Computer simulations of the ferromagnetic-antiferromagnetic bilayer system

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Abstract

Computer simulation of bilayer spin system is performed. The first layer is a ferromagnetic film. The second layer is an antiferromagnetic film. The exchange interaction acts between the films. The Ising model is used for modeling. The Wolf cluster algorithm is used for calculations. The dependence of the bias field on the exchange interaction between the films is determined. The dependence is the linear.

1 Introduction

Computer modeling of spin systems is actively used to identify patterns in the magnetic substances behavior. Bilayer systems consisting of ferromagnetic and antiferromagnetic films are actively used in spintronics devices. The main property of such systems is to magnetize the ferromagnetic film with an antiferromagnetic film [1, 2, 3]. This bias is based on the exchange interaction at the boundary of the two films. Bias allows you to fix the state of the ferromagnet. Layered antiferromagnets are actively used in this role [4].

The displacement of the ferromagnetic film hysteresis loop is due to the presence of bias [5, 6, 7, 8]. The offset value is called the bias field [9, 10, 11, 12]. Experimental exchange bias found in compounds FeF_2/Fe and MnF_2/Fe [13, 14, 15]. In this article, computer simulation of exchange bias in a two-layer FM/AFM structure within the Ising model is performed. Research carried out by computer modeling, which has proven itself well in similar tasks [16, 17, 18].

2 System model

The bilayer system is modeled as a cellular automat. Each cell can take one of two values $+1/2$ or $-1/2$. The state of the cell number i denotes S_i. State of cell corresponds to value of spin in real magnetic substance. Such systems correspond to the Ising model. We're looking at a rectangular lattice with two layers. The dimensions of each layer along the OX and OY axes are L. L is the number of cells arranged in one direction. Along the OZ axis, both films have a thickness d of cells. The system is considered a thin film if inequality $d \ll L$ is performed. Periodic boundary conditions are used along the OX and OY axes to simulate endless films. The system geometry is shown in Figure 1.
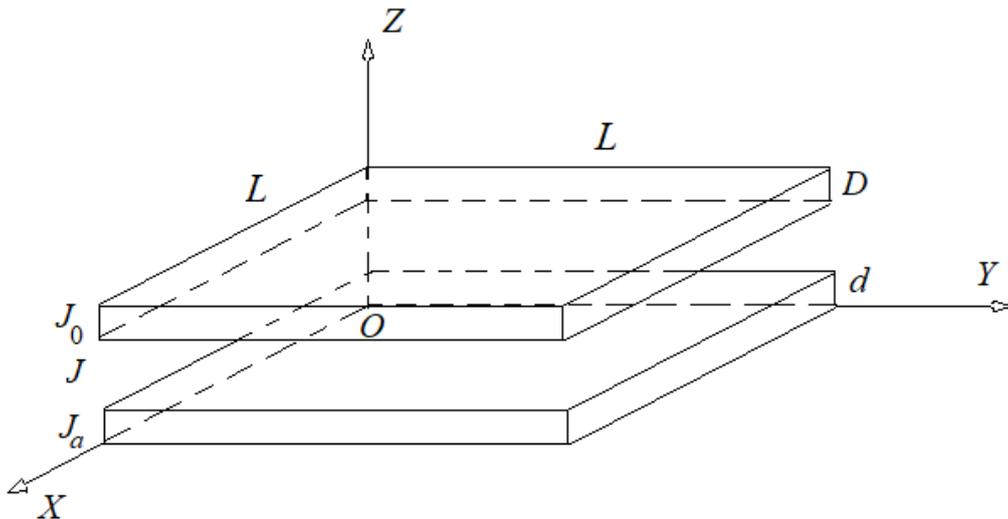
Figure 1: The system geometry.

Each cell communicates only with its nearest neighbors. Two films belong to different types of magnetic substances. The amount of cell interaction is different. In the first film, the amount of interaction is indicated by J_a ($J_a > 0$). Cells of one layer interact with energy $-J_a$. Cells in adjacent layers interact with the value J_a. Cells of one layer are energetically advantageous to have the same value. Cells of adjacent layers are energetically advantageous to have opposite values. Such model corresponds to layered antiferromagnets. In the second film, all cells interact with the same value $-J_0$. Cells of the second layer are energetically advantageous to have the same values. Such model corresponds to ferromagnetic materials. Between cells at the boundary of two films, interaction occurs with energy $-J$. It is energetically advantageous to have the same meanings. Complete ordering of the system is hindered by the thermal molecules movement. Thermal motion is modeled by random forces. It puts cells at an energy disadvantage. Intensity of thermal motion is determined by temperature t.

