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Properties of a superlattice composed of identical ferromagnetic films with antiferromagnetic interfacial coupling

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Abstract. We present theoretical studies of the magnetization, phase transition and twist angles of a superlattice composed of identical ferromagnetic films with antiferromagnetic coupling at the interfaces. The numerical results show there are some interesting properties of the superlattice.

(i) There is a plateau on the magnetization–temperature curve for the period $P = 4$, and the curve has a peak at a definite temperature for $P > 4$ and a suitable external field.

(ii) For a given external field and interfacial-coupling parameter the twist angles are sensitive to temperature, and the phase transition temperature from the twist state to the spin-parallel state does not change monotonically with the period of the superlattice.

Some of the theoretical results are in agreement with the experimental results qualitatively.

1. Introduction

In the last few years, superlattices or multilayered films such as Co/Ru, Fe/Cr and Co/Cu have attracted much attention [1–10]. Studies of these superlattices or multilayered films have resulted in the discovery of some interesting behaviour, e.g. the giant magnetoresistance effect and antiferromagnetic coupling between adjacent ferromagnetic films across the spacer layer [1–6] and in particular the oscillation behaviour of the magnetoresistance and coupling with the spacer-layer thickness in Fe/Cr, Co/Cr, Co/Ru and Gd/Y superlattices [6, 10]. Theoretically, a better theoretical model describing the field dependence of the magnetoresistance was presented in [2]. Although there has been some theoretical work [11–13] on the magnetic properties of the superlattice with antiferromagnetic interfacial coupling, adjacent ferromagnetic films in the superlattice used differ greatly in their exchange constants and spin quantum numbers ($J_a/J_b = 0.0355$ and $S_a/S_b = \frac{7}{2}$). Recently the zero-temperature magnetic properties of multilayered films composed of identical ferromagnetic films with antiferromagnetic interfacial coupling was discussed [9, 14] but, as far as we know, there has not been any work on the magnetic properties of the corresponding superlattice at finite temperatures. In addition, the interfacial-coupling parameter changes with the spacer-layer thickness, so that the dependences of the magnetic properties on this parameter are also interesting.

In this paper, we discuss, for various interfacial-coupling parameters, the temperature and field dependences of the relative magnetization and twist angles, as well as the phase transitions of the superlattice constructed of the identical ferromagnetic films with antiferromagnetic coupling at the interfaces. The superlattices in this paper can be considered to be practical superlattices, such as Fe/Cr and Co/Cr. If we apply the isotropic Heisenberg model, the Hamiltonian of the superlattice with a BCC lattice structure is described by

$$H = -\sum_{\langle ij\rangle} J_{ij} S_i S_j - h \sum_i S_i \tag{1}$$

where the sum in the first term is over sites i and nearest neighbours j, h is a reduced external field and the exchange constant is

$$J_{ij} = \begin{cases} J > 0 & \text{in any ferromagnetic film} \\ J_1 < 0 & \text{between two adjacent ferromagnetic films.} \end{cases}$$

According to the mean-field approximation, for any temperature and external field, the average value of any atomic spin in the ith atomic plane which is parallel to the interfaces can be written as

$$\langle S_i \rangle = SB(y_i) \tag{2}$$

with

$$y_i = (S/k_B T)[h \cos\theta_i + 4J_{i-1,i}\langle S_{i-1}\rangle \cos(\theta_i - \theta_{i-1}) + 4J_{i+1,i}\langle S_{i+1}\rangle \cos(\theta_{i+1} - \theta_i)] \tag{3}$$

where k_B is the Boltzmann constant, $B(y)$ is the Brillouin function and θ_i is the twist angle through which any atomic spin in the ith atomic plane rotates from the direction of the external field. The angle depends on the directions and magnitudes of the atomic spins in the $(i-1)$th atomic plane and the $(i+1)$th atomic plane. If we have the coordinate system where the x–z plane is parallel to the interfaces, all atomic spins are in the x–z plane and the external field is in the direction of the z axis, θ_i is given by

$$\theta_i = \tan^{-1}[h_x(i)/h_z(i)] \tag{4}$$

with

$$h_x(i) = 4\langle S_{i-1}\rangle J_{i-1,i} \sin\theta_{i-1} + 4\langle S_{i+1}\rangle J_{i+1,i} \sin\theta_{i+1} \tag{5}$$

$$h_z(i) = h + 4\langle S_{i-1}\rangle J_{i-1,i} \cos\theta_{i-1} + 4\langle S_{i+1}\rangle J_{i+1,i} \cos\theta_{i+1}. \tag{6}$$

