Localized magnetism in a superlattice

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We study a magnetic superlattice in which one of the inner atomic layers has been modified. We use the Ising model in the mean-field approximation. We find that if the modified exchange constant J_0 is greater than that in the bulk, localized magnetism occurs, with the magnetization decaying in both directions for the infinite superlattice. The transition temperatures for finite and infinite systems are calculated for both uniform and alternating superlattices.

I. INTRODUCTION

Over the years, the magnetic properties of solids and artificially fabricated superlattices have been widely studied. The effects of a surface on the magnetic behavior have also been investigated by assuming one or more layers of surface atoms with exchange constants (interactions) different from those in the bulk.[1-9] It was found that if the surface exchange constants are above some critical values, the surface will order at a temperature $T_s > T_0$ (Curie temperature for the bulk); and in the region $T_0 < T < T_s$, we have surface magnetic structure, with the magnetization decaying exponentially into the bulk with a characteristic length. This surface magnetism has been confirmed by recent experimental results.[10-13] In the earlier theoretical works, the semi-infinite limit is chosen, but some recent works have also considered uniform[7] and alternating[9] finite superlattices.

The theoretical interests are undoubtedly stimulated by recent advances in epitaxial-growth techniques, where it is nowadays possible to grow magnetic films of controllable thickness, or even magnetic monolayers atop nonmagnetic substrates.[14-18]

In the present paper, we study a magnetic superlattice in which one of the inner atomic layers has a different exchange constant J_0. For simplicity, we assume the modified layer to be exactly in the center of the superlattice. We will show that as long as J_0 is larger than that in the bulk, localized phase transition can occur at a temperature $T_l > T_0$, and the magnetization decays in both directions with a characteristic length. We will use the Ising model in the mean-field approximation, and study the uniform[7] and alternating[9] superlattices for both the finite and infinite cases. Many of the results will be expressed in terms of determinants introduced in Refs. 7 and 9.

II. UNIFORM SUPERLATTICE WITH ONE MODIFIED INNER LAYER

We consider a lattice of localized spins with spin equal to one-half. The interaction is of the nearest-neighbor ferromagnetic Ising type, and the exchange constant is plane dependent. In the mean-field approximation, the mean value M_i of the spin variable at each plane is determined by[8,9]

$$M_i = \tanh[\beta(z_0 J_{ii} M_i + zJ_{i,i+1} M_{i+1} + zJ_{i,i-1} M_{i-1} + h)] , \quad (1)$$

where z_0, z are the numbers of nearest neighbors in the plane and between the planes, respectively, and $J_{\alpha,\beta}$ is the exchange constant between plane α and β.

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

$$\underline{A}\mathbf{M} = 0 , \quad (2)$$

where the matrix $\underline{A}$ has elements

$$A_{mn} = [k_B T - z_0 J_{m,m}]\delta_{m,n} - zJ_{m,n}[\delta_{m+1,n} + \delta_{m,n+1}] . \quad (3)$$

Let us consider the uniform model of Fig. 1(a). Here $J_{i,i} = J_{-i,-i} = J_A$ for $i = 1, 2, \ldots, n$ and $J_{0,0} = J_0$. The interlayer exchange is assumed to have the same value J.

Let us use the dimensionless quantities $t = k_B T/(zJ)$, $j_\alpha = z_0 J_\alpha/(zJ)$, $\alpha = A$, B or 0, $x_\alpha = t - j_\alpha$, and introduce the variables $m_i = M_i + M_{-i}$, $i > 0$, and $m_0 = 2M_0$, for reason of symmetry.

