MONTE CARLO SIMULATION OF MAGNETIZATION REVERSAL VIA DOMAIN-WALL MOTION IN Fe SESQUILAYERS ON W(110)

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ABSTRACT

Iron sesquilayers are ultrathin films with coverages between one and two atomic monolayers. They consist of an almost defect-free monolayer with compact islands of a second atomic layer on top. This variation of the film thickness results in a strong interaction between domain walls and the island structure. It makes these systems an ideal laboratory to study the dynamics of domain walls driven by weak external fields. We present computer simulations which provide insight into the role of the thermally activated nucleation processes by which a driven domain wall overcomes the obstacles created by the islands.

INTRODUCTION

Iron sesquilayers with coverages between one and two atomic monolayers grown at room temperature on the (110) surface of tungsten are extremely interesting systems, both from the experimental and theoretical point of view. There have been continuous experimental efforts [1–11] to understand the physics of these films, and surprising results still emerge [1, 2]. Below their critical temperatures, these films are uniaxial in-plane ferromagnets which may belong to the Ising universality class [2, 3, 4]. As a function of coverage, their coercivity exhibits a pronounced maximum located around 1.4 atomic monolayers [5, 6, 7]. Recently, a spin reorientation transition was observed in freshly prepared samples at temperatures above the Curie point of a monolayer [1]. The origin of these unusual magnetic properties lies in the film morphology. These ultrathin films consist of a nearly perfect atomic monolayer which supports compact islands of the second monolayer [8], as is illustrated in Fig. 1. The island structure results in a varying film thickness which causes a domain wall to prefer certain configurations. That the morphology can be controlled by the film thickness and that the surface can be precisely mapped by STM make sesquilayers ideal systems in which to study the role of disorder in domain-wall propagation.

Recently, we developed a computer model for iron sesquilayers and utilized it to simulate domain-wall motion in a magnetic field [12]. This enabled us to describe the dependence of the coercivity on the film thickness, the temperature, and the frequency of the field. The success of the model motivated us to look more closely at the processes involved in domain-wall motion. This is the subject of the present work. We address questions concerning the functional dependence of the domain-wall velocity on the driving field. There are different models used in the literature which differ significantly [13–16], and there is no generally accepted opinion on the field dependence of the activation volumes and energies involved in
domain-wall motion driven by weak fields. Therefore, we use Monte Carlo simulations to obtain information about the interaction between a domain wall and the pinning environment of rough films. We concentrate on quantities which have not yet been directly observed in experiments. In simulations it is possible to identify the metastable domain-wall configurations, the energy barriers which separate them, the activation volumes controlling the thermally activated domain-wall motion, and the Barkhausen volumes. Our results suggest that quantities such as the activation volume or energy must be used with great care because what is observed in experiments are effective quantities reflecting a complex interplay between disorder, temperature, driving field and, possibly, the history of the sample.

COMPUTER MODEL OF AN Fe SESQUILAYER FILM

In this section, we describe our computational model of iron sesquilayers as developed in Ref. [12]. It is based on the fact that the film is a highly anisotropic uniaxial ferromagnet [10]. Therefore, the kinetic Ising model is a reasonable approximation which can capture the important physics of the system. The Hamiltonian of the model is that of the usual nearest-neighbor Ising ferromagnet subject to an external field $H$:

$$
\mathcal{H} = -J \sum_{(ij)} s_i s_j - \mu H \sum_i s_i .
$$

The two-state variables $s_i$ describe the two preferred orientations of the local magnetization and are defined on a computational lattice which faithfully reflects the morphology of a real
sesquilayer film. Data necessary to create simulational lattices for various coverages were obtained by digitizing STM pictures of iron sesquilayers published by Bethge et al. [8]. The morphology of the computational lattice is illustrated in Fig. 1. We have chosen the computational spin $s_i$ to represent an area of a monolayer of size $6\text{Å} \times 6\text{Å}$. One and two layers of a square lattice were used for the mono- and double-layer parts of the film, respectively, and the spin-spin interaction, $J = 8.73\text{ meV}$, was fixed such that the critical temperature of a perfect monolayer (230K [3]) is reproduced. The size of the computational lattice was $195 \times 102 \times 1(2)$, corresponding to $1170 \times 612\text{ Å}^2$. To fix the coupling to the external field we use the bulk magnetic moment for an iron atom. Thus, our computational spins each carry a magnetic moment of $\mu = 11.43\mu_B$. In this work, we only present data for the coverage 1.26 atomic layers at the temperature of 184 K.

