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Order parameters and hysteresis behavior of a ferromagnetic Blume–Capel thin film: The role of the crystal field interactions

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ABSTRACT

As a complementary work of a recent study (Physica B 433 (2014) 96), ferromagnetic thin films in simple cubic lattice structure described by a spin-1 Blume–Capel Hamiltonian have been considered within the framework of effective-field theory (EFT). Thermal variations of bulk and surface order parameters (i.e. magnetization and quadrupolar moments), as well as hysteresis loops in the presence of modified surface interactions, and crystal fields have been examined. We have found that depending on the type of the phase transition (i.e. ordinary or extraordinary), bulk and surface order parameters may exhibit fairly non-monotonous and quite exotic profiles. Regarding the bulk and surface hysteresis loops, at a fixed set of system parameters, both the bulk and surface hysteresis loops exhibit the same coercivity whereas remanence of a bulk (surface) loop is greater than that of a surface (bulk) loop in ordinary (extraordinary) case.

1. Introduction

Magnetism in the presence of free surfaces with modified exchange interactions has attracted a considerable amount of attention over the past three decades [1] and the research of thin film magnetism is a current topic of critical phenomena [2–5]. In magnetic systems with thin film geometry, due to their reduced coordination number, the surface atoms may have a lower symmetry in comparison with that of the inner atoms, meanwhile, the exchange interactions between the surface atoms may be different from those between the corresponding bulk counterparts, leading to a phenomenon known as surface enhancement in which the surface may exhibit an ordered phase even if the bulk itself is disordered. This phenomenon has already been experimentally observed [6–8].

In this context, an extraordinary case is defined as the transition at which the surface becomes disordered at a particular temperature T_c^s which is larger than the bulk transition temperature T_c^b. From the academic point of view, although the Heisenberg model gives more realistic description of these systems, due to the fact that many thin films such as the Fe/Ag(100) system [9] exhibit a strong uniaxial anisotropy, phase transition characteristics of thin ferromagnetic films are often modeled by several extensions of an Ising type spin Hamiltonian [10]. A qualitative comparison of Heisenberg model and Ising model in Blume–Capel model can be found in very recent work [11]. It is theoretically predicted that there exists a critical value of surface to bulk ratio of exchange interactions R_c above which the surface effects are dominant and the transition temperature of the entire film is determined by the surface magnetization whereas below R_c, the transition characteristics of the film are governed by the bulk magnetization. The critical value R_c itself is called as the special point, and the numerical value of this point has been examined within various theoretical techniques for spin-1/2 case [12–22]. We note that, ordinary and extraordinary phase transition characteristics are different in equilibrium and nonequilibrium systems [23].

The problem has also been handled for higher spins using a number of techniques [24–30]. Among these works, using extensive Monte Carlo (MC) simulations, the effect of surface exchange enhancement on ultrathin spin-1 films has been studied by Tucker [26], and it was concluded that the R_c value is spin dependent. However, in a recent work [28], using MC simulations, the influence of crystal field interaction (or single ion anisotropy) on the critical behavior of a magnetic spin-1 film has been studied, and it has been argued that R_c is independent of the crystal field interaction. Apart from these, within the framework of effective-field theory (EFT), Saber and co-workers [29] have examined the phase diagrams, the layer longitudinal magnetizations and quadrupolar moments of a spin-1 film as functions of the ratio of the surface exchange interactions to the bulk ones, transverse fields, and film thickness. However, they did not include important crystal field effects in their calculations. Moreover, theoretical studies based on EFT are completely focused on the effect of surface and bulk transverse fields in the absence of crystal fields.

