Computer simulation of three-layer systems based on ferromagnetic nanofilms

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Abstract. Computer modeling of magnetization behavior of thin ferromagnetic Ising films separated by antiferromagnetic film was carried out. Metropolis ’s algorithm was used for the simulation. Finite-dimensional scaling theory has been used. Phase transition temperatures were determined by Binder cummulants. Systems with different number of layers in ferromagnetic and antiferromagnetic film have been investigated. Temperatures of phase transitions in ferromagnetic and antiferromagnetic films are determined. A phase diagram of the system has been constructed. There are four phases on the phase diagram. Phase for implementation the spintronic devices is defined. The distribution of magnetization and chess magnetization across the layers of the system in different phases has been investigated.

1. Introduction

Ferromagnetic multilayer films are important materials. It has interesting physical properties: giant magnetic resistance [1-3], magnetic anisotropy [4-5], magnetic resistance of tunneling [6] and giant magnetic reflection [7-9]. These properties are very sensitive to the microstructure of the multilayer film. The presence of ferromagnetism in multilayer films makes it possible to control the magnetic resistance and magneto-optical properties the external magnetic field. Most ferromagnetic multi-layer films exhibit high sensitivity to specific electrical resistance in a relatively small external magnetic field on the order 50 E or less. Multilayer ferromagnetic nanostructures can be used in creating miniature ultrafast and ultra-sensitive magnetic sensors.

The conductivity dependence on the outer magnetic field can be derived from the Landau-Lifschitz equation. This approach allowed modeling the resistance changes in different structures [10,11]. For three-layer structures, obtaining analytical solutions is difficult. In this case, the finite element method is used. In article [12] finite element calculations is used to determine the combination of magnetic and non-magnetic layers for maximizing magnetic resistance characteristics in sandwich structures. The results show that optimal behavior is expected when the thickness of the non-magnetic layer is equal thickness of the magnetic layer. In the article [13], magnetic resistance in a three-layer bimagnetic film structure is theoretically investigated. The structure consists of soft and rigid magnetic films separated by a highly conductive non-magnetic layer. The model for describing the effect of
magnetic resistance in a film structure is suggested. This model is based on the simultaneous solution of Maxwell’s linearized equations and the Landau-Lifschitz equation. The magnetostatic coupling between the magnetic layers results in asymmetry in the field dependence of the film resistance. The magnetostatic coupling is described in terms of the effective displacement field occurring in the soft magnetic layer. Calculated field and frequency relationships of film impedance are qualitatively consistent with previous experimental results for asymmetric magnetic impedance in film structures NiFe/Cu/Co. In the article [14], the effect of giant magnetic resistance in amorphous ultrathin ferromagnetic films was simulated using the Monte Carlo method within the Ising model. This model explores the effect of temperature and concentration on the magnetic properties of the system, such as magnetization, critical temperature, hysteresis loop, coercive, and magnetic resistance effect. Electric conductivity and frequency dependence ratio of giant magnetic resistance are considered. In the article [15] three-layer and spin-valve magnetic structures with effects of giant magnetic resistance by Monte Carlo methods based on application the anisotropic Heisenberg model to description the magnetic properties of thin ferromagnetic films are investigated. For ferromagnetic and antiferromagnetic configurations these structures there are obtained dependence of magnetic characteristics on temperature and external magnetic field. A technique has been developed for determining the magnetic resistance coefficient using the Monte Carlo method. Giant magnetic resistance values were calculated for three-layer and spin-valve structures at different thickness of ferromagnetic films.

Computer modeling of three-layer systems based on two ferromagnetic films and one antiferromagnetic is performed in this article. The Ising model is used for modeling.

2. Description of the system

We explore systems with three unlimited films (Fig. 1). Two extreme films of the same ferromagnetic material with D spin layers. Medium film of antiferromagnetic material with d spin layers. Arrange the films parallel to the plane OXY.

