Surface Magnetic Effects in an Alternating Superlattice

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We investigate the surface magnetism of the alternating superlattice with localized spin-1/2. Using the mean-field approximation method, we discuss not only the correlation between the critical value j_{0C} of the exchange constant in the surface layer and interlayer exchange constants, but also the connection between j_{0C} and the bulk exchange constant j_A. The calculated results are in good agreement with the former theoretical calculations. Based on the solutions, we show the relations between the critical parameter $c = J_S/J_A$ and the bulk exchange constants as well as the surface transition temperature. J_S is the exchange constant in the first two surface layers. Comparing with the earlier theoretical works, our results show the effect of the surface modification more gradual.

Key words: Surface Transition; Alternating Magnetic Superlattice.

1. Introduction

It is widely accepted that the magnetic properties of a surface differ from those in the bulk of a solid. This is expected since the surface atoms are embedded in a different environment and additionally the exchange constants between atoms associated with these surface are different from those in the bulk [1, 2]. It was found that if the surface exchange constants are smaller than certain critical values, the surface will order at the same transition temperature T_0 as the bulk, namely the Curie temperature of the bulk. But if the surface exchange constants are above these critical values, the surface will order at a temperature $T_S > T_0$; and in the temperature range $T_0 < T < T_S$, we have a surface magnetic structure. In the last case, the magnetization decays exponentially into the bulk with a characteristic length [3, 4].

The study of magnetic effects in an alternating superlattice is still of current interest because of a great potentiality of technological applications and the theoretical interests are undoubtedly stimulated by modern vacuum science, and particularly, epitaxial-growth techniques. It is easy to grow very thin magnetic films of controllable thickness or even monolayers atop nonmagnetic substrates [1, 5, 6]. In theory, the problem of surface magnetism has also attracted much attention [2 – 4, 7 – 11].

Considering an alternating superlattice of $2n+2$ layers, as shown in Figure 1, in the layers $i = 0$ and 1 are atoms with exchange constants J_S. The layers $i = 2, 4, \ldots, 2n$ consist of atoms A with exchange constant J_A and the layers $i = 3, 5, \ldots, 2n+1$ of atoms B with exchange constant J_B. All interlayer exchange constants $J_{i,i+1}$ are J except for that between layers $i = 0$ and 1, and $i = 1$ and 2, which are J_{01} and J_{12}, re-

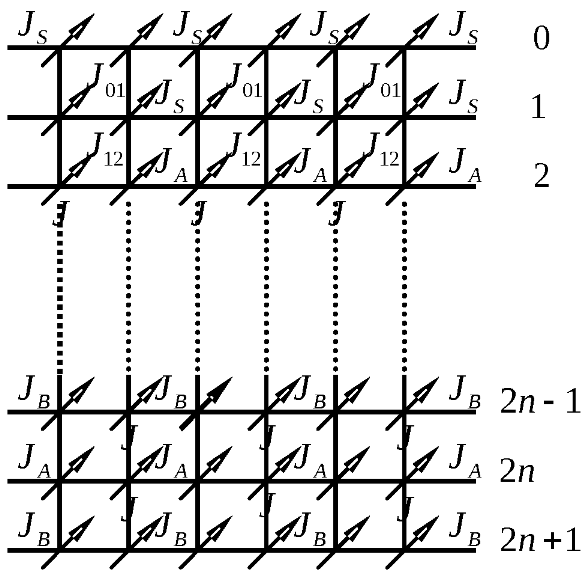

Fig. 1. Schematic illustration of an alternating superlattice with surface layer. Layers $i = 0$ and 1 consist of atoms with exchange constant J_S. The interlayer exchange constant between $i = 0$ and 1 is J_{01}, and J_{12} is the interlayer exchange constant between $i = 1$ and 2.

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spectively. Two cases have been considered: (i) In the first two surface layers, the exchange constant J_S and the interlayer exchange constant J_{01} are modified and (ii) we not just consider the modification of surface exchange constants, but also take into account interlayer exchange constants both J_{01} and J_{12}.

