Study the bias field in bilayer film by computer simulation

S V Belim¹² and I B Larionov

¹Omsk State Technical University, 11, Mira ave., Omsk, 644050, Russia
²Siberian State Automobile and Highway University, Omsk, Russia

Abstract. Computer modeling of two-layer system from antiferromagnetic and ferromagnetic films is carried out. The Ising model is used. Wolf’s cluster algorithm is used for calculations. Phase transition temperatures are determined. A state with an ordered antiferromagnetic film and a disordered ferromagnetic film is selected for examination. Dependence the ferromagnetic film magnetization on parameters of antiferromagnetic film is determined. Computer simulation of ferromagnetic film behavior in external magnetic field is performed. The value of the antiferromagnetic bias field is determined from the comparison these two experiments. The dependence of the bias field on the exchange integral value at the film boundary is determined.

1. Introduction

Two-layer films with ferromagnetic and layered antiferromagnetic materials are used in spintronic devices. This use is based on the effect of exchange bias [1,2]. In a two-layer system, an effective internal magnetic field occurs. This magnetic field causes the hysteresis loop to shift. The amount this effective magnetic field depends on the state of the antiferromagnetic film [3,4]. The magnetization effect is used in spin valves to fix the magnetic moment direction in one of the ferromagnetic layers [5,6]. Studying the bias field also allows the study spintronic effects in antiferromagnetic [7-10].

As experimental studies have shown, exchange magnetization can be different [11]. Two-layer films with ferromagnet and antiferromagnet layers have been investigated in various systems: Co/LaFeO₃/SrTiO₃ (001) [12], CoFe/NiO(111) [13], Co/NiO(001) [14], MnPd(001)/Fe/MgO(001) [15], FeMn/Co [16], and IrMn(002)/Fe/MgO(001) [17]. Exchange bias field can change when antiferromagnetic parameters change [11]. Any factor affecting the joint behavior of ferromagnets and antiferromagnets can change the exchange bias field. [11, 18]. For example, film thickness [19, 20], temperature [21, 22], intermediate gasket [23, 24] are such parameters.

In this article the effect the antiferromagnetic film on ferromagnetic film magnetization by means of exchange interaction at medium boundary was studied. The studies were carried out by computer simulation, which is well established in similar tasks [25-27].
2. Description of a system

Computer simulations were performed for a two-layer system consisting the layered antiferromagnetic film and the ferromagnetic film. The ferromagnetic film has \( D \) layers. The exchange integral between the spines of the ferromagnetic is \( J_0 \). Antiferromagnetic film has \( d \) layers. The interaction between the spines in one layer was ferromagnetic and determined by the exchange integral \( J_a \). Antiferromagnetic forces act between adjacent layers. The exchange integral has the same magnitude and opposite sign. The spin interaction on the boundary of two films is ferromagnetic. The exchange integral of the interaction at the film boundary equal \( J \). The films are parallel to the \( OXY \) plane. The system configuration is shown in Figure 1.

\[
H = J_a \sum_{0 \leq z < D} (-1)^\sigma S_i S_j - J_0 \sum_{D \leq z < D+d} S_i S_j - J \sum_{z = D} S_i S_j.
\]

In all components, the summation is performed on the nearest neighbors. The \( \sigma \) parameter is equal 0 if spins are in one plane, and is equal 1 if spins in the neighbors planes.

For computer modeling, the transition to relative values is more convenient.

\[
R_a = J_a / J_0, R = J / J_0.
\]

In this case, the system temperature was determined in units \( J_0 \).

\[
T = k T / J_0. \quad (k \text{ – Boltzmann constant}.)
\]
We record the Hamiltonian in relative values.

\[
H / J = R \sum_{0 \leq z < D} (-1)^\sigma S_i S_j - \sum_{D \leq z < D+1} S_i S_j - R \sum_{z = D} S_i S_j.
\]

For comparison, the behavior a single ferromagnetic film with thickness \(D\) layers in the external magnetic field \(h\) was investigated. We write down the Hamiltonian of such system in relative values.

\[
H / J = - \sum_{0 \leq z < D} S_i S_j - h \sum_{0 \leq z < D} S_i.
\]

To describe the spin’s ordering in a ferromagnetic film, we use magnetic moment \(m\), calculated as the sum of spins in unit volume.

\[
m = \sum S_i / N.
\]

Value \(N\) is number of spins in the ferromagnetic film. For antiferromagnetic film, we use the Neel order parameter calculated as the magnetization difference of the even and odd layers for the system in unit volume.

\[
m_a = \left( \sum_{\text{even}} S_i - \sum_{\text{odd}} S_i \right) / N_a.
\]

Value \(N_a\) is number of spins in the antiferromagnetic film.