Then Eqs. (2) and (3) can be written as

$$\underline{B}\mathbf{m} = 0 ,$$

where the $(n+1)\times(n+1)$ matrix $\underline{B}$ is

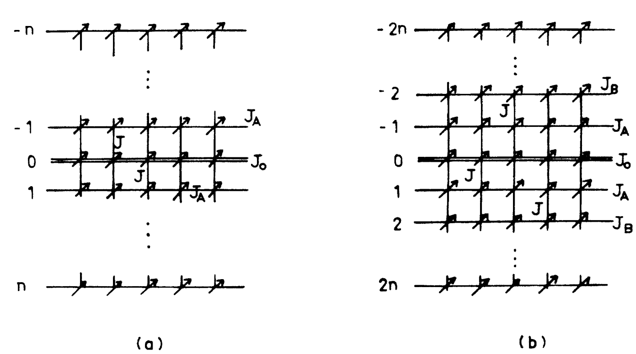

FIG. 1. (a) Uniform superlattice with one modified layer. (b) Alternating superlattice with one modified layer.

$$\underline{B}=\begin{pmatrix} x_0/2 & -1 & 0 & 0 & & & & \\ -1 & x_A & -1 & 0 & & & & \\ 0 & -1 & x_A & -1 & & & & \\ 0 & 0 & -1 & x_A & & & & \\ & & & & \ddots & & & \\ & & & & & x_A & -1 & 0 \\ & & & & & -1 & x_A & -1 \\ & 0 & & & & 0 & -1 & x_A \end{pmatrix}_{(n+1)\times(n+1)} \tag{4}$$

The transition temperature is given by

$$\det\underline{B}=(x_0/2)\mathcal{B}_n-\mathcal{B}_{n-1}=0\ , \tag{5}$$

where the determinant

$$\mathcal{B}_m(T)=\det\begin{pmatrix} x_A & -1 & 0 & 0 & & & & \\ -1 & x_A & -1 & 0 & & & & \\ 0 & -1 & x_A & -1 & & & & \\ 0 & 0 & -1 & x_A & & & & \\ & & & & \ddots & & & \\ & & & & & x_A & -1 & 0 \\ & & & & & -1 & x_A & -1 \\ 0 & & & & & 0 & -1 & x_A \end{pmatrix}_{m\times m}$$

has been[7] evaluated as

$$\mathcal{B}_m(T)=\sinh[(m+1)\phi]/\sinh\phi\ , \tag{6a}$$

with

$$\cosh\phi=x_A/2 \quad \text{for } x_A\ge 2\ . \tag{6b}$$

For $x_A<2$, ϕ becomes $i\theta$ and the hyperbolic functions become trigonometric functions of θ.

For a finite value of n, Eq. (5) with (6) can be solved numerically for the transition temperature.

In the limit $n\to\infty$,

$$\frac{m_{i+1}}{m_i}=\frac{\mathcal{B}_{i+1}}{\mathcal{B}_i}=\gamma\le 1\ ,$$

where γ satisfies[8]

$$x_A-\left[\gamma+\frac{1}{\gamma}\right]=0\ . \tag{7}$$

Using Eqs. (5) and (7) we have the analytical results

$$t=j_A+[4+(j_0-j_A)^2]^{1/2}\ ,$$

and

$$\gamma=\tfrac{1}{2}[x_A-(x_A^2-4)^{1/2}],\quad \lambda=-\ln\gamma\ . \tag{8}$$

Equation (8) shows that as long as $j_0>j_A$, $t>j_A+2=t_0$, the bulk Curie temperature; and the magnetization de-

