ISSN 0027-1349, Moscow University Physics Bulletin, 2019, Vol. 74, No. 6, pp. 646–649. © Pleiades Publishing, Ltd., 2019.
Russian Text © The Author(s), 2019, published in Vestnik Moskovskogo Universiteta, Seriya 3: Fizika, Astronomiya, 2019, No. 6, pp. 71–74.

CONDENSED MATTER PHYSICS

The Influence of a Magnetic Field on Phase Transition in Antiferromagnetic Films: Computer Modeling Research

S. V. Belim[1*] and I. B. Larionov[1]

[1]*Dostoevsky Omsk State University, Omsk, 644077 Russia*

Received August 12, 2019; revised September 2, 2019; accepted September 4, 2019

Abstract—The influence of an external magnetic field on the phase-transition temperature for antiferromagnetic thin films is investigated. The computer modeling method for the antiferromagnetic Ising model with a thin film geometry is used. Films with thicknesses from 4 to 16 layers have been investigated. It is shown that the temperature of the antiferromagnetic phase transition decreases according to the square law as the external magnetic intensity increases. The rate of decrease of the phase-transition temperature depends on the film thickness and on the relationship between the exchange integrals on the surface and the bulk of the system. For each system, there is a limit value of the magnetic intensity such that no antiferromagnetic phase transition occurs if it is exceeded. The dependence of the limit value of the magnetic intensity on the relationship between the exchange integrals obeys the square law as well.

Keywords: Ising model, think films, Neel temperature, antiferromagnetics.

DOI: 10.3103/S0027134919060067

1. INTRODUCTION

The character of phenomena observed under phase transitions in thin antiferromagnetic films differs from that of phenomena in infinite or semi-infinite systems. Unlike infinite systems, thin films have two free surfaces, which leads to the necessity to take the surface antiferromagnetism into account. In semi-infinite systems, the situation is similar. However, the phase transition in the bulk of a semi-infinite system is the same as that for an infinite one because the contribution of a free surface to total-system thermodynamic parameters is infinitesimal. The only possible antiferromagnetic effect occurs when the spin-ordering temperature on the surface differs from the Neel temperature. As a result, an additional phase and the corresponding two phase transitions appear on the phase diagram. A qualitatively different situation is observed in thin films. The total number of layers is low and two surface layers substantially affect the thermodynamic functions of the entire system.

Two main distinctions of spins located on the surface from spins located in the bulk of the system can be noted. First, a surface that spins has a lower number of nearest neighbors. In all spin models, only the nearest neighbors are taken into account because exchange integrals decrease very rapidly as the distance increases. As a result, less thermal-motion energy is required to flip the spin. Secondly, the exchange-coupling energy on the surface might differ from that in the bulk of the system. As an example, the interatomic distance for Gd, computed in [1], is equal to 3.52 Å in the crystal bulk and to 3.64 Å on the surface. As a result, the exchange integral is equal to $J_S = 1.25$ on the surface and to $J_B = 1.51$ in the crystal bulk.

The computer modeling of ferromagnetic and antiferromagnetic films (see [2] and [3], respectively) shows that no phase transition is observed for thin films: the system as a whole passes from the paramagnetic phase to the antiferromagnetic one. The corresponding increase of the surface exchange integral leads to the growth of the Neel temperature. The growth of the phase-transition temperature is a decreasing function of the film thickness. This effect is caused by the higher spin-ordering temperature of surface spins. Ordered structures on the surface affect close layers substantially (see [4, 5]). However, due to the small thickness of the film all of the layers are close to the surface.

The influence of external magnetic fields to phase transitions in antiferromagnetic systems is substantial (see [6, 7]). For infinite antiferromagnetic systems, the increase of the magnetic field leads to the the decrease of the phase-transition temperature. The

*E-mail: sbelim@mail.ru

Neel temperature depends quadratically on the intensity of the magnetic field (see [8–10]). This motivates the investigation of the joint influence of the value of the surface exchange integral and of the magnetic field on the phase-transition temperature in antiferromagnetic films.

The goal of the present paper was to investigate phase transitions in the antiferromagnetic Ising model with a thin-film geometry via computer modeling.

