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LETTER TO THE EDITOR

On surface amorphization and observation of surface magnetization in a semi-infinite ferromagnet

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Abstract. Some relationships between surface amorphization and magnetization at or near surface are clarified by using a semi-infinite simple cubic spin-½ Ising ferromagnet with a free surface. Depending on the measuring depth in spin-polarized LEED or Mössbauer spectroscopy, it is discussed how the magnetization changes for the two cases where the surface is coupled ferromagnetically or antiferromagnetically to the bulk.

Recently, magnetization at or near surface has been obtained experimentally by various techniques, such as spin-polarized low energy electron diffraction (LEED) and Mössbauer spectroscopy. The thermal variation of magnetization near a surface can be measured by these methods. In particular, amorphous materials are considered to be well suited to give an insight into the magnetic properties near the surfaces. In these systems, the asymmetry factor of spin-polarized LEED becomes proportional to the magnetization near the surface in the whole temperature region.

On the other hand, it is also interesting to cover a large surface with an amorphous layer, since the formation of an amorphous layer at a surface may be effective in improving the mechanical, magnetic and corrosive resistances of a material with a free crystalline surface. Theoretical work [1, 2] is the major interest for the magnetic problems. Some recent work [3–5] indicates that surface (or interface) amorphization actually happens in some magnetic materials and gives rise to interesting magnetic phenomena.

The purpose of this letter is to clarify some of the relationships between the surface amorphization and the behaviour of magnetization near the surface, when the surface magnetization is observed by spin-polarized LEED or Mössbauer spectroscopy. The same theoretical framework as given in [1] is also applied in the following, except that in [1] the magnetization at the surface is obtained by means of the three-layer approximation but in this work the better (or four-layer) approximation is used.

The Hamiltonian of the system is given by

$$H = -\sum_{ij} J_{ij} S_i^z S_j^z \tag{1}$$

where $S_i^z = \pm 1$ and the summation is carried out only over nearest-neighbour pairs of spins. J_{ij} is the exchange interaction, which has the value $\bar{J}_s$ on the surface, the value $\bar{J}_1$ between the surface and the next (first) layer and J otherwise. The system is a semi-infinite simple cubic ferromagnet with a (100) surface. The surface exchange interaction

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$\bar{J}_s$ and the perpendicular interaction $\bar{J}_1$ are assumed to be randomly distributed according to the probability distribution functions

$$\begin{aligned} P(\bar{J}_s) &= \tfrac{1}{2}[\delta(\bar{J}_s - J_s - \Delta J_s) + \delta(\bar{J}_s - J_s + \Delta J_s)] \\ P(\bar{J}_1) &= \tfrac{1}{2}[\delta(\bar{J}_1 - J_1 - \Delta J_1) + \delta(\bar{J}_1 - J_1 + \Delta J_1)] \end{aligned} \tag{2}$$

with

$$\delta_\alpha = \Delta J_\alpha / J_\alpha \quad \alpha = \mathrm{s\ or\ 1} \tag{3}$$

where δ_α (or ΔJ_α) reflect the structural fluctuations due to the surface amorphization. That is, for the surface amorphization the lattice model of amorphous magnets [6] is used.

At this point, by the use of the framework given in [1] we can formulate the surface magnetization σ_s and each layer magnetization $\sigma_\nu(\nu \geq 1)$ of the present system. Experimentally, the magnetic properties near the surface of a semi-infinite magnet can be obtained by spin-polarized LEED or Mössbauer spectroscopy. For instance, depending on the energy of input polarized electrons, spin-polarized LEED can measure the magnetic behaviour of a few layers near the surface. Therefore, it is worth investigating the thermal variations of subsequent magnetizations as well as surface magnetization σ_s;

