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Magnetic Properties of the Spin-$\frac{1}{2}$ Ising Ferromagnetic Thin Films with Alternating Superlattice Configuration

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The magnetic properties in a finite ferromagnetic superlattice are studied. The spin-$\frac{1}{2}$ Ising model with alternating intralayer parameters is used within the effective field theory, which is based on a probability distribution technique that accounts for the self-correlation function. The transition temperatures are calculated as a function of the intra- and interlayer exchange interactions and of the surface exchange interaction. The magnetization profiles are also studied.

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I. Introduction

Over the years, there has been considerable effort devoted to the preparation and explantation of composite systems formed from alternating layers of different materials. By a layer we mean N ferromagnetic atomic layer, whereas by an atomic layer we mean a separate sheet of atoms. If the ferromagnetic layer is thin enough (N is small) to behave like a 2D system, we can approximately model each individual ferromagnetic layer by a 2D lattice (atomic layer). Superlattice structures composed of two different ferromagnetic layers, for example, monolayers of cobalt (Co) [1, 2], iron (Fe) [3, 4], and nickel (Ni) [5] have been grown on copper (Cu); iron (Fe) has been grown on gold (Au) [6], and gadolinium (Gd) monolayer has also been grown on tungsten (W) [7]. The critical properties of such systems have been studied, either experimentally or theoretically. Ferromagnetic order in some of these materials has been reported. It is thus reasonable to envisage, and to study theoretically, magnetic superlattices that consist of L ferromagnetic layers in which the atoms vary from one layer to another. A study of surface effects on magnetic properties of superlattice configured Ising thin films (SCITF) has already been made in Refs. [8] and [9] within the mean field theory (MFT), where the top and bottom surfaces exchange interactions are allowed to change. The Curie temperatures were calculated as a function of thickness of the superlattice for various coupling strengths. In Ref. [10] almost the same model as in [8, 9] has been examined, but in the effective-field theory approach. The transition temperatures of an infinite superlattice with two layers in a unit cell and a finite one with a modified surface were calculated. In Ref. [11] for the case of an alternating superlattice, the transition temperatures are calculated as a function of the film thickness and of the intra- and interlayer exchange constants within the framework of the effective field theory.

From the theoretical point of view, one of the models more widely used to study the magnetic properties of ferromagnetic systems is the Ising model. The purpose of this paper is to consider the magnetic properties of a finite superlattice with alternating ferromagnetic layers thin enough to behave two-dimensionally. We approximate this finite superlattice by a SFITF consisting of L completely filled and well ordered alternating two-dimensional layers separated by nonmagnetic layers by taking into account surface effects and deviation of the interlayer interaction J_{ab} from the intralayer one.

II. Formalism

We consider a superlattice consisting of a set of alternating atomic layers A and B in the structure $(ABABA....BA)$ as is depicted in Fig. 1. For simplicity we restrict our attention to the case of simple cubic structures. The coupling strength between nearest-neighboring spins in $A(B)$ is denoted by $J_a(J_b)$ and takes the value J_s, if both spins are nearest neighbors with the surface layer (top and the bottom surfaces) while J_{ab} stands for the exchange coupling between the nearest neighbor spins in layers A and B. The Hamiltonian of the system is given by

$$H = -\sum_{(i,j)} J_{ij} S_{iz} S_{jz} \tag{1}$$

where the sum runs over all nearest-neighbor spin pairs. S_{iz} denotes the z component of a quantum spin $\vec{S_i}$ of magnitude S = 1/2 at site i, J_{ij} stands for one of the three exchange interactions depending on where the spin pair is located.