2. SYSTEM DESCRIPTION

The Hamiltonian of the system for thin antiferromagnetic films in the magnetic field described by the Ising model has the form

$$H = -J_B \sum_B S_i S_j - J_S \sum_S S_i S_j - J_S \sum_{SB} S_i S_j + \mu h_v \sum S_i,$$

where S_i is the spin in the ith node ($+1/2$ or $-1/2$), J_B is the exchange integral in film layers that differ from boundary layers, J_S is the exchange integral free surfaces of the film and interaction of surface spins and spins of the first subsurface layer, h_v is the intensity of the external magnetic field, and μ is the Bohr magneton. In the initial three terms of the free energy, only pairs of nearest neighbors are taken into account under the summing. In the first term, spin pairs such that no spin is located on the free surface of the thin film are considered. In the second term, spin pairs such that each both spins are located on a same free surface are considered. In the third term, spin pairs such that one spin is located on a free surface and another one is located in the first subsurface layer are summed. Dimensionless relative values

$$R = J_S/J_B \quad \text{and} \quad h = \mu h_v/J_B$$

are more convenient for computer modeling. In this case, the Hamiltonian takes the form

$$H/J_B = -\sum_B S_i S_j - R \sum_S S_i S_j - R \sum_{SB} S_i S_j + h \sum S_i.$$

It is more convenient to consider the dimensionless value

$$T = kt/J_B,$$

where k is the Boltzmann constant, instead of the temperature t.

For the computer modeling, thin films with linear dimensions $L \times L \times D$, where D is the film thickness, are used. The system is located between the $\{z = 0\}$ and $\{z = D - 1\}$ planes. Periodic boundary-value conditions are used along the directions of the OX and OY axes. The Metropolis algorithm is used to perform the computer modeling.

To describe the magnetic properties of the system, two order parameters (volume one and surface one) are introduced. The surface order parameter m_S is computed as the chess magnetization of spins located in the plane $\{z = 0\}$. By virtue of the system symmetry, it is pointless to introduce the second surface parameter for the plane $\{z = D - 1\}$. A volume parameter m computed as the chess magnetization as well is used to describe the collective behavior of the remaining spins located outside surfaces.

For both order parameters, the dependence of the fourth-order Binder cumulants (see [11]) on the temperature is computed:

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

where angular brackets denote the thermodynamic averaging over system states.

Due to the finite-dimensional scaling theory (see [12]), the values of the Binder cumulants at the phase-transition temperature do not depend on the system parameters. To find the phase-transition temperature, graphs of the dependence of the Binder cumulant are constructed for systems of various sizes; then their intersection point corresponding to the phase-transition temperature is found. To find the Neel temperature T_{N}, the cumulants U are used; the temperature T_S of the surface phase transition is determined on the base of U_S.

3. COMPUTER EXPERIMENT: RESULTS

In the computer experiment, systems with linear dimensions from $L = 20$ to $L = 36$ with a step $\Delta L = 4$ are investigated. Films of thicknesses from $D = 4$ to $D = 16$ with a step $\Delta D = 4$ are considered. The number of Monte-Carlo steps per spin is equal to 8×10^5. The magnetic field varies from $h = 0$ to $H = 5.0$ with step $\Delta H = 0.5$. The relationship between the exchange integrals varies from $R = 0.7$ to $R = 1.8$ with step $\Delta R = 0.1$.

According to the computations for the phase transition in thin antiferromagnetic films, the Neel temperature depends quadratically on the intensity of the external magnetic field. From the qualitative viewpoint, the system demonstrates the same regularities as infinite and semi-infinite antiferromagnetic systems. Figure 1 demonstrates a typical dependence of the phase-transition temperature T_{N} on the intensity h of the external magnetic field under the assumption that the thickness of the antiferromagnetic film is

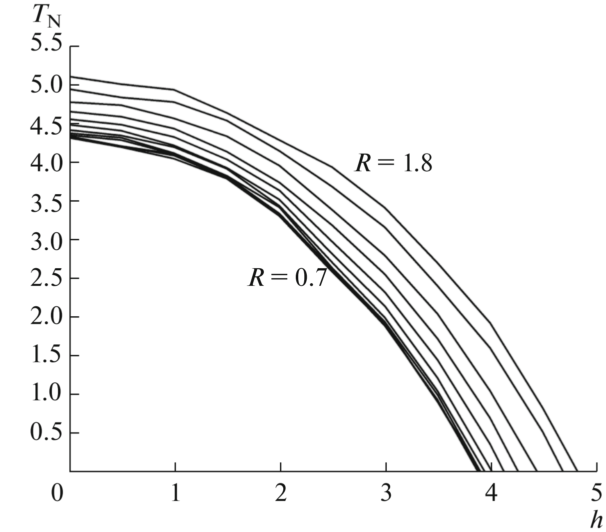

Fig. 1. The dependence of the phase-transition temperature T_N on the intensity of the external magnetic field h for the antiferromagnetic film of thickness $D = 12$, where the relationships of the exchange integral vary from $R = 0.7$ to $R = 1.8$.

