PHASE TRANSITION IN FERROMAGNETIC SUPERLATTICE NANOWIRES

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The critical behavior of a superlattice nanowires consisting of two different ferromaganets is examined within the framework of the molecular-field theory approach. The transition temperature T_c for the nanowires which is modeled as having a hexagonal cross section are calculated as a function of inter-and intralayer exchange constant by the transfer matrix method. The results are illustrated numerically for a particular choice of parameters.

Keywords: A. Nanowires, superlattice, spin-waves, phase transition.
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INTRODUCTION

The interesting phenomena and practical benefits discovered in the magnetic materials with magnetic properties modulated in the nanometer scale have led to considerable attention [1-3]. In the recent past many experimental and theoretical research have been focused on the properties of magnetic systems in the nanometer scale [4-6]. With the advance of modern vacuum science, it is possible to artificially fabricate such structures.

Theoretically, various superlattice and nanowires can be modeled as having a chosen shape and size cross section (in the x-y plane) with a finite number spins arranged [7-9]. At comparation of bulk systems one can see that both superlattice and nanowires systems show novel magnetic and electronic features. The critical behavior of magnetic films and superlattice have been examined, either experimentally or theoretically [10-12]. On the other hand, considerable effort has been recently devoted to phase transition in nanowires [13,14].

MODEL AND FORMALISM

As indicated in fig. 1. we consider (l,r) hexagonal ferromagnetic superlattice nanowire (SLNW) model in which the l atomic layers of material *a* alternate with r atomic layers of material *b*, having exchange constant J_a and J_b in intralayer, and Y_a and Y_b in interlayer, respectively. On the other hand corresponding exchange constants between spins at the surface shell are J_{as} and J_{bs} in intralayer, and Y_{as} and Y_{bs} in interlayer, respectively. The exchange interactions between neighboring spins on two adjacent *a* and *b* materials are Y and Y_s. Lattice constant of the SLNW is $(l+r)a$.

The Ising Hamiltonian of the system can be written in the form

$$H = -\sum_{\substack{n,\tau,\tau', \\ (\tau\neq\tau')}} J_{n,n}^{\tau,\tau'}(S_n^{\tau}S_n^{\tau'}) - \sum_{n,\tau}\left(Y_{n,n-1}^{\tau,\tau}(S_n^{\tau}S_{n-1}^{\tau}) + Y_{n,n+1}^{\tau,\tau}(S_n^{\tau}S_{n+1}^{\tau})\right) \quad (1)$$

where the first term describes exchange interactions inside atomic layer, the second term describes exchange interactions between neighboring atomic layers. The external magnetic field is neglected for simplicity. Here, n is the index of atomic layer, τ describes the position of a lattice site in this layer. The axis z of the coordinate system is along the nanowires under study.

According to the molecular-field model the mean spins $m_n^{\tau} = \langle S_n^{\tau}\rangle$ $(\tau = 1, 2, ...7)$ are determined by the set of equations

$$m_n^{(\tau)} = B_S\left[\left(\sum_{\tau'} J_{n,n}^{\tau,\tau'} m_n^{(\tau')} + Y_{n,n+1}^{\tau,\tau} m_{n+1}^{(\tau)} + Y_{n,n-1}^{\tau,\tau} m_{n-1}^{(\tau)}\right)\Big/ kT\right] \quad (2)$$

where *k* is Boltzmann constant, $B_S(x)$ is the Brillouin function

$$B_S(x) = \frac{2S+1}{2S}\coth\left(\frac{2S+1}{2S}x\right) - \frac{1}{2S}\coth\left(\frac{1}{2S}x\right) \quad (3)$$

