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

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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 the critical value of reduced exchange interaction (surface to bulk ratio) $R_c$ at which the critical temperature becomes independent of film thickness $L$ has been also taken into consideration. The average magnetizations of each layer is reversed in these regimes. Based on the results, we have confirmed that the system represents a crossover behavior in between ordinary to extraordinary transition in the presence of surface exchange enhancement.

Keywords: Monte Carlo simulations, Magnetic thin-film, Surface magnetism, Surface enhancement phenomenon

I. 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].

Applied oscillating magnetic fields, depending on the competition between the two time scales, namely the oscillation period $P$ of the external perturbation and the relaxation time $\tau$ of the sample, a dynamic symmetry breaking may take place causing 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 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 dynamic paramagnetic behavior. The relaxation time $\tau$ can be controlled by supplied energy with several different ways: The agency of an adjustable parameter such as the field amplitude, strength itself, the type of the exchange interactions, and the temperature. The DPT point can be controlled by tuning mentioned competing factors together with the time period of external field.

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]. Violbabosa and coworkers found that the formation of the blocks of layers with robust magnetic structure 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 also found that Gd films exhibit a magnetic surface transition which occurs at about above the bulk Curie temperature [18].

In 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 were 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 belongs to 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.

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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 \cite{22}. 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 \cite{23}. 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 Taucner and Pleimling \cite{24}. 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. In this present paper, the DPT properties in the presence of external oscillatory field of the system are studied by MC simulation. 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.

\section{Simulation}

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

\[ \mathcal{H} = - \sum_{\langle ij \rangle} J_{ij} s_i s_j - h(t) \sum_i s_i \]  

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 all nearest neighbor interactions whereas the summation in the second term is carried out over all lattice sites. In the second term, \( h(t) = h_0 \sin(\omega t) \) represents the oscillating magnetic field, where \( h_0 \) and \( \omega \) 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 \cite{25,26} 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 selected some 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 each time step (a time step is defined as an MC step per site or simply MCS). Data were generated over 50 independent sample realizations by running the simulations for 50000 MCS per site after discarding the first 25000 steps. This amount of transient steps is found to be sufficient for thermalization for the whole range of the parameter sets. Throughout the analysis, oscillation period of the external field is kept fixed as \( P = 100 \).

Our program calculates the instantaneous values of the bulk and surface magnetizations \( M_s \) and \( M_b \), and the total magnetization \( M_T \) at time \( t \). These quantities are defined as

\[ M_s(t) = \frac{1}{N_s} \sum_{i=1}^{N_s} s_i, \quad M_b(t) = \frac{1}{N_b} \sum_{j=1}^{N_b} s_j, \]

\[ M_T(t) = \frac{N_s M_s(t) + N_b M_b(t)}{N_s + N_b} \]  

where \( N_s \) and \( N_b \) denote the number of spins in the surface and bulk layers, respectively. From the instantaneous magnetizations, we obtain the related order parameters as follows \cite{27}:

\[ Q_s = \frac{1}{P} \oint M_s(t) dt, \quad Q_b = \frac{1}{P} \oint M_b(t) dt, \]

\[ Q_T = \frac{1}{P} \oint M_T(t) dt \]  

Using Eq. (1), we calculate the total energy per spin

\[ E_{tot} = \frac{1}{P(N_s + N_b)} \oint \mathcal{H} dt \]  

Consequently, the specific heat is defined as

\[ C = \frac{dE_{tot}}{dT}. \]

We also note that the value of the bulk exchange interaction \( J_b \) is fixed to unity, and we also use the normalized surface to bulk ratio of exchange interactions \( R = J_s/J_b \), as well as the reduced field amplitude \( H_0 = h_0/J_b \), and reduced temperature \( \Theta = k_B T/J_b \).
III. RESULTS AND DISCUSSION

Based on the results, we mainly focus on the effect of external oscillatory field amplitude in surface enhancement phenomenon. First, in order to obtain a general insight on DPT characteristics, we plot Fig. 1 and 2 respectively. In Fig. 1 the thermal variations of surface, bulk and total order parameters for the films with thickness $L = 3$ are shown. Following this, total dynamical order parameters for the films with three different thicknesses are shown in Fig. 2. We restrict our discussions for two value of reduced exchange $R = 0.25$ and 2.75. Both in Fig. 1 and 2, the transition point increases with reduced exchange interaction at constant values of the other system parameters. Hence, relatively more thermal agitation is needed to make the system dynamically disordered for more interaction. Moreover, at a constant temperature, surfaces are weakly ordered due to the scarcity of dipole-dipole interaction per site for $R = 0.25$ value. For $R = 2.75$, surfaces dominate against bulk due to the surface enhancement. From Fig. 1, we see that both surfaces and bulk layers of magnetic thin-films exhibit a phase transition at a certain critical temperature independently from the value of $R$.