$$M_1 = \tfrac{1}{2}(\sigma_s + \sigma_1) \tag{4}$$

$$M_2 = \tfrac{1}{3}(\sigma_s + \sigma_1 + \sigma_2) \tag{5}$$

$$M = \tfrac{1}{4}(\sigma_s + \sigma_1 + \sigma_2 + \sigma_B) \tag{6}$$

where σ_B is the bulk magnetization of simple cubic spin-$\tfrac{1}{2}$ Ising ferromagnet ($\sigma_B = \sigma_{\nu\to\infty}$). The replacement $\sigma_3 = \sigma_B$ in (6) implies that the four-layer approximation is applied to the numerical evaluation of coupled equations for layered magnetizations, instead of the three-layer ($\sigma_2 = \sigma_B$) approximation given in [1]. Here, notice that in the region of the surface magnetization σ_s the four-layer approximation gives the same result as that for the three-layer approximation, while the first-layer magnetization σ_1 is a little different from its corresponding three-layer approximation.

Figure 1 shows typical results of σ_s, M_1 and M for the semi-infinite ferromagnet with $J_s = J_1 = J$ and $\delta_1 = 0.0$, when the surface amorphization ($\delta_s = 1.6$) is applied to the system with a crystalline free (100) surface ($\delta_s = 0.0$). For the system with $J_s = J_1 = J$ and $\delta_1 = 0.0$, the change of σ_s due to the surface amorphization ($\delta_s \neq 0.0$) is examined in detail in figure 6 of [1]. As discussed in [1], our formulation (EFT) is equivalent to the Zernike approximation [7] and hence, when $J_s < J_{sc}$ ($J_{sc} = 1.307J$ is the critical value for surface ordering), the surface and bulk transition temperatures (T_c^s and T_c^b) are given by

$$k_B T_c^\alpha / J = 5.073 \qquad \alpha = \mathrm{s\ or\ b} \tag{7}$$

for $\delta_s = \delta_1 = 0.0$.

Now, as is seen from figure 1, the surface magnetization σ_s (full curve labelled $\sigma_s(0.0)$) of a free crystalline surface changes linearly with temperature in the vicinity of T_c^b. Such behaviour has been observed in many semi-infinite ferromagnets [8]. The magnetizations M_1 and M (chain curves) lie between σ_s and the bulk magnetization σ_B (broken curve). They can also be observed by spin-polarized LEED; by decreasing the penetrating depth of polarized electrons, the surface magnetization curves (M and M_1) approach the true surface magnetization curve (σ_s), such as the ferrimagnetic Fe_3O_4 [9].

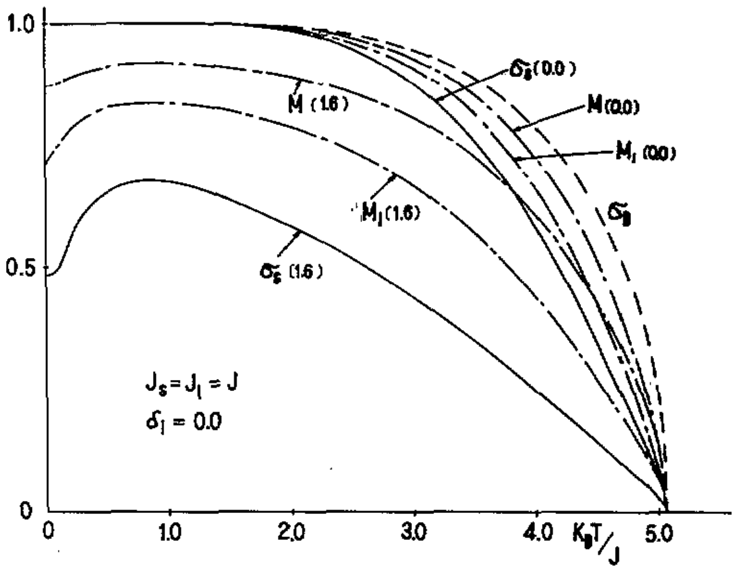

Figure 1. Thermal variations of σ_s, M_1 and M for the semi-infinite ferromagnetic system with $J_s = J_1 = J$ and $\delta_1 = 0.0$, when the value of δ_s is taken as $\delta_s = 0.0$ (the case of crystalline free surface) and $\delta_s = 1.6$ (the case of surface amorphization). Broken curve represents the bulk magnetization σ_B. The surface amorphization ($\delta_s > 1.0$) expresses that the frustration effect is set in the surface (see figure 6 in [1]).