For Ising-1/2 spins we obtain, within the effective field theory, a set of a simultaneous equations describing the layer magnetization of our system. The method we use is described in [12-14], that employed the probability distribution technique to account for the single-site spin correlations. For the site magnetization m_s of the top surface we get:

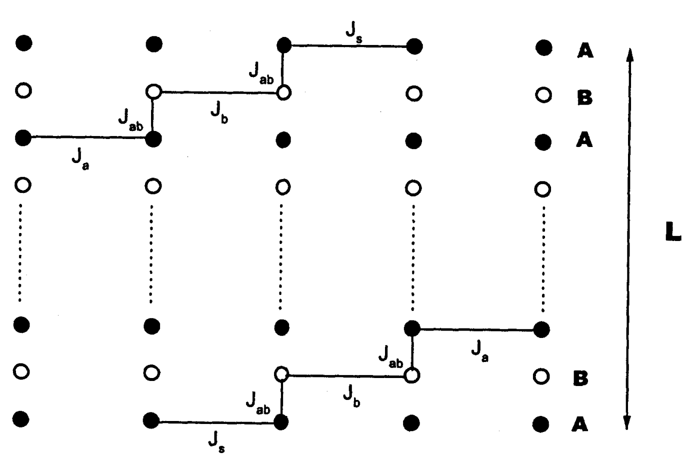

FIG. 1. Sketch of a unit cell of the superlattice.

$$m_s = 2^{-N-N_0} \sum_{\mu=0}^{N} \sum_{\mu_1=0}^{N_0} \sum_{i=0}^{\mu} \sum_{j=0}^{N-\mu} \sum_{k=0}^{\mu_1} \sum_{l=0}^{N_0-\mu_1} C_\mu^N C_{\mu_1}^{N_0} C_i^\mu C_j^{N-\mu} C_k^{\mu_1} C_l^{N_0-\mu_1}$$
$$(-1)^{i+k} 2^{i+j+k+l} m_s^{i+j} m_2^{k+l} F\Big[-\frac{1}{2}\{(2\mu - N)J_s + (2\mu_1 - N_0)J_{ab}\}\Big] \tag{2}$$

For the site magnetization m_2 of the next layer (layer B) we get:

$$m_2 = 2^{-N-2N_0} \sum_{\mu=0}^{N} \sum_{\mu_1=0}^{N_0} \sum_{\mu_2=0}^{N_0} \sum_{i=0}^{\mu_1} \sum_{j=0}^{N_0-\mu_1} \sum_{k=0}^{\mu} \sum_{l=0}^{N-\mu} \sum_{p=0}^{\mu_2} \sum_{q=0}^{N_0-\mu_2} C_\mu^N C_{\mu_1}^{N_0} C_{\mu_2}^{N_0} C_i^{\mu_1}$$
$$C_j^{N_0-\mu_1} C_k^\mu C_l^{N-\mu} C_p^{\mu_2} C_q^{N_0-\mu_2} (-1)^{i+k+p} 2^{i+j+k+l+p+q} m_s^{i+j} m_2^{k+l} m_3^{p+q} \tag{3}$$
$$F\Big[-\frac{1}{2}\{(2\mu_1 - N_0)J_{ab} + (2\mu - N)J_b + (2\mu_2 - N_0)J_{ab}\}\Big]$$

And the site magnetization m_n $(3 \quad n \quad L-2)$ of the layers is given by:

$$m_n = 2^{-N-2N_0} \sum_{\mu=0}^{N} \sum_{\mu_1=0}^{N_0} \sum_{\mu_2=0}^{N_0} \sum_{i=0}^{\mu_1} \sum_{j=0}^{N_0-\mu_1} \sum_{k=0}^{\mu} \sum_{l=0}^{N-\mu} \sum_{p=0}^{\mu_2} \sum_{q=0}^{N_0-\mu_2} C_\mu^N C_{\mu_1}^{N_0} C_{\mu_2}^{N_0} C_i^{\mu_1}$$
$$C_j^{N_0-\mu_1} C_k^\mu C_l^{N-\mu} C_p^{\mu_2} C_q^{N_0-\mu_2} (-1)^{i+k+p} 2^{i+j+k+l+p+q} m_{n-1}^{i+j} m_n^{k+l} m_{n+1}^{p+q} \tag{4}$$
$$F\Big[-\frac{1}{2}\{(2\mu_1 - N_0)J_{ab} + (2\mu - N)J + (2\mu_2 - N_0)J_{ab}\}\Big]$$

where J is $J_a(J_b)$ when m_n is the magnetization of the layer $A(B)$. In general, if we get a set of L atomic layers $(ABA.....BA)$ and for $(0 \quad i \quad (L-1)/2)$:

$$m_{L-i} = m_{i+1} \tag{5}$$

where $m_1 = m_s$.