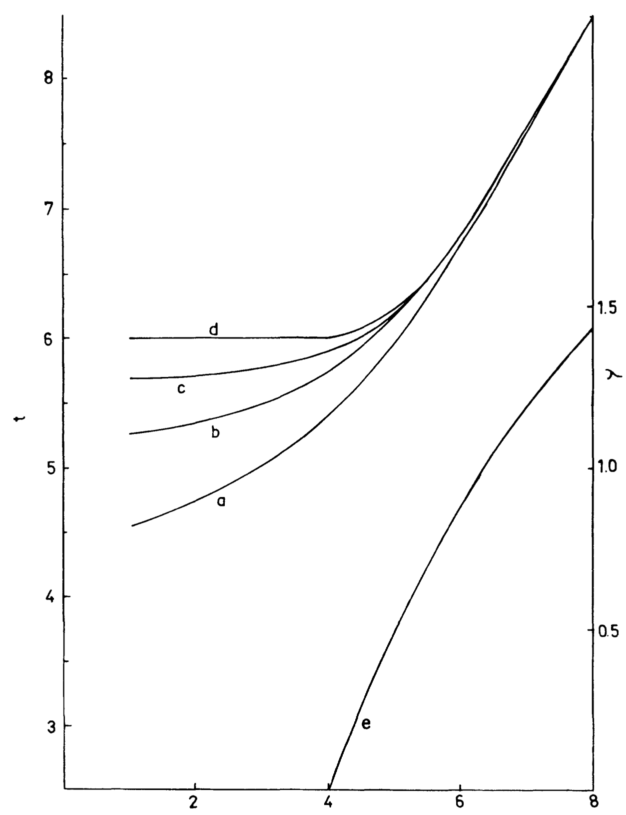

FIG. 2. Dependence of t on j_0 for a, $n=1$; b, $n=2$; c, $n=4$; and d, $n=\infty$ for the uniform superlattice. The dependence of λ on j_0 for $n=\alpha$ is shown in curve e.

cays with the characteristic length λ^{-1}.

In Fig. 2 we have plotted the Curie temperatures t obtained from Eq. (5) as a function of j_0. We have chosen $j_A=4$, and shown the results for $n=1$, 2, and 4, as well as $n=\infty$. We have also plotted λ vs j_0 for the $n=\infty$ case. Note that in this case, for $j_0<j_A$, all the layers order at t_0 except for the modified one. However, as $j_0>j_A$, $t>t_0$ and localization of magnetization occurs.

III. ALTERNATING SUPERLATTICE WITH ONE MODIFIED INNER LAYER

We next consider the alternating model, Fig. 1(b). Here $J_{2i,2i}=J_{-2i,-2i}=J_B$, $J_{2i-1,2i-1}=J_{-(2i-1),-(2i-1)}=J_A$ for $i=1,2,\ldots,n$, and $J_{0,0}=J_0$. $J_{m,m+1}$ is again J.

With use of the variables m_i and m_0 as before, Eq. (2) becomes

$$\underline{F}=\begin{bmatrix} x_0/2 & -1 & 0 & 0 & & & \\ -1 & x_A & -1 & 0 & & & \\ 0 & -1 & x_B & -1 & & & \\ 0 & 0 & -1 & x_A & & & \\ & & & & \ddots & & \\ & & & & x_B & -1 & 0 \\ & & & & -1 & x_A & -1 \\ & & & & 0 & -1 & x_B \end{bmatrix}_{(2n+1)\times(2n+1)}, \tag{9}$$

where we are using the same dimensionless quantities.

The transition temperature is given by

$$\det\underline{F}=(x_0/2)\mathcal{D}_{2n}-\mathcal{C}_{2n-1}=0\ , \tag{10}$$

by expanding about the first row.

The two determinants $\mathcal{D}_{2m}$ and $\mathcal{C}_{2m-1}$, defined as

$$\mathcal{D}_{2m}(T)=\begin{vmatrix} x_A & -1 & 0 & 0 & & & \\ -1 & x_B & -1 & 0 & & & \\ 0 & -1 & x_A & -1 & & & \\ 0 & 0 & -1 & x_B & & & \\ & & & & \ddots & & \\ & & & & x_B & -1 & 0 \\ & & & & -1 & x_A & -1 \\ & & & & 0 & -1 & x_B \end{vmatrix}_{2m\times 2m}$$

and

$$\mathcal{C}_{2m-1}(T)=\begin{vmatrix} x_B & -1 & 0 & 0 & & & \\ -1 & x_A & -1 & 0 & & & \\ 0 & -1 & x_B & -1 & & & \\ 0 & 0 & -1 & x_A & & & \\ & & & & \ddots & & \\ & & & & x_B & -1 & 0 \\ & & & & -1 & x_A & -1 \\ & & & & 0 & -1 & x_B \end{vmatrix}_{(2m-1)\times(2m-1)},$$

have been determined[9] for $\alpha \geq 2$, as

$$\mathcal{D}_{2m} = \frac{1}{\sinh\phi}\{\sinh[(m+1)\phi]+\sinh(m\phi)\} , \qquad (11a)$$

$$\mathcal{C}_{2m-1} = \frac{2}{x_A \sinh\phi}[\cosh\phi+1]\sinh(m\phi) , \qquad (11b)$$

where

$$\alpha = x_A x_B - 2 = 2\cosh\phi . \qquad (12)$$

Again, the trigonometric functions are to be used for $\alpha < 2$.

