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Computer simulation of three-layer ferromagnetic nanosystems in magnetic field

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Computer simulation of three-layer ferromagnetic nanosystems in magnetic field

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Abstract. A computer modelling of magnetization behavior in ultrathin ferromagnetic films, divided by antiferromagnetic film is carried out. The exchange integral value is different for each ferromagnetic films. One of the films is magnetohard, the second one is magnetosoft. The situation where magnetosoft film has the exchange integral value twice smaller than the value of magnetohard film is investigated. Heisenberg model is used. Calculations are made using Metropolis algorithm. The phase transition temperature is obtained for all three films. The magnetic field was applied along the film plane. The simulation showed that magnetizations of ferromagnetic films first become perpendicular to the direction the staggered magnetization vector in the antiferromagnetic film. With a higher magnetic field value, the magnetization vectors of the ferromagnetic films become mutually perpendicular. Thus, in these multi-layer systems, it is possible to control the orientation of the substances spins, which is an important property for implementing spintronics devices.

1. Introduction

Ferromagnetic multilayer nanofilms have found wide application in spintronics devices [1,2]. The wide use of multilayer nanofilms is due to the phenomenon of the giant magnetic resistance in them [3]. Today, the design of sensors and spin valves is based on ferromagnetic nanofilms separated by non-magnetic material. An additional external antiferromagnetic layer is used in the spin valves to stabilize the magnetization in one of the ferromagnetic films. Recently, however, the direction related to the creation of spintronics devices with antiferromagnetic materials has been actively developing. This is due to some advantages of antiferromagnets compared to ferromagnets: good resistance to disturbances, absence of parasitic fields, ultra-fast dynamics and large magneto-transport effects [4-6]. These properties allow the creation of ultra-fast memory devices at room temperature [7.8].

Typically, a configuration of two ferromagnetic films (F) separated by a non-magnetic material (N) is used for spin valves. The F/N/F multilayer structures are easily controlled by a small external magnetic field. The thickness of the non-magnetic layer is selected to provide antiferromagnetic coupling between the ferromagnetic layers. Such coupling provides a different direction of magnetization in the ferromagnetic layers. The different orientation of the magnetic layers results a large electrical resistance due to the effect of the giant magnetic resistance.

The non-magnetic material between the ferromagnetic films can be replaced with an antiferromagnetic film (AFM). The F/AFM/F multi-layer structure is more capable of controlling magnetization orientation. As with the F/N/F system in the F/AFM/F multi-layer film, the ferromagnetic layers must be made of different materials. Two ferromagnetic films must have different resistance to the external magnetic field. One layer has to be magnetically soft and the other layer has to be magnetically soft.

Computer modelling of three-layer systems based on two ferromagnetic films with antiferromagnetic interlayer was performed in this article.

2. Description of the system

We will explore systems from three layers. There are two films from ferromagnetic materials with number of layers D and medium film from antiferromagnetic material with number of layers d. Arrange the films parallel to the OXY plane. All three films have a simple cubic crystal lattice. We 'll use the Heisenberg model. The Hamiltonian of such a system in the magnetic field is:

$$H = -J\sum_{0\le z<D} S_i S_j - J_{a1}\sum_{z=D} S_i S_j + J_a \sum_{D<z<D+d} S_i S_j - J_{a2}\sum_{z=D+d} S_i S_j - J_1 \sum_{D+d<z<2D+d} S_i S_j + \mu h_0 \sum S_i . \quad (1)$$

Here via S_i is denoted spin in i node. J is exchange integral in magnetohard ferromagnetic layer. J_a is exchange integral in antiferromagnetic layer of the system. J_1 is exchange integral in magnetosoft ferromagnetic layer. J_{a1} is exchange interaction integral between spins in hard ferromagnetic layer and spins in antiferromagnetic layer along plane their contact. J_{a2} is exchange interaction integral between spins in soft ferromagnetic layer and spins in antiferromagnetic layer along plane of their contact, h0 - magnetic field intensity. μ is Bohr magneton. Ferromagnetic films have different exchange integral values. It has different magnetic susceptibilities. A material with higher magnetic susceptibility is magnetosoft. The material with lower magnetic susceptibility is magnetohard. In computer modelling it is more convenient to work with dimensionless relative values:

$$R = J_1/J,\ R_a = J_a/J,\ R_{a1} = J_{a1}/J,\ R_{a2} = J_{a2}/J,\ h = \mu h_0/J. \quad (2)$$