From Fig. 2, one can easily see the effect of external field amplitude $H_0$ for fixed value of the system parameters from the panel (a) to (c) and (d) to (f). Critical temperature exhibits a decreasing behavior with increasing $H_0$ as a consequence of the well-known following physical mechanism: For small amplitude values, the energy supplied by the external oscillatory field cannot break the ferromagnetic energy induced order due to the nearest-neighbor exchange coupling through the system at low temperatures. Hence, a DPT cannot be observed unless a relatively large amount of thermal energy is supplied to the system. As the field amplitude increases, it becomes dominant against the ferromagnetic nearest-neighbor bonds, and a DPT can be observed at low temperatures. When we fixed rest of the parameters except reduced exchange and compared the strength of the order parameters for the films with different thicknesses in two different value of $R$ (namely $R = 0.25$ and 2.75), we see the hierarchically sequence reversal in Fig. 2 (from (a) to (d) and (b) to (e) and (c) to (f)). In between these two value, there should be a critical point of the reduced exchange at which all the layers seem to oscillate in phase independently from the thickness.

![FIG. 1.](image1)

**FIG. 1.** (Color online) Surface, bulk and total order parameters for a film $L = 3$ layers for two different regime of reduced exchange interaction.

![FIG. 2.](image2)

**FIG. 2.** (Color online) Average magnetization in static case (a) and (d), and the total order parameters for the films with three different thicknesses $L = 3, 4, 5$. and for three different values of $H_0$. In order to make the aforementioned phenomenon more clear, we plot the dynamical order parameters of each layers for a film with $L = 20$ in Fig. 3. For this purpose, we choose a constant temperature value at which the system is well-below the transition point and the thermal fluctuations can be ruled out. The magnetization $M(t)$ cannot follow the external field $h(t)$ ($\tau > P$ case) for each selected field amplitude values $H_0$, consequently the dynamic ferromagnetism is enhanced. Reduced exchange varies from $R = 1.0$ to 2.0 including the critical value of itself. So, we have qualitatively different two regimes: $R < R_c$ and $R > R_c$. Below $R_c$ the in-
surface type of magnetic ordering. The opposite of the
differ from the bulk one. This regime corresponds to a
change constant between atoms in the surface region may
become more difficult to follow the external field for any
there are relatively more neighboring per magnetic sites
ner layers are highly ordered compare to surfaces. This
section can be briefly explained as follows: In middle of the film,
are relatively more neighboring per magnetic sites
which causes locally larger magnetic interaction. So it
becomes more difficult to follow the external field for any
Surface spins are embedded in an environment of
lower symmetry than that of the inner atoms. The
exchange constant between atoms in the surface region may
differ from the bulk one. This regime corresponds to a
surface type of magnetic ordering. The opposite of the
above scenarios can be considered also. Above \( R_c \), in
the inner layers, although there are more neighboring,
there are far fewer exchange constant per magnetic sites
which causes relatively smaller magnetic interaction than
that of the surface one. \( R_c \) plays the main role to obtain
the frontier of this crossover. The free surface cannot
break the translational symmetry since magnetic prop-
erties of the free surfaces exactly overlap with the bulk
one at \( R_c \). We can say more generally that the deficiency
of the interaction per surface spin can be compensated
by increasing the modified exchange interaction strength.
Moreover, the effect of external field can be also seen by
following the panels from (a) to (c).