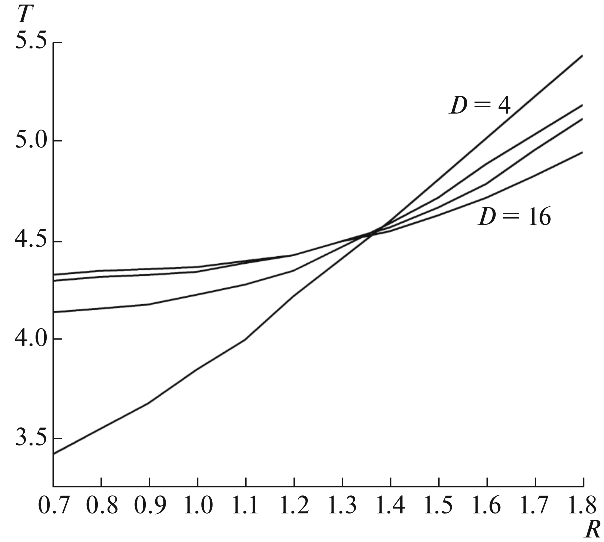

Fig. 2. The dependence of the phase-transition temperature T_0 in the zero external magnetic field on the relationship R of the exchange integral for films with thicknesses that vary from $D = 4$ to $D = 16$.

equal to $D = 12$, while the value R of the relationship between the exchange integrals varies. For other values of the film thickness D, the dependencies of the temperature on the magnetic field are qualitatively the same.

The general dependence of the phase-transition temperature T_N on the intensity h of the magnetic field can be described by the relationship

$$T_N = T_0(R, D)\left(1 - \left(\frac{h}{h_0(D, R)}\right)^2\right),$$

where $T_0(D, R)$ the phase-transition temperature for the film of thickness D with the relationship R of the exchange integrals in the zero external magnetic field, while $h_0(D, R)$ is the limit value of the external magnetic field such that the phase-transition is equal to zero. In the zero magnetic field, the dependence of the phase-transition temperature on the relationship R of the exchange integrals is provided (for films of various thicknesses D) in Fig. 2.

From Fig. 2, we see that the phase-transition temperature grows as the value of the relationship between the exchange integrals grows. This dependence is explained by the influence of the surface energy of interactions of spins on the system as a whole. We also note that the growth rate of the temperature decreases as the film thickness increases. This dependence is explained as follows: in the depth of the sample, the influence of boundary layers on the ordering of spins decreases. In the limit case of semi-infinite and infinite systems, the Neel temperature of the bulk does not depend on the spin-interaction on the surface. In such a system, the surface layer begins to behave as an independent system with its own temperature of the surface phase transition. In the thin films considered in the present paper no surface phase transition is observed. The smallest film thickness that provides the surface phase transition is still an open problem.

Figure 3 displays the dependence of the limit value of the external magnetic field on the relationship between the exchange integrals (for films of various thicknesses).

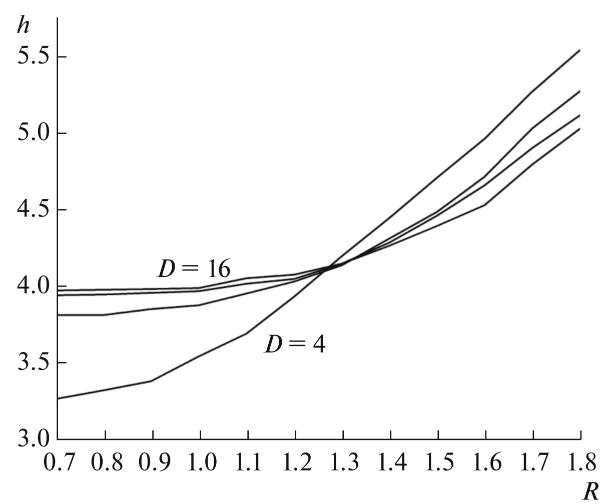

Fig. 3. The dependence of the limit value of the intensity h_0 of the external magnetic field on the relationship R of the exchange integral for films with thicknesses that vary from $D = 4$ to $D = 16$.