In these equations, N and N_0 denote the numbers of nearest neighbors in the plane and between adjacent planes, respectively, and C_k^l are the binomial cœfficients, $C_k^l = \frac{l!}{k!(l-k)!}$. For the case of a simple cubic lattice which we will consider here, one has $N = 4$, $N_0 = 1$. The function F is described in Ref. [15].

The condition for the Curie temperature T_c/J_a (in the case $J_a < J_b$) and T_c/J_b (in the case $J_b < J_a$) of our system results from the linearization of equations (2) to (5). As a result of the linearization, we obtain a set of L linear equations for the system with thickness L. The determinant of this set of equations should be equal to zero and this condition yields L different solutions for the temperature. The largest solution can be interpreted as the Curie temperature of the system [16, 17].

III. Results and discussion

The calculations were carried out to investigate the effect of film thickness, different ratios exchange parameters $R_b = J_b/J_a$, $R_{ab} = J_{ab}/J_a$ in the case $J_a < J_b$ and the effect of different

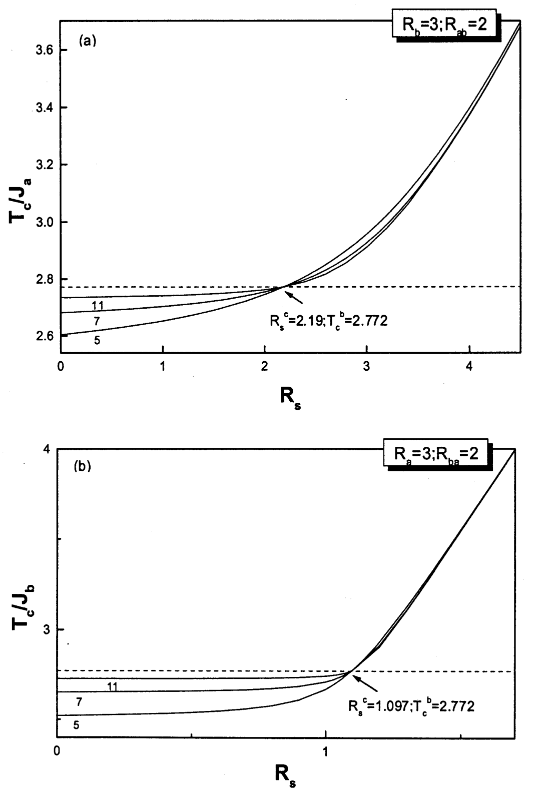

FIG. 2. The Curie temperature of the system as a function of the parameter R_s for three values of film thickness that are indicated by the numbers. (a) $J_a < J_b$, (b) $J_b < J_a$.