In obtaining the critical frontiers depicted in
(k\( T_c /J - R \)) plane, we evaluated the thermal variation of
specific heat for a given set of system parameters. A
typical example is shown in Fig. 4 for the films with dif-
ferent thicknesses as \( L = 3, 4, 5 \). The temperature values
corresponding to the maxima of specific heat curves are
the transition temperatures. From the panel (a) to (c)
and (d) to (f), field amplitude \( H_0 \) changes. Also, from
(a) to (d), (b) to (e) and (c) to (f) reduced exchange has two different value. DPT points shift towards the
lower temperature with increasing field values as well
as they shift towards higher temperature with increasing
reduced exchange. The related detailed story has been
explained above. Similarly, the effect of reduced
exchange on specific heat peaks is easy to understand:
The stronger dipole-dipole interaction make more con-
tribution to total energy. Hence, more thermal agitation is
needed to make the system dynamically disordered. In
Fig. 4, the crossover behavior can be seen easily when
\( R \) changed from \( R < R_c \) to \( R > R_c \) (namely, from (a)
to (d), (b) to (e) and (c) to (f)). Below \( R_c \), thicker film
has more nearest-neighbor interaction per site, this cre-
ates more contribution to energy. Consequently, both
strength of the peak and corresponding critical temper-
atures are relatively higher than the others.

In order to obtain a general overview of the non-
equilibrium phase diagram in (k\( T_c /J - R \)) planes. For
this purpose, in Fig. 4 we plot the critical temperature
versus \( R \) with selected film thickness values \( L = 3, 4, 5 \)
and for three selected values of field amplitude \( H_0 \). Since,
the temperature values at which the specific heat curves
exhibit a sharp maximum correspond to the transition
temperature of thin film, critical temperature values have
been obtained by examining the thermal variation of spe-
cific heat curves (a selected set has been given in Fig.
4). Fig. 5 represents a characteristic phenomenon
peculiar to thin film systems. Namely, due to the exis-
tence of reduced surfaces, there exists a special value of
surface to bulk ratio of exchange interactions \( R_c \) at which
the transition temperature of the film becomes indepen-
dent of thickness \( L \). Simply we can say that the curves
with different film thicknesses intersect each other. This
fully supports a recent study \[19\] where in the framework
of an EFT the existence of a special transition point was
predicted. The critical temperature value of crossover
point for \( H_0 = 0.0 \) (static case) is in a good agreement
with previous studies \[19, 22, 29\]. However, variation of
\( R_c \) as a function of \( H_0 \) is very slow according to Fig. 5,
and we see that the location of \( R_c \) barely deviates from
its equilibrium value with increasing \( H_0 \). This deviation
has been reported before by Yüksel \[12\]. The discussion
on existence of this kind of deviation is an academic is-
ssue and this may be due to insufficient data and cannot
be located accurately with such an approach with less
effort. This was also reported in a MC simulation treat-
ment of surface critical phenomena by Hasenbusch \[29\].
From panel (a) to (c) the effect of field amplitude \( H_0 \) on
the transition characteristics of the film can be seen and
it is also straightforward as stated before: Greater the
amplitude $H_0$ means more energy transferred to the system over half cycle by the external oscillatory field and this makes transition from dynamically ordered to disordered phase more easy. For $R < R_c$, we have ordinary transition behavior where the bulk magnetism is dominant against the surface magnetism whereas for $R > R_c$, the surface may exhibit enhanced magnetic behavior in comparison with bulk. This is called extraordinary transition. Moreover, as shown in Fig. 4, for $R < R_c$, thicker films have greater transition temperatures while for $R > R_c$, the transition temperature of the film decreases with increasing thickness. The results indicate that the well-known surface enhancement properties of the system may change its characteristics in the presence of an external oscillatory field.

**IV. CONCLUSION**

In conclusion, we have applied MC simulations to study the DPT characteristics in thin ferromagnetic films in the presence of oscillating magnetic fields. The foremost results obtained from simulation data can be summarized as follows: We first investigate the thermal variations of related order parameters for the films with different thicknesses. The effect of the field amplitude and reduced exchange on the previous standard arguments for static case has been propounded. In the vicinity of the dynamic ferromagnetic-paramagnetic phase transition temperature, specific heat curves exhibit a sharp peak which becomes more apparent for sufficiently high reduced exchange values ($R > R_c$ regime) values. The thinner films in the absence of enhanced surfaces ($R < R_c$ regime) with high field amplitudes exhibit a weak peak in relatively lower temperatures.

