Modelling study of magnetic and concentration phase transition in ultrathin antiferromagnetic films

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Abstract. Using the method of the “average spin” a modelling study of magnetic and concentration phase transition in ultrathin antiferromagnetic of different crystalline structure has been carried out. It has been shown, that relative change of Neel temperature is subject to the power law with negative index which doesn’t depend on the film’s crystal kind. The calculation of the dependence of phase transition critical concentration in diluted magnetic material on the film thickness has been made out. The legitimacy of the use of the method developed for modelling of magnetic and concentration phase transition in different nanostructures is certified by accordance between the results of calculations and the experimental data.

1. Introduction
Increasing of magnetic phase transition temperature in antiferromagnetic ultrathin films with growth of its thickness was marked in many researches [see, for example, 1 - 4]. And also, as was shown in the work [2], experimentally observable dependence of Neel temperature $T_N$ on the thickness of the film $N$ can be described with the help of the following correlation:

$$\varepsilon(D) = \frac{T_N(D \rightarrow \infty) - T_N(D)}{T_N(D \rightarrow \infty)} = \left(\frac{\xi_0}{D}\right)^\lambda$$

where $T_N(N \rightarrow \infty)$ is the temperature of “lump sample”, $\xi_0$ is the correlation length at $T = 0\ K$, the argument $\lambda$ is related with critical value of spin magnetic moments correlation $\nu$ as $\lambda = 1/\nu$. It should be marked out also that the critical temperature of magnetic phase transition in diluted magnetic materials depends very much on the concentration of “magnetic atoms” [3, 5].

A modeling study of effect of finiteness of the film thickness and the concentration of “magnetic atoms” on the temperature of magnetic phase transition $T_{Neel}$ in diluted antiferromagnetic material has been carried out by us in this article. For solution of the problem let us use the model of “average spin” developed by us [5, 6], the basic provision of which are formulated below.

2. The model
- Ultrathin film consist of $N$ monolayers of diluted magnetic material with the concentration of “magnetic atoms” $p$;
The direct exchange interaction occurs only between the nearest neighbors; moreover, the interaction fields \( h \) between the spin magnetic moments of the atoms are distributed in a random manner;

- Spin magnetic moments are oriented along an axis \( Oz \) (approximation of the Ising model).

According to the approximation of the above model, the equations defining the temperature of magnetic phase transition \( T_{\text{Neel}} \) in antiferromagnetic ultrathin film can be put in the following form:

\[
1 = \sum_{k_1=0}^{z_{11}} \sum_{l_1=0}^{k_1} \sum_{k_2=0}^{z_{12}} \sum_{l_2=0}^{k_2} c_{k_1}^{l_1} c_{k_2}^{l_2} \left( (2l_1 - k_1) + (2l_2 - k_2) \right) \tanh \left( \frac{(2l_1 - k_1) + (2l_2 - k_2)}{t_{\text{Neel}}} \right)
\]

where

\[
\sum_{k_1=0}^{z_{11}} \sum_{l_1=0}^{k_1} \sum_{k_2=0}^{z_{12}} \sum_{l_2=0}^{k_2} c_{k_1}^{l_1} c_{k_2}^{l_2} \left( (2l_1 - k_1) + (2l_2 - k_2) \right) \tanh \left( \frac{(2l_1 - k_1) + (2l_2 - k_2)}{t_{\text{Neel}}} \right) = \sum_{k_1=0}^{z_{n,n-1}} \sum_{l_1=0}^{k_1} \sum_{k_2=0}^{z_{n,n-1}} \sum_{l_2=0}^{k_2} c_{k_1}^{l_1} c_{k_2}^{l_2} \left( (2l_1 - k_1) + (2l_2 - k_2) \right) \tanh \left( \frac{(2l_1 - k_1) + (2l_2 - k_2)}{t_{\text{Neel}}} \right)
\]

Using the correlation (2) we can investigate the effect of the “magnetic atoms” concentration \( p \), the film thickness \( N \) and its crystalline structure on the Neel temperature.

It’s remarkable that the simultaneous equations (2) can be resolved using the Newton method. The equations (2), notwithstanding their complicated form, have been put in an algorithmically comfortable form, allow to carry out modeling studies of magnetic properties of the materials basing on the knowledge of the film’s crystalline structure and the numerical value of the exchange integral \( J_{m,k} \) only. The rule for selecting of nearest neighbours of each atom \( z_{m,k} \) is an important part of the method. When changing of this rule we can easily correct the modeling method for magnetic systems with different crystallographic structure.