In this case, the Hamiltonian will take the form:

$$H/J = \sum_{0\le z<D} S_i S_j - R_{a1}\sum_{z=D} S_i S_j - R_a \sum_{D<z<D+d} S_i S_j - R_{a2}\sum_{z=D+d} S_i S_j + R \sum_{D+d<z<2D+d} S_i S_j + h \sum S_i . \quad (3)$$

Instead the temperature t, it is more convenient to consider a dimensionless value $T = kt/J$, where k is a Boltzmann constant.

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

An order parameter is entered for each of the films to describe the magnetization behaviour. For ferromagnetic films the total value of magnetic moment per spin m_1, m_2 and projection of magnetization on coordinates axis m_{1x}, m_{1y}, m_{2x}, m_{2y} was calculated. For antiferromagnetic film order parameter m_a was calculated as the staggered magnetization in unit volume. Projections of the order parameter on the coordinate's axis max, may were also determined for the antiferromagnetic film.

The phase transition temperature was determined for all three films. For this purpose, the fourth order Binder cummulants [10] were determined as a function on temperature:

$$U_1 = 1 - \frac{\langle m_1^4 \rangle}{3\langle m_1^2 \rangle^2},\ U_2 = 1 - \frac{\langle m_2^4 \rangle}{3\langle m_2^2 \rangle^2},\ U_a = 1 - \frac{\langle m_a^4 \rangle}{3\langle m_a^2 \rangle^2}. \quad (4)$$

The angle brackets denote thermodynamic averaging by system states. According to the finite-dimensional scaling theory [10], the Binder cummulants values at the phase transition temperature do not depend on the size of the system. To determine the phase transition temperature, Binder cummulants graphs dependence was plotted for systems with different sizes. The intersection point of the graphs corresponds to the phase transition temperature. Phase transition temperatures of T_1 and T_2 for ferromagnetic films and temperature T_N for antiferromagnetic film were determined. Next, the system behaviour at temperatures substantially below the phase transition point was discussed.

3. Behaviour of the system in the magnetic field

To determine the temperature of phase transitions in a computer experiment we use systems with a linear size in the *OXY* plane from L=20 to L=36 with a step ΔL=4. Films with the number of ferromagnetic layers $D = 4$ and the number of antiferromagnetic layers $d = 4$ were considered. The values [11] were selected for the exchange integral ratio:

$$R=0.5,\ R_a=1.0,\ R_{a1}=0.1,\ R_{a2}=0.1. \qquad (5)$$

As the variations these parameters have shown qualitatively, the pattern of behaviour the system in the magnetic field remains unchanged. This result was previously obtained for conventional single film systems [12,13]. Only parameter values change. Number of Monte Carlo steps per spin 8×10^5. At these values the phase transitions temperatures are $T_1 = 1.29$, $T_2 = 0.65$, $T_N = 1.29$.

The system's behaviour in the magnetic field was investigated for linear dimension $L = 36$ and temperature $T = 0.5$. The magnetic field was applied along the *OX* axis. The magnetic field value changed from h=0.1 to h=0.5 with step Δh=0.01.

The system was brought into a state of thermodynamic equilibrium at zero magnetic field. After it an external magnetic field was applied and later system was again put into equilibrium. The change of order parameter and its components along *OX* and *OY* axes were calculated. Figure 1 shows the dependence the order parameters for all three films in the system on the external magnetic field value.

As can be seen from Figure 1, the external magnetic field results the ordering of the ferromagnetic films and has weak effect on the order parameter from the antiferromagnetic film. The ordering takes place mainly in the *XY* plane. Figure 2 shows the dependence of the projection values of the film order parameters on the *OXY* plane on the external magnetic field value.

From the data in Figure 2 it can be seen that in the absence of a magnetic field and in weak magnetic fields, the order parameters are oriented in an arbitrary direction. No complete rotation of all spins along the *OX* axis is observed. The component along the *OZ* axis remains. When the magnetization is averaged by a large number of configurations in a computer experiment, saturation occurs at a value lower than one. The magnetic field oriented along the *OX* axis turns the spins in the ferromagnetic films, orienting them predominantly parallel to the *OXY* plane. Orientation of spins in the antiferromagnetic film is not affected by magnetic field. Figure 3 shows the dependency of the order parameter component along the *OX* axis.