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Based on the results of the works mentioned above, investigation of critical phenomena in thin films with higher spins requires particular attention due to several reasons. First of all, thermal variation of the order parameters as functions of the system parameters, especially crystal field interactions was not provided by existing studies using well-known techniques such as MC simulations [26,28] or EFT [29]. Moreover, the result concluded in Ref. [28] which states that R_c is independent of the crystal field interactions is rather implausible. It is well established that magnetic properties observed in the systems (finite or bulk systems) described by a spin-1 BC model are expected to reduce to those corresponding to conventional two-state Ising model in the highly anisotropic limit. This can be achieved by letting $D\to\infty$ in the calculations where D denotes the crystal field interactions. This fact should reveal itself in the numerical values of critical parameters. Namely, the transition temperature of spin-1 BC model should converge to spin-1/2 value in the limit $D\to\infty$. Moreover, in Ref. [26], using MC simulations, it was found that for the spin-1 Ising films, R_c=1.45 value is significantly below the value R_c=1.52 obtained by MC simulation for the spin-1/2 system [18]. In this regard, our recent study [31] qualitatively supports these observations within the framework of EFT. According to us, considered crystal field values in Ref. [28] are rather small values to observe the expected variation in R_c as a function of crystal field strength.

An earlier milestone approach on the surface magnetism dates back to the work of Mills [12,13], approximately four decays ago from present. On the basis of the mean field theory (MFT), Mills proved that thin film systems exhibit ordinary and extraordinary transition behaviors in the presence of modified surfaces. This outcome was also proven by more sophisticated techniques such as series expansion methods and Monte Carlo simulations [18]. In the pioneering work of Binder and Hohenberg [15], it was shown that Mills's prediction has a quite general applicability, and the phenomenon of surface ordering is not restricted to only mean field level, but the series expansions and MC simulations also yield the same qualitative picture. Therefore, the expected difference between the results of various techniques is quantitative subject of matter. For example, series yield R_c=1.6 [18] whereas mean field theory predicts R_c=1.25 [14] for spin-1/2. Therefore, the qualitative behavior of the system is expected to be the same within the framework of various techniques whereas the numerical values of critical temperatures and critical exponents may vary. On the other hand, although the thermal fluctuations are partially considered in the formalism, EFT method offers rich physical phenomena with tractable mathematics which presents qualitatively similar results in comparison with MC simulations. Despite its mathematical simplicity, EFT systematically includes the single-site correlations in the calculations, hence the obtained results are expected to be more accurate than those obtained by MFT.

In a very recent work [31], by means of EFT, we have examined the critical phenomena and universality behavior of ferromagnetic thin films described by a spin-1 Blume–Capel (BC) Hamiltonian for various thickness values ranging from 3 to 40 layers. As a complementary study, in the present paper, our purpose is to investigate the crystal field dependence of order parameters and hysteresis loops of a ferromagnetic BC thin film with modified surface exchange interactions, and to give some preliminary ideas for the future works based on much more sophisticated techniques such as MC simulations. The recent developments of theoretical studies on hysteresis in magnetic model systems can be found in Refs. [32,33]. For this aim, we organized the paper as follows: In Section 2 we briefly present the formulations. The results and discussions are presented in Section 3, and finally Section 4 contains our conclusions.

2. Formulation

We consider a ferromagnetic thin film with thickness L described by conventional BC Hamiltonian [34]

$$\mathcal{H}=-\sum_{\langle ij\rangle}J_{ij}S_iS_j-D\sum_i(S_i)^2-h\sum_i S_i, \tag{1}$$

where $J_{ij}=J_s$ if the lattice sites i and j belong to one of the two surfaces of the film, otherwise we have $J_{ij}=J_b$ where J_s and J_b denote the ferromagnetic surface and bulk exchange interactions, respectively. The first term in Eq. (1) is a summation over the nearest-neighbor spins with $S_i=\pm1,0$, the second term represents the crystal field energy on the lattice, and the third term is the Zeeman energy.

The magnetizations and quadrupolar moments (i.e. $m_i=\langle S_i\rangle$ and $q_i=\langle (S_i)^2\rangle, i=1,\ldots,L$) perpendicular to the surface of the film corresponding to L parallel distinct layers can be obtained by conventional EFT formulation based on differential operator technique and decoupling approximation (DA) [35],