Phase transition temperatures were determined for both systems. For the ferromagnetic film, the Curie temperature in the zero external magnetic field was calculated. The external field blurs the phase transition. For the two-layer system, the Neel temperature of the phase transition in the antiferromagnetic film was determined.

Phase transition temperatures were determined based on fourth order Binder cummulants [28].

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

Angle brackets are used to denote thermodynamic averaging. Binder cummulants have the same value for all system sizes at the phase transition point [28]. We built the Binder cummulants dependence on temperature and determined their point of intersection. The intersection point of the graphs corresponds to the phase transition temperature.

To determine the magnetization field value, the system parameters were selected such that the antiferromagnetic film was in the low temperature phase and the ferromagnetic film in the paramagnetic phase. System temperature selected according to inequality \(T_c < T < T_N\).

The first computer experiment examined the dependence of the ferromagnetic film magnetization on the external magnetic field at some selected temperature \(T > T_c\). The magnetic moment value in ferromagnetic film at the same temperature was determined in a two-layer system with a layered antiferromagnet. The thickness \(D\) of the ferromagnetic film was the same. For the antiferromagnetic film, the own exchange integral \(J_a\), the exchange integral of the boundary interaction \(J\) and the film
thickness $d$ were changed. The magnetic film magnetization in the two-layer system was used to determine a magnetic field having the same effect on the isolated ferromagnetic film. The resulting value was taken as a bias field.

Wolf’s cluster algorithm was used for modeling. Systems with linear $L \times L$ sizes were investigated. We used periodic boundary conditions.

3. Computer experiment

Systems with linear sizes from $L=20$ to $L=36$ with a step $\Delta L=4$ were investigated for determination the phase transitions temperature. Thickness of ferromagnetic film is $D=4$. Values $d=4$, $d=6$ and $d=8$ were selected for the antiferromagnetic film. The graph for ferromagnetic film magnetization $m$ versus the value boundary exchange integral $R$ at different values antiferromagnetic exchange integral $R_a$ is shown in Figure 2.

![Figure 2](image_url)

**Figure 2.** Dependence of ferromagnetic film magnetization $m$ on boundary exchange integral $R$ at different antiferromagnetic exchange integral $R_a$ ($D=4$, $d=4$, $T=4.0$).

The ferromagnetic film magnetization depends on the exchange integral at the boundary of the films. The dependence of magnetization on antiferromagnetic exchange integral is weak. The main effect on the ferromagnetic film is the spin layer contacting the antiferromagnetic. The antiferromagnetic exchange integral affects the ordering of spines in the layer contacting the ferromagnetic. However, the antiferromagnetic film is in an ordered phase, so the growth of the antiferromagnetic exchange integral has little effect on the magnetic moment of the near-surface layer.
Dependence of magnetization for single ferromagnetic film on external magnetic field is shown in Figure 3.

**Figure 3.** Dependence of magnetization for ferromagnetic film $m$ on external magnetic field $h$. ($D=4$, $T=4.0$)

We built the bias field dependency from the graph comparison in Figures 2 and 3. The result is shown in Figure 4.

**Figure 4.** The dependence of the bias field $h_a$ on the boundary exchange integral $R$ at different values of the antiferromagnetic exchange integral $R_a$. ($D=4$, $d=4$, $T=4.0$)
4. Conclusion

The effective bias field of the antiferromagnetic depends substantially on the boundary interaction exchange integral. The bias field is weakly dependent on the internal exchange integral of the antiferromagnetic. Experiments with different thickness of antiferromagnetic film were carried out. The bias field remains unchanged as the film thickness increases. This effect is due to the fact that the bias field is determined by the ordering of spins in the boundary layer.