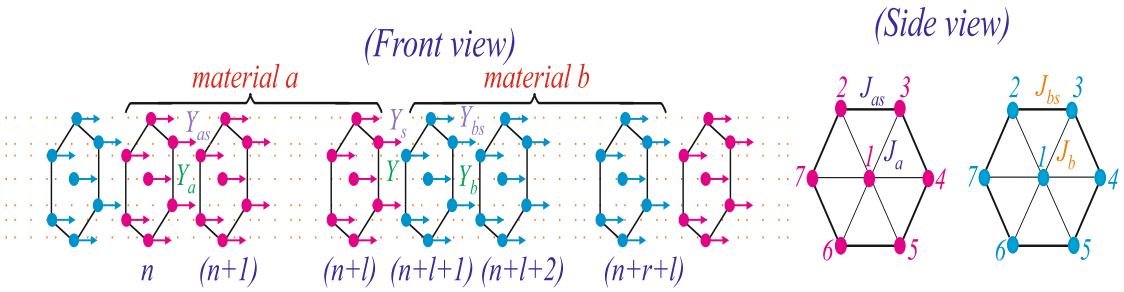

Fig.1. Model of hexagonal ferromagnetic nanowires in which the l atomic layers of material *a* alternate which r atomic layers of material *b*. The nanowires are infinite in the direction perpendicular to the axes z.

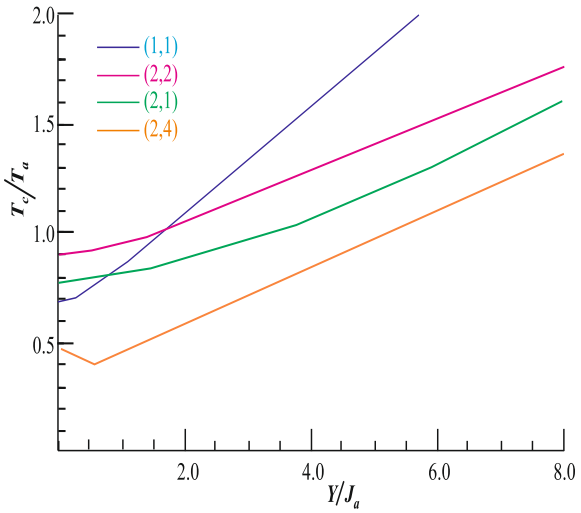

Fig2. Critical temperatures as a function of Y/J_a for $J_{as}/J_a=1$, $Y_a/J_a=1$, $Y_{as}/J_a=1$, $J_b/J_a=1.5$, $J_{bs}/J_a=1.5$, $Y_b/J_a=1.5$, $Y_s/Y=1$, $Y_{bs}/J_a=1.5$.

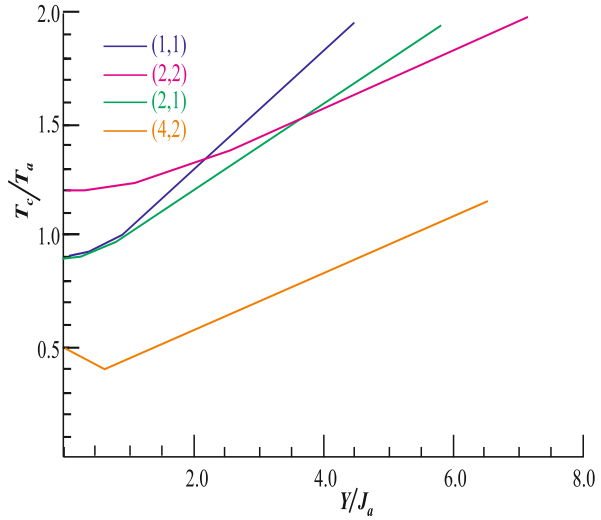

Fig.3. Critical temperatures as a function of Y/J_a for $J_{as}/J_a=1.2$, $Y_a/J_a=1$, $Y_{as}/J_a=1.5$, $J_b/J_a=2$, $J_{bs}/J_a=2.2$, $Y_b/J_a=1.8$, $Y_s/Y=1.2$, $Y_{bs}/J_a=2.1$.