For computer modeling of the system, it is necessary to define its Hamiltonian.

$$H = J_a \sum_{0 \leq z < d} (-1)^b S_i S_j - J \sum_{z=d} S_i S_j - J_0 \sum_{d \leq z < 2d} S_i S_j + h_v \sum S_i.$$

Only the nearest neighbors are summed. The external magnetic field h_v is also taken into account here. $b = 1$ if S_i and S_j are in the same layer. $b = 0$ if S_i and S_j are located in adjacent layers.

We use relative values in computer modeling.

$$R_a = J_a/J_0, \quad R = J/J_0, \quad h = h_v/J_0.$$

We write Hamiltonian using relative quantities.

$$H/J_0 = R_a \sum_{0 \leq z < d} S_i S_j - R \sum_{z=d} S_i S_j - \sum_{d \leq z < 2d} S_i S_j + h \sum S_i.$$

We introduce a relative temperature.

$$T = kt/J_0.$$

k is Boltzmann's constant.

We performed a computer simulation for the two thin films system with dimensions $L \times L \times d$. Computer modeling was carried out using the Wolf cluster algorithm.

The order parameter is entered to describe the collective behavior of the system. Different order parameters are used for different films. The average spin value m is used for the ferromagnetic film.

$$m = \left[\sum_{d \leq z < 2d} S_i \right] \Big/ (L^2 d).$$

The difference in the spins of the even and odd layers was used for the antiferromagnetic film.

$$m_a = \left[\sum_{0 \leq z < d, z \ mod2 = 0} S_i - \sum_{0 \leq z < d, z \ mod2 = 1} S_i \right] \Big/ (L^2 d).$$

The phase transition can occur in the system when the temperature changes. During the phase transition, spin values are ordered. Fourth order Binder cummulants [19] are used to determine the phase transition temperature.

$$U = 1 - \frac{\langle m^4 \rangle}{3 \langle m^2 \rangle^2}, \ U_a = 1 - \frac{\langle m_a^4 \rangle}{3 \langle m_a^2 \rangle^2}.$$

Averaging by system states is indicated by angle brackets. Binder cummulants depend on temperature. Finite dimensional scaling theory[19] shows that Binder cummulants of systems with different sizes intersect at one point. The crossing point corresponds to the phase transition temperature. Phase transition temperatures vary from film to film. The phase transition temperature depends on the intensity of the interaction between the spins.

The computer modeling purpose is to determine the effect of the antiferromagnetic film on the ferromagnetic film. The antiferromagnetic film can be replaced by an external magnetic field. This field is called the bias field. The task is to determine the dependence of the bias field on the interaction intensity at the film boundary.

3 Results of computer simulation

Systems with a linear size from $L = 16$ to $L = 32$ with a step of $\Delta L = 4$ were investigated in a computer experiment. We considered films with thickness $d = 4$. The antiferromagnetic film had a parameter $R_a = 2.0$. The temperature of the phase transitions was determined in the first experiment. Phase transition temperatures $T_C = 3.51$ and $T_N = 7.02$ are obtained for ferromagnetic and antiferromagnetic films respectively. Temperature $T = 4.0$ is selected for further experiments. The antiferromagnetic film is ordered and the ferromagnetic film is disordered at this temperature.

The isolated ferromagnetic film in the external magnetic field was simulated in the first experiment. The magnetic field varied from $h = 0.0$ to $h = 2.0$ in increments $\Delta h = 0.1$. Dependence of ferromagnetic film order parameter on external magnetic field is shown in Figure 2.

The bilayer system in the zero external magnetic field was simulated in the second experiment. Interaction at the boundary of two films varied from $R = 1.0$ to $R = 2.0$ in increments $\Delta R = 0.1$. Dependence of ferromagnetic film order parameter on interaction value at film boundary R shown in Figure 3.