Acknowledgments

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

References

[1] Gomonay H, Loktev V, 2008 J. Magn. Soc. Jpn. 32 535.
[2] Cheng R, Xiao D, Brataas A, 2016 Phys. Rev. Lett. 116 207603.
[3] Sürgers C, Fischer G, Winkel P, Löhneysen H V, 2014 Nature Commun. 5 3400.
[4] MacDonald A H, Tsoi M, 2011 Philos. Trans. R. Soc. A Math. Phys. Eng. Sci. 369 3098.
[5] Gomonay E V, Loktev V M, 2014 Low Temp. Phys. 40 17.
[6] Gomonay O, Jungwirth T, Sinova J, 2017 Phys. Status Solidi RRL 1 (2017)
[7] Garello K, Miron I M, Avci C O, Freimuth F, Mokrousov Y, Blügel S, Auffret S, Boulle O, Gaudin G, Gambardella P, 2013 Nature Nanotechnol. 8 587.
[8] Chernyshov A, Overby M, Liu X, Furdya J K, Lyanda-Geller Y, Rokhinson L P, 2009 Nature Phys. 5 656.
[9] Zhang X, Liu Q, Luo J-W, Freeman A J, Zunger A, 2014 Nature Phys. 10 387.
[10] Park B G, Wunderlich J, Martí X, Holý V, Kurosaki Y, Yamada M, Yamamoto H, Nishide A, Hayakawa J, Takahashi H, Shick A B, Jungwirth T, 2011 Nature Mater. 10 347.
[11] Zhang W, Krishnan K M, 2016 Mat. Sci. Eng. R 105 1.
[12] Nolting F, Scholl A, Stöhr J, Seo J W, Fompeyrine J, Siegwart H, Locquet J-P, Anders S, Lüning J., Fullerton E E, Toney M F, Scheinfein M. R, Padmore H A, 2000 Nature 405 767
[13] Zhu W, Seve L, Sears R, Sinkovic B, Parkin S S P, 2001 Phys. Rev. Lett. 86 5389
[14] Ohldag H, Scholl A, Nolting F, Anders S, Hillebrecht F U, Stöhr J 2001 Phys. Rev. Lett. 86 2878
[15] Blomqvist P, Krishnan K M, Ohldag H 2005 Phys. Rev. Lett 94 107203
[16] Bali R, Nelsoncheeseman B B, Scholl A, Arenholz E, Suzuki Y, Blamire M G, 2009 J. Appl. Phys. 106 277
[17] Zhang W, Bowden M E, Krishnan K M, 2011 Appl. Phys. Lett. 98 092503
[18] Shi Z, Du J, Zhou S M, 2014 Chin. Phys. B 23 02 7503
[19] Park B G, Wunderlich J, Martí X, Holý V, Kurosaki Y, Yamada M, Yamamoto H, Nishide A, Hayakawa J, Takahashi H, Shick AB, Jungwirth T, 2011 *Nature Mater.* **10** 347

[20] Wu J, Choi J, Scholl A, Doran A, Arenholz E, Hwang C and Qiu Z Q, 2009 *Phys. Rev. B* **79** 212411

[21] Reichlova H, Novák V, Kurosaki Y, Yamada M, Yamamoto H, Nishide A, Hayakawa J, Takahashi H, Maryško M, Wunderlich J, Marti X, Jungwirth T, 2016 *Mater. Res. Express* **3** 076406

[22] Zhang W, Krishnan K M, 2012 *Phys. Rev. B* **86** 054415

[23] Gruyters M, Schmitz D, 2008 *Phys. Rev. Lett* **100** 077205

[24] Normile P S, Toro J A D, Muñoz T, González J A, Andrés J P, Muñiz P, Galindo R E, Riveiro J M, 2007 *Phys. Rev. B* **76** 104430

[25] Belim S V, Trushnikova E V, 2019 *Journal of Physics: Conf. Series.* **1210** 012011

[26] Belim S V, Trushnikova E V, 2018 *Letters on Materials* **8** 440

[27] Belim S V, Larionov I B, 2019 *Moscow University Physics Bulletin* **74**(6) 646

[28] Binder K, 1981 *Phys. Rev. Lett.* **47** 693