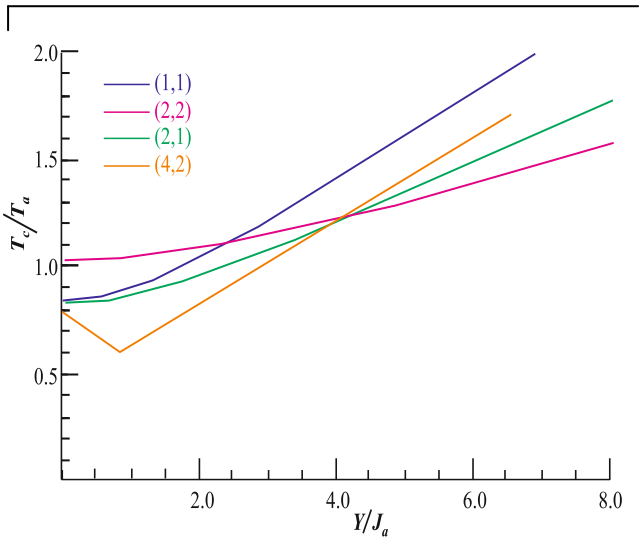

Fig.4. Critical temperatures as a function of Y/J_a for $J_{as}/J_a=0.7$, $Y_a/J_a=1.2$, $Y_{as}/J_a=0.5$, $J_b/J_a=2$, $J_{bs}/J_a=1.5$, $Y_b/J_a=1.8$, $Y_s/Y=0.5$, $Y_{bs}/J_a=1.3$.

As the temperature becomes higher than the critical temperature T_c the whole system becomes demagnetized and the mean atomic magnetization approaches zero. Near the critical temperature T_c mean spins m_n^{τ} become small. For small arguments of Brillouin function all terms order higher than linear can be neglected, and one has the expansion:

$$B_S(x)\approx\frac{S+1}{3S}x \qquad (4)$$

It is necessary to take into account that all six spins are in the same orientation according to the spin labeled by 1, therefore

$$m_n^{(2)}=m_n^{(3)}=m_n^{(4)}=m_n^{(5)}=m_n^{(6)}=m_n^{(7)}$$

in intralayer. Using (4) the system of equations (2) can be solved by recurrence relation technique [12] to relate the different spins at the first and second atomic layer of elementary unit cell

$$\begin{pmatrix} m_{n+l+2}^{(1)} \\ m_{n+l+2}^{(2)} \\ m_{n+l+1}^{(1)} \\ m_{n+l+1}^{(2)} \end{pmatrix} = D_{ab} D_a^{l-2} \begin{pmatrix} m_{n+1}^{(1)} \\ m_{n+1}^{(2)} \\ m_n^{(1)} \\ m_n^{(2)} \end{pmatrix} = R^{(a)} \begin{pmatrix} m_{n+1}^{(1)} \\ m_{n+1}^{(2)} \\ m_n^{(1)} \\ m_n^{(2)} \end{pmatrix} \tag{5}$$

the matrixes D_a and D_{ab} have the form:

$$D_a = \begin{pmatrix} d_a & -E \\ E & 0 \end{pmatrix}, \quad d_a = \begin{pmatrix} Tk_a/Y_a & -6J_a/Y_a \\ -J_a/Y_{as} & (Tk_a - 2J_{as})/Y_{as} \end{pmatrix}, \quad D_{ab} = \begin{pmatrix} d_{ab}^{(11)} & d_{ab}^{(12)} \\ d_{ab}^{(21)} & d_{ab}^{(22)} \end{pmatrix} \tag{6}$$

$$d_{ab}^{(11)} = \begin{pmatrix} \left(6YJ_aJ_b + Y_s\left(T^2k_ak_b - Y^2\right)\right)/YY_bY_s & 6\left(YJ_bk_aT + Y_sJ_ak_bT - 2YJ_{as}J_b\right)/YY_bY_s \\ \left(YJ_a\left(2J_{bs} - k_bT\right) - Y_sJ_bk_aT\right)/YY_{bs}Y_s & \left(Y\left(2J_{bs} - k_bT\right)\left(2J_{as} - k_aT\right) + 6J_aJ_bY_s - YY_s^2\right)/YY_{bs}Y_s \end{pmatrix},$$

