Computer Simulation of Exchange Bias Field at the Ferromagnetic-Antiferromagnetic Boundary

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Abstract. This paper presents computer simulation results for a bilayer system with ferromagnetic and antiferromagnetic films. The dependence of the exchange bias field on the external magnetic field for this system is calculated. The Heisenberg model and the Wolf cluster algorithm are used for calculations. The reason for the appearance of the bias field is the interaction between spins at the films interface. An increase in the external magnetic field leads to a nonlinear increase in the bias field. There are two reasons for nonlinearity. First, the external magnetic field suppresses antiferromagnetic ordering. Second, an external magnetic field-dependent ferromagnetic has an inverse effect on the antiferromagnetic film.

1. Introduction
Spin electronics is an important technology. It is used for spin valves. This use is based on giant magnetoresistance and tunnel magnetoresistance [1-5]. Devices based on spin valves consist of a free antiferromagnetic (AFM) layer and a fixed ferromagnetic (FM) layer. The fixation is due to the exchange bias between the FM layer and the AFM layer. Exchange bias has been studied experimentally in a large number of articles for systems such as CoFe/MnN [2,6], FeMn/NiFe [7], etc. In the AFM/FM system, the exchange bias results from the magnetic coupling between adjacent FM and AFM atomic layers at the interface. The exchange bias results in a hysteresis loop shift. This shift is due to the magnetic bias field [8,9]. The value of the exchange bias field depends on the method of manufacturing the bilayer system. Bilayer systems are sprayed at high temperature and then cooled in an external magnetic field. The exchange bias field depends on the magnetic field magnitude during cooling [10,11].

To date, several theoretical models for exchange bias have been proposed [12,13,14]. In article [13] authors discuss the possibility of forming domain walls or incomplete domain walls parallel to the films interface. In article [14] authors examine the effect of boundary defects on the exchange bias field. Despite a large number of works, the complete theory for exchange bias does not exist.

In this work, we examine the dependence of the exchange bias field on the external magnetic field magnitude by computer modeling.

2. Methods
We're looking at a system of two thin parallel films. Both films are described by the Heisenberg model. We examine films with a simple cubic crystal lattice. In the lattice nodes are three-dimensional spin vectors \( \vec{S} = (S_x, S_y, S_z) \). \( |\vec{S}| = 1/2 \). We are limited to short-range forces. Interaction occurs only
between the nearest neighbors. The films are parallel to the plane OXY. The first film is a layered antiferromagnetic. This film has $d$ layers. Interaction between spins in one layer is ferromagnetic. The exchange integral for this interaction is $J_a$. Interaction between spins in adjacent layers is antiferromagnetic. The exchange integral for this interaction is negative and equal to $-J_a$.

The second film is a ferromagnetic. This film has $D$ layers. The exchange integral for the interaction between all spins is $J_0$. Interaction between films occurs only at the boundary of their contact. The interaction is exchange. We consider the case of ferromagnetic exchange interaction between the contacting layers. The exchange integral for this interaction is $J$. The system geometry is shown in Figure 1.

![Figure 1. The system geometry.](image)

We record the Hamiltonian for this in an external magnetic field.

$$H = J_a \sum_{0 \leq z < d} (-1)^z \vec{S}_i \cdot \vec{S}_j - J_0 \sum_{d \leq z < D + d} \vec{S}_i \cdot \vec{S}_j - J \sum_{z = d} \vec{S}_i \cdot \vec{S}_j + \mu_B \vec{h}_{ext} \sum_{0 \leq z < d} \vec{S}_i.$$  

Summation is performed only on the nearest neighbors in all terms. The first sum is the interaction energy between the spins in the antiferromagnetic. $\sigma$ is 1 if the spins are on the same layer and 0 if the spins are on different layers. The second sum describes the interaction between the films. The third sum is the energy of the ferromagnetic. $\vec{h}_{ext}$ is the external magnetic field. $\mu_B$ is the Bohr magneton. We use relative quantities in computer simulation.

$$R_a = J_a / J_0; \quad R = J/J_0; \quad h = \mu_B \vec{h}_{ext} / J_0.$$  

We write the Hamiltonian for redefined quantities.

$$H / J = R_a \sum_{0 \leq z < d} (-1)^z \vec{S}_i \cdot \vec{S}_j - \sum_{d \leq z < D + d} \vec{S}_i \cdot \vec{S}_j - R \sum_{z = d} \vec{S}_i \cdot \vec{S}_j + \vec{h} \sum_{0 \leq z < d} \vec{S}_i.$$  

We also use relative temperature.

$$T = k t / J_0.$$  

$k$ is the Boltzmann's constant.

