm}=\sigma\mp\sigma_d(n^{+}-n^{-})/2=\sigma\mp\sigma_d P_0(n^{+}+n^{-}+n_{sp})/2. \qquad (3)$$

The scattering cross section $\sigma=1/\lambda$ for unpolarized V is obtained as a best fit to the data; see dashed line in Fig. 1, lower panel. The value of the scattering cross section per d hole $\sigma_d=0.72\ \mathrm{nm}^{-1}$ is taken from Ref. 12. The product $P(d)I(d)=I^{+}-I^{-}$ is calculated for increasing V thickness d by adding the contributions from the substrate and subsequent individual layers of the V film using Eqs. (1)–(3). The band polarization P_0 is taken constant within each atomic layer of V and treated as a free parameter. The calculation is performed layer by layer and it is assumed that P_0 of a given layer does not change upon adsorption of subsequent layers. These basic assumptions make the analysis rather speculative but still might provide a first approximation. We further note that the ranges of partly filled layers are modeled as continuous variation of the thickness which is a reasonable simplification in the present case. Best fit to the experimental data reveals the band polarization and hence an estimate of the magnetic moment in each layer of the V film. The result of this analysis is presented in Fig. 2, lower panel. The corresponding calculated PI is shown as solid line in Fig. 2, upper panel. In order to gain confidence in the choice of the two parameters σ and σ_d we vary $1/\sigma$ between 4.0 and 4.6 Å and independently σ_d between 0.5 and 0.9 nm^{-1} and test the effect on the magnetization profile. In both cases the changes are quite small and fall within the hatched areas on Fig. 2, lower panel.

When studying Auger electrons of the adsorbate, on the other hand, Eq. (1) considerably simplifies. The substrate contributions $I_s^{\pm}$ vanish, and the spin dependence of the attenuation length is very weak and can be neglected since the electrons are emitted at much higher energies. The resulting Auger polarization $P_{\mathrm{Auger}}(d)$ then is a weighted average of contributions from varying depth of the V film giving rise to

$$P_{\mathrm{Auger}}=\frac{\int_0^d P(z)I(z)\exp(-z/\lambda)dz}{\int_0^d I(z)\exp(-z/\lambda)dz}, \qquad (4)$$

where $P(z)$ and $I(z)$ are the emitted Auger-electron polarization and intensity, respectively, at a depth z below the adlayer surface. For a homogeneous adlayer $I(z)$ is constant

and thus cancels in (4). Using model depth profiles $P(z)$ in Eq. (4) and comparing to the measured Auger polarization versus film thickness again yields a magnetization depth profile of the adlayer. However, no reliable absolute value of the magnetization of V can be extracted from the particular $L_3M_{23}M_{45}$ Auger emission used in this study. This transition has been chosen because of its high intensity. It leaves behind one hole in each the $3p$ and the $3d$ states, and the spectrum basically reflects the valence-band density of states in the presence of a $3p$ hole. For Fe and Ni this line has been shown to exhibit a spin polarization which is parallel to the magnetic moment and of the same magnitude as that of the $L_3M_{45}M_{45}$ Coster-Kronig transition.[16] It therefore can be used for element specific magnetometry at surfaces. As a test we have integrated the magnetic depth profile $P(z)$ obtained from SPSEE, shown in Fig. 2, using Eq. (4). The polarization of the first ML is kept fixed at -3.4% and $P(z)$ is scaled accordingly. The result of (4) is shown as solid line in Fig. 4. It exhibits fair agreement with the experimental data. We note that the depth resolution of SPAES is reduced in comparison with SPSEE because of the larger attenuation length. However, we can definitely rule out a magnetization profile where only the first layer at the interface is magnetized, like in Ru/Fe (100).[6] Such a profile would yield an overall negative polarization P_{Auger}, shown as dashed line in Fig. 4.

We have shown that the presence of the Fe interface induces a large spin polarization in thin V adlayers. For the particular structure of epitaxially grown V on Fe (100) at room temperature we find that a V adlayer of up to 1 ML thickness has an induced magnetization of $-0.3\pm0.08\ \mu_B$ per atom which is oriented antiparallel to the Fe surface magnetization. The entire result presented in Fig. 2 can be regarded as magnetic depth profile of V on Fe (100), but only with some reservation. The analysis is valid under the following two assumptions: (i) the magnetization of any V layer does not alter upon evaporation of further V layers, and (ii) the growth is strictly layer by layer. Generally, the first assumption might or might not be justified, while the second most likely is not. We emphasize, however, that in the range of submonolayer coverage both assumptions are valid. The determination of the magnetic moment of the first ML of V on Fe (100) therefore is a firm result. It quantitatively corresponds to a state-of-the-art computational result for a V adlayer of the same geometry: Handschuh and Blügel[9] find $-0.6\mu_B$ in a first-principles calculation.

When going to thicker V adlayers we observe the sign of the induced magnetization to change in the second layer, and the third layer to carry a magnetic moment parallel to the Fe surface magnetization. In subsequent layers the induced magnetization eventually disappears. Comparison with calculated profiles might be obscured by the above mentioned shortcomings of the analysis. However, the observed profile qualitatively corresponds to the one predicted by Vega *et al.*[8] As a further model we tried a layer-by-layer antiferromagnetic ordering superimposed on the noncommensurate magnetization profile of Fig. 2. Such an antiferromagnetic structure might be expected when comparing with Cr or Mn. As a test case we use a modulation amplitude of $0.15\mu_B$ with antiparallel coupling to the Fe substrate. The calculated spin polarizations of secondary and Auger electrons using Eqs. (1)–(3) and (4), respectively, are shown as dashed-dotted lines in Fig. 2, lower panel, and Fig. 4, respectively. We find that such a model cannot be ruled out with the present experiment.

For the magnetization of Fe at the interface, on the other hand, we are able to determine an upper bound $(M_{\mathrm{bulk}}-M_{\mathrm{interface}})/M_{\mathrm{bulk}}<0.2$ of the relative demagnetization upon V adsorption. This clearly is at variance with computations[7,8] as well as with Mössbauer studies,[11] which detect hyperfine fields rather than magnetizations.

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