On the other hand, the magnetization curves M and M_1 for the surface amorphization ($\delta_s = 1.6$) are rather largely deviated from its surface magnetization curve σ_s, in comparison with the results of a free crystalline surface. Thus, when the surface magnetization is measured by spin-polarized LEED (or Mössbauer spectroscopy), it indicates that a more careful analysis of its data is required, depending on the measuring depth when the frustration effect ($\delta_s > 1.0$) occurs in the surface.

As is observed in Gd(0001) on a W(110) substrate [10], the magnetization at a surface is often coupled antiferromagnetically to the bulk ferromagnet because of the surface magnetic reconstruction. In figure 2, therefore, for the system with the same parameters as figure 1 the surface magnetic behaviour is examined by taking $J_1 = -J$ where the surface is coupled antiferromagnetically to the bulk. Here, notice that surface magnetization and each layer magnetization are given by the same values as those for the ferromagnetic case ($J_1 = J$) of figure 1, except that the value of σ_s becomes negative. However, the thermal variations of M_1, M_2 and M show completely different behaviour when comparing the results with those in figure 1. For the free crystalline surface ($\delta_s =$ 0.0), M takes the saturation value $M = 0.5$, since $\sigma_s = -1.0$ and $\sigma_1 = \sigma_2 = \sigma_B = 1.0$ at $T = 0$ K. But, M_2 takes $M_2 = \frac{1}{3}$ and M_1 reduces to zero at $T = 0$ K. In this way, depending on the measuring depth, one can observe the change of magnetization near the surface, namely from M to M_1. In particular, when one measures the true surface magnetization, a discontinuous change from M_1 to $|\sigma_s|$ may be observed. Similar behaviour is also seen in the curves of the surface amorphization with $\delta_s = 1.6$. In other words, if the surface is coupled antiferromagnetically to the bulk and $J_s < J_{sc}$, the thermal variations of magnetization at or near the surface should exhibit similar behaviour to those shown in figure 2.

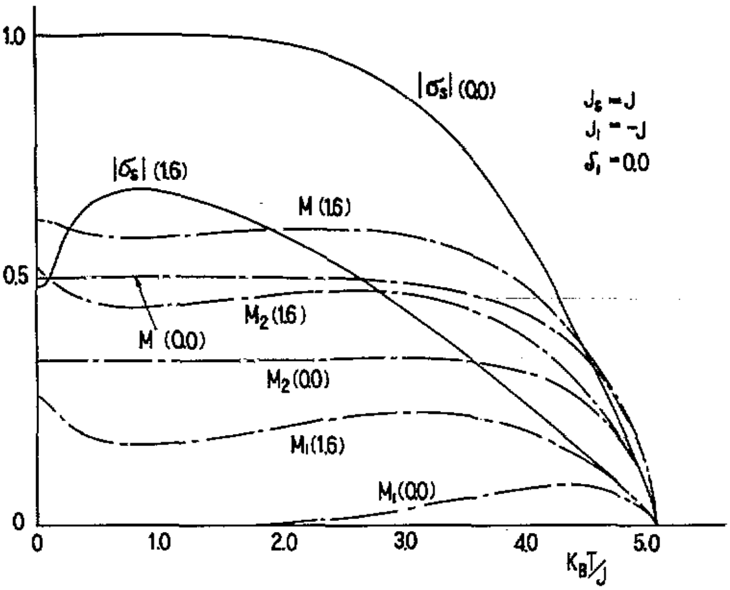

Figure 2. Temperature dependences of $|\sigma_s|$, M_1, M_2 and M for the same system as that of figure 1, when the surface is coupled antiferromagnetically ($J_1 = -J$) to the bulk; the value of δ_s is selected as $\delta_s = 0.0$ and $\delta_s = 1.6$.