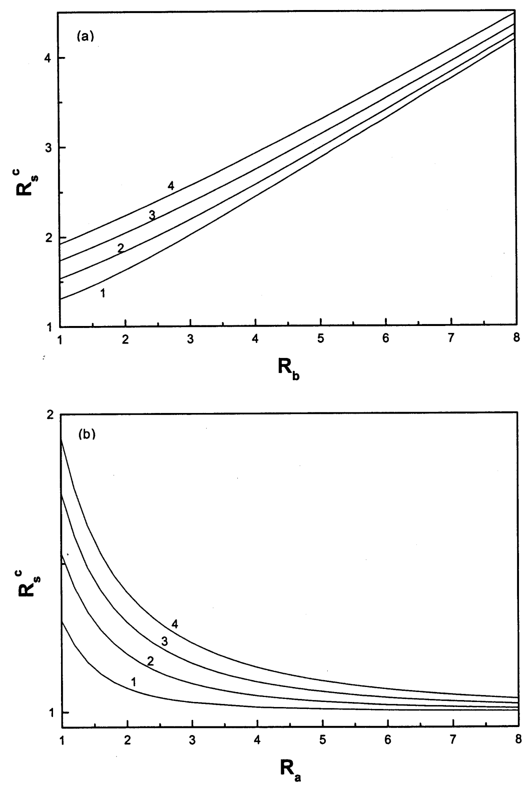

FIG. 3. Critical values R_s^c as a function of (a) $R_b(J_a < J_b)$, (b) $R_a(J_b < J_a)$, for different values of R_{ab} and R_{ba}, respectively, indicated by a value attached to each curve.

ratios exchange parameters $R_a = J_a/J_b$, $R_{ba} = J_{ab}/J_b$ in the case $J_b < J_a$, and at last, the enhancement (or reduction) of the surface exchange interaction, on the temperature versus $R_s = J_s/J_a$, $R_a(R_b)$, $R_{ab}(R_{ba})$ phase diagrams.

We first consider the case with $J_a < J_b$. In Fig. 2(a), we show the Curie temperature T_c/J_a of the system as a function of the surface exchange interaction R_s presented with different values of thickness labeled by a number in the case with R_{ab} = 2 and R_b = 3. The dashed line is the Curie temperature of the corresponding infinite superlattice system denoted by T_c^b/J_a. It is very interesting to see that, there exists a critical surface exchange coupling R_s^c such that, the critical temperature remains constant for every thickness L and is equal to T_c^b/J_a. For $R_s < R_s^c$, the critical temperature T_c/J_a of the alternating superlattice is smaller than the critical temperature T_c^b/J_b of the corresponding infinite superlattice system. T_c/J_a increases with L and approaches the T_c^b/J_a asymptotically as the number of the layers becomes large. For $R_s > R_s^c$, the critical temperature of the system is greater than T_c^b/J_a and decreases with L. We obtain a similar results also in the case $J_b < J_a$ as it is shown in Fig. 2(b).

Fig. 3(a) plots the critical value of R_s^c as a function of R_b for different values of R_{ab} as indicated by a number attached to each curve (when $J_a < J_b$). We see that R_s^c in all cases is greater than 1.0 regardless of the value of R_{ab}. The characteristic property of the curves in the figure is an increase of the critical value R_s^c when the exchange parameter R_b between atoms B increases.

Fig. 3(b) plots the critical value of R_s^c as a function of R_a for different values of R_{ba} as indicated by a number attached to each curve (when $J_b < J_a$). We see, for large values of R_a, that R_s^c is quite dependent of R_{ba} and approaches 1.0. The characteristic property of the curves in the figure is a decrease of the critical value R_s^c when the exchange parameter R_a between atoms A increases. This behavior has a tendency opposite to the first case ($J_a < J_b$). These two figures show also an increase of R_s^c when $R_{ab}(R_{ba})$ increases for a fixed value of $R_b(R_a)$.

The Curie temperature of the alternating superlattice system with thickness L = 5 and the corresponding infinite one (dashed line) as a function of $R_b(R_a)$ are exhibited in Fig. 4(a), 4(b) where we take several values of R_s. In Fig. 4(a), the curves referring to $R_s < R_s^c \in [1.54, 4.25]$ (R_s^c = 1.54 (4.25) when $R_b = 1$ and R_{ab} = 2 (R_b = 8 and R_{ab} = 2)) show an increase of the

