Modelling of the size effect’s influence on the critical temperature of the nanowires’ phase transition

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Abstract. Influence of the size effect on the magnetic phase transition’s temperature and magnetic moment of the nanowires was modelled based on “average spin” method. As it was shown that Curie temperature was increased with nanowires’ sizes increase. The calculated value of the critical exponent of the spin-spin correlations $\nu = 0.737$ is close to experimental value.

1. Introduction

Magnetic phase transition’s temperature varies by noticeable amount for nanoparticles (NPs) [1-2], nanowires [3] and ultrathin films [4-5] compared with the bulk material. This is due to the nanostructure’s size is commensurable number with the spin-spin correlation size. In this case nanodivides influence on the physical properties of the nanostructures so what is called size-effects to affect.

There are many experimental and theoretical studies about nanostructures’ size-dependent magnetic properties of the phase transitions. So experimental studies of the size-dependent Curie temperature of EuS NPs were shown in [1, 2]. Measurements were shown decreasing of the phase transition temperature with decreasing NPs size based on magnetic isotherms method. The authors of [3] came to this conclusion used scaling correlation of Curie temperature’s dependence on the nanowire diameter:

$$ \varepsilon = \frac{T_c(d \to \infty) - T_c(d)}{T_c(d \to \infty)} = \left( \frac{\xi_0}{d} \right)^{1/\nu}, $$

and measured spin-spin correlations’ critical exponent $\nu = 0.8 \pm 0.1$ and correlation’s length $\xi_0 = 1.7 \pm 0.5 \ \text{nm} \ \text{at} \ T = 0 \ \text{K}$. It should be noted ultrathin films’ experimental studies [4] wherein the correlation (1) was used to calculate experimental data for $\nu$.

Theoretical studies of the size-effect’s influence on the phase transition’s critical temperature based on d-f model and using Creen’s function technique [6], Monte-Carlo method [7-11] and average spin method [12-13] are in agreement with experimental data.

The aim of this work is to study the influence of the nanowire’s size on the magnetic phase transition temperature. The study was based on “average spin” method developed earlier [12, 14-15] and it main principles are given below.
2. The model

Here we can consider two types of the nanowires: continuous and hollow in which the atoms are distributed over the side surface. Size-effect is determined only by the length of the hollow nanowire in the approximation of the nearest neighbours. We can consider the model of the hollow nanowire:

- Nanowire has the shape of a regular right prism with the height La where a is a lattice constant, L are the whole numbers;
- the atoms of the ferromagnetic are distributed uniformly over sites of simple square lattice with constant a and located over the side surface with magnetic moments \( m_{nk} \);
- fields of interaction \( h \) between atom’s spin magnetic moments are distributed randomly and there is direct exchange interaction between nearest neighbours only;
- atom’s spin magnetic moments are oriented along axis oz perpendicular to the base of the prism (in the approximation of the Ising model).

According to [12, 14-15] the distribution function of random fields of exchange interaction \( h \) with \( n - th \) atom is determined as:

\[
W_n(h) = \int \delta \left( h - \sum_{\{k\}_n} \varphi_k(m_k, r_k) \right) \prod_{\{k\}_n} \Phi(m_k, r_k) dm_k dr_k , \tag{2}
\]

where \( \{k\}_n \)- the nearest neighbors set with number \( n \), \( \varphi_k = \varphi_k(m_k, r_k)- field at the origin of the coordinates created by atoms with magnetic moments \( m_k \) located at the coordinates \( r_k \), \( \Phi(m_k, r_k) \)- the distribution function for the magnetic moments and coordinates. In the case of identical atoms with magnetic moment \( m_{k0} \) distributed over crystalline lattice sites it is:

\[
\Phi(m_k, r_k) = \delta(r_k - r_{k0})[\alpha_k \delta(\theta_k) + \beta_k \delta(\theta_k - \pi)]
\]

\[
[(1 - p)\delta(m_k) + p\delta(m_k - m_{k0})] , \tag{3}
\]

where \( r_{k0} \)- the coordinates of lattice sites, \( \alpha_k \)- the relative probability of the spin orientation along axis oz (\( \theta_k = 0 \)); \( \beta_k = 1 - \alpha_k \)- the relative probability of the spin orientation against axis oz (\( \theta_k = \pi \)); \( \theta_k \)- the angle between \( m_k \) and axis oz.

There is the characteristic function written with equation (2) and (3):

\[
A_n(\rho) = \prod_{\{k\}_n} (1 - p) + p[\alpha_k \exp(i\rho \varphi_k(m_{k0}, r_{k0})) + \beta_k \exp(-i\rho \varphi_k(m_{k0}, r_{k0}))], \tag{4}
\]

and then we can write the distribution function \( W_n(h) = \int A_n(\rho) \exp(i\rho h) d\rho \). According to “average spin” method we replace instantaneous values \( \alpha_k \) and \( \beta_k \) in equation (4) to their assembly average \( \langle \alpha_k \rangle = \int \alpha_k W_n(h) dh \) and \( \langle \beta_k \rangle = \int \beta_k W_n(h) dh \). Such replacement allow us to write self-consistent equations connecting magnetic moment \( \mu_n \) with neighbor’s magnetic moments defined by \( W_n(h) \):

\[
\mu_n = \langle \alpha_n \rangle - \langle \beta_n \rangle = \int \tanh \left( \frac{m_{R0} h}{k_B T} \right) W_n(h) dh. \tag{5}
\]

A system of equations can be represented as follow to determine the Curie temperature using the approach [13]:

\[
x_n = \sum_{\{l\}} \int \text{Tanh} \left( \frac{h}{f T} \right) \frac{\partial W_n}{\partial \mu_l} x_l dh , \tag{6}
\]

where \( x_n = \{\partial \mu_n / \partial \mu_1\}_{T=T_c} \), the summation is over the nearest neighbours in (6), \( t = k_B T / m_0 \) - the relative temperature; \( f \)- the exchange interaction constant.

Equation systems (5) and (6) allow us to study the dependence of the average magnetic moment on the temperature and Curie temperature dependence on the nanowire’s length.
3. Results

The temperature dependence of the atomic average magnetic moment $m$ is represented on the figure 1 for nanowire with length $L$ calculated with (6) in the approximation that the exchange interaction constants are the same between atoms.

![Figure 1](image1.png)

Fig 1. The dependence of the average magnetic moment $m$ on the temperature $t$ for nanowires with different lengths $L$ measured in monolayers.

As could be expected the phase transition temperature $T_c$ increases with $L$ increasing as in ultrathin films [12, 13]. The above-mentioned property is associated with the nearest neighbours’ number increasing with nanowire’s length increasing.

The dependence of the relative change of Curie temperature $\varepsilon(L)$ on the nanowire’s length (in monolayers) is represented in figure 2 and followed by (1) where $\xi_0 = 0.87 ML$ and $\lambda = 1.36$ are the correlation legth at $T = 0$ and inverse value of the spin-spin correlations’ critical exponent $\nu = 1/\lambda = 0.735$ respectively.

![Figure 2](image2.png)

Fig 2. Dependence of the relative change of Curie temperature $\varepsilon(L)$ on the nanowire’s length (in monolayers) in logarithmic scale.

4. Conclusion

Reducing of the nanowire’s size leads to increased surface role resulting in a decrease in the number of nearest neighbors as a reduction of the thickness of ultrathin films [4, 5], and hence the
phase transition temperature to drop. The critical exponent of the spin-spin correlations $\nu = 0.735$ is in agreement with experimental data.

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