According to our findings, an increment of the field amplitude causes a decreasing in corresponding temperature coordinate of the crossover point in $(k_B T_c / J_b - R)$ planes. Critical value of surface to bulk ratio of exchange interactions $R_c$ at which the transition temperature is independent of film thickness is not apparently responsive to varying field amplitude values, but exhibits slow variation as a function of $H_0$. We confirmed the general trend was generated by using EFT calculations before [19]. Hence, we can say that the evolution of a crossover is not from the limitation of EFT.

We hope that this study will shed light on further investigations of the dynamic nature of critical phenomena.
in pure crystalline ferromagnetic thin films and will be beneficial from both theoretical and experimental points of view.

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[1] E. Schierle, E. Weschke, A. Gottberg, W. Söllinger, W. Heiss, G. Springholz, and G. Kaindl, Phys. Rev. Lett. 101, (2008) 267202.
[2] M. Ahlberg, M. Marcellini, A. Taroni, G. Andersson, M. Wolff, and B. Hjörvarsson, Phys. Rev. B 81, (2010) 214429.
[3] C. E. ViolBarbosa, H. L. Meyerheim, E. Jal, J.-M. T Tannerre, M. Przybylski, L. M. Sandratskii, F. Yildiz, U. Staub, and J. Kirschner, Phys. Rev. B 85, (2012) 184414.
[4] A. Berger, O. Idigoras, and P. Vavassori, Phys. Rev. Lett. 111, (2013) 190602.
[5] B.-Y. Wang, J.-Y. Hong, K.-H. O. Yang, Y.-L. Chan, D.-H. Wei, H.-J. Lin, and M.-T. Lin, Phys. Rev. Lett. 110, (2013) 117203.
[6] O. Yalçın, Ş. Ünlüer, S. Kazan, M. Özdemir, Y. Öner, JMMM 373 (2015) 144.
[7] M. Saber, A. Ainane, F. Dujardin, B. Stb, Journal of Non-Crystalline Solids 250 (1999) 735.
[8] A. Oubelkacem, A. Ainanea, J. J. de Miguel, J. Ricardo de Sousa, M. Saber, Physica A 358 (2005) 160.
[9] S. Tuleja, J. Kecer, and V. Ilkovi, Phys. Stat. Sol. (b) 243, (2006) 1352.
[10] A. Zaim, M. Kerouad, Y. EL Amraoui, D. Baldomir, JMMM 316 (2007) e306.
[11] Ü. Akınç, JMMM 329 (2013) 178.
[12] Y. Yüksel, Phys. Lett. A 377 (2013) 2494.
[13] Ü. Akınç, JMMM 368 (2014) 36.
[14] Ü. Akınç, Thin Solid Films 550 (2014) 602.
[15] Y. Yüksel, Ü. Akınç, Physica B 433 (2014) 96.
[16] Y. Yüksel, Physica A 396 (2014) 9.
[17] C. Waldfried, T. McAvoy, D. Welipityia, P. A. Dowben, E. Vescovo, Europhys. Lett. 42 (1998) 685.
[18] R. Skomski, C. Waldfried, P. A. Dowbeny, J. Phys.: Condens. Matter 10 (1998) 5833.
[19] B. O. Aktaş, Ü. Akınç, H. Polat, Thin Solid Films 562 (2014) 680.
[20] O. Canko, E. Kantar, M. Keskin, Physica A 388 (2009) 28.
[21] M. Ertaş, M. Keskin, Chin. Phys. B 22 (2013) 120507.
[22] H. Park, M. Pleimling, Phys. Rev. Lett. 109, (2012) 175703.
[23] H. Park, M. Pleimling, Phys. Rev. E 87, (2013) 032145.
[24] K. Taucher, M. Pleimling, Phys. Rev. E 89, (2014) 022121.
[25] K. Binder, Monte Carlo Methods in Statistical Physics, Springer, Berlin, 1979.
[26] M. E. J. Newman, G. T. Barkema, Monte Carlo Methods in Statistical Physics, Oxford University Press, 2001.
[27] T. Tome, M. J. de Oliveira, Phys. Rev. A 41, (1990) 4251.
[28] T. Kaneyoshi, J. Phys. Condens. Matter 3 (1991) 4497.
[29] M. Hasenbusch, Phys. Rev. B 84, (2011) 134405.