On the other hand, when $J_{sc} > J_s$ and the surface amorphization is not large, the surface ordering temperature T_c^s becomes larger than the bulk transition temperature T_c^b even for the surface coupled antiferromagnetically to the bulk. Figure 3 shows two such cases, namely the crystalline free surface ($\delta_s = \delta_1 = 0.0$) and the surface with amorphization ($\delta_s = \delta_1 = 0.6$), when the values of J_s and J_1 are selected as $J_s = 2.0J$ ($J_s > J_{sc}$) and $J_1 = -J$. For each case, the surface magnetization $|\sigma_s|$ takes a finite value in the temperature region $T_c^b < T < T_c^s$, while the surface amorphization ($\delta_s = \delta_1 = 0.6$) acts to prohibit the magnetic ordering at the surface in the region. In the figure, the behaviour of $|M|$ in the vicinity of T_c^b are also depicted. At first sight, we may consider that $|M|$ reduces to zero at T_c^b. In order to clarify the behaviour of M in the vicinity of $T = T_c^b$, the inset expresses the thermal variations of $|M|$ and σ_B for the two cases by taking a larger scale. The results clearly show that the compensation point ($T = T_{comp}$) is obtained at a temperature a little lower than the bulk T_c^b. In particular, notice that for the surface amorphization ($\delta_s = \delta_1 = 0.6$) the compensation point is found at a temperature a little higher than that for the free crystalline surface ($\delta_s = \delta_1 = 0.0$). At this point, it may be worth noting that a similar phenomenon ($T_{comp} < T_c^b$) is found in recent experiments for Gd(0001) and Tb(0001) on W(110) substrates [10, 11].

In this letter, we have studied the effects of surface amorphization on magnetizations at or near the surface in the semi-infinite simple cubic spin-$\frac{1}{2}$ Ising ferromagnet. Some work [3–5] indicates that surface amorphization may be important for analysing some characteristic phenomena at the surface (or interface). Then, only the random anisotropy model was considered. As is noted in [3, 5] the effects of random exchange interactions studied in this letter may also play an essential role for the analyses. In particular, the relation between the measuring depth and the magnetization at or near

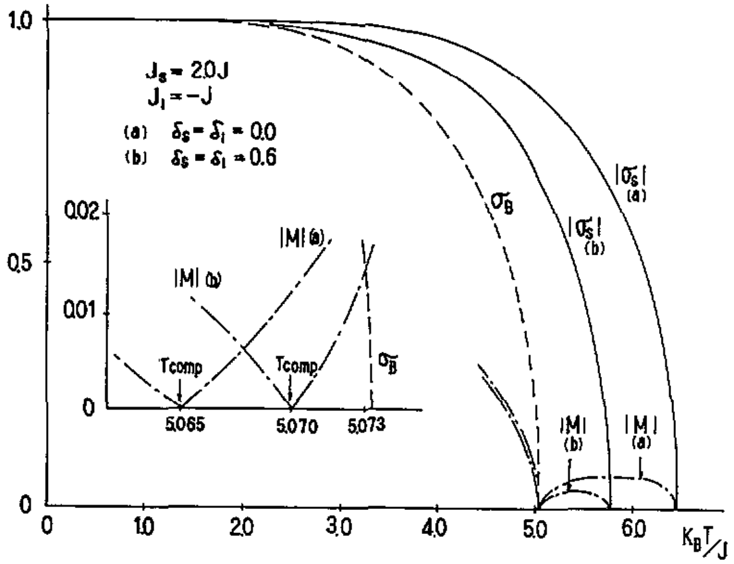

Figure 3. Thermal variations of $|\sigma_s|$ and $|M|$ for the system with $J_s = 2.0J$ ($J_s > J_{sc}$), when the surface is coupled antiferromagnetically ($J_I = -J$) to the bulk and the two values of δ_α($\delta_s = \delta_I = 0.0$ and $\delta_s = \delta_I = 0.6$) are selected. Broken curve represents the bulk magnetization σ_B. The inset shows the behaviour of $|M|$ in the vicinity of T_c^b where the compensation point is observed in the region ($T_{comp} < T_c^b$).

the surface discussed in this letter becomes important when one observes the surface magnetization by means of spin-polarized LEED or Mössbauer spectroscopy.

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