$$\begin{aligned}
m_1&=[1+m_1B_1+q_1(A_1-1)]^z[1+m_2B_2+q_2(A_2-1)]F_1(x)|_{x=0},\\
m_p&=[1+m_pB_2+q_p(A_2-1)]^z[1+m_{p-1}B_2+q_{p-1}(A_2-1)],\\
&\quad+[1+m_{p+1}B_2+q_{p+1}(A_2-1)]F_1(x)|_{x=0},\\
m_L&=[1+m_LB_1+q_L(A_1-1)]^z[1+m_{L-1}B_2+q_{L-1}(A_2-1)]F_1(x)|_{x=0},\\
q_1&=[1+m_1B_1+q_1(A_1-1)]^z[1+m_2B_2+q_2(A_2-1)]F_2(x)|_{x=0},\\
q_p&=[1+m_pB_2+q_p(A_2-1)]^z[1+m_{p-1}B_2+q_{p-1}(A_2-1)],\\
&\quad+[1+m_{p+1}B_2+q_{p+1}(A_2-1)]F_2(x)|_{x=0},\\
q_L&=[1+m_LB_1+q_L(A_1-1)]^z[1+m_{L-1}B_2+q_{L-1}(A_2-1)]F_2(x)|_{x=0},
\end{aligned} \tag{2}$$

where $2\le p\le L-1$, z is the coordination number of the lattice, and the coefficients A_i and B_i are defined as $A_1=\cosh(J_s\nabla)$, $A_2=\cosh(J_b\nabla)$, $B_1=\sinh(J_s\nabla)$ and $B_2=\sinh(J_b\nabla)$. In the present work, we will focus on the ferromagnetic films in a simple cubic lattice structure with z=4 where z is the intra-layer coordination number. The functions $F_1(x)$ and $F_2(x)$ in Eq. (2) are then given by

$$F_1(x)=\frac{2\sinh[\beta(x+h)]}{2\cosh[\beta(x+h)]+\exp(-\beta D)},$$
$$F_2(x)=\frac{2\cosh[\beta(x+h)]}{2\cosh[\beta(x+h)]+\exp(-\beta D)},$$

where β is the inverse of the reduced temperature.

With the help of the Binomial expansion, Eq. (2) can be written as follows:

$$\begin{aligned}
m_1&=\sum_{i=0}^{z}\sum_{j=0}^{i}\sum_{k=0}^{1}\sum_{l=0}^{k}K_1^{(1)}(i,j,k,l)m_1^jm_2^lq_1^{i-j}q_2^{k-l},\\
m_p&=\sum_{i=0}^{z}\sum_{j=0}^{i}\sum_{k=0}^{1}\sum_{l=0}^{k}\sum_{n=0}^{1}\sum_{t=0}^{n}K_2^{(1)}\\
&\quad\times(i,j,k,l,n,t)m_{p-1}^lm_p^jm_{p+1}^tq_{p-1}^{k-l}q_p^{i-j}q_{p+1}^{n-t},\\
m_L&=\sum_{i=0}^{z}\sum_{j=0}^{i}\sum_{k=0}^{1}\sum_{l=0}^{k}K_1^{(1)}(i,j,k,l)m_L^jm_{L-1}^lq_L^{i-j}q_{L-1}^{k-l},\\
q_1&=\sum_{i=0}^{z}\sum_{j=0}^{i}\sum_{k=0}^{1}\sum_{l=0}^{k}K_1^{(2)}(i,j,k,l)m_1^jm_2^lq_1^{i-j}q_2^{k-l},\\
q_p&=\sum_{i=0}^{z}\sum_{j=0}^{i}\sum_{k=0}^{1}\sum_{l=0}^{k}\sum_{n=0}^{1}\sum_{t=0}^{n}K_2^{(2)}(i,j,k,l,n,t)\\
&\quad\times mp-1lm_p^jm_{p+1}^tq_{p-1}^{k-l}q_p^{i-j}q_{p+1}^{n-t},\\
q_L&=\sum_{i=0}^{z}\sum_{j=0}^{i}\sum_{k=0}^{1}\sum_{l=0}^{k}K_1^{(2)}(i,j,k,l)m_L^jm_{L-1}^lq_L^{i-j}q_{L-1}^{k-l},
\end{aligned} \tag{3}$$

with the coefficients

$$\begin{aligned}
K_1^{(\alpha)}(i,j,k,l)&=\binom{z}{i}\binom{i}{j}\sum_{x=0}^{i-j}\sum_{y=0}^{k-l}\binom{i-j}{x}\binom{k-l}{y}\\
&\quad\times(-1)^{i+k-j-l-x-y}\Theta_\alpha(x,j,y,l),
\end{aligned}$$