2. Theory

We start with a lattice of localized spins with value 1/2. The interaction can be described with the nearest-neighbour ferromagnetic Ising model, and the exchange constant is modulated to reflect a superlattice structure and a surface modification. In the mean-field approximation, the mean value M_i of the spin variable at each plane is determined by [12–14]

$$M_i = \tanh[\beta(Z_0 J_{ii} M_i + Z J_{i,j+1} M_{i+1} + Z J_{i,i-1} M_{i-1} + h)], \tag{1}$$

where Z_0 and Z are the numbers of nearest neighbours in the plane and between the planes, respectively.

Near the transition temperature, the order parameters M_i are small, and in the absence of an external field h, (1) reduces to

$$\underline{A}M = 0. \tag{2}$$

where

$$\underline{A_{mn}} = (k_B T - Z_0 J_{mm})\delta_{m,n} - Z J_{mn}(\delta_{m+1,n} + \delta_{m,n+1}). \tag{3}$$

The transition temperature is given by the determinant equation,

$$\det \underline{A} = 0. \tag{4}$$

According to the theory above, determinants can be obtained:

$$\underline{A} = \begin{bmatrix} X_S & -C_1 & & & \\ -C_1 & X_S & -C_2 & & \\ & -C_2 & X_A & & \\ & & & X_B & \\ & & & & \ddots \end{bmatrix}_{(2n+2)\cdot(2n+2)},$$

$$C_{2n-1} = \begin{bmatrix} X_B & -1 & & \\ -1 & X_A & -1 & \\ & -1 & X_B & \\ & & & \ddots \end{bmatrix}_{(2n-1)\cdot(2n-1)},$$

$$D_{2n} = \begin{bmatrix} X_A & -1 & & \\ -1 & X_B & -1 & \\ & -1 & X_A & \\ & & & \ddots \end{bmatrix}_{2n\cdot 2n},$$

where

$$\frac{k_B T - Z_0 J_A}{ZJ} = X_A, \quad \frac{J_S}{J} = C_1, \quad \frac{k_B T - Z_0 J_S}{ZJ} = X_S, \quad \frac{k_B T - Z_0 J_B}{ZJ} = X_B, \quad \frac{J_{12}}{J} = C_2.$$

Expanding the first two rows, we obtain

$$X_S\left[X_S D_{2n} - {C_2}^2 C_{2n-1}\right] - {C_1}^2 D_{2n} = 0. \tag{5}$$

The determinants C_{2n-1} and D_{2n} satisfy the recurrence relations,

$$D_{2n} = X_A C_{2n-1} - D_{2n-2}, \quad C_{2n-1} = X_B D_{2n-2} - C_{2n-3}. \tag{6}$$

The bulk transition is obtained by taking the limits $n \to \infty$, $D_{2n-2}/D_{2n} \to 1$, and $D_{2n-4}/D_{2n-2} \to 1$ in (6).

Finally it can be written

$$X_A X_B = 4, \quad k_B T_0 = \frac{1}{2}\left\{Z_0(J_A + J_B) + [{Z_0}^2(J_A - J_B)^2 + 16Z^2J^2]^{1/2}\right\}. \tag{7}$$

We will consider an exponentially decaying solution in the semi-infinite limit, $n \to \infty$.

Then $D_{2n-2}/D_{2n} = D_{2n-4}/D_{2n-2} = \gamma < 1$, and from (6) the results are given by

$$C_{2n-1}/D_{2n} = \frac{1}{X_A}(1+\gamma), \quad \gamma^2 - \alpha\gamma + 1 = 0, \tag{8}$$

where

$$\alpha = X_A X_B - 2. \tag{9}$$

Substituting the ratio C_{2n-1}/D_{2n} in (5) and eliminating γ using (8), we obtain the equation

$$\left(2\frac{{X_S}^2 X_A - C_1^2 X_A}{{C_2}^2 X_S} - X_A X_B\right)^2 - {X_A}^2 {X_B}^2 + 4X_A X_B = 0. \tag{10}$$