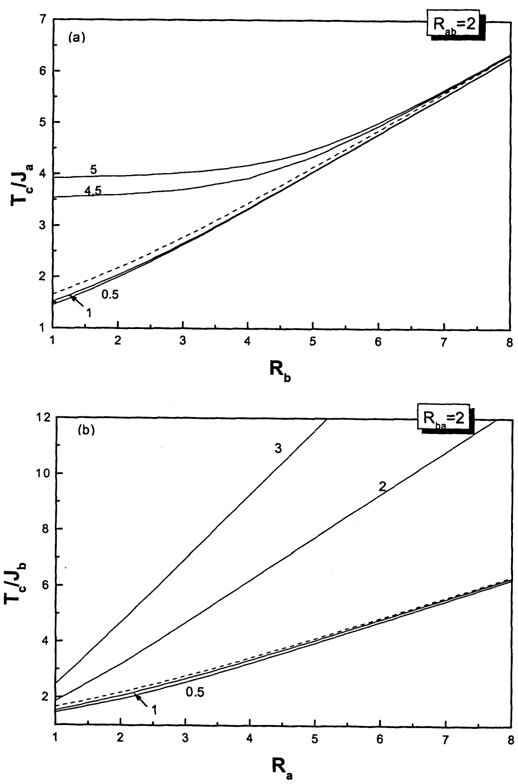

FIG. 4. The system critical temperature as a function of parameters (a) R_b ($J_a < J_b$), (b) R_a ($J_b < J_a$), for different values of surface exchange interaction indicated by a number attached to the curves.

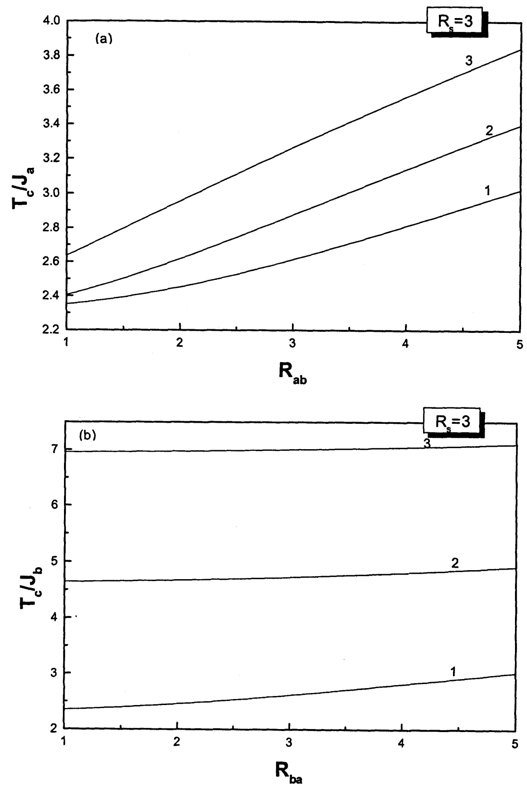

FIG. 5. The Curie temperature of the system as a function of parameters (a) R_{ab} ($J_a < J_b$), (b) R_{ba} ($J_b < J_a$), for different values of intralayer coupling parameters R_b and R_a, respectively. The film thickness is L = 5 and the surface exchange parameter is R_s = 3.

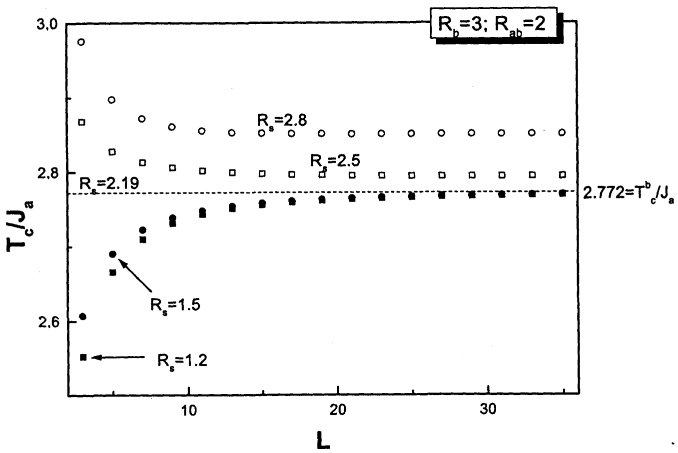

FIG. 6. The dependence of the critical temperature T_c/J_a on the thickness L of the film for R_b = 3 and R_{ab} = 2. The number accompanying each curve denotes the value of R_s.