Table 1. The values of the coefficients $A(D)$ and $B(D)$

D	$A(D)$	$B(D)$
4	2.72 ± 0.02	0.87 ± 0.04
8	3.21 ± 0.03	0.59 ± 0.02
12	3.28 ± 0.02	0.57 ± 0.03
16	3.32 ± 0.01	0.55 ± 0.01

From the graphs in Fig. 3, we see that the limit value of the intensity of the magnetic field increases as the relationship between the exchange integrals increases. If the film thickness increases, then the curve of the growth of the limit value of the magnetic-field intensity tends to the horizontal line $h_0 = 4.0$ typical for infinite systems. The curve of the dependence of h_0 on R can be approximated (with high accuracy) by the quadratic function

$$h_0(D, R) = A(D) + B(D)R^2.$$

The values of the coefficients $A(D)$ and $B(D)$ are provided in Table 1.

CONCLUSIONS

Thus, the influence of an external magnetic field on a thin film is the same as its influence on each antiferromagnetic system. Under the action of a magnetic field, the Neel temperature decreases quadratically. The dependence of the rate of decrease of the temperature on the intensity of the magnetic field depends on the film thickness. The dependence of the rate of increase of the Neel temperature under the growth of the surface exchange integral depends on the film thickness as well. This effect was experimentally observed in [13–15]. In all these experiments, the phase-transition temperature increases as the film width becomes larger, which corresponds to values $R < 1.38$.

A decreasing effect for the phase-transition temperature in antiferromagnetic films under the action of an external magnetic field has been experimentally confirmed as well. As an example, it was shown in [16] that the Neel temperature decreases in thin films of $BiFe_{0.9}Zn_{0.1}O_3$ from the value of 630 K to room temperatures under the action of a magnetic field. A phase diagram for the antiferromagnetic film of FeF_2 in an external magnetic field was experimentally obtained in [17]. The dependence of the Neel temperature on the external magnetic field qualitatively coincides with the results of the present paper; its form is close to a quadratic function.

REFERENCES

1. C.-Yu. Lin, J.-L. Li, Y.-H. Hsieh, et al., Phys. Rev. X **2**, 021012 (2012).
2. M. Hamedoun, K. Bouslykhane, H. Bakrim, et al., J. Magn. Magn. Mater. **301**, 22 (2006).
3. S. V. Belim and E. V. Trushnikova, Lett. Mater. **8**, 440 (2018).
4. S. V. Belim and E. V. Trushnikova, Phys. Met. Metallogr. **119**, 441 (2018).
5. S. V. Belim and E. V. Trushnikova, J. Surf. Invest.: X-Ray, Synchrotron Neutron Tech. **12**, 923 (2018).
6. J. L. Monroe, Phys. Rev. E **64**, 016126 (2001).
7. X. N. Wu and F. Y. Wu, Phys. Lett. A **144**, 123 (1990).
8. H. W. J. Blote and X. N. Wu, J. Phys. A **23**, L627 (1990).
9. X.-Z. Wang and J. S. Kim, Phys. Rev. Lett. **78**, 413 (1997).
10. A. A. Tarasenko, L. Jastrabik, F. Nieto, et al., Phys. Rev. B **59**, 8252 (1999).
11. K. Binder, Phys. Rev. Lett. **47**, 693 (1981).
12. D. P. Landau and K. Binder, Phys. Rev. B **17**, 2328 (1978).
13. K. Yadav, H. K. Singh, K. K. Maurya, et al., Appl. Phys. A **124**, 66 (2018).
14. K. Yadav, M. P. Singh, F. S. Razavi, et al., Mater. Chem. Phys. **137**, 323 (2012).
15. E. Dagotto, T. Hotta, and A. Moreo, Phys. Rep. **344**, 1 (2001).
16. A. A. Amirov, Y. A. Chaudhari, S. T. Bendre, et al., Eur. Phys. J. B **91**, 63 (2018).
17. A. S. Carricco, R. E. Camley, and R. L. Stamps, Phys. Rev. B **50**, 13453 (1994).

Translated by A. Muravnik