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1993 J. Phys.: Condens. Matter 5 5459

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Substrate-induced magnetic ordering of rare-earth overlayers: II*

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Received 22 March 1993, in final form 6 May 1993

Abstract. In earlier studies, it was found that for terbium overlays on Ni(111) and Fe(100), the substrates induced some ferromagnetic ordering in the rare-earth film, at temperatures above the Tb Curie temperature. A study is given of the magnetization of ferromagnetic films on ferromagnetic substrates, at temperatures below both Curie temperatures. Expansions are developed for the magnetization within the film as a power series in the distance z to the interface, using Ginzburg–Landau theory. Empirical data for Tb and gadolinium films are found to be consistent with the general form of the expressions found from the theory. Relations are derived for the observed expansion coefficients in terms of the Ginzburg–Landau parameters of the film material. The form a/z for the magnetization is predicted to represent the magnetization well, for z located in an experimentally accessible range of values; data for the magnetization are consistent with this form.

1. Introduction

In a previous paper [1], we modelled the spatially dependent magnetization $M(r)$, as determined by the $5p_{3/2}$ shallow core level branching ratios in different photoemission geometries. We found that the mean-field Ginzburg–Landau theory could be used to explain our results for Tb on Ni(111) and the results of Paul *et al* [2] for Tb on Fe(100), considering in both cases results for the case $T > T_C$, where T_C is the Curie temperature for Tb.

Data have also been obtained for the relative magnetization, as a function of thickness, for Tb overlayers on Ni(111) [1, 3] and for Tb overlayers on Fe(100) [2], for $T < T_C$ of Tb. We wish to ascertain whether these experimental data can also be readily modelled using Ginzburg–Landau theory. There are a number of theoretical studies in which the spatially dependent magnetization $M(r)$ has been described for films, alloys, and ferromagnetic multilayers by applying the Ginzburg–Landau formulation [1, 4–15]. In particular, Schwenk *et al* [14] have computed the magnetization profile in periodic alternating layers, made up of two ferromagnetic materials of differing transition temperatures. Analytical results are presented over the entire temperature range, and for thicknesses including the case of ultrathin layers. Also, Camley and Tilley [11] apply the Ginzburg–Landau theory to a sandwich of two ferromagnetic materials, which couple anti-ferromagnetically at the interface. They study the magnetic superlattices formed, applying their results to $T = 0$. However, only a few examples exist where experimental data for simple metal overlayers

* Part I appeared as [1].

have been successfully modelled in this manner [1, 3, 4, 16–19]. Of particular interest to us are rare-earth overlayers on ferromagnetic substrates.

The starting point of the Ginzburg–Landau theory is the expansion of the free-energy density in a power series in the order parameter. For our case, the order parameter is the magnetization vector $M(r)$. In order that the expansion be valid, it might appear necessary that the magnetization be reasonably small, i.e. that the temperature be not far from T_C [20]. Nonetheless, the theory has been applied successfully over a wide temperature range to a diversity of physical systems, as noted in the preceding paragraph. It has been found that truncation of the expansion, at say, the fourth power of the magnetization vector, still allows a good modelling of data, at temperatures well below the transition. A purpose of this study is to examine how well the magnetization data below the transition temperature for Tb overlays can be modelled by Ginzburg–Landau theory.

2. Experiment

The experiments were performed in an ultra high vacuum (UHV) system equipped with a hemispherical analyser for angle-resolved photoemission and a retarding-field analyser for low-energy electron diffraction as described previously [21]. The light source for the photoemission studies was the 1 GeV ring at the Synchrotron Radiation Center, dispersed by 3 m and 6 m toroidal grating monochromators. The energy resolution (analyser and monochromator) of the photoemission spectra collected by the hemispherical analyser varied from 0.15 to 0.3 eV full width at half maximum.

The incidence angle of the light is defined with respect to the surface normal. A normal light incidence angle (zero degrees) has a vector potential completely parallel to the surface (s-polarized) while glancing-incidence light has a large component of the vector potential normal to the surface (p-polarized). Photoelectrons were collected throughout this work normal to the surface to preserve symmetry selection rules.

The manner in which the Tb or Gd 5p core levels depend on light polarization was measured qualitatively on a relative scale from the ratio of 5p_{1/2} intensity divided by the 5p_{3/2} intensity for p-polarized and s-polarized light (β_p/β_s) as previously described [1]. This is denoted as the p-level anisotropy. The photon energy was typically about 20 eV above threshold (60 eV) to enhance the 5d–5p final state effects [21, 22].

The p-level anisotropy is not normally expected to deviate from unity for non-magnetic systems [1, 3, 22] but some deviations, as a result of crystal field effects, have been noted [1]. The major deviation from unity of the p-level anisotropy, as noted before [1], is a result of magnetic ordering.