2. Results and discussion

For a given temperature and external field, solving numerically equations (2)–(6), one can obtain the values of θ_i and $\langle S_i\rangle$. Thus the relative magnetization M/M_0 (M_0 is the value of the saturation magnetization at $T = 0$ K) of the superlattice is given simply by

$$M/M_0 = \frac{1}{SP} \sum_{i=1}^{P} \langle S_i \rangle \cos\theta_i \tag{7}$$

where S is the spin quantum number and P is the period of the superlattice. In this paper,

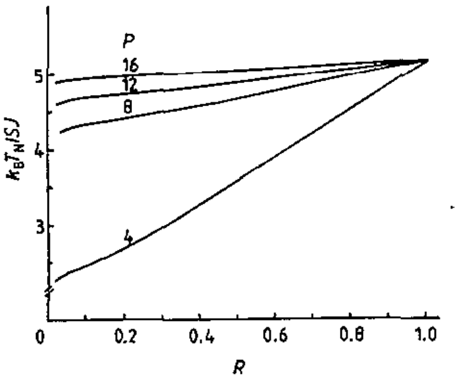

Figure 1. Critical temperature T_N as a function of the interfacial coupling parameter R for different periods of the superlattice. Here P represents the period.

our parameters have the values $S = 1$, $R(= -J_1/J) = 0.01, 0.02, 0.04, 0.06, 0.08$ and 0.1, and $P = 4, 8, 12$ and 16.

2.1. Transitions

There are three possible ground states in this superlattice.

(i) For $h = 0$, the spins in a ferromagnetic film are antiparallel to the spins in its adjacent ferromagnetic films, and this state is called an antiferromagnetic state.

(ii) For $h_c > h > 0$, the spins in any atomic plane which is parallel to the interfaces are at the same angle with respect to the external field. Generally, for different atomic planes, the angles are different. This state is called the twist state.

(iii) For $h > h_c$, all spins in the superlattice are aligned with the external field. The state is called the spin-parallel state.

In this paper, h_c represents the critical field.

For $h = 0$, as the temperature is increased from zero, the sublattice magnetizations decrease. When $T = T_N$, $\langle S_i \rangle = 0$. Therefore, when $T \to T_N$, $\langle S_i \rangle$ ($i = 1, 2, 3, \ldots, P$) is very small so that $B(y)$ in (2) can be expanded in series. Having neglected the non-linear terms, we can obtain the critical temperature T_N as a function of the interfacial-coupling parameter R. Figure 1 shows that T_N depends on R more sensitively for the superlattice with a smaller period, but the influence of R on T_N is weaker for a larger period.

For $h \neq 0$, there are two possible states: a twist state and a spin-parallel state. As h increases and exceeds h_c, the state of the superlattice changes from the twist state to the spin-parallel state. Figure 2 shows how h_c changes with R for different temperatures and periods. It can be seen that, for $T = 0$ and a superlattice with a smaller period, the relations between h_c and R are linear approximately; when the temperature or the period is increased, the relations are distorted slightly and h_c decreases obviously for a given value of R.

2.2. Temperature and field dependences of relative magnetization

In figure 3, we give a few examples of how the magnetization changes with the external field at different temperatures for various interfacial-coupling parameters. This figure shows that the relations between the magnetization and the external field are linear for