$$d_{ab}^{(12)} = \begin{pmatrix} -Y_ak_bT/YY_b & 6Y_{as}J_b/Y_sY_b \\ Y_aJ_b/YY_{bs} & Y_{as}\left(2J_{bs} - k_bT\right)/Y_{bs}Y_s \end{pmatrix}, \quad d_{ab}^{(21)} = \begin{pmatrix} k_aT/Y & -6J_a/Y \\ -J_a/Y_s & \left(k_aT - 2J_{as}\right)/Y_s \end{pmatrix},$$

$$d_{ab}^{(22)} = \begin{pmatrix} -Y_a/Y & 0 \\ 0 & -Y_{as}/Y_s \end{pmatrix}$$

where $k_{a(b)} = 3kS_{a(b)}/\left(S_{a(b)} + 1\right)$ and E is two- dimensional unit matrix. The matrices $D_a^{\,l-2}$ can be expressed by D_a using similarity transformation [15].

$$D_a^{l-2} = \begin{pmatrix} C_{l-2} & 0 \\ 0 & C_{l-2} \end{pmatrix} D_a - \begin{pmatrix} C_{l-3} & 0 \\ 0 & C_{nl3} \end{pmatrix} = \begin{pmatrix} C_{l-1} & -C_{l-2} \\ C_{l-2} & -C_{l-3} \end{pmatrix}. \tag{7}$$

$$C_n^{(a)} = u \begin{pmatrix} \alpha_n^{(1)} & 0 \\ 0 & \alpha_n^{(2)} \end{pmatrix} u^{-1}, \quad \alpha_n^{(j)} = \sin\left(n\theta_a^{(j)}\right)/\sin\left(\theta_a^{(j)}\right), \quad j = 1, 2.$$

$$u_{11} = Y_{as}\left(2\cos\theta_a^{(2)} + k_aT/Y_a\right)/J_a, \quad u_{12} = Y_{as}\left(2\cos\theta_a^{(1)} + k_aT/Y_a\right)/J_a, \, u_{21} = u_{22} = 1.$$

Here, $\theta_a^{(1)}$ and $\theta_a^{(2)}$ are defined from the following expression with the minus and plus sign, respectively.

$$2\cos\theta_a^{(1,2)} = \left[k_aT\left(Y_a + Y_{as}\right) - 2Y_aJ_{as} \pm \sqrt{4Y_aY_{as}\left(6J_a^2 - k_aT\left(k_aT - 2J_{as}\right)\right) + \left(\left(k_aT - 2J_{as}\right)Y_a + k_aTY_{as}\right)^2}\right]\Big/2Y_aY_{as} \tag{8}$$

The 4x4 martix $R^{(a)}$ is given by following expression

$$R_{11}^{(a)} = \left[6J_a\left(YJ_b\rho_{n-1} - k_bTY_s\varphi_{n-1}\right) + 6YJ_b\left(\varphi_{n-1}\left(2J_{as} - k_aT\right) + Y_{as}\varphi_{n-2}\right) - Y_s\left(Y_ak_bT\rho_{n-2} + \left(Y^2 - k_ak_bT^2\right)\rho_{n-1}\right)\right]/YY_bY_s,$$

$$R_{21}^{(a)} = \left[J_bY_s\left(Y_a\rho_{n-2} - k_aT\rho_{n-1}\right) + Y\left(\left(2J_{as} - k_aT\right)\left(2J_{bs} - k_bT\right) - Y_s^2\right)\varphi_{n-1} + YY_{as}\left(2J_{bs} - k_bT\right)\varphi_{n-2} + \right.$$
$$\left. + J_a\left(6J_bY_s\varphi_{n-1} + Y\left(2J_{bs} - k_bT\right)\rho_{n-1}\right)\right]/YY_{bs}Y,$$

$$R_{31}^{(a)} = \left[k_aT\rho_{n-1} - Y_a\rho_{n-2} - 6J_a\varphi_{n-1}\right]/Y, \quad R_{41}^{(a)} = \left[\left(k_aT - 2J_{as}\right)\varphi_{n-1} - J_a\rho_{n-1} - Y_{as}\varphi_{n-2}\right]/Y_s,$$