For Gd on Cu(100), the results shown in this work are a summary of more conventional dichroism measurements obtained from constant-initial-state spectroscopy as described previously [21, 22]. Such measurements have been typically applied to deeper core levels of the rare earth than the 5p levels [23–25].

3. The differential equations for the magnetization

We begin with the differential equations satisfied by M_{\parallel} and M_{\perp} in the Ginzburg–Landau formulation [20, 26, 27]:

$$-C \frac{d^2 M_{\parallel}(z)}{dz^2} + AM_{\parallel}(z) + BM_{\parallel}(z)M(z)^2 = H_{\parallel}^m \quad (1)$$

$$-C \frac{d^2 M_{\perp}(z)}{dz^2} + AM_{\perp}(z) + BM_{\perp}(z)M(z)^2 = H_{\perp}^m \quad (2)$$

where the magnetization vector is $M(r) = M_{\parallel}(r)\hat{e}_{\parallel} + M_{\perp}(r)\hat{e}_{\perp}$, so that M_{\parallel} and M_{\perp} are the components of M that are parallel and perpendicular to the interface, respectively. The coordinate z is the distance of the considered plane in the overlayer film to the interface. Hence, $0 \leq z \leq D$, where D is the film thickness. The symbols H_{\parallel}^m and H_{\perp}^m in equations (1) and (2) denote the parallel and perpendicular components, respectively, of the demagnetization field. The coefficients A , B and C are temperature-dependent parameters; it shall be assumed that their spatial dependence is negligible. In order that the free energy have a minimum, it is necessary that both B and C be positive. For $T > T_C$, A is positive; for $T < T_C$, A is negative. The latter case will apply in this study.

Equations (1) and (2) are derived by starting from the Ginzburg-Landau expansion of the Helmholtz free-energy density $f(r)$ as a power-series in the components of the magnetization $M(r)$ and its spatial derivatives. It is then required that the free energy F attain minimal value when $M(r)$ reaches thermal equilibrium.

If terms in $f(r)$ beyond the fourth power of M are ignored, equations (1) and (2) are obtained for the static magnetization $M(r)$. This truncation is quite prevalent in the literature [11, 14, 20, 26, 27] for temperature both below and above the Curie temperature.

Since the lateral dimensions x and y of the overlayer greatly exceed the film thickness D , we can properly assume that M depends on z , but not on x or y . Furthermore, experimental studies of ultra-thin ferromagnetic films [17, 28] suggest that experimental investigations of Tb overlayers [1-3] sample only a single domain consistent with spin-polarized photoemission of Gd [29]. If the sample also includes a ferromagnetic substrate with a single domain, the magnetization vector $M(r)$ is along the easy axis of magnetization of the substrate. We are here assuming that the film is a linear magnetic material with its magnetization parallel to the inducing field of the substrate as is consistent with spin-polarized photoemission studies [29].

Equations (1) and (2) can be simplified. Since the applied field $H = 0$, we can concern ourselves solely with the demagnetization field H^m given by

$$H^m = B - 4\pi M(r) \quad (3)$$

where the vector B is the magnetic induction vector.

The relevant Maxwell's equations become

$$\nabla \times H^m = 0 \quad (4)$$

and

$$\nabla \cdot B = 0 = \nabla \cdot (H^m + 4\pi M). \quad (5)$$

These equations are identical to those of Schwenk *et al* [14]. Since M , B and H^m can depend upon z but not x or y , the most general solutions to these Maxwell's equations are that

$$H^m = (0, 0, -4\pi M_{\perp}) + C \quad (6)$$

where C is a spatially constant vector. Schwenk *et al* [14] tacitly assume $C = 0$. If $C \neq 0$, then H^m and B would be non-zero for $z \rightarrow \infty$.

We shall also assume that the magnetization for Tb films on Ni(111) and Fe(100) is in-plane. There is particularly strong evidence for this result in our experimental study of paramagnetic Tb overlayers; there is no evidence of a substrate-induced normal component [1]. For paramagnetic Tb [1-3], as $z \rightarrow \infty$, $M(z) \rightarrow 0$; this would not occur if the substrate-induced field applied to the overlayer had a substantial component normal to the surface, since

$$M = m_B^2 BN(E_F). \quad (7)$$

This experimental results for paramagnetic Tb is not surprising since for both Fe(100) and Ni(111), these surfaces also represent the 'hard' (magnetization) directions while the other low-index faces are also the directions that are 'easy' [30]. Thus the magnetization for these surfaces lies 'in-plane' [1]. Secondly, the measurements for Tb on Fe(100) by Paul, Landolt and coworkers [2, 18] are sensitive only to in-plane magnetization. It may also be remarked that experiments for Ni on Cu(111) [31] and for Fe on Au(100) [32] find in-plane magnetizations.