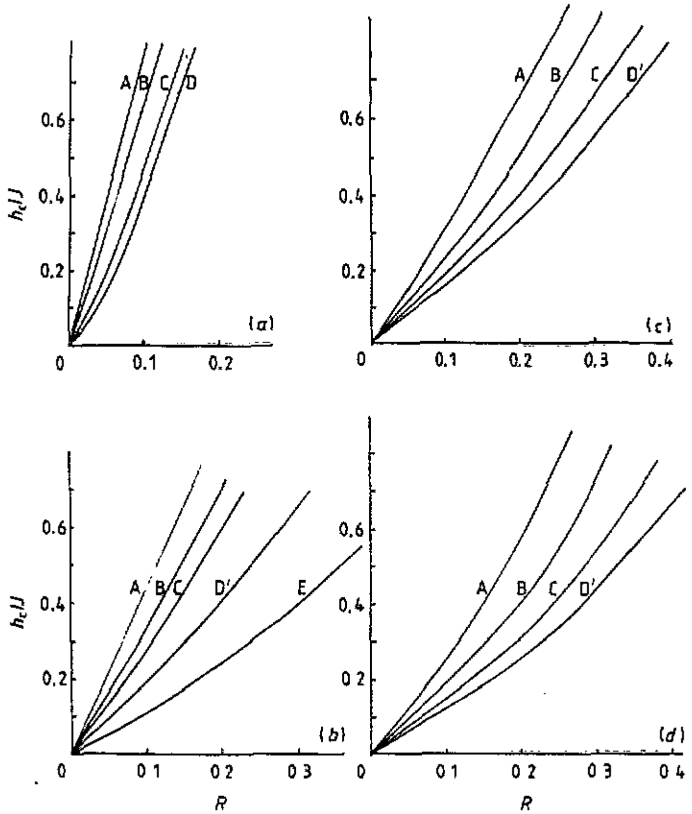

Figure 2. Critical field as a function of the interfacial coupling parameter for periods P of (*a*) 4, (*b*) 8, (*c*) 12 and (*d*) 16 at various temperatures T' ($= k_BT/SJ$): curves A, $T' = 0$; curves B, $T' = 2.0$; curves C, $T' = 2.5$; curve D, $T' = 2.64$; curves D′, $T' = 2.86$; curve E, $T' = 3.0$.

a smaller period, smaller values of R and $h < h_c$; the magnetization does not increase obviously with increase in the external field for a larger period and $h > h_c$, as figures 3(*b*) and 3(*b*′) show; however, the magnetization increases more clearly with increase in the external field for a smaller period and $h > h_c$, which is demonstrated in figures 3(*a*) and 3(*a*′). Comparing figures 3(*b*) and 3(*b*′) with the experimental figures [4], [6], we can see that the theoretical results are in agreement with the experimental results qualitatively. Of course, we should note the difference between the temperatures used in the theoretical calculations and experiments.

Studying the relative magnetization as a function of temperature, we find some interesting information about the superlattice. For different periods of the superlattice, the calculations show that there are three types of magnetization curve as can be seen in figure 4.

(i) For a given value of R and the period $P = 4$, the magnetization curve has a plateau in a suitable external field (see figure 4(*a*)). The height and length of the plateau are determined by R and h. According to our numerical results, at $T = 0$, the superlattice is in the twist state for the given values of R and h. In addition, the magnitudes of $\langle S_i \rangle$ or θ_i in different atomic layers are equal at any temperature. As the temperature is increased from $T = 0$, the magnitudes of $\langle S_i \rangle$ and θ_i decrease, but the contributions of the decreases

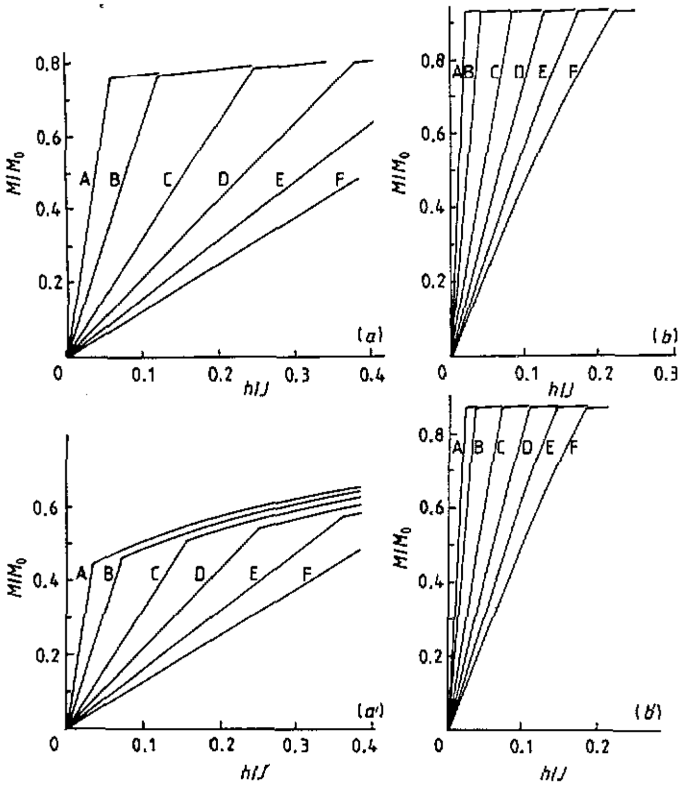

Figure 3. Relative magnetization as a function of the external field for periods P of (a), (a') 4 and (b), (b') 12 at various R: T' ($=k_BT/SJ$) of (a), (b) 2.0 and (a'), (b') 2.5; curves A, R = 0.01; curves B, R = 0.02; curves C, R = 0.04, curves D, R = 0.06; curves E, R = 0.08; curves F, R = 0.1. The values of the external field corresponding to the turning points of the curves are the critical fields h_c.