We use the Wolf algorithm for computer modeling [15]. We investigate systems with linear dimensions $L \times L \times d$ and $L \times L \times D$. Periodic boundary conditions apply along axes $OX$ and $OY$. The magnetization value per spin $\vec{m}$ is used as the order parameter for the ferromagnetic film.

$$\vec{m} = \sum_{d \leq z < D + d} \vec{S}_i / N.$$
Difference of two sub-lattices magnetizations $\vec{m}_a$ is used as order parameter for the antiferromagnetic film. The first sub-lattice includes even layers. The second sub-lattice includes odd layers.

$$\vec{m}_a = \left( \sum_{\text{even}} \vec{S}_i - \sum_{\text{odd}} \vec{S}_i \right) / N_a.$$ 

We investigate the behavior of the system in a magnetic field perpendicular to the films plane.

$$h_x=0, \quad h_y=0, \quad h_z=h.$$ 

Therefore, only projections of the order parameters on the OZ axis are studied.

Phase transition temperatures $T_C$ and $T_N$ are calculated for both films. Fourth order Binder cummulants [16] are used to determine phase transition temperatures.

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

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

Angle brackets denote thermodynamic averaging by system states. Graphs for Binder cummulants dependence on temperature are built for systems with different linear dimensions $L$. These graphs intersect at one point. The crossing point of the graphs corresponds to the phase transition temperature [17]. The phase transition temperature is proportional to the exchange integral $J_0$. The proportionality factor depends on the systems geometry. Phase transition temperatures are different in ferromagnetic and antiferromagnetic films. We investigate systems in which the antiferromagnetic exchange integral is larger than the ferromagnetic one $J_a > J_a$. For these systems, the temperature for the antiferromagnetic phase transition is greater than the temperature for the ferromagnetic phase transition $T_a > T_c$.

To study the effect of antiferromagnetic film on ferromagnetic, a temperature $T$ slightly higher than the Curie temperature is selected, but lower than the Neel temperature $T_C < T < T_N$. For this temperature, the first film is in the antiferromagnetic phase and the second film is in the paramagnetic phase. The boundary layer of the antiferromagnetic film affects the spins ordering in the ferromagnetic film by exchange interaction. This effect increases the magnetization on the ferromagnetic film. Action of antiferromagnetic film is equivalent to some external magnetic field $h_b$. This is the magnetic field of exchange bias $h_b$.

We investigate the behavior the bilayer system in the external magnetic field $h$. For ferromagnetic film, final magnetic field $h_f$ is equal to sum of two fields.

$$h_f = h + h_b.$$ 

The external magnetic field changes the state not only the ferromagnetic film, but also the antiferromagnetic one. Exchange bias depends on the external magnetic field $h_a = h_a(h)$. The computer modeling purpose is to determine the dependence of exchange bias on an external magnetic field.

3. Computer simulation results

We are investigating a system with the same film thickness $d=4$ and $D=4$. The systems linear dimensions vary from $L=16$ to $L=36$ in increments $\Delta L=4$. We chose the values of the exchange integrals ratio close to experimental data. We used the results of the article [18] to determine the exchange integrals ratio in the simulation. We use the value $R_a=2.0$. We use two values $R_0=R_a/2$ and $R_0=R_a$ for the film interaction parameter. We calculated phase transition temperatures for both films.
$T_c=1.43$ and $T_s=2.86$. Further studies are performed at temperature $T=1.6$. External magnetic field changes $h=0.0$ to $h=1.0$ in increments $\Delta h=0.1$.

Figure 2 shows graphs for dependence of isolated ferromagnetic film magnetization and ferromagnetic film in bilayer system on external magnetic field at different values of $R$.

Figure 2 shows that the antiferromagnetic film has a significant effect on the ferromagnetic film’s magnetization. Equality of magnetizations is used to define the exchange bias field.

\[ m(h_s) = m(h+h_b). \]

Figure 2. Dependence of the ferromagnetic film’s magnetization on the external magnetic field. a) Isolated ferromagnetic film. b) $R=R_a/2$. c) $R=R_a$.