Let $F^m(M)$ denote the contribution to the free energy F due to the demagnetization field H^m ; then $F^m(M)$ is given by the expression

$$F^m(M) = -\frac{1}{2} \int M \cdot H^m d^3r. \quad (8)$$

Inserting $H^m = (0, 0, -4\pi M_\perp(z))$ into this integral results in

$$F^m(M) = -\frac{1}{2} \int M_\perp H_\perp^m d^3r = 2\pi \int M_\perp^2 d^3r. \quad (9)$$

This integral is never negative and is smallest when $M_\perp = 0$. If the anisotropy energy can be ignored, then equation (9) contains the dominant dependence of the free energy on M_\perp ; hence $M_\perp = 0$. Thus the magnetization is in-plane. From equation (6), using $C = 0$, the result $H^m = 0$ is attained. The arguments encompassing the discussion from equation (3) to equation (9) are similar to those of Schwenk *et al* [14]. The geometry differs somewhat from that of the present experiments in that their concern is that of a periodic series of multilayers, while we have undertaken our experiments for simple overlayers [1]. None the less, in both geometries, the fact that the magnetization is independent of x and y is clear; the equilibrium results $H^m = 0$ and $M_\perp = 0$ follow.

The anisotropy contribution to the free energy could include terms such as

$$F_{\text{anis}}(M) = L \int (\hat{n} \times M)^2 d^3r \quad (10)$$

with L a positive constant and \hat{n} as the unit vector normal to the interface. This would favour lining M up along the normal to the plane to make $F_{\text{anis}}(M) = 0$ (its smallest value) if L is positive. For ferromagnetic Gd on W(110), there are strong indications that this anisotropy is very small [17, 29] and is insufficient to orient M along the surface normal on this paramagnetic substrate. Estimates of this anisotropy energy for other ferromagnetic overlayers also suggest this energy to be quite small, some 0.5 meV or less [31, 33]. It is reasonable that the substrate field will swamp out such an anisotropy since the substrate has more moments, is ferromagnetic, and the film must grow atom by atom.

With the above assumption that M is in-plane, equation (2) can be ignored and we can rewrite equation (1) as

$$-C \frac{d^2 M_\parallel(z)}{dz^2} + A M_\parallel(z) + B M_\parallel(z)^3 = 0. \quad (11)$$

Henceforth, we shall replace $M_\parallel(z)$ by $M(z)$.

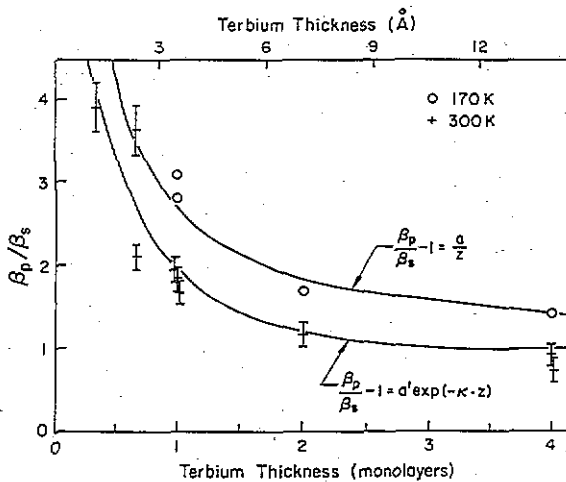


Figure 1. The p-level anisotropy data for Tb on Ni(111) at room temperature (+) and at 170 K (○) as a function of film thickness, as given in [1]. For $T > T_C$ the data are fitted to an exponential profile while for $T < T_C$, $M(z) = a/z$, with a as a constant (see equation (24) and the discussion following it).

4. Formal solution of the differential equation

It is convenient to replace $M(z)$ in equation (11) by the dimensionless magnetization $m(z)$ defined by

$$m(z) = \frac{M(z)}{M(\infty)} = (B/|A|)^{1/2} M(z) \tag{12}$$

where, $M(\infty)$ is the bulk magnetization of the material of the film and is given by $(|A|/B)^{1/2}$. That this is so follows immediately from the solution for $M(r)$ obtained by deleting the first term of equation (11). The latter equation is now

$$(1/\kappa^2) d^2m/dz^2 + m - m^3 = 0 \tag{13}$$

with κ defined by $\kappa^2 = (|A|/C)$. The parameter B is absent from equation (13) but maintains its presence via equation (12). Note that $m(\infty) = 1$; hence if data for large z are available for any quantity proportional to M , the data allow determination of $m(z)$ for all z covered by the experiments. The proportionality constant need not be known.

The first integral is

$$(1/\kappa^2)(dm/dz)^2 + m^2 - m^4/2 = s/2 \tag{14}$$

where $s/4$ is the integration constant obtained by integrating equation (13).

Then, the formal solution of equation (13) for $T < T_C$ follows by taking the second integral:

$$\kappa z = \pm \sqrt{2} \int_{m(z)}^{m(0)} \frac{dm}{(m^4 - 2m^2 + s)^{1/2}} \tag{15}$$

(noting that $z = 0$ is the interface plane). The data for Tb on Ni(111) [1] and for Tb on Fe(100) [2], presented in figures 1 and 2 respectively, show that $m(0) > m(z)$ and that $m(z)$ monotonically decreases with z . As a result, equation (15) requires the positive sign on the right hand side, for these data.