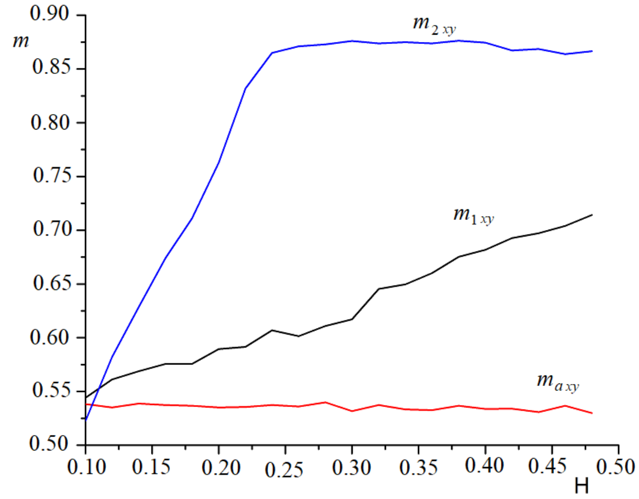

Figure 1. Dependence the order parameters for the three films of the system on the external magnetic field. m_1 is magnetization for magneto-hard ferromagnetic film. m_2 - magnetization for magnetic soft ferromagnetic film. m_a is the staggered magnetization of the antiferromagnetic film.

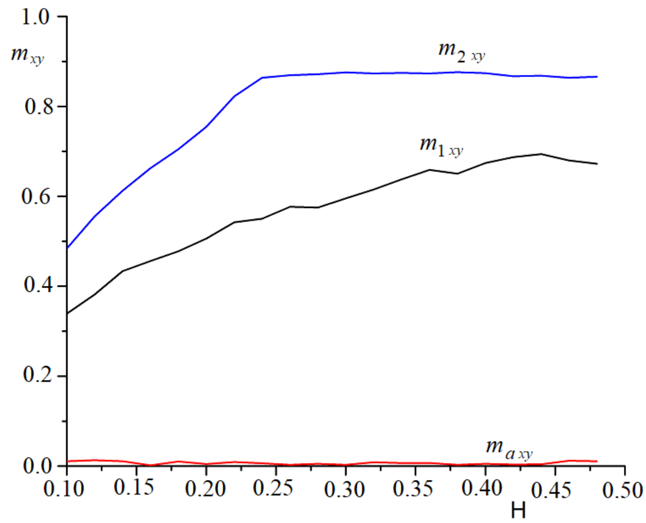

Figure 2. Dependence the projection values of film order parameters on OXY plane on external magnetic field value. m_1 is magnetization for magneto-hard ferromagnetic film. m_2 - magnetization for magnetic soft ferromagnetic film. m_a is the staggered magnetization of the antiferromagnetic film.

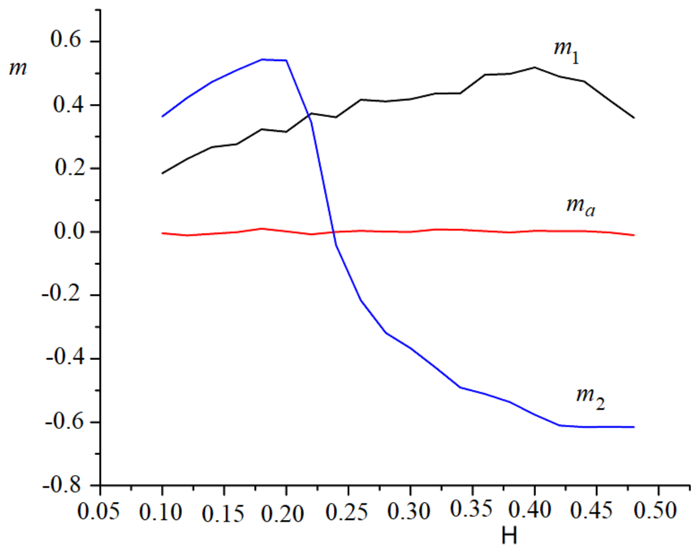

Figure 3. Dependence the projection values for film order parameters on OXY plane on external magnetic field value. m1 is magnetization for magneto-hard ferromagnetic film. m2 - magnetization for magnetic soft ferromagnetic film. ma is the staggered magnetization of the antiferromagnetic film.