The hypothesis about the linear dependence the bias field H_{bias} on the interaction at the border of films R was tested.

$$H_{bias} = bR.$$

We applied the least squares method to determine the coefficient a. We obtained the values of these values from the computer experiment results.

$$a = 0.23, \quad H_{bias} = 0.23R.$$

4 Conclusion

The computer experiment was performed for the study the bilayer systems. It has been shown that the effect of the antiferromagnetic layer on the ferromagnetic layer is similar to the external magnetic bias field. The dependence of the bias field on the amount of interaction at the layer boundary is obtained. Dependency is linear.
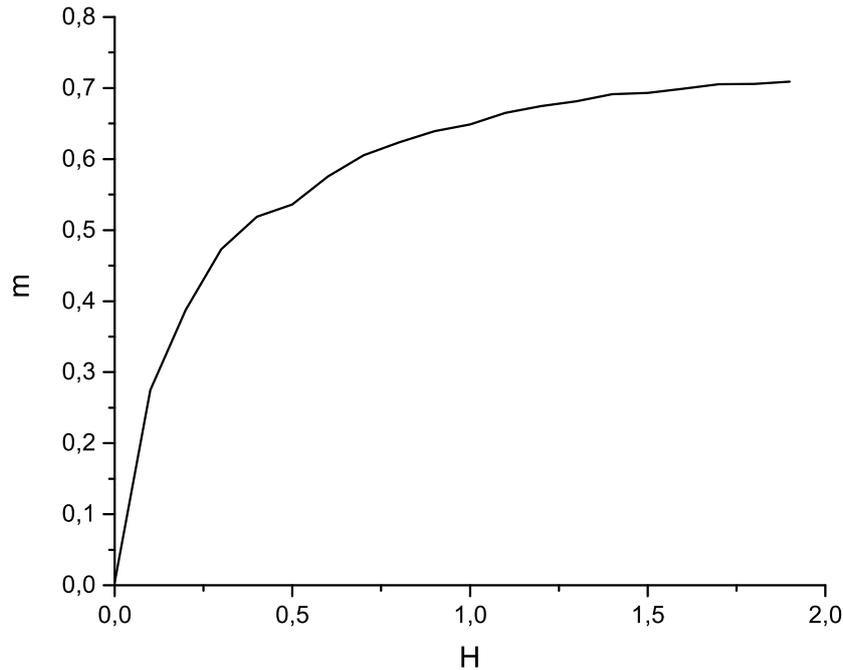
Figure 2: Dependence of ferromagnetic film order parameter on external magnetic field

5   Acknowledgements

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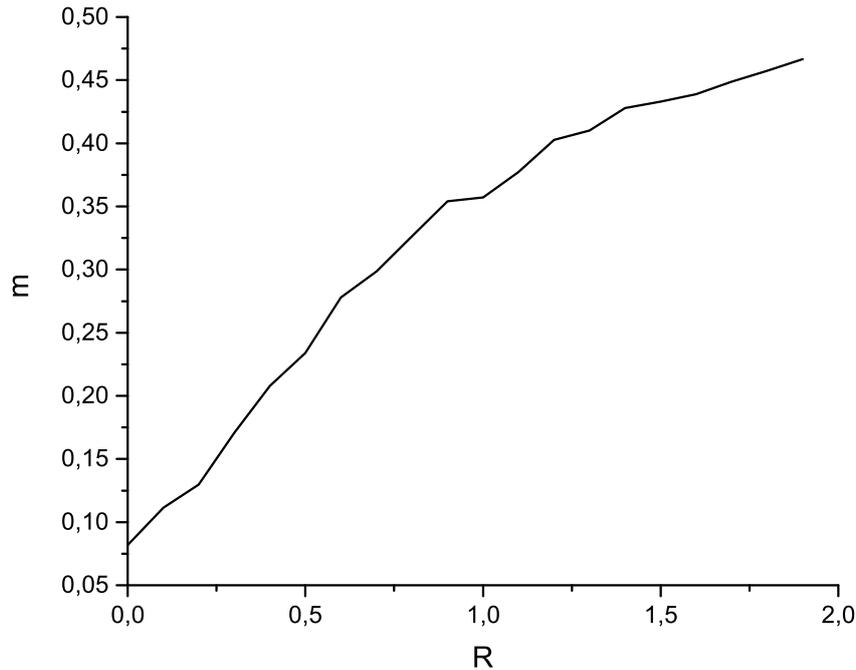
Figure 3: Dependence of ferromagnetic film order parameter on interaction value at film boundary R

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