Curie temperature of the system when the exchange parameter between atoms B increases. On the other hand, from curves referring to $R_s > R_s^c$, the dependence of the critical temperature on the R_s is significant only for small values of R_b. However, for larger values of R_b, the infinite limit of the corresponding superlattice is approached rapidly and it is the same for every R_s. In Fig. 4b, The Curie temperature T_c/J_b increases with R_a for every values of R_s. The curves for $R_s > R_s^c$ show an important dependence of the Curie temperature on the R_s only for large values of R_a.

In Fig. 5(a) and Fig. 5(b) we plot the Curie temperature of the system with thickness L = 5 as a function of R_{ab} and R_{ba}, respectively. The influence of the intralayer coupling parameters R_b and R_a for both the cases ($J_a < J_b$ and $J_b < J_a$) on the Curie temperature of the system is presented. The surface exchange parameter is R_s = 3. The curves refer to different intralayer coupling parameters (numbers attached to each curve). We see from Fig. 5(a), that the critical temperature T_c/J_a increases with R_{ab} and R_b. Fig. 5(b) shows that for a fixed value of R_a, T_c/J_b increases slightly with increasing R_{ba}. On the other hand, the Curie temperature depends sensibly on R_a.

Figure 6 shows the variation of the critical temperature T_c/J_a as a function of the film thickness L for R_b = 3, R_{ab} = 2 and different values of R_s attached to each curve. For $R_s = R_s^c$, T_c/J_a remains constant for any thickness L represented by a dashed line in the figure (which represents the bulk critical temperature). When the thickness L increases and $R_s < R_s^c$, the transition temperature T_c/J_a increases and approaches the bulk critical temperature value of the corresponding infinite system. On the other hand, for $R_s > R_s^c$, T_c/J_a of the film decreases as L increases and approaches a value depending on the degree of the reduced exchange coupling R_s. These results are in agreement with those of Fig. 2(a).

In Fig. 7, the magnetization profiles at various temperatures are shown for the case with an enhanced surface exchange interaction R_s = 3.5 (Fig. 7(a)), a reduced surface exchange interaction R_s = 1.5 (Fig. 7(b)). The exchange parameters have the values R_b = 3 and R_{ab} = 2 ($J_a < J_b$). We see from Fig. 7(a) that larger magnetization m_n appears on layers lying near surfaces. As the

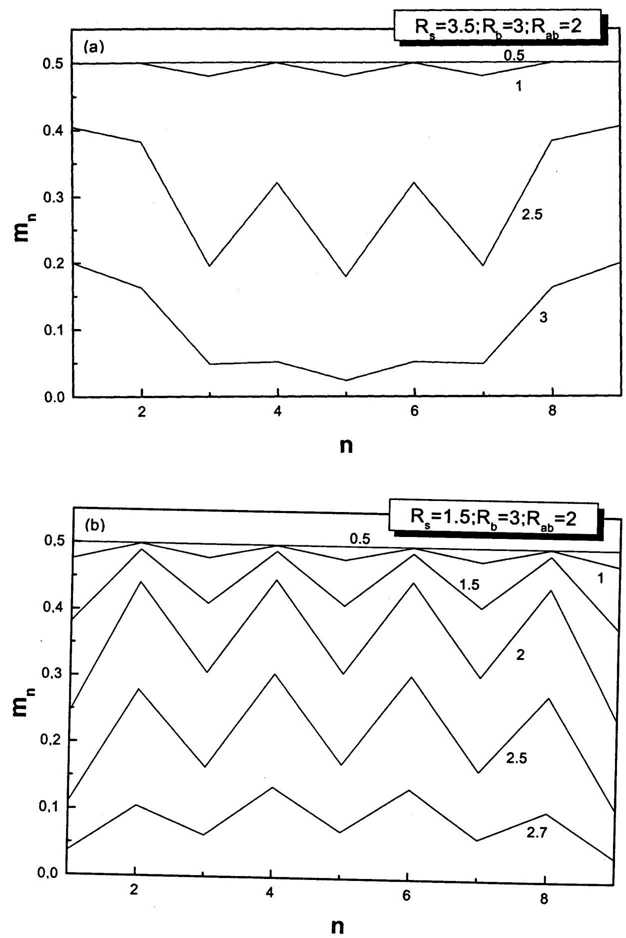

FIG. 7. magnetization profiles for various temperatures attached to each curve. The exchange parameters have the values $R_b = 3$, $J_a = 1$, $R_{ab} = 2$ ($J_a < J_b$). (a) Enhanced surface exchange interaction R_s = 3.5, (b) reduced surface exchange interaction R_s = 1.5.

temperature increases (the values of the temperature are attached to each curve), the magnetization profile changes from oscillatory to non-oscillatory behavior.