It can be seen from Figure 3 that the magnetic moment for the magnetohard component remains oriented along the positive direction the *OX* axis. This fastening effect is related to the presence the antiferromagnetic film and is used in spin valves with AFM/F/N/F configuration. At low field values, the magnetization direction is also fixed by means of an antiferromagnetic film. But at $h > 0.2$ there is a rapid reversal the spin direction along the *OX* axis with a slight increase in the external magnetic field. Figure 4 shows the relationship of the angle between the magnetization directions for the two ferromagnetic layers in the *OXY* plane to the external magnetic field.

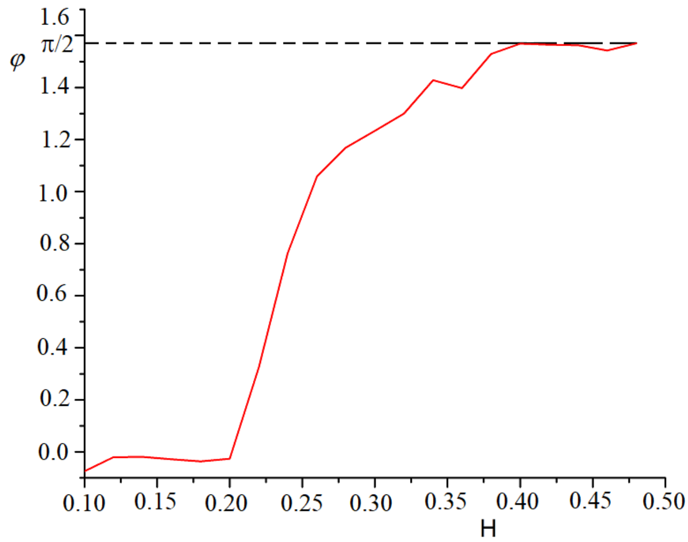

Figure 4. Dependence of angle between magnetization directions for two ferromagnetic layers on external magnetic field.

4. Conclusion

From the obtained results it is possible to draw conclusions on the behaviour of a system of two ferromagnetic layers separated by an antiferromagnetic film. With small magnetic fields, the spins of all three layers are oriented mainly along the OZ axis. When the magnetic field is turned on along the OX axis, spins in ferromagnetic films are rotated and preferably the spines have directions lying in the OXY plane. The spines in the antiferromagnetic layer remain oriented along the OZ axis. Thus, at any magnetic field value, there is a difference in directions in the ferromagnetic and antiferromagnetic layers. This property results in the realization of giant magnetic resistance in the investigated system. With further increase of magnetic field in magnetsoft layer spins turn along OX axis. As a consequence, magnetisations become mutually perpendicular in ferromagnetic layers. This reversal leads to additional increase of the electrical resistance of the system.

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References

[1] Ennen I, Kappe D, Rempel T et al 2016 *Sensors* **16** 904
[2] Xu C, Ostler T A, Chantrell R W 2016 *Phys. Rev.* B **93** 054302
[3] Baibich M N, Broto J M, Fert A et al 1988 *Phys. Rev. Lett.* **61** 2472
[4] Gomonay O, Jungwirth T and Sinova J 2017 *Phys. Status Solidi-R* **11** 1700022
[5] Jungwirth T, Marti X, Wadley P and Wunderlich J 2016 *Nature Nanotech.* **11** 231
[6] Zhang W, Jungfleisch M B, Jiang W et al 2014 *Phys. Rev. Lett.* **113** 196602
[7] Marti X et al 2014 *Nature Mater.* **13** 367
[8] Cherifi R O et al 2014 *Nature Mater.* **13** 345
[9] Núñez A S et al 2006 *Phys. Rev. B* **73** 214426
[10] Landau D P and Binder K 1978 *Phys. Rev. B* **17** 2328

[11] Prudnikov V V, Prudnikov P V, Romanovskii D E 2015 *JETP Lett.* **102** 668
[12] Belim S V, Trushnikova E V 2019 *Journal of Physics: Conf. Series*. **1210** 012011
[13] Belim S V, Trushnikova E V 2018 *Letters on Materials* **8** 440