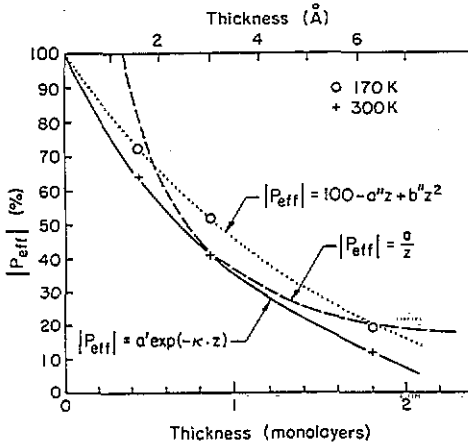


Figure 2. The Ginzburg-Landau model fitted to the Auger electron polarization data for Tb on Fe(100), taken from [2]. Data for room temperature (+) and 170 K (O) have been plotted. The measured quantity $|P_{eff}|$ is proportional to the magnetization $m(z)$. The data at 300 K are modelled by equation (25), while those taken at 170 K are modelled by equations (16), (17) and (18).

As is the case for $T > T_C$, for $T < T_C$, the solution of equation (15) can be cast in the form of incomplete elliptic integrals $F(\phi, k)$ of the first kind. The forms are given in the appendix.

Khan [34] has derived a result equivalent to equation (15) and has also expressed the integral in terms of Jacobi θ functions. Our results in the appendix are formally equivalent to those of Khan. In addition, Winternitz *et al* [35] have obtained exact solutions of the three-dimensional analogue of equation (11). These latter solutions are important for cases in which lateral-plane symmetry (corresponding to the geometries considered here) is not present.

The formal solutions just cited admit a power-series expansion:

$$m(z) = \sum_{j=0}^{\infty} m_j z^j. \tag{16}$$

Equating coefficients of z^j for $j = 0, 1$ yields

$$m_1 = \pm(\kappa m_0^2 / \sqrt{2})(1 - 2/m_0^2 + s/m_0^4)^{1/2} \tag{17}$$

$$m_2 = (\kappa^2 / 2)m_0^3(1 - 1/m_0^2). \tag{18}$$

The lower sign in equation (17) is applicable to the data for the reasons cited below equation (15).

Measurements of the magnetization profile allows extraction of values for κ and s , using equations (17) and (18), provided there are extensive data for large z . As already noted, $m(z)$ is the magnetization in units of that of the bulk. Analysis of the data allows values for m_0, m_1 and m_2 to be obtained.

Equations (17) and (18) yields $\kappa = (|A|/C)^{1/2}$ and s , while $|A|/B$ can be obtained from inspection of data for the magnetization curve $M(T)$ for bulk Tb, using $M(T) = (|A|/B)^{1/2}$.

Note that thermal equilibrium data for the magnetization of Tb films or for bulk Tb cannot be used (in the absence of an externally applied magnetic field) to ascertain values for A, B and C separately; the differential equation for $M(z)$ is sensitive only to the ratios $|A|/B$ and $|A|/C$.

The meaning of the integration constant s can be clarified by first noting that $s \rightarrow 1$ as $D \rightarrow \infty$. The latter fact can be seen from inspection of equation (14); let $z \rightarrow \infty$ and note that $m(z) \rightarrow 1$ and $dm/dz \rightarrow 0$. Now, for $D < \infty$, note that at the free surface of the film, the number of nearest neighbours of the atoms is reduced; exchange energies are altered. For this reason, $m(z, D)$ may have a weak dependence on D , for fixed z . (Here, $m(z, D)$ denotes $m(z)$ for films of thicknesses D , and $z \leq D$.) Inspecting equation (15) shows a weak dependence of either s or $m(0)$ on the thickness D .

Since the value of $m(0)$ is likely to be dominated by the magnetization of the substrate relative to film-material bulk magnetization, s must be dependent on D . If $m(z, D)$ decreases as D decreases (z fixed), then s must slowly increase to keep the left hand side of equation (15) unaltered.

A simple form for $m(z)$, valid over a restricted (but accessible) range of z , can be derived by writing equation (16) in the form

$$m(z) = -(m_0^2/m_1 z)(1 + J/z + Nz + Qz^2 + \dots)^{-1} \quad (19a)$$

where $J = -m_0/m_1$ and $N = (m_2 m_0 - m_1^2)/m_0 m_1$.

If z can be restricted to a range of values for which $J/z \ll 1$ and also $Nz \ll 1$, then

$$m(z) = a/z \quad (20)$$

with

$$a = (\sqrt{2}/\kappa)(1 - 2/m_0^2 + s/m_0^4)^{-1/2}. \quad (21)$$

If s does not greatly deviate from unity, then $a \simeq \sqrt{2}/\kappa$ is obtained, since $m_0 > 1$.

