Temperature dependence of the magnetisation in a magnetically inhomogeneous surface

1989 J. Phys.: Condens. Matter 1 7983

(http://iopscience.iop.org/0953-8984/1/42/022)

J. Phys.: Condens. Matter 1 (1989) 7983–7987. Printed in the UK

LETTER TO THE EDITOR

Temperature dependence of the magnetisation in a magnetically inhomogeneous surface

J Mathon and M S Phan
Department of Mathematics, The City University, London EC1V 0HB, UK

Received 3 August 1989

Abstract. The temperature dependence of the surface magnetisation for a highly inhomogeneous surface is calculated. The surface atoms are assumed to be coupled only to the atoms below the surface, not to their neighbours in the surface plane. It is demonstrated that the surface magnetisation obeys an approximate Bloch law, provided the surface-to-bulk exchange link J' is not too weak. The prefactor in the Bloch law depends strongly on J'. The present model is compared with previous calculations for a perfect surface with a weaker surface-to-bulk exchange and with recent experimental results obtained by magnetometry with spin-polarised electrons.

A new development in surface magnetism is the discovery that the surface-to-bulk exchange coupling in a ferromagnet can be determined from the temperature dependence of the surface magnetisation (Siegmann *et al* 1988, Mathon 1989). The method is based on a recent theoretical result of Mathon and Ahmad (1988) which states that the surface magnetisation $M_s(T)$ obeys in the spin-wave regime an approximate Bloch Law $M_s(T)/M_s(0) = 1 - kCT^{3/2}$ with a prefactor k that is directly related to the strength of the surface-to-bulk exchange (C is the bulk prefactor). The unique spatial resolution of magnetometry with spin-polarised electrons (Siegmann *et al* 1988) allows accurate measurements of $M_s(T)$ to be made and, therefore, the precise value of the prefactor k can be determined. Using this method, the strength of surface-to-bulk exchange was already determined for $NiFeB_{0.5}$ glass (Mauri *et al* 1988) and also for permalloy (Siegmann *et al* 1988). It is found that the surface-to-bulk exchange depends strongly on the physical and chemical properties of the surface and is weaker than the bulk exchange even for clean surfaces. In particular, it has been demonstrated that adsorbates such as Ta on permalloy can reduce the surface to bulk exchange to values as low as 10% of the bulk exchange (Siegmann *et al* 1988, Mauri *et al* 1988).

It is tacitly assumed when interpreting measurements of $M_s(T)$ on the basis of a spin-wave theory (Mathon and Ahmad 1988, Mathon 1988) that the translational symmetry in the surface plane is preserved. This condition is clearly not satisfied for contaminated or irregular surfaces. The purpose of this Letter is to investigate how magnetic inhomogeneities in the surface plane influence $M_s(T)$.

To examine this problem we consider here the most inhomogeneous case of a surface magnetic atom which has exchange bonds only to its neighbours below the surface, and no exchange bonds to the neighbours in the surface plane. Such a model clearly applies to a magnetic atom surrounded by non-magnetic neighbours or to an atom with missing

0953-8984/89/427983 + 05 $02.50

neighbours in the surface plane. Our model is, therefore, equivalent to that of a magnetic adatom above a perfect ferromagnetic surface. The model of the magnetic adatom and that of a translationally invariant surface already investigated in Mathon and Ahmad (1988) and Mathon (1988) are clearly the most extreme cases. Real surfaces lie somewhat in between.

For simplicity, we assume that an adatom is in an atop position and is coupled to the substrate by an exchange bond J'. As for the substrate, it is sufficient to assume at this stage that it is described by an unspecified exchange Hamiltonian with spin S.

The spin deviation on the adatom $\Delta = M_s(0) - M_s(T)$ is given in the spin-wave approximation by

$$\Delta = \int_0^\infty 2\mu_B N_a(E)[\exp(E/kT) - 1]^{-1}\, dE \tag{1}$$

where μ_B is the Bohr magneton and $N_a(E)$ is the spin-wave density of states (DOS) projected on the adatom. $N_a(E)$ can be expressed as

$$N_a(E) = \pi^{-1} \operatorname{Im} G_a(E) \tag{2}$$

where $G_a(E)$ is the diagonal element of the spin-wave Green function on the adatom. The Green function is defined by

$$G = (W - H)^{-1} \tag{3}$$

where H is the total exchange Hamiltonian of the coupled adatom–substrate system. To calculate G, we first assume that the adatom–substrate exchange J' is switched off. The spin-wave Green function G^S of a semi-infinite substrate can be easily determined (see Mathon and Ahmad 1988). Given G^S, we switch J' on and calculate the exact G from the Dyson equation $G = G^S + S^S W G$, where the perturbation W due to the adatom–substrate exchange is given by

$$W_{a0} = -SJ' \qquad W_{aa} = SJ' \qquad W_{00} = SJ' \tag{4}$$

(it is assumed that the only substrate atom that is coupled to the adatom is at the origin). Solving the Dyson equation, we obtain

$$G^{-1} = E - W_{aa} - W_{a0}^2 G_{00}^S (1 - W_{00} G_{00}^S)^{-1} \tag{5}$$

where G_{00}^S is the diagonal element of the substrate Green function on the atom sitting below the adatom.

