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## Investigation of critical phenomena of the hard/soft magnetic bilayer model by the Monte-Carlo method



ALLOYS AND COMPOUNDS

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#### 1. Introduction

#### ABSTRACT

A model for the description of thermodynamic properties of hard/soft magnetic bilayer is proposed. We perform a thorough research of critical phenomena of this model by the Monte-Carlo method. Critical exponents of the heat capacity  $\alpha$ , magnetization  $\beta$ , susceptibility  $\gamma$ , and correlation radius  $\nu$  are calculated using the finite-size scaling theory. Obtained values of critical exponents agree with the theoretical predictions for the XY-model.

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### The creation of layered nanocomposite materials has opened a new section in the physics of magnetism [1–5]. The exchange interaction at the interface between layers of different magnetic order forms completely new ground state of a heterophase magnet, radically changes the behavior of spins, and leads to appearing a number of unusual phenomena, such as the formation of an external magnetic field of a one-dimensional heterophase spin spring (exchange-spring behavior). Skomski and Coey [3,5] explored the theory of exchange coupled films and predicted that a giant energy product to be of 120 MGOe. All these effects and the ability to obtain a structure with desired magnitude and sign of the interlayer exchange lead to the fact that these materials gain great technological significance from application as a permanent magnet to use as advanced media.

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#### 2. Hard/soft magnetic bilayer

The preparation of exchange coupled thin-layer structures is a highly labor-intensive process which requires a controlled growth of nanometer hard and soft magnetic layers, a formation of perfect structures and interfaces.

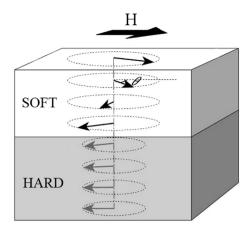
The growth of such films, their incorporation into suitable magnetic heterostructures, and understanding of their magnetic reversal behavior is a whole area to which a lot of investigations are devoted [1-24]. A schematic drawing of hard/soft bilayer is shown in Fig. 1 [7].

The fundamental concept and strong attraction of hard/soft bilayers are provided by the suggestion that a hard layer is entirely stiff with larger anisotropy and in a soft bilayer the anisotropy fails to exist at all. In the external magnetic field directed against the magnetization vector of a hard layer (Fig. 1), the magnetization of the soft layer remains co-directional and parallel to the magnetization of the hard layer close to values of an external field [19]:

$$H_{ex} = \pi^2 J_s / 2M_s t^2,$$

where  $J_s$  is the exchange constant between spins inside the soft layer, *t* is the thickness of the soft layer,  $M_s$  is the magnetization of





**Fig. 1.** Scheme of a hard/soft bilayer and illustration of an exchange-spring behavior (a spin spring) in a hard-magnetic/soft-magnetic bilayer.

the soft layer saturation.

When the value of applied field *H* becomes higher than  $H_{ex}$ , the spins in the soft layer exhibit continuous rotation as in a Bloch wall, and the farther spins in the soft layer from the hard layer are, the higher the rotation is. The magnetization of the soft layer is reversible and approaches saturation as  $(H/H_{ex})^{-0.5}$ . Both predictions are consistent with experimental studies of NiFe/NiCo bilayers, and with subsequent studies of Sm–Co/NiFe [20], Sm–Co/Co–Zr [21,22], and CoFe<sub>2</sub>O<sub>4</sub>/(MnZn)Fe<sub>2</sub>O<sub>4</sub> [23] exchange-coupled bilayers.

So, magnetic exchange-spring hard/soft structures are unique structures and appear to be attractive to researches. Unfortunately, thermodynamic properties of hard/soft bilayers, nowadays, have received almost no attention, and much less there are no investigations on critical properties of the bilayers. Apparently, this is due to the difficulties of performing experimental researches of this kind.