From Fig. 7(b), we can see that smaller magnetization m_n appears on layers lying near surfaces and the profile of magnetization has an oscillatory character up to the Curie temperature of the system T_c = 2.772 for thickness L = 9.

VI. Conclusion

In this paper, we have developed a theory of the spin-$\frac{1}{2}$ Ising ferromagnetic thin films with alternating superlattice configuration based on the effective field theory. We have examined the transition temperatures and the magnetization profiles for several sets of material parameters. The most interesting results are:

- There exists a critical value of the surface exchange coupling above which the surface magnetism appears.
- It is interesting to note that the influence of the surface exchange coupling R_s for both surfaces on the curie temperature is very significant only for small values of R_b (if $J_a < J_b$, and for large values of R_a (if $J_b < J_a$).
- The magnetizations are large (small) on layers near the surfaces when $R_s > R_s^c$ ($R_s < R_s^c$).

The formalism can be used for studying a superlattice-configured thin film of various thickness, structures and topology. Investigation of magnetic properties of the mentioned systems in which atoms vary from one layer to another will be most useful and enlightening. At the moment, iron and cobalt may be the best candidates for alternating superlattices, although superlattices of alternating magnetic monolayers have not been studied experimentally yet. Since these are itinerant magnets with nearly isotropic magnetic interaction, one can use an itinerant model, or, at least, a Heisenberg model, to describe the system properly.

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References

[1] R. Miranda, D. Chandesris and J. Lacante, Surf. Sci. **130**, 269 (1983).
[2] D. Pescia, G. Zamperi, M. Stampanoni, C. L. Bona, R. F. Willis and F. Meier, Phys. Rev. Lett. **58**, 933 (1987).
[3] M. F. Onellion, C. L. Fu, M. A. Thompson, J. L. Erskine and A. J. Freeman, Phys. Rev. Lett. B **33**, 7322 (1986).
[4] D. Pescia, M. Stampanoni, C. L. Bona, A. Vaterlaus, R. F. Willis and F. Meier, Phys. Rev. Lett. **58**, 2126 (1987).
[5] M. A. Thompson and J. L. Erskine, Phys. Rev. Lett. B, **31**, 6832 (1987).
[6] W. Durr *et al*., Phys. Rev. Lett. **58**, 511 (1987).
[7] M. Farle and K. Baberschke, Phys. Rev. Lett. **58**, 511 (1987).
[8] H. K. Sy, Phys. Rev. B **45**, 4454 (1992).
[9] H. K. Sy and M. H. Ow, J. Phys.: Condensed Matter **4**, 5891 (1992).
[10] Q. D. Chen and S. M. Zheng, Phys. Stat. Sol. (b) **200**, 217 (1997).
[11] Y. M. Seidov and G. R. Shaulov, J. Phys.: Condensed Matter **6**, 9621 (1994).
[12] Cheng Jia and Xuan-Zhang Wang, J. Phys.: Condens. Matter **8**, 5745 (1996).
[13] A. Saber *et al.*, J. Phys.: Condens. Matter **12**, 43 (2000).
[14] A. Saber *et al.*, J. Phys.: Condens. Matter **11**, 2087 (1999).
[15] A. Saber *et al.*, Physica A **269**, 329 (1999).
[16] A. R. Ferchmin and S. Krompiewski, J. Phys. C **8**, 1901 (1975).
[17] T. Balcerzak, J. Magn. Magn. Mater. **129**, 279 (1994).