The condition on the validity of equation (20) can be rewritten:

$$m_0^{-1} \ll \kappa z / \sqrt{2} \ll m_0. \quad (22)$$

The discussions of equations (11)–(22) apply to $T < T_C$ for magnetizations *in plane*, appropriate for the data considered in this study. However, for the magnetization normal to the surface, i.e., $H_{\perp}^m \neq 0$, there exists a special solution for $M(z)$ in this geometry that can be noted. Equation (11) can be replaced by

$$-C(d^2 M_{\perp}(z)/dz^2) + A M_{\perp}(z) + B M_{\perp}^3(z) = -4\pi M_{\perp}(z) \quad (23)$$

from substitution of equation (6) into equation (2). Clearly, $M_{\perp}(z) = h/z$ is a solution to this differential equation if $A = -4\pi$ and if the constant h satisfies $2C = B h^2$. This result is consistent with the results of Tuszynski and coworkers [15, 36].

5. Comparison with data

The results for Tb films plotted in figures 1 and 2 are obtained by photoemission or Auger spectroscopy. These are surface-sensitive probes under the conditions employed [1, 2]. The simplest assumption is that $M_{\parallel}(z = D, D)$ was measured. Here, $M_{\parallel}(z, D)$ is the in-plane magnetization at plane z , for a film of thickness D . We add the plausible assumption that $M_{\parallel}(z, D)$ depends dominantly on z , and only weakly on D . This assumption is buttressed

by the fact that the data encompass only a narrow range (five monolayers, at most) of values of D . Thus, $M(z) = M_{\parallel}(z, D)$ can be approximated by the measured values of $M_{\parallel}(z, z)$.

For an explicit comparison between theory and data, we first note that we have recently introduced a technique for probing local magnetic ordering using conventional angle-resolved photoemission spectroscopy [1, 3, 21, 22] without spin detection of the photoelectrons. By measuring the 5p core levels in different photoemission geometries, the magnetic ordering of Gd [19, 20] and Tb [1, 3] overlayers has been characterized.

The initial state eigenspinors of the Tb $5p_{3/2}$ level $m_j = \pm 3/2$, are of well-defined electron spin character, while the $5p_{1/2}$ and $5p_{3/2}$, $m_j = \pm 1/2$ eigenspinors have mixed electron spin character. As a result of these differences, there are differences in the final state valence 5d interactions with these shallow core levels. These changes in the final state interactions are easily observed in angle-resolved photoemission by changing the incident light polarization [21, 22]. The strongest manifestation of this 5d–5p coupling is a change in the 5p branching ratio with changes in the incident light polarization. Changing the incident light polarization selectively excites different symmetry states in the initial state eigenspinors. This can occur even without alignment of the spatial coordinate system with the magnetic coordinate system [1, 21, 22].

This probe of the magnetic ordering can be quantified on a relative scale by the ratio of the 5p branching ratios for p and s polarized light (β_p/β_s), which we denote as the p-level anisotropy [1, 3]. The p-level anisotropy has been measured and plotted for a variety of Tb film thicknesses at temperatures well above (300 K) and well below (170 K) the Tb Curie temperature (220 K). These results are summarized in figure 1, for Tb overlayers on Ni(111) [1, 3].

The p-level anisotropy is unity with no magnetic ordering (and neglecting crystal-field effects) [1]. Thus

$$\beta_p(z)/\beta_s(z) - q = pM_{\parallel}(z) \quad (24)$$

where p is an appropriate scaling constant, and q is unity with no crystal-field effects. It should be noted that experimental studies indicate that q could vary from 0.82 to 1.2 [1], but for this discussion, this possible crystal-field effect will be ignored.

In an earlier work we showed, using Ginzburg–Landau theory, that for $T > T_C$

$$M_{\parallel}(z) \simeq R \exp(-\kappa z) \quad (25)$$

where κ^{-1} is the correlation length and is equal to $(C/A)^{1/2}$ [1] and R is a constant. The magnetization dependence of equation (25) can be related to the p-level anisotropy; it is fitted to the experimental data as also seen in figure 1.

For $T < T_C$, we can model the p-level anisotropy by using equations (20) and (24), as seen in figure 1, because $M(0)$ is relatively large and z is large. These models can also be applied to the results for Tb on Fe(100) by Auger electron polarization studies by Paul and coworkers [2] as discussed in detail elsewhere for several temperatures at $T < T_C$ [18]. Their experimental results for $T > T_C$ have been fitted to equation (25) as seen in figure 2. For $T < T_C$ their results cannot be fitted to equation (20) (as has been done for Tb on Ni(111)) because the data exist only for small values of z . Rather, the data are better modelled by equations (16)–(18); the comparison is given in figure 2.