These difficulties in preparation and study of hard/soft magnetic bilayers can be overcome by means of numerical investigations using high-efficient Monte-Carlo methods. Monte-Carlo methods efficiency for such investigations was repeatedly shown in papers [25–30] considering phase transitions and critical phenomena in magnetic nanostructure models.

In paper [31], we proposed a hard/soft magnetic bilayer model and investigated the temperature dependence of thermodynamic parameters by the Monte-Carlo method. Double peaks resulted from two phase transitions occurring in the system are found on the temperature dependences of the heat capacity and susceptibility. The first transition is associated with the behavior of the hard layer and the second is stemmed from the behavior of the soft layer. The dependence of thermodynamic properties on system dimensions is considered. The present work is devoted to the thorough and comprehensive investigation of critical properties of the hard/soft magnetic bilayer model.

#### 3. Model and method

In the most of hard/soft magnetic bilayers, including (Sm–Co)/ Fe, (Sm–Co)/Co structures there is strong in-plane anisotropy and magnetic moments lie in plane of bilayers [7], as shown in Fig. 1. Moreover for (Sm–Co)/Fe exchange-spring systems the in-plane ordering of magnetic moments was detected during the whole magnetization reversal process by means of layer-resolved Mössbayer spectroscopy [32]. Therefore thermodynamic properties of magnetic hard/soft bilayer can be estimated using a simple model integrating the standard XY-model. The Hamiltonian of the system is written as:

$$H = -\frac{1}{2} \sum_{i,j} J \left( S_i^x S_j^x + S_i^y S_j^y \right) - \sum_i K \left( S_i^x \right)^2, \tag{1}$$

where the first sum allows for the exchange interaction of each magnetic atom with nearest neighbors inside layers with  $J = J_h$  and  $J = J_s$  exchanges in hard and soft layers, correspondingly, and an interlayer interaction with  $J = J_i$  parameter; the second sum is a contribution of the anisotropy into a system energy;  $K = K_h$  and  $K = K_s$  are anisotropy constants of hard and soft layers, respectively;  $S_i^{x,y}$  are spin projections localized on a site *i*.

Calculations were performed by the standard Metropolis algorithm of the Monte-Carlo method [33] for the systems with linear sizes  $L \times L \times L$ , where  $L = 8 \div 40$ . And the thicknesses of hard and soft magnetic layers were L/2. Periodic boundary conditions were applied over the system in two directions (along *x*- and *y*-directions), i.e. we considered thin hard and soft layers with open surfaces from the other side opposite [31].

### 4. Critical properties of the hard/soft magnetic bilayer

It is well known that values of critical exponents are highly sensitive to a critical temperature. Therefore, the choice of a critical temperature for the estimation of critical properties of the magnetic system is a very important and vital procedure. For a precise determination of a critical temperature, where a phase transition would occur in the hard/soft bilayer system, we used the Binder cumulant method [34] which allowing for the estimation of phase transition temperatures with sufficiently high accuracy. According to this method, all cumulants determined by formulae [34]:

$$U_L = 1 - \frac{\langle M^4 \rangle_L}{3 \langle M^2 \rangle_l^2},\tag{2}$$

for various *L* must intersect at one point at  $T = T_c$ . Fig. 2 presents the dependence of  $U_L$  cumulants on linear sizes of the studied system [31]. The arrow points at the phase transition temperature.

Next, we calculated critical exponents of heat capacity  $\alpha$ , magnetization  $\beta$ , susceptibility  $\gamma$  and the correlation radius  $\nu$  by means of the finite-size scaling theory [35,36]. The finite-size scaling theory was first developed by Ferdinand and Fisher

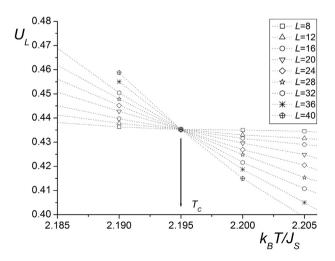


Fig. 2. Determination of a phase transition temperature for hard/soft magnetic bilayer model.

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