Consider the case with two spins states ($S=1/2$ or $S=-1/2$). Such systems are described by the Ising model. The Hamiltonian of system contains three components characterizing each of the films.

$$H = J \sum_{0 \leq z \leq D} S_i S_j - J_d \sum_{D \leq z \leq D+d} S_i S_j + J \sum_{D+d \leq z \leq 2D+d} S_i S_j.$$

![Figure 1. Configuration of the three-layer system.](image-url)
$S_i$ is the spin in $i$ node, $J$ is exchange integral in ferromagnetic layers of the system, $J_a$ is exchange integral in antiferromagnetic layers of the system. In computer modeling it is more convenient to work with dimensionless relative values.

$$R = J_a / J.$$ 

In this case, the Hamiltonian is recorded in a simpler form.

$$H / J = \sum_{0 \leq z < D} S_i S_j - R \sum_{D \leq z < D+d} S_i S_j + \sum_{D+d \leq z < 2D+d} S_i S_j.$$ 

Instead the temperature $t$ it is more convenient to consider a dimensionless value

$$T = k t / J.$$ 

$k$ – Boltzmann constant.

Computer simulations were performed for three-layer systems with linear film sizes $L \times L$. The system was placed between two planes $z=0$ and $z=2D+d-1$. Periodic boundary conditions were used along the directions OX and OY axes. Computer simulations were performed using the Metropolis algorithm.

Four order parameters were introduced to describe the magnetic properties of the system. Two order parameters $m_1$ and $m_2$ describe magnetic ordering in ferromagnetic films. The order parameter $m_a$ describes antiferromagnetic ordering in the middle film. Parameter $m$ describes the magnetic ordering in the middle film. The parameters $m_1$, $m_2$ and $m$ were calculated as the sum of spins in the film unit volume. The order parameter $m_a$ was calculated as the chess magnetization of the spins in unit volume of the antiferromagnetic film.

For all order parameters the Binder cummulants dependence on temperature was calculated [16].

$$U_1 = 1 - \left\langle m_1^4 \right\rangle / 3 \left\langle m_1^2 \right\rangle^2,$$

$$U_2 = 1 - \left\langle m_2^4 \right\rangle / 3 \left\langle m_2^2 \right\rangle^2,$$

$$U_a = 1 - \left\langle m_a^4 \right\rangle / 3 \left\langle m_a^2 \right\rangle^2.$$ 

The angle brackets denote thermodynamic averaging by system states. According to the finite-dimensional scaling theory [17], the values of Binder cummulants at the phase transition temperature do not depend on the size of the system. To determine the phase transition temperature, Binder cumulant dependence plots were plotted for systems with different sizes. The intersection point in the graphs corresponds to the phase transition temperature. The phase transition temperatures for the ferromagnetic films $T_1$, $T_2$ and the temperature $T_a$ for the antiferromagnetic film were determined. Magnetization distribution in the three-layer system at temperatures below the phase transition was investigated.

3. System phase diagram

Systems with linear dimensions from $L=20$ to $L=36$ with a step $\Delta L=4$ in the OXY plane were investigated in a computer experiment. Films with the number of ferromagnetic layers $D$ and the number of antiferromagnetic layers’ $d$ were considered. Number of Monte Carlo steps per spin is $8 \times 10^5$. The relation of exchange integrals changed from $R=0.7$ to $R=1.3$ with a step $\Delta R=0.1$. 
According to the calculation the phase transition temperatures in the ferromagnetic layers $T_1$ and the antiferromagnetic layer $T_a$ are independent of each other. Both phase transition temperatures depend on the number of layers. The temperature of the antiferromagnetic phase transition depends on the exchange integrals ratio $R$. The dependence of $T_1$ and $T_a$ on the number of layers at $R = 1$ is shown in Figure 2. At $R = 1$, the equation $T_1 = T_a$ is performed.

![Figure 2](image.png)

**Figure 2.** The dependence of the phase transition temperatures in the ferromagnetic films $T_1$ on the number of spin layers $D$.