Both sets of thickness-dependent magnetization data [1–3] can be modelled by equation (19) if the reciprocal of the magnetization, $1/m(z)$, is plotted versus z ; the graph is displayed in figure 3. Such modelling indicates the validity of using mean-field theory in

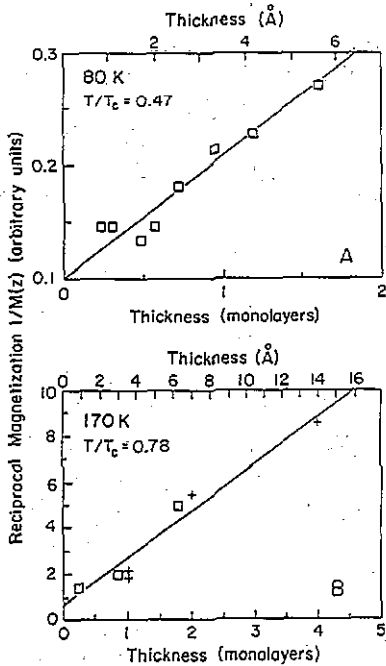


Figure 3. The reciprocal magnetization data (A) for Tb on Fe(100) (taken from [18]) at 80 K and (B) for Tb on Fe(100) [2] (□) and Ni(111) [1] (+) at 170 K plotted versus film thickness for $T < T_C$.

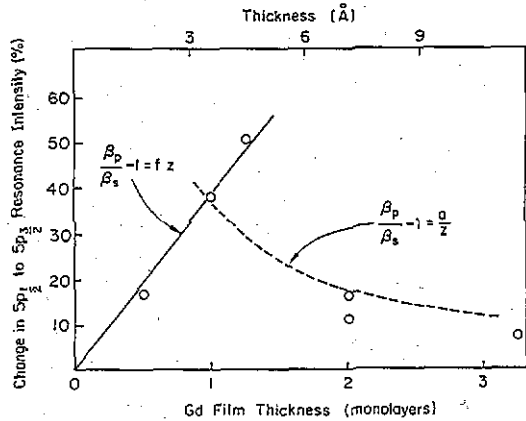


Figure 4. The constant initial state (CIS) spectroscopy equivalent to the p-level anisotropy (less than unity) for Gd on Cu(100) taken from [21] and [22]. These data are similar to dichroism data obtained for 2p rare-earth core levels [23, 25]. Ginzburg-Landau theory has been used to model this data, shown as the curves. The data do not imply long-range magnetic order, as an experimental arrangement sensitive only to short-range order was employed.

predicting magnetization since for Tb it does seem clear that $n(z) = 1/m(z)$ varies linearly with z , and from equation (19a)

$$n(z) \simeq n_1 z + m^{-1}(0) \quad n_1 = -m_1/m_0. \quad (19b)$$

The data for Tb on Ni(111) and on Fe(100), for $T < T_C$, are in good agreement when plotted in this manner. Note that equations (17) and (18) predict signs for the linear and quadratic terms in z , in the small- z expansion of $m(z)$. The coefficient of the linear term is negative; for the quadratic term it is positive. As can be seen in figure 2, the best fit to the data of Tb on Fe(100) for this form has coefficients which agree with both signs.

Consider ferromagnetic overlayers on paramagnetic substrates, such that a single monolayer exhibits enhanced magnetization, and the magnetization is restricted to be in plane. Then a simple model is to assume that the magnetization will go as $M_{\parallel}(z) = hz$ for z less than one monolayer thickness and $M_{\parallel}(z) = a/z$ for z greater than one monolayer thickness. (The constants h and a are related by the fact that $hz = a/z$ at z corresponding to one monolayer thickness.) Such a model is a result of the linear increase in moments up to one monolayer (following a simple summation of moments) and the inverse decay beyond one monolayer that results from the analysis above, treating one monolayer as the ferromagnetic substrate. Enhanced magnetization for very thin films is not unknown and this model may be very applicable [37, 38].

Such characteristic behaviour has been observed for Gd overlayers on Cu(100) at $T < T_C$ (220 K) [21, 22] as seen in figure 4. Such a result also suggests that for this system that the magnetization is in-plane, though some experimental indications exist suggesting that M has a component (albeit small) that is normal to the surface in this system [29]. Ferromagnetic overlayers on ferromagnetic substrates will not agree with the Ginzburg–Landau model in the very-thin-film limit [18]. The failure to model overlayers *much less* than a monolayer could be associated with percolation and interface magnetization effects.

6. Conclusion

In summary, in spite of a large number of assumptions, the Ginzburg–Landau theory qualitatively describes the thickness dependence of the surface magnetization within the overlayer for rare-earth overlayers on ferromagnetic substrates. This model can be applied to ultrathin films (less than 10 monolayers thick). The agreement is surprisingly good. As noted in a brief report [18] failure of this mean-field theory (away from T_C) only appears to occur in the very-thin-film limit (approximately $\frac{1}{2}$ monolayer for the rare earths).