$$R_{12}^{(a)} = R_{11}^{(a)}\{\rho \to \gamma, \varphi \to \psi\}, \qquad R_{13}^{(a)} = -R_{11}^{(a)}\{n \to n-1\},$$
$$R_{14}^{(a)} = -R_{11}^{(a)}\{\rho \to \gamma, \varphi \to \psi, n \to n-1\},$$
$$R_{22}^{(a)} = R_{21}^{(a)}\{\rho \to \gamma, \varphi \to \psi\}, \qquad R_{23}^{(a)} = -R_{21}^{(a)}\{n \to n-1\},$$
$$R_{24}^{(a)} = -R_{21}^{(a)}\{\rho \to \gamma, \varphi \to \psi, n \to n-1\},$$

Where

$$\rho_{n-1} = \left(u_{11}\alpha_{n-1}^{(1)} - u_{12}\alpha_{n-1}^{(2)}\right)/\left(u_{11} - u_{12}\right), \quad \gamma_{n-1} = Y_{as}u_{11}u_{12}\left(\alpha_{n-1}^{(2)} - \alpha_{n-1}^{(1)}\right)/J_a\left(u_{11} - u_{12}\right),$$
$$\varphi_{n-1} = J_a\left(\alpha_{n-1}^{(1)} - \alpha_{n-1}^{(2)}\right)/Y_{as}\left(u_{11} - u_{12}\right), \quad \psi_{n-1} = \left(u_{11}\alpha_{n-1}^{(2)} - u_{12}\alpha_{n-1}^{(1)}\right)/\left(u_{11} - u_{12}\right).$$

The matrices $R^{(a)}$ and $R^{(b)}$ combine to yield a transfer matrix $R = R^{(b)}R^{(a)}$, which relate spins of left hand first and second atomic layers of neighbor elementary unit cell:

$$\begin{pmatrix} m_{n+l+r+2}^{(1)} \\ m_{n+l+r+2}^{(2)} \\ m_{n+l+r+1}^{(1)} \\ m_{n+l+r+1}^{(2)} \end{pmatrix} = R \begin{pmatrix} m_{n+1}^{(1)} \\ m_{n+1}^{(2)} \\ m_{n}^{(1)} \\ m_{n}^{(2)} \end{pmatrix} \qquad (9)$$

The matrix elements of $T^{(b)}$ are obtained from the elements of $T^{(a)}$ when $a \to b$ and $b \to a$. Note that determinant of the transfer matrix R is equal to unit.

There is a symmetry in the system under study, which allows us write $m_{n+l+r+2}^{(1,2)} = m_{n+1}^{(1,2)}$ and $m_{n+l+r+1}^{(1,2)} = m_{n}^{(1,2)}$. Then the following equation can be obtained to derive transition temperature

$$Det(R - E) = 0 \qquad (10)$$

where E is 4x4 unit matrix.

RESULTS AND DISCUSSION

The formalism of transition temperature derivation obtained above is universal and can be used various number atomic layers of SLNW under study. In Fig.2- 4, we have shown the results for the (1,1), (2,1), (2,2) and (2,4) SLNWs. The transition temperature (in unit $T_a = 8J_a/k_a$) is plotted as function of Y/J_a. In Fig. 2, the curves, corresponding to all exchange constants for each material, are same. These are $J_a = J_{as} = Y_a = Y_{as}$, $J_b = J_{bs} = Y_b = Y_{bs}$, $J_b = 1.5J_a$ and $Y = Y_s$. When $Y/J_a < 1.5$, then critical temperature for all cases $T_c/T_a < 1$. . Fig. 3 shows the curves when exchange constants between surface shell spins are smaller than between once and core spins. Fig. 4 shows the case when these are greater, respectively. Analysis shows that critical temperature increases with the layer number in one elementary unit cell increases and it decrease when the difference of numbers of atomic layers, belonging to deferent materials, increases.

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