The critical value of the surface exchange constant above for which the decaying solution exists is obtained by the condition $T_S = T_0$, or $\gamma = 1$. This gives

$${X_S}^2 X_A - {C_2}^2 X_S - ({C_1}^2 X_A + {C_2}^2 X_S) = 0. \tag{11}$$

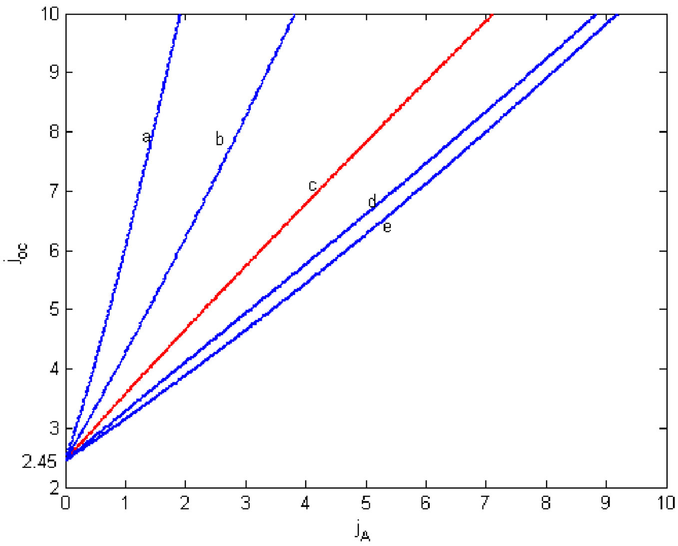

Fig. 2. The dependence of j_{0C} on j_A for j_B/j_A equal to (a) 4, (b) 2, (c) 1, (d) 1/2, and (e) 1/4. For the case (c), a linear relation can be obtained. As j_A increases, for the ratio of $j_B/j_A = 4$, the value of j_{0C} rapidly increases.

Equation (11), with T_0 from (7), gives the relation between J_{12} and the critical value of exchange constant in the surface.

For general discussion and numerical works, it is convenient to introduce the dimensionless quantities

$$j_A = \frac{Z_0 J_A}{ZJ}, \quad j_B = \frac{Z_0 J_B}{ZJ}; \\ t_0 = \frac{k_B T_0}{ZJ} = \frac{1}{2}\left\{(j_A + j_B) + \sqrt{(j_A - j_B)^2 + 16}\right\}. \tag{12}$$

Then (11) becomes

$$\frac{k^2}{16} {j_{0C}}^2 (t_0 - j_{0C})(t_0 - j_B) \\ -2(t_0 - j_{0C})^2 + \frac{1}{8} {j_{0C}}^2 = 0, \tag{13}$$

where

$$k = \frac{J_{12}}{J} \text{ and } j_{0C} = \frac{Z_0 J_S}{ZJ}.$$

j_{0C} is the critical value of exchange constant in the surface. k is an important parameter, which has a striking effect on the value of j_{0C}.

3. Results and Discussion

In Figure 2, we have plotted j_{0C} as a function of j_A for $k = 1$ and ratios of j_B/j_A equal to (a) 4, (b) 2, (c) 1, (d) 1/2, and (e) 1/4. For case (c) when the bulk lattice is uniform, that means $j_A = j_B$, a linear dependence is obtained. However, for our alternating lattice structure, case (a), case (b), case (d) and (e), the dependence of j_{0C} on j_A has been modified by (13). All results are based on the special case of a simple cubic lattice, $Z_0 = 4$, $Z = 1$.

In Figure 3, we have shown j_{0C} as a function of k, for $j_B = 1$, and the ratios of j_B/j_A equal to (a) 4, (b) 2, (c) 1, (d) 1/2, and (e) 1/4. It is very interesting that if the values of parameter k are near 6, the values of j_{0C} approach 1 for all cases of $j_B/j_A \cdot j_{0C}$ gradually decreases with increasing parameter k, which indicates that the interlayer exchange constant J_{12} has an important effect on the surface transition. For the case of $k = 0$, the two "surface layers" behave like a quasi-two-dimensional system, this result agrees with earlier works [12, 15, 16].