Acknowledgments

The authors would like to thank Dave LaGraffe, Dongqi Li and Marshall Onellion who assisted in this study. The authors would also like to acknowledge helpful discussions with M Landolt (ETH, Zürich) and to thank M Landolt and W Hürsch for sharing with us their ideas and their data. This work was funded by the US DOE.

Appendix

As pointed out below equation (15), the formal solution for the dimensionless magnetization $m(z)$, given in equation (15), can be re-expressed in the form of incomplete elliptic integrals $F(\phi, k)$. For this purpose, it is necessary to consider separately three ranges of values of s .

Case 1: $s > 1$. Use of standard identities (see, for example, [39–41]) yields for $s > 1$ the result

$$\beta z = F(\alpha_z, r) - F(\alpha_0, r) \quad (\text{A1})$$

where $\beta = (\frac{1}{2})s^{1/4}\kappa$ and with α_z defined by

$$\cos \alpha_z = [m^2(z) - s^{1/2}]/[m^2(z) + s^{1/2}]. \quad (\text{A2})$$

Also,

$$r = (\frac{1}{2} + \frac{1}{2}s^{-1/2})^{1/2}. \quad (\text{A3})$$

The values of r are confined to the range $2^{-1/2} \leq r \leq 1$.

Case 2: $0 \leq s \leq 1$. For this case, equation (15) transforms into the form

$$kz = F(\phi_0, w) - F(\phi_z, w) \quad (\text{A4})$$

with

$$k = (\kappa/\sqrt{2})(1\sqrt{1-s})^{1/2}. \quad (\text{A5})$$

Also, ϕ_z is defined by

$$\sin \phi_z = m(z)/(1\sqrt{1-s})^{1/2} \quad (\text{A6})$$

while w is given by

$$w = [s^{-1}(1 - \sqrt{1-s}) - \frac{1}{2}]^{1/2} \quad (\text{A7})$$

and is restricted to the range $0 \leq w \leq 2^{-1/2}$.

Case 3: $s < 0$. Since $s \rightarrow 1$ as $D \rightarrow \infty$, this case is only possible for very thin films. If $s < 0$, then equation (15) can be restated as follows:

$$\eta z = F(\xi_z, t) - F(\xi_0, t) \quad (\text{A8})$$

with η defined by

$$\eta = \kappa(1-s)^{1/2}. \quad (\text{A9})$$

The variable ξ_z is determined by

$$\sin^2 \xi_z = 2\sqrt{1-s}/[\sqrt{1-s} - 1 + m^2(z)] \quad (\text{A10})$$

and the variable t is

$$t = (1 - 1/\sqrt{1-s})^{1/2}. \quad (\text{A11})$$

Note that use of equations (A1), (A4), or (A8), together with tabulated values of $F(\phi, k)$ allows for exact numerical integration of equation (13). A best-fit comparison between data and the numerical solution then enables extraction of κ . Such a procedure is an alternative to the power-series expansion procedures described in the text.

References

- [1] Dowben P A, LaGraffe D, Li Dongqi, Miller A, Zhang L, Dotti L and Onellion M 1991 *Phys. Rev. B* **43** 3171
- [2] Paul O, Toscano S, Hürsch W and Landolt M 1990 *J. Magn. Magn. Mater.* **84** L7
- [3] LaGraffe D, Dowben P A and Onellion M 1990 *Phys. Lett.* **147A** 240
LaGraffe D, Dowben P A, Miller A and Onellion M 1990 *Mater. Res. Soc. Symp. Proc.* vol 187 (Pittsburgh, PA: Materials Research Society) p 225
- [4] Mathon J 1986 *J. Phys. F: Met. Phys.* **16** L217
- [5] Mathon J 1986 *J. Phys. F: Met. Phys.* **16** 669
- [6] Mathon J and Bergmann G 1986 *J. Phys. F: Met. Phys.* **16** 887
- [7] Binder K and Hohenberg P C 1972 *Phys. Rev. B* **6** 3461