in the magnitudes of $\langle S_i \rangle$ and θ_i to the magnetization cancel each other until θ_i is equal to zero. Then, as the temperature is increased further, the decrease in $\langle S_i \rangle$ results in a rapid decrease in the magnetization.

(ii) For the superlattice with a longer period in the same field, the magnetization, as a function of temperature, differs from those shown in figure 4(a) and is shown in figure 4(b). The magnetization curves each have a maximum at corresponding temperatures for some given values of R.

(iii) There is another type of magnetization curve in an appropriate external field, for instance the curves for $R = 0.01$ and 0.02 in figure 4(b). The curves resemble the spontaneous magnetization curves of ordinary ferromagnets. The reason is that, at $T = 0$, all atomic spins in the superlattice are in the direction of the external field and the arrangement of the spins is similar to that in ferromagnets.

Curves of the types (ii) and (iii) in the above paragraph have been obtained in experiments with the $(Gd_{10}\text{–}Y_{10})_{225}$ superlattice [10], and the theoretical curves and experimental curves are very similar.

The comparison of magnetization–temperature curves of superlattices with different periods is given in figure 5. It shows the period dependence of the magnetization–temperature curve.

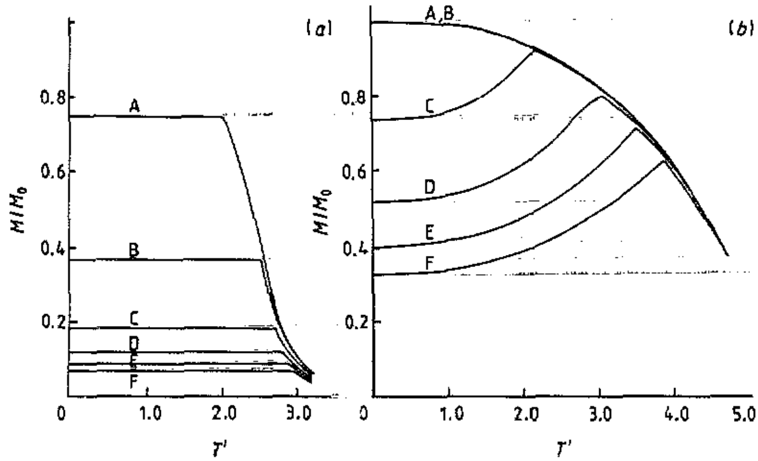

Figure 4. Relative magnetization as a function of temperature T' $(=k_BT/SJ)$ for the given external field $h/J = 0.06$ and periods P of (*a*) 4 and (*b*) 16 at various R: curves A, $R = 0.01$; curves B, $R = 0.02$; curves C, $R = 0.04$; curves D, $R = 0.06$; curves E $R = 0.08$; curves F, $R = 0.1$.

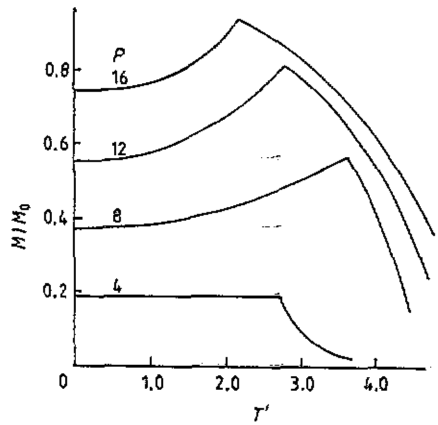

Figure 5. Relative magnetization as a function of temperature for $h/J = 0.06$ and $R = 0.04$ at various periods P.

2.3. *Temperature and field dependences of twist angles*

From our calculations for the superlattices with the periods $P = 4, 8, 12$ and 16, we find that, for $R \leqslant 0.1$, the difference between the twist angles of two arbitrary spins in the same ferromagnetic film is less than 2°. Thus we use $\bar{\theta}$ to represent the average value of the twist angles in the ferromagnetic film, while in the adjacent ferromagnetic films the average value of the twist angles is equal to $-\bar{\theta}$.