For the numerical works, the choice $J_S = cJ_A$ can be taken into account by a single parameter for the surface modification. Then (11) becomes an equation for the critical parameter c,

$$c^2(t_0 - c j_A)(t_0 - j_B) - 2(t_0 - c j_A)^2 + \frac{1}{8} {j_A}^2 = 0. \tag{14}$$

In Figure 4, c is considered as a function of j_A for ratios of j_A/j_B equal to (a) 1, (b) 2, (c) 3, and (d) 4. For all cases of j_A/j_B, including the uniform one, c starts at $\sqrt{2}$ for $j_A = 0$, and decreases as j_A increases. This is because $j_A = 0$ corresponds to non-vanishing interlayer exchange constants and exchange constants in the first two "surface layers". When the value of

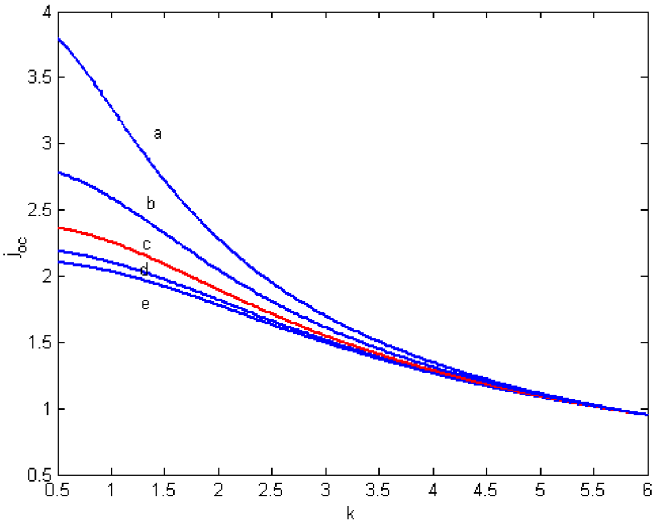

Fig. 3. The dependence of j_{0C} on k for j_B/j_A equal to (a) 1/4, (b) 1/2, (c) 1, (d) 1, and (e) 4. From this figure, it can be seen that if the value of parameter k is near 6, the values of j_{0C} approach 1 for all cases of j_B/j_A.

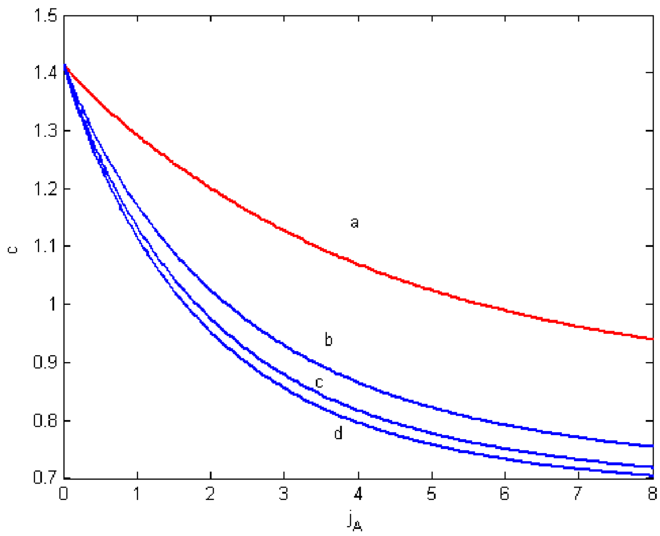

Fig. 4. The dependence of c on j_A for j_A/j_B equal to (a) 1, (b) 2, (c) 3, and (d) 4. It shows the correlation between critical parameter c and exchange constant j_A, as well as the gradual trend of surface modification. For all cases of j_A/j_B, including the uniform one, c starts at $\sqrt{2}$ for $j_A = 0$, and decreases as j_A increases.

j_A/j_B equals 1, with j_A increasing c is well close to 0.95, not 1.1 as in early result [12].