- [8] Edwards D M, Mathon J and Wohlfarth E P 1975 *J. Phys. F: Met. Phys.* **5** 1619
- [9] Edwards D M, Mathon J and Wohlfarth E P 1973 *J. Phys. F: Met. Phys.* **3** 161
- [10] Coutinho S, Edwards D M and Mathon J 1983 *J. Phys. F: Met. Phys.* **143** L143
- [11] Camley R E and Tilley D R 1988 *Phys. Rev. B* **37** 3413
- [12] Camley R E 1987 *Phys. Rev. B* **35** 3608
- [13] Fishman F, Schwabl F and Schwenk D 1987 *Phys. Lett.* **121A** 192
- [14] Schwenk D, Fishman F and Schwabl F 1988 *Phys. Rev. B* **38** 11618
- [15] Tuszynski J A 1989 *Mater. Res. Soc. Symp. Proc.* vol 151 (Pittsburgh, PA: Materials Research Society) p 265
- [16] Taborelli M, Allenspach R, Boffa G and Landolt M 1986 *Phys. Rev. Lett.* **56** 2869
- [17] Farle M, Berghaus A and Baberschke K 1989 *Phys. Rev. B* **39** 4838
- [18] Dowben P A, Hürsch W and Landolt M 1993 *J. Magn. Magn. Mater.* to be published
- [19] Chen Qibiao, Onellion M, Wall A, Li Dongqi and Dowben P A 1992 *J. Phys.: Condens. Matter* **4** 7985
- [20] Kadanoff L P *et al* 1967 *Rev. Mod. Phys.* **39** 395
Landau L D and Lifshitz E M 1978 *Statistical Physics* 3rd edn, ed E M Lifshitz and L P Pitaevskii (Oxford: Pergamon) section 142
- [21] Dowben P A, LaGraffe D and Onellion M 1989 *J. Phys.: Condens. Matter* **1** 6751
- [22] LaGraffe D, Dowben P A and Onellion M 1989 *Phys. Rev. B* **40** 970
- [23] Sacchi M, Sakho O, Sirotti F, Jin X and Rossi G 1991 *Surf. Sci.* **251/252** 346
Sacchi M, Sakho O and Rossi G 1991 *Phys. Rev. B* **43** 1276
- [24] Thole B T, van der Laan G and Sawatzky G A 1985 *Phys. Rev. Lett.* **55** 2086
van der Laan G, Thole B T, Sawatzky G A, Goedkoop J B, Fuggle J C, Esteve J M, Karnatak R, Remeika J P and Dabkowska H A 1986 *Phys. Rev. B* **34** 6529
Thole B T and van der Laan G 1988 *Phys. Rev. B* **38** 3158
van der Laan G and Thole B T 1988 *Phys. Rev. Lett.* **60** 1977
- [25] Goedkoop J B 1989 *PhD Thesis* Katholiek Universiteit te Nijmegen
Goedkoop J B, Grioni M and Fuggle J C 1991 *Phys. Rev. B* **43** 1179
- [26] Dowben P A, LaGraffe D, Li Dongqi, Miller A, Zhang L, Dotti L and Onellion M 1991 *Phys. Rev. B* **43** 3171, equations (3) (3') and (3'')
- [27] Mills D L 1971 *Phys. Rev. B* **3** 3887
Suhl H 1975 *Appl. Phys.* **8** 217
- [28] Robins J L, Celotta R J, Unguris J, Pierce D T, Jonker B T and Prinz G A 1988 *Appl. Phys. Lett.* **52** 1918
Scheinfeln M R, Unguris J, Blue J L, Coakley K J, Pierce D T and Celotta R J 1991 *Phys. Rev. B* **43** 3395
- [29] Li Dongqi, Zhang Jiandi, Dowben P A and Garrison K 1993 *J. Phys.: Condens. Matter* **5** L73
- [30] Kittel C 1976 *Introduction to Solid State Physics* 3rd edn (New York: Wiley) p 487
- [31] Ballentine C A, Fink R L, Araya-Pochet J and Erskine J L 1990 *Phys. Rev. B* **41** 2631
- [32] Durr W, Taborelli M, Paul O, German R, Gudat W, Pescia D and Landolt M 1989 *Phys. Rev. Lett.* **62** 206
- [33] Gay J G and Richter R 1986 *Phys. Rev. Lett.* **56** 2728
- [34] Kahn W I 1986 *J. Phys. C: Solid State Phys.* **19** 2969
- [35] Winternitz P, Grundland A M and Tuszynski J A 1988 *J. Phys. C: Solid State Phys.* **21** 4933; 1991 *Phys. Rev. B* **44** 10040
- [36] Skierski M, Grundland A M and Tuszynski J A 1988 *Phys. Lett.* **133A** 213
- [37] Li Chun, Freeman A J and Fu C L 1990 *J. Magn. Magn. Mater.* **83** 51
- [38] Wu Ruqian and Freeman A J 1991 *J. Magn. Magn. Mater.* **99** 81
Wu Ruqian, Li Chun, Freeman A J and Fu C L 1991 *Phys. Rev. B* **44** 9400
- [39] Gradshteyn I S and Ryzhik I M 1980 *Tables of Integrals, Series, and Products* corrected and enlarged edition (New York: Academic) p 260, formula 3.165, no 2
- [40] Gradshteyn I S and Ryzhik I M 1980 *Tables of Integrals, Series, and Products* corrected and enlarged edition (New York: Academic) p 246, formula 3.152, nos 6, 7
- [41] Gradshteyn I S and Ryzhik I M 1980 *Tables of Integrals, Series, and Products* corrected and enlarged edition (New York: Academic) p 906, formula 8.117, no 1; 8.118, no 1