Physics Letters A 377 (2013) 2494–2504

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Monte Carlo simulations of dynamic phase transitions in ultrathin Blume–Capel films

Yusuf Yüksel *

Department of Physics, Dokuz Eylül University, TR-35160 Izmir, Turkey

A R T I C L E   I N F O

Article history:
Received 22 June 2013
Received in revised form 31 July 2013
Accepted 1 August 2013
Available online 8 August 2013
Communicated by R. Wu

Keywords:
Dynamic phase transition
Monte Carlo simulation
Magnetic thin film
Surface magnetism

A B S T R A C T

Dynamic phase transition phenomena in ultrathin films described by the Blume–Capel model have been investigated using Monte Carlo simulations. Hysteresis loops, micromagnetic structures, and hysteresis loop area curves, as well as dynamic correlation between the magnetization and the external field have been studied as functions of the field, as well as the film parameters. The variation of critical coupling of the modified film surface at which the transition temperature becomes independent of film thickness has been clarified for varying system parameters. Frequency dispersion of hysteresis loop area has been found to obey a power law for low and moderate frequencies for both ordinary and enhanced surfaces.

1. Introduction

Recently, magnetic materials with finite sizes such as thin films have attracted considerable amount of interest both in theoretical and experimental manner and the research of thin film magnetism is a current topic of critical phenomena [1–5]. 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 addition to the fundamental purpose, thin film materials have great importance in technological applications. For instance, ultrathin Au/Co/Au magnetic films, CoPt-alloy films, CoNi/Pt and Tb/Fe multilayers are considered as potential candidates of raw materials in ultrahigh-density magneto-optical recording devices [9].

Due to the presence of modified exchange couplings at the surface, magnetic thin film systems may exhibit an extraordinary phase transition at which the surface transition temperature is higher than that of the bulk whereas in the ordinary case, the transition temperature of the film is mainly determined by the bulk region. In order to investigate the thermal and magnetic properties of thin films, the models based on an Ising type spin Hamiltonian are well suited since many thin films such as the Fe/Ag(100) system [10] exhibit a strong uniaxial anisotropy. A great many theoretical efforts have shown 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 at which the transition temperature of the film becomes independent of thickness, and the numerical value of this point has been examined within various theoretical techniques for spin-1/2 case [11–19]. On the other hand, the problem has also been extended to higher spins using a number of techniques [20–26]. 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 [22], and it was concluded that the R_c value is spin dependent. However, in a recent work [24], 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. This latter outcome clearly contradicts with that reported in a very recent study based on the effective-field theory (EFT) [27]. Moreover, Wang et al. [28] have studied the magnetic properties and critical behavior of a molecular-based magnetic film within the framework of MC simulations. They have acquired two special points at which the compensation and critical temperatures are independent of the layer thickness and the surface single-ion anisotropy.

Apart from these, in contrast to the large number of works concerning the equilibrium behavior of thin films, there are very few

* Corresponding author. Tel.: +90 2324119518; fax: +90 2324534188.
E-mail address: yusuf.yuksel@deu.edu.tr.

0375-9601/$ – see front matter
http://dx.doi.org/10.1016/j.physleta.2013.08.001

studies in the literature devoted to the investigation of nonequilibrium phase transition characteristics of thin film systems [29], and there exist several uncertain points remaining to be clarified in the latter case. For instance, the effect of a time dependent perturbation such as the presence of an oscillating external field on the magnetic behavior of film should be clarified. When a ferromagnetic material is subjected to a periodically oscillating magnetic field, the response of the ferromagnet may be delayed depending on the competition between the period of the external field and the relaxation time of the system. This competition shows itself as a phase lag between the external perturbation and response (i.e. magnetization) of the system. It has been previously shown by Acharyya [30] that for bulk systems near the transition point, the phase lag gives a peak by achieving its maximum value. Critical phenomena in nonequilibrium bulk systems have been clarified using several techniques such as MC simulations [30–32], mean-field theory (MFT) [33], and recently EFT [34]. In addition, related to this nonequilibrium phenomena, a few theoretical studies have been devoted to the investigation of dynamical aspects of phase transition properties of finite systems such as cylindrical Ising nanowire and nanotube systems [35,36], as well as ferrimagnetic nanoparticles [37]. Moreover, using MC simulations, Laosiritaworn [38] has investigated the thickness dependence of hysteresis properties in Ising thin films, and it has been found that the calculated hysteresis properties significantly change due to the stronger ferromagnetic coupling in thicker films. It has also been shown that hysteresis properties obey the universal power law relations for varying thickness and field parameters. However, effects of the presence of modified surface exchange interactions were ignored in the aforementioned work. Recently, Park and Pleimling [39] have shown that nonequilibrium surface exponents do not coincide with those of the equilibrium critical surface.