The ferromagnetic film may be in ordered phase (FO) and disordered phase (FN). The antiferromagnetic film also can be in ordered phase (AO) and disordered phase (AN). In the absence of a magnetic field, four phases may exist in the system: FO/AO, FO/AN, FN/AO, FN/AN. The phase diagram for the layer ratio system $(D, d) = (6, 6)$ is shown in Figure 3.

Systems in the FO/AN phase can be used when creating spintronic devices. In other phases, the effect of the giant magnetic resistance will either not be observed or will be reduced by one of the magnetic sublattice in the antiferromagnetic. Hence it can be concluded that it is necessary to select materials with the ratio of exchange integrals $R<1.0$. 
Figure 3. The phase diagram for the layer ratio system \((D, d) = (6,6)\).

Figure 4 shows the distribution of magnetization and chess magnetization across the layers in the phase FO/AN at \(R=0.8, T=3.7\) and \((D, d) = (6,6)\). A similar distribution in the FO/OA phase at \(R = 0.8, T = 2.7\) and \((D, d) = (6,6)\) is shown in Figure 5.

Figure 4. The distribution of magnetization and chess magnetization across the layers in the phase FO/AN at \(R=0.8, T=3.7\) and \((D, d) = (6,6)\).
4. Conclusion

The behavior of three-layer systems with two ferromagnetic films separated by an antiferromagnetic film differs from systems with a non-magnetic film in the middle. The antiferromagnetic film completely shields the ferromagnetic films from each other. Phase transitions in all three films occur similarly to transitions in conventional films not included in the system [18,19]. Four independent phases can be implemented on the system phase diagram. For spintronic devices, the system must be in the FO/AN phase.

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References

[1] Camley R E 2015 Thermal properties of magnetic multilayers and nanostructures: applications to static and dynamic behavior Magnetism of Surfaces, Interfaces, and Nanoscale Materials (Handbook of Surface Science vol 5) ed R E Camley et al (Amsterdam: North-Holland) Chapter 6

[2] Xu C, Ostler T A, Chantrell R W. 2016 *Phys. Rev. B* **93** 054302

[3] Locatelli N, Naleto V, Grollier J, de Loubens G, Cros V, Deranlot C, Ulysse C, Faini G, Klein O and Fert A, 2011 *Appl. Phys. Lett.* **98** 062501

[4] Rizal C, Moa B, Wingert J and Schyrp J, 2015 *IEEE Transactions on Magnetics* **51** 6

[5] Rizal C, Ueda Y, 2009 *IEEE Transactions on Magnetics* **45** 2399
[6] Ikeda S, Hayakawa J, Lee Y M, 2005 Japan. J. Appl. Phys. 44 L1442
[7] Armelles G, Cebollada A, García-Martín A and González M U, 2013 Adv. Opt. Mat. 1 10
[8] Lodewijks K, Maccaferri N, Pakizeh T, Dumas R K, Zubritskaya I, Akerman J, Vavassori P, Dmitriev A, 2014 Nano Lett. 14 7207
[9] Maksymov I S, 2016 Reviews in Physics 1 36
[10] Dong C, Chen S, Hsu T Y, 2002 J. Magn. Magn. Mater. 250 288
[11] Dong C, Chen S, Hsu T Y, 2003 J. Magn. Magn. Mater. 263 78
[12] García-Arribasa A, Fernández E, Svalov A, Kurlyandskaya G V, Barandiaran J M, 2016 J. Magn. Magn. Mater. 400 321
[13] Buznikov N A, Antonov A S, 2016 J. Magn. Magn. Mater. 420 51
[14] Nakhaei H, Rezaei G, 2017 Journal of Alloys and Compounds 723 5 401
[15] Prudnikov V V, Prudnikov P V, Romanovskii D E, 2015 JETP Lett. 102 668
[16] Binder K, 1981 Phys. Rev. Lett. 47 693
[17] Landau D P, Binder K. 1978 Phys. Rev. B 17 2328
[18] Belim S V, Trushnikova E V, 2019 Journal of Physics: Conf. Series. 1210 012011
[19] Belim S V, Trushnikova E V, 2018 Letters on Materials 8 440