In the infinite limit $n \to \infty$,

$$\frac{m_{2i+1}}{m_{2i}} = \frac{\mathcal{D}_{2i+2}}{\mathcal{D}_{2i}} = \gamma, \quad \frac{m_{2i+1}}{m_{2i-1}} = \frac{\mathcal{C}_{2i+1}}{\mathcal{C}_{2i-1}} = \gamma ,$$

where the decay ratio $\gamma \leq 1$ is given by

$$\gamma^2 - \alpha\gamma + 1 = 0 . \qquad (13)$$

By writing[8] the ratio

$$\frac{\mathcal{C}_{2n-1}}{\mathcal{D}_{2n}} = \frac{1}{x_A}(1+\gamma) , \qquad (14)$$

Eqs. (10) and (13) give

$$x_A x_0^2 = 2x_B(x_A x_0 - 2) . \qquad (15)$$

Equation (15) is a cubic equation in t, but it shows that if $j_0 > j_B$, then $t > t_0' =$ the alternating lattice[8] bulk Curie temperature, and

$$\gamma = \tfrac{1}{2}[\alpha - (\alpha^2 - 4)^{1/2}], \quad \lambda = -\ln\gamma . \qquad (16)$$

Equations (10) and (15) [together with Eqs. (11) and (12)] can be solved numerically for t. For our numerical works, we have chosen $j_A = 2$, $j_B = 1$, $t_0' = 3.562$.

In Fig. 3 we have plotted t vs j_0, for $n = 1,2$ corresponding to five and nine layers, as well as the infinite case. The decay constant λ is also shown. Again, for $j_0 > j_B$, in the infinite case, all the layers order at t_0' except for the modified one. However, for $j_0 > j_B$, $t > t_0'$ and there is localization of magnetization about the modified plane.

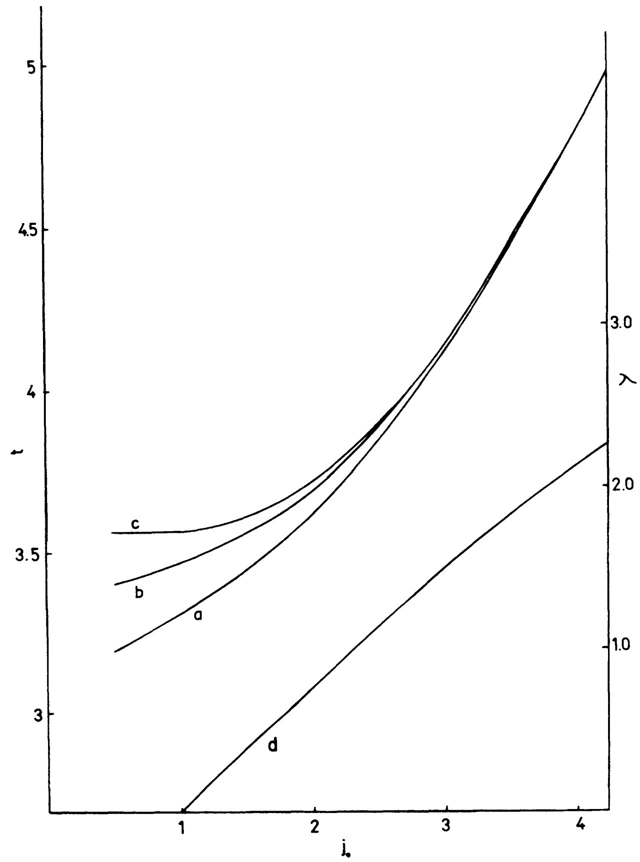

FIG. 3. Dependence of t on j_0 for a, $n=1$; b, $n=2$; and c, $n=\infty$ for the alternating superlattice. The dependence of λ on j_0 is shown in curve d.

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