In Figure 5, we have shown the typical dependence of k_BT_S on the surface modification parameter c. For different values of J_A/J_B, we have choosen $J = 1/2(J_A + J_B)$ and used the simple cubic lattice, with $Z_0 = 4$, $Z = 1$. The unit $J_B = 1$ is used. The four curves are depicted for ratios of j_A/j_B equal to (a) 2, (b) 1.5, (c) 1, and (d) 0.5, respectively. As c increases, the surface transition temperatures increase linearly, which reflects the gradual effect of the surface modification. In addition, under the condition of $c = 1$, we can obtain the bulk transition temperatures that have been denoted in Figure 5.

4. Conlusion

In summary, we have investigated a spin-1/2 Ising model in an alternating superlattice. In the first case, J_S for the first two surface layers and the interlayer exchange constant J_{01} have been modified. Through numerical calculations, we found that the critical exchange constant j_{0C} for surface magnetism depends on the bulk exchange constants, which undoubtedly indicates that surface transition relies on the bulk exchange constants. The linear relation between j_{0C} and j_A is true for any lattice structure, and for any interlayer exchange constant J.

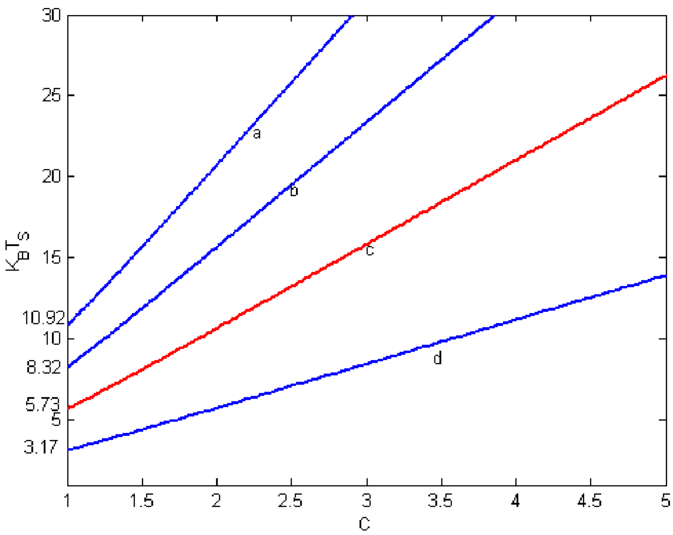

Fig. 5. The relation between surface transition temperature k_BT_S and critical parameter c for j_A/j_B equal to (a) 2, (b) 1.5, (c) 1, and (d) 0.5. Under the condition of $c = 1$, the bulk transition temperatures obtained are 10.92, 8.32, 5.73, and 3.17 corresponding to cases of (a), (b), (c), and (e), respectively.

In the second case, we have presented the dependence of j_{0C} on k ($\propto J_{12}$). Especially when $k = 0$ ($J_{12} = 0$) the first two "surface layers" behave like a quasi-two-dimensional system. Under the condition of $k \geq 6$, the value of j_{0C} approaches the constant 1 and is independent of the interlayer exchange constant. We have also discussed the connection between critical parameter c and bulk exchange constant; for all values of the ratio j_B/j_A, the critical values of c start at $\sqrt{2}$ for $j_A = 0$, which corresponds to non-vanishing interlayer exchange constants and exchange constants in the first two "surface layers". As j_A increases, for the case of $j_A/j_B = 1$, c is well close to 0.95. The surface transition temperatures in Figure 5 are specially sensitive to the critical parameter c, particularly for large value of j_A/j_B, which provides the possibility for us to calculate the value of c by measuring T_S in the experiment. A comparison with some theoretical works that only consider modification of exchange constant J_S and neglect the effect of exchange constants J_{01} and J_{12}, indicates that the effect of the surface modification is more gradual in our model.

Although a superlattice of alternating magnetic monolayers has not been studied very well today in experiments, with the progress of techniques, we believe such systems can be studied well both theoretically and experimentally. Therefore, it is worth investigating such systems further by using more elaborate theoretical frameworks and techniques of fabrication.

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