### 3. Modelling study of magnetic phase transition in undiluted \((p = 1)\) antiferromagnetic material

The calculation results for dependence of critical temperature of phase transition on the thickness of ultrathin undiluted \((p = 1)\) antiferromagnetic film, the crystalline structure and the orientation of crystallographic axes are shown at the figure 1. According to expectations, with increasing of monolayers number the Neel temperature rather quickly reaches the values adequate to a “lump sample”. For example for a simple cubic lattice the extreme relative Neel temperature \( t_N (N \to \infty) = \)
5.05, for a body-centered lattice it is \( t_N(N \to \infty) = 7.01 \) and for a face-centered is \( t_N(N \to \infty) = 11.04 \).

**Figure 1.** The dependence of relative Neel temperature \( t_N = k_B T_N / (m_1 f_{1,1}) \) on the films thickness \( N \) (in monolayers) for different crystalline lattice and crystallographic axes directions.

The results represented at the Figure 1, can be put in a logarithmic scale (see the Figure 2), where \( \varepsilon(N) = (T_N(N \to \infty) - T_N(N))/T_N(N \to \infty) \) is a relative change of the Neel temperature.

Evidently, the relative change of the Neel temperature \( \varepsilon(N) \) can be well described with the help of the correlation (1) with the argument \( \lambda \) values presented in the table below. It results from the table that the values of \( \lambda \) calculated by us, are rather close to the experimental data obtained in respect of the films CoO/SiO\(_2\) in which CoO has a crystalline structure kind of NaCl with a FCC lattice.

**Table 1.** The theoretical and experimental values of \( \lambda \).

| Crystalline lattice         | Calculated values | Argument \( \lambda \) |
|-----------------------------|-------------------|------------------------|
| Simple cubic (SU (100))     | 1.802             |                       |
| Body-centered (BCC (100))   | 1.599             |                       |
| Body-centered (BCC (110))   | 1.609             |                       |
| Face-centered (FCC (100))   | 1.581             |                       |
| Face-centered (FCC (111))   | 1.585             |                       |
| Experimental values obtained in respect of the films CoO/SiO\(_2\) | \( \lambda_{exp} = 1.55 \pm 0.05\)\([1]\), \( \lambda_{exp} = 1.60 \pm 0.1\)\([2]\) | |

4. A modelling study of magnetic phase transition in diluted antiferromagnetic material

The investigations results for concentration dependence of the magnetic phase transition temperature for films of different thickness and crystalline lattice are represented at the Figure 3. The picture illustrates quite a natural result: while decreasing the concentration of “magnetic atoms” the interaction between them falls down, and as a consequence the Neel temperature decreases. Moreover, under some critical concentration the Neel temperature falls down to zero and the system transits from an ordered state to an unordered (paramagnetic) state.
Figure 3. The dependence of the reduced Neel temperature on the concentration of “magnetic atoms” and on the films thickness $N$ (in monolayers) for different crystalline lattice (the lower line: $N = 2$, the middle line: $N = 3$, the upper lines $N = 5$ and $N = 8$ coincide).

Figure 4. The dependence of the critical concentration on the films thickness $N$ (in monolayers) for different crystalline lattice.

From the figure 4 we can see that the critical concentration depends on the film thickness and its crystalline lattice, that is related with changing of the number of the nearest neighbors. Therefore, while increasing the number of monolayers the curve $p_c = p_c (N)$ asymptotically approach to the percolation thresholds of the relative lattices: $p_c (N \to \infty) = 0.31$ for a simple cubic lattice, $p_c^{BSN} (N \to \infty) = 0.25$ for a body-centered lattice and $p_c^{FCC} (N \to \infty) = 0.167$ for a face-centered lattice [1, 7].

5. Conclusion
A modeling study of magnetic phase transition in diluted magnetic materials has been carried out in the framework of a rather simple model developed by us earlier [6]. The efficiency of the model is defined both by the small number of varying parameters ($J_{m,k}, z_{m,k}$ и $p$) and by the simple procedure of choosing of the nearest neighbors $z_{m,k}$ and the values of exchange integrals $J_{m,k}$.

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