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Monte Carlo simulations of dynamic phase transitions in ferromagnetic thin-films

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HIGHLIGHTS

- Dynamical ferromagnetic Ising-type thin films have been examined.
- Thermal variations of dynamical order parameters have been plotted.
- The profiles of average magnetizations on each layers have been presented.
- Dynamic phase boundaries have been plotted in related planes.
- The variation of crossover point with varying oscillating field amplitude has been presented.

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ABSTRACT

By means of detailed Monte Carlo (MC) simulations, we have presented dynamic phase transition (DPT) properties of ferromagnetic thin-films. Thermal variations of surface, bulk and total dynamical order parameters (DOP) for a film and total order parameter for the films with different thicknesses have been examined. Opposite regimes of reduced exchange interaction (surface to bulk ratio values in $R < R_c$ and $R > R_c$ regimes where R_c is the critical value at which the critical temperature becomes independent of film thickness L) have also been taken into consideration. The average magnetizations with varying temperature of each layer are reversed in these two regimes. Based on the results, we have confirmed that the system represents a crossover behavior between ordinary and extraordinary transition in the presence of surface exchange enhancement.

1. Introduction

Magnetic properties of free surfaces drastically differ from the bulk material, because the free surface breaks the translational symmetry (i.e. surface atoms are embedded in an environment of lower symmetry than that of the inner atoms and consequently the exchange constants between atoms in the surface region may differ from the bulk value). The surface enhancement phenomenon in finite magnetic materials has attracted considerable amount of interest for both experimentalists [1–6] and theorists [7–16].

Depending on the competition between the two time scales, namely the oscillation period P of the external oscillating magnetic field and the relaxation time τ of the sample, a dynamic symmetry loss breaking could cause a DPT. There are two cases due to the competition between these time scales: $P < \tau$ and $P > \tau$. In the first case, the system cannot relax within

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a complete cycle of the magnetic field oscillation, hence the instantaneous magnetization $M(t)$ oscillates in time around a nonzero value corresponding to dynamically ordered state (i.e. dynamic ferromagnetic phase). In other case, $M(t)$ can follow the external field with some delay, and the system exhibits a dynamically disordered behavior. The core of DPT properties is the relation between relaxation time τ and the other competing factors: The agency of an adjustable parameter such as the field amplitude, the type of the exchange interactions, and the temperature. The DPT point can be controlled by tuning these competing factors together with the time period of external field.

In experimental point of view, Schierle and coworkers observed that the magnetizations of the outermost layers in EuTe(111) films decrease significantly differently from those of bulk layers [1]. ViolBarbosa and coworkers presented the robust magnetic structure formation of the blocks of layers whereas the interblock interactions are relatively weak in fcc-Fe on Cu(001) film [3]. Moreover, the enhanced surface magnetism has been the focus of such systems. For instance, Gd film has been investigated experimentally. The thickness-dependent spin-polarized electronic structure of strained ultrathin and thin films of Gd has been investigated by Waldfried et al. [17]. They found that the surface magnetic structure dominates the magnetic ordering of the ultrathin Gd films. With decreasing thickness some bulk bands exhibit increasingly more passive magnetic behavior. Skomski and coworkers found that Gd films exhibit a magnetic surface transition which occurs above the bulk Curie temperature [18].

In the sense of dynamic phase transitions, a great deal of theoretical efforts has also been devoted to the investigation on such systems. The details of surface enhancement phenomenon for the films subjected to an external oscillatory field have been intensively propounded by Aktaş et al. by using effective-field theory (EFT) [19]. The general trend of frequency dispersion that belongs to a critical temperature coordinate of the special point for different frequency and amplitude values has been demonstrated in their work. Nonequilibrium phase transition in the kinetic Ising model on a two-layer square lattice has been examined by Canko et al. [20]. Dynamic phase diagrams have been constructed in the plane of the reduced temperature versus the amplitude. Similarly, dynamic magnetic behavior of a mixed Ising system on a bilayer square lattice has been investigated by Ertaş and Keskin [21]. They presented the dynamic phase diagrams in the reduced temperature and magnetic field amplitude plane and the effects of interlayer coupling interaction on the critical behavior of the system have been investigated in their work. Later, the kinetic phase transition in the semi-infinite Ising model, in the presence of a time-dependent oscillating external field, is studied within the framework of the mean-field approximation (MFA) [22].

In recent series of works by Pleimling and coworkers, surface criticality at a DPT and surface phase diagram of the three-dimensional kinetic Ising model has been elucidated. In the first one of these studies, Park and Pleimling found that the nonequilibrium surface exponents do not coincide with those of the equilibrium critical surface [23]. In addition, in three space dimensions, the surface phase diagram of the nonequilibrium system differs markedly from that of the equilibrium system. The values of the critical exponents have been determined through finite-size scaling by Park and Pleimling in their followup investigation [24]. Their results have showed that the studied nonequilibrium phase transition belongs to the universality class of the equilibrium three-dimensional Ising model. The surface phase diagram of the three-dimensional kinetic Ising model below the equilibrium critical point subjected to a periodically oscillating magnetic field has also been presented by Taucher and Pleimling [25]. They presented that surface phase diagram that in parts strongly resembles the corresponding equilibrium phase diagram, with an ordinary transition, an extraordinary transition, and a surface transition. These three lines meet at a special transition point. For weak surface couplings, however, the surface does not order.

In this regard, our task in the present work is to shed some light on the DPT properties – especially the evolution of crossover point with field amplitude – of ferromagnetic thin-films in the presence of ac driving fields. The layout of the work is as follows: Section 2 describes the model and the MC simulation scheme, the numerical results are reported in Section 3, the paper ends with concluding remarks in Section 4.

2. Methodology

We consider a ferromagnetic thin film with thickness L described by spin-1/2 Hamiltonian

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} s_i s_j - h(t) \sum_i s_i \quad (1)$$

where $s_i = \pm 1$ is a two-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 summation in the second term is carried out over all the lattice sites. In the second term, $h(t) = h_0 \sin(\omega t)$ represents the oscillating magnetic field, where h_0 and ω are the amplitude and the angular frequency of the applied field, respectively. The period of the oscillating magnetic field is given by $P = 2\pi/\omega$. If the lattice sites i and j belong to one of the two surfaces of the film we have $J_{ij} = J_s$, otherwise $J_{ij} = J_b$, where J_s and J_b denote the ferromagnetic surface and bulk exchange interactions, respectively.

In order to simulate the system, we employ the Metropolis MC simulation algorithm [26,27] to Eq. (1) on an $N \times N \times L$ simple cubic lattice where $N = 70$ and we apply periodic (free) boundary conditions in direction(s) parallel (perpendicular) to film plane. We have studied ultrathin-films with thickness $L = 3, 4, 5$ together with a relatively thicker thin-film $L = 20$ to observe average magnetizations of each layer for some selected system parameters. For simplicity, the exchange couplings are restricted to the ferromagnetic case.

Configurations were generated by selecting the sites in sequence through the lattice and making single-spin-flip attempts, which were accepted or rejected according to the Metropolis algorithm, and $N \times N \times L$ sites are visited at