The ferromagnetic film magnetization in bilayer system is determined for specified value of external magnetic field $h$. After that, the magnetic field $h_s$ is determined, which leads to the same magnetization value in the isolated ferromagnetic film. The exchange bias field $h_b$ is the difference between these two values.

\[ h_b = h_s - h. \]

Figure 3 shows the dependence of the exchange bias field $h_b$ on the external magnetic field $h$ at $R=R_a/2$ and $R=R_a$. 

\[ h_b = h_s - h. \]
Figure 3. Dependence of exchange bias field $h_b$ on external magnetic field $h$ at $R=R_a/2$ and $R=R_a$.

4. Conclusion
The dependence of the exchange bias field on the external magnetic field is non-linear (Figure 3). The reason for nonlinearity is the change in the antiferromagnetic state in the magnetic field. The external magnetic field suppresses antiferromagnetic spins ordering. With the growth the magnetic field, the ferromagnetic spins ordering in the antiferromagnetic film appears and increases. We have plotted the dependence of projection on $OZ$ axis the antiferromagnetic order parameter and magnetization for antiferromagnetic film (Figure 4).

Figure 4. Dependence of antiferromagnetic order parameter and magnetization the antiferromagnetic film on external magnetic field.

The graph in Figure 4 shows that at $h < 0.7$ antiferromagnetic spin ordering dominates. Ferromagnetic spins ordering in antiferromagnetic film dominates at $h>0.7$. Changing the spin ordering type affects the dependence of exchange bias on the external magnetic field. At the dominant ordering changes point ($h=0.7$) is the maximum of the function $h_b(h)$. The maximum magnetization of
the spin layer in antiferromagnetic at the border with the ferromagnetic is also at the point \( h = 0.7 \) (Figure 5).

![Figure 5. Dependence of magnetization for boundary layer in antiferromagnetic film on external magnetic field.](image)

The boundary spin layer of the antiferromagnetic film creates exchange bias in the ferromagnetic film. The behavior of this layer determines the magnetization processes.

Increasing the exchange integral for the interaction between ferromagnetic and antiferromagnetic films leads to a decrease in the growth rate the bias field with an increase in the external magnetic field (Figure 3). This effect is due to the inverse effect the ferromagnetic film on the antiferromagnetic film. The external magnetic field increases the ferromagnetic film magnetization. The ferromagnetic film affects the magnetization of the antiferromagnetic film through exchange interaction. Effect of ferromagnetic film increases with increase \( R \). The change in the state of the antiferromagnetic film affects the bias field \( h_b \) created by it.

5. References

[1] Chappert C, Fert A, Van Dau N 2007 *Nature Mater.* 6 813
[2] Zilske P et al. 2017 *Appl. Phys. Lett.* 110 192402
[3] Chang H W et al. 2019 *AIP Advances* 9 035330
[4] Akbulut A, Akbulut S, Yildiz F. 2016 *J. Magn. Magn. Mater.* 417 230
[5] Pan C, Gao T, Itohawa N et al. 2019 *Sci. China Technol. Sci.* 62 2009
[6] Meinert M et al. 2015 *Phys. Rev. B* 92 144408
[7] Nogues J, Schuler I K 1999 *J. Magn. Magn. Mater.* 192 203
[8] Mishra S K et al. 2010 *Phys. Rev. B* 81 212404
[9] O'Grady K, Fernandez-Outon L E, Vallejo-Fernandez G 2010 *J. Magn.* *Magn. Mater.* 322 883
[10] Chang H W et al. 2016 *Surface & Coatings Technology* 303 148
[11] Coutrim L T et al. 2016 *Phys. Rev. B* 93 174406
[12] Kiwi M, 2001 *J. Magn. Magn. Mater.* 234 584
[13] Garcia G et al. 2010 *J. Magn. Magn. Mater.* 322 3329
[14] Stiles M D, McMichael R D 1999 *Phys. Rev. B* 59 3722
[15] Wolff U, 1989 *Physical Review Letters.* 62 361
[16] Binder K 1981 *Phys. Rev. Lett.* 47 693
[17] Landau D P, Binder K 1978 *Phys. Rev. B* 17 2328
[18] Barco-Rhos H, Rojas-Calderyn E, Restrepo-Parra E 2010 *TecnoLygicas*, 2010 26 133
Acknowledgments

The reported study was funded by RFBR, project numbers 20-07-00053.