In figure 6 we present examples of how $\bar{\theta}$ changes with the external field for different temperatures, superlattice periods, $R = 0.01$ and 0.04. Figure 7 describes the temperature dependences of $\bar{\theta}$ for $h = 0.06$, and $R = 0.01$ and 0.04. For the superlattice in the twist state at $T = 0$, as the temperature is increased, $\bar{\theta}$ decreases; further, when the

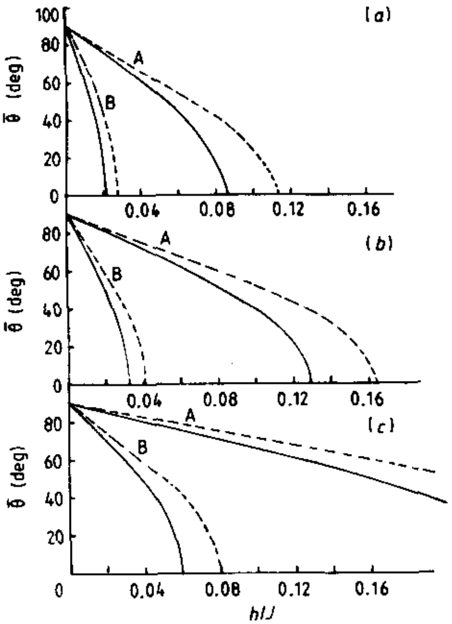

Figure 6. Average value of the twist angles as a function of the external field for periods P of (a) 12, (b) 8 and (c) 4 and temperatures $T'(=k_BT/SJ)$ of 0.0 (– – –) and 2.0 (——) at two values of R: curves A, $R = 0.04$; curves B, $R = 0.01$.

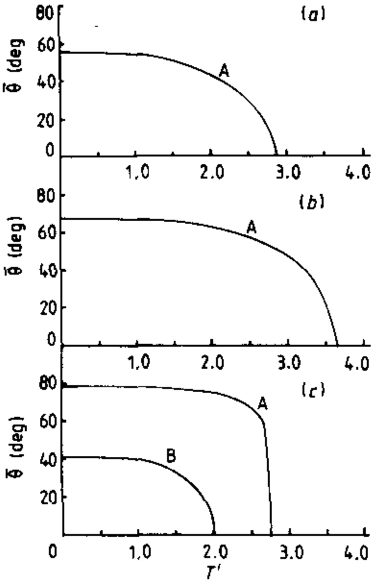

Figure 7. Average value of the twist angles as a function of temperature $T'(=k_BT/SJ)$ for $h/J = 0.06$ and periods P of (a) 12, (b) 8 and (c) 4 at two values of R: curves A, $R = 0.04$; curves B, $R = 0.01$. In (a) and (b), when $R = 0.01$, the superlattices are in the spin-parallel state ($\bar{\theta} = 0$).

temperature is equal to a certain value, $\bar{\theta}$ is equal to zero. This value of temperature is the phase transition temperature T_c from the twist state to the spin-parallel state. An unusual behaviour is that this phase transition temperature does not change with the period of the superlattice monotonically. According to our calculations, for $P = 8$, the phase transition temperature has the maximal value as figure 6(b) shows for the same value of R. Then, as P increases, the phase transition temperature decreases. This case is known from figure 5 too.

3. Conclusion

We have investigated the temperature and field dependences of the relative magnetization and spin configurations of the superlattice formed from identical ferromagnetic films with antiferromagnetic coupling at the interfaces. Because we have used the isotropic Heisenberg model for the superlattice, the results are suitable principally for practical superlattices with interfacial coupling which is much stronger than the anisotropies, e.g. Fe/Cr and Co/Ru superlattices [6, 14]. We see that the magnetization–temperature and magnetization–field curves are in agreement with the experimental curves [6, 10] qualitatively. At the same time, we obtain some interesting properties.

(i) There is a plateau on the magnetization–temperature curve of the superlattice with the period $P = 4$, and the curve has a peak at a definite temperature for $P > 4$ and an appropriate external field.

(ii) For a given external field and interfacial coupling, the twist angles are sensitive to temperature, and the phase transition temperature T_c from the twist state to the spin-parallel state does not change monotonically with the period of the superlattice. According to our numerical results, the superlattice with the period $P = 8$ has the highest phase transition temperature T_c.

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