On the experimental side, a dynamic phase transition (DPT) occurring for the high-frequency magnetic fields was studied by Jiang et al. [40] using the surface magneto-optical Kerr-effect technique for epitaxially grown ultrathin Co films on a Cu (001) surface. For a [Co(4 Å)/Pt(7 Å)] multilayer system with strong perpendicular anisotropy, an example of DPT has been observed by Robb et al. [41]. They found that the experimental nonequilibrium phase diagrams strongly resemble the dynamic behavior predicted from theoretical calculations of a kinetic Ising model. It is clear from these works that there exists strong evidence of qualitative consistency between theoretical and experimental studies.

Another important feature in nonequilibrium phase transitions is the hysteretic response of the system to the periodically oscillating magnetic fields. In dynamic systems (i.e. the systems in the presence of ac fields), the hysteresis phenomenon is related to a dynamic phase lag between instantaneous magnetization and periodic external magnetic field [37]. In contrast to the behavior observed in static models (i.e. the systems with dc magnetic fields), where the strength of the external field does not change with time explicitly, dynamic hysteresis in nonequilibrium phase transitions is observed in dynamically paramagnetic phase. In other words, in the presence of dc magnetic fields, a ferromagnetic material exhibits a nonzero coercivity. By the agency of a tunable parameter, such as increasing the temperature, this coercive field reduces to zero in the vicinity of ferromagnetic–paramagnetic phase transition region. However, the situation is clearly different in the presence of an ac field. Namely, at high oscillation frequencies of the external field, the relaxation time of the system is relatively much larger than the oscillation period of the external perturbation. Therefore, the system is not able to follow the driving field which results in a dynamic symmetry loss leading to asymmetric hysteresis curves. In this case, coercivity is not applicable since the magnetization never reaches to zero. As the field frequency decreases or the amplitude of the external field increases, the system approaches to dynamic paramagnetic phase, and we observe symmetric hysteresis loops with nonzero coercivity [30,31,33].

Explanation of static hysteresis behavior observed in the bulk magnetic systems in the presence of dc fields has been well established [42]. Jiles and Atherton [43] proposed a theory for explaining the magnetization process in ferromagnetic materials based on the two fundamental mechanisms. Namely, the propagation of domain walls under the influence of an applied field, and rotation of aligned moments within a domain towards the field direction. They have also compared their theory [44] with experimental results for ferromagnetic steel by considering the various types of magnetization curves such as the anhysteretic, initial magnetization curve, and families of major hysteresis loops. In all cases they found an excellent agreement. Zapperi et al. [45] investigated the motion of a ferromagnetic domain wall driven by an external magnetic field through a disordered medium and observed remarkable agreement with experiments on $Fe_{21}Co_{64}B_{15}$ amorphous alloy. Similar analysis has also been performed for hysteresis in ferroelectric materials based on the domain-wall theory [46]. On the other hand, for the systems in thin film geometry, Haas et al. [47] performed a comprehensive experimental study on the late stages of phase separation in thin polymer solution films with thicknesses 1.5 and 10 μm, and estimated the average domain size as a function of the film thickness. Weir et al. [48] determined a value for the domain-wall energy and investigated the magnetization reversal of CoNi/Pt multilayers supporting perpendicular magnetization. They have also shown that CoNi/Pt multilayers support irregular fine-scale domain structures. Nowak [49] described the magnetic hysteresis behavior in thin ferromagnetic films with in plane anisotropy within the framework of Stoner–Wohlfarth model and obtained very realistic shapes of hysteresis loops. Moreover, a detailed review of comprehensive works on field-induced magnetization reversal in ultrathin ferromagnetic films can be found in [50].

It is clear from above discussions that the equilibrium phase transition properties, as well as the dc hysteresis process in thin films are well known. However, in nonequilibrium case, the problem deserves particular attention. Therefore, in the present Letter, we have extended the model of Tucker [22] by taking into account a time dependent perturbation in the thin film system described by spin-1 Blume–Capel Hamiltonian. For this purpose, we have calculated the phase diagrams and dynamic specific heat curves, as well as several characteristic quantities peculiar to kinetic models such as hysteresis loop area and dynamic correlation between magnetization and ac fields, and we consider the effect of the system parameters on these quantities. We have also discussed the micromagnetic structure of the system for selected system parameters at certain stages of the oscillating field.

The Letter is organized as follows: In Section 2, we describe the model and its related dynamic quantities which have been calculated throughout the analysis. Section 3 contains the numerical results and discussions. Finally, Section 4 is devoted to our conclusions.

2. Formulation

We consider a ferromagnetic thin film with thickness L described by conventional spin-1 Blume–Capel Hamiltonian [51,52]

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

where $S_i = \pm 1, 0$ is a three-state spin variable, and J_{ij} is the nearest neighbor interaction energy. The summation in the first term is taken over only the nearest neighbor interactions whereas the sums in the second and third terms are carried out over the all