Separating the real and imaginary parts of $G_{00}^S(E) = R(E) + iI(E)$, we obtain the local DOS on the adatom

$$N_a(E) = (1/\pi) W_{a0}^2 I(E)[(E - ESJ'R(E) - W_{aa})^2 + (SJ'EI(E))^2]^{-1}. \tag{6}$$

The initial behaviour of $N_a(E)$ which determines the Bloch law for the magnetisation is obtained by expanding the denominator in (6) in powers of E. To the lowest order in E, we have

$$N_a(E) = N_S(E)(1 + O(E)) \tag{7}$$

where $N_S(E) = (1/\pi) \operatorname{Im} G_{00}^S(E) \propto E^{1/2}$ is the surface DOS for a perfect semi-infinite ferromagnet.

We have thus proved a quite general result that the loss of magnetic neighbours in the surface plane has no effect on the initial Bloch law for the adatom. The local

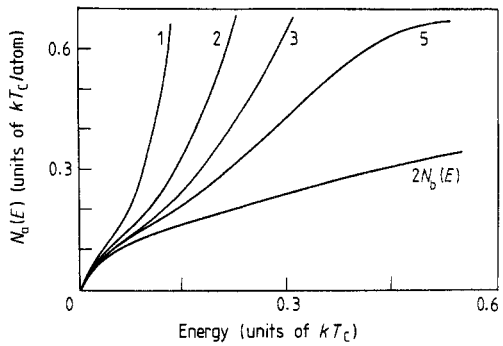

Figure 1. Density of spin-wave states projected on an adatom for adatom–substrate exchange J'/J: 1.0, 2.0, 3.0 and 5.0. The energy is measured in units of kT_C (T_C is the substrate Curie temperature; $J/kT_C \simeq 0.5$).

magnetisation $M_a(T)$ decreases with temperature as if the adatom were incorporated in a perfect surface, i.e. twice as fast as in the bulk (Rado 1957, Mills and Maradudin 1967). It might seem that surface roughness or contamination have no effect on the temperature dependence of the surface magnetisation. However, guided by our results (Mathon and Ahmad 1988, Mathon 1988) for a perfect surface with a weaker surface-to-bulk exchange, we expect that this initial behaviour (classical law) breaks down almost immediately. To demonstrate this, we need to evaluate $N_a(E)$ at higher energies. This requires the knowledge of $G^S_{00}(E)$ for a specific substrate model.

For simplicity, we consider a (100) surface and model the substrate by a simple cubic (SC) nearest-neighbour Hamiltonian with spin S and exchange J. The spin-wave Green function in the mixed Bloch–Wannier representation $G^S_{00}(E, q_\parallel)$ was obtained for such a surface in Mathon and Ahmad (1988). The required matrix element $G^S_{00}(E)$ on the atom '0' below the adatom is, therefore, given by

$$G^S_{00}(E) = (N_\parallel^{-1}) \sum_{q_\parallel} G^S_{00}(E, q_\parallel) \tag{8}$$

where $q_\parallel$ is the two-dimensional wavevector parallel to the surface, the summation is over the surface Brillouin zone and $N_\parallel$ is the number of atoms in the surface plane.

The adatom DOS can be now easily computed from (6) and (8) but it is first necessary to discuss the choice of J'. It might seem that $J' = J$ should hold in our model (the adatom is of the same type as the substrate atoms). However, this is not necessarily so for two reasons. Firstly, the adatom wave function on a metallic substrate is much more atomic-like than in the bulk and, therefore, the effective J' may be very different from J (see Afsharnaderi and Mathon 1988). Secondly, an adatom in other than atop position is coupled to more than one neighbour in the substrate. One can show in this case (Mathon 1983) that the adatom Green function G_a is again given by (6) but the adatom–substrate exchange now needs to be replaced by an effective J' larger than J. It is, therefore, reasonable to expect that realistic J' range from J to about 5–6J depending on the number of magnetic atoms that are adatom nearest neighbours.

The curves $N_a(E)$ computed for such values of J' are shown in figure 1. As expected, all $N_a(E)$ for small E fall on the universal curve $N_S(E) \simeq 2N_b(E) \propto E^{1/2}$ ($N_b(E)$ is the bulk DOS) but this initial behaviour is obtained at energies so low that it is of academic interest only. At experimentally relevant energies, i.e. between 1% and 40–50% kT_C (the spin-wave regime), the adatom DOS deviates rapidly upwards from the universal law and depends very strongly on J'. This behaviour is reminiscent of the DOS for a perfect surface with a weak surface to bulk exchange (Mathon and Ahmad 1988). We,

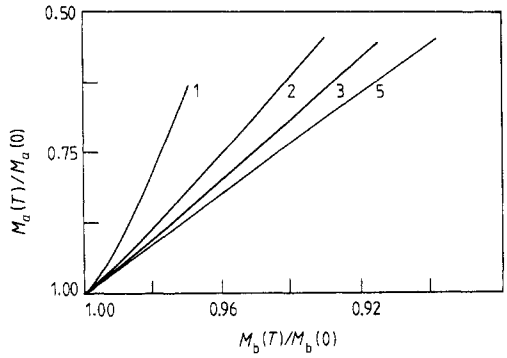

Figure 2. Plots of the adatom magnetisation $M_a(T)/M_a(0)$ against the Bloch law for the bulk $M_b(T)/M_b(0)$. The values of J'/J are indicated. The highest temperature in these plots is $0.4\,kT_C$.

therefore, expect that $M_a(T)$ computed from (1) will decrease with temperature much faster than the classical law predicts. However, it needs to be clarified whether $M_a(T)$ obeys an approximate $T^{3/2}$ law which has been observed for contaminated surfaces (Siegmann *et al* 1988, Mauri *et al* 1988). To test this, we have plotted in figure 2 the curves $M_a(T)$ calculated from (1) and (6) against the true Bloch law for the bulk $M_b(T)$.

It can be seen from figure 2 that a very good Bloch law holds in the case $J'/J \simeq 5$ up to $T \simeq 0.4\,kT_C$ with $k \simeq 4$ ($M_a(T)$ decreases with temperature four times as fast as in the bulk). Much higher values of k are obtained for smaller J' but the Bloch law is not so well obeyed over the whole temperture range shown. However, one can fit good straight lines to the curves corresponding to $J'/J = 2, 3$ between $T/T_C \simeq 0.1$ and 0.4 and this is precisely the temperature range in which the surface magnetisation was measured by Siegmann *et al* (1988) and Mauri *et al* (1988).

The physical reason why a good Bloch law is obtained for larger values of J' is easy to understand. It is clear from (6) that there is always a spin-wave virtual bound state on the adatom for E satisfying $E - ESJ'R(E) - W_{aa} = 0$. This means that $N_a(E)$ has always a maximum (this is visible in figure 1 for $J' = 5J$). The DOS curves which initially rise steeply must, therefore, eventually turn downwards and it is this behaviour which leads to an approximate $T^{3/2}$ law at temperatures before the maximum (a curve $E^{1/2}$ can be fitted to $N_a(E)$ locally). For small J', the inflection point on the DOS curve occurs for values of $N_a(E)$ so high that the approximation of non-interacting spin waves breaks down (this is the reason why all curves in figure 2 terminate for $\Delta \simeq 0.5$).

To conclude, we wish to make several observations. Our calculation indicates that an approximate $T^{3/2}$ law holds even for magnetically inhomogeneous surfaces. It appears that the surface geometry alone has little influence on the $T^{3/2}$ law. It is the strength of the effective exchange link between surface atoms and the bulk which is crucial. This is in accord with the results of experiments on artificially contaminated surfaces (Mauri *et al* 1988).

There appears to be a theoretical upper bound $k \simeq 5$ on the prefactor in the $T^{3/2}$ law. In fact, it can be seen from figure 1 of Mathon and Ahmad (1988) that it would be difficult to achieve a faster decrease of $M_S(T)$ for a homogeneous surface layer. A much faster decrease of $M_S(T)$ can be easily obtained for an inhomogeneous surface but good $T^{3/2}$ law is no longer obeyed.

Finally, we wish to point out that our results for $M_a(T)$ are far more general than the simple model we employed might seem to imply. Although we approximated the substrate surface Green function $G^S_{00}(E)$ by that of a SC ferromagnet with nearest-neighbour exchange, one can easily show that the only essential result needed to evaluate

the adatom DOS from (6) is that Im $G^{S}_{00}(E) \propto E^{1/2}$. This clearly holds for any ferromagnet at the bottom of the spin-wave band.

References

Afsharnaderi M and Mathon J 1988 *J. Physique Coll.* **49** C8 1641–2
Mathon J 1983 *J. Phys. F: Met. Phys.* **13** 1281–9
—— 1988 *Physica* B **149** 31–6
—— 1989 *Proc. 2nd Int. Workshop Magnetic Properties of Low-Dimensional Systems* (Berlin: Springer) at press
Mathon J and Ahmad S B 1988 *Phys. Rev.* B **37** 660–3
Mauri D, Scholl D, Siegmann H C and Kay E 1988 *Phys. Rev. Lett.* **61** 758–61
Mills D L and Maradudin A A 1967 *J. Phys. Chem. Solids* **28** 1855–74
Rado G T 1957 *Bull. Am. Phys. Soc.* **2** 127
Siegmann H C, Mauri D, Scholl D and Kay E 1988 *J. Physique Coll.* **49** C8 9–16