SIMULATIONS AND MEASURED QUANTITIES

In order to obtain detailed information on the dynamics of a domain wall, we set up a computer experiment with a propagating domain wall driven by the field. We start with the lattice magnetized as shown in the upper panel of Fig. 1(a). A narrow strip along one short side of the lattice is initialized in the stable phase, while the rest of the system is in the metastable phase. An external field is applied, and quantities related to the motion of the domain wall are recorded as the wall propagates. Results are averaged over on the order of 100 runs for each value of $H$. Two important quantities are the average probability that the volume of the stable phase will grow, $g(n)$, or shrink, $s(n)$, in the next Monte Carlo step. They are sampled for each value of the stable-phase volume (measured by the number $n$ of spins in the stable state). Since the magnetization reversal occurs via domain-wall motion, $n$ translates into an “average” position of the wall. These growth and shrinkage probabilities carry information relevant for describing the dynamics of the domain wall. In particular, they allow us to calculate the average time the domain wall needs to travel a certain distance, which can be checked against the directly measured times. The good agreement indicates that the growth and shrinkage probabilities can be used reliably to investigate the motion of the wall.

DYNAMICS OF THE DOMAIN-WALL MOTION

The island structure of the second atomic monolayer creates regions where the domain-wall exchange energy is about twice as large as in a monolayer. Thus, there is a complicated free-energy landscape for the domain-wall configurations. As the wall propagates in this disordered environment, it prefers to stay in metastable configurations that minimize the interface free energy. To proceed to the next favorable position, the domain wall must cross a region where it has an increased interface free energy. Such regions are usually related to the islands and represent obstacles or barriers to be overcome before the domain wall can move forward. The mechanism which allows these obstacles to be overcome is provided by thermal fluctuations of the domain wall. Like in ordinary nucleation phenomena [17], if a fluctuation into a region where the interfacial free energy is unfavorable is sufficiently large, the free-energy reduction obtained by further increasing the volume of the stable phase just outweighs the cost of creating more interface. The probability for the fluctuation to grow even further then becomes larger than the probability to shrink. Such a fluctuation is called critical. Typically, the system needs many “attempts” to create a critical fluctuation, and
Figure 2: (a): The average time spent by the domain wall at positions with a given number \( n \) of overturned spins (volume of the stable phase) for several driving fields. The curves from top to bottom correspond to fields \( H = 0.03, 0.04, 0.05, 0.06 \) and \( 0.07 \) (in units of \( J \)). (b): The ratio of the average shrinkage and growth probabilities of the stable phase, \( s(n)/g(n) \). In regions with values greater than one the domain wall tends to recede, whereas in regions where this ratio is less than one the domain wall tends to advance. The curves were obtained for fields \( 0.03 \) and \( 0.04 \) \( J \). The weaker the field, the stronger the “oscillations” of the curve. Examples of the activation volume, \( V_A \), and of the corresponding Barkhausen volume, \( V_B \), are shown.

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pinning centers is deformed by the field. Therefore, the metastable configurations contain more of the stable phase in stronger fields.

An important conclusion following from observation of the residence times is that the waiting times in individual metastable configurations (the weights of the residence-time peaks) are broadly distributed. Another notable observation is that the relative weights of the residence-time peaks change with the field. This indicates that the pinning effectiveness of a given local environment depends on its wider vicinity and perhaps on the history of the domain wall (for different values of $H$, the domain wall can enter a given region from different directions, thereby experiencing different detailed environments).

The distance between neighboring residence-time peaks is the Barkhausen volume. This can, under suitable conditions, be an experimentally observable quantity [14]. However, it must not be confused with the activation volume. To see the latter, one must examine the growth and shrinkage probabilities. Figure 2(b) shows the ratio $s(n)/g(n)$ for two different field strengths in the vicinity of the most pronounced peaks in Fig. 2(a). The domain wall tends to retreat from positions in which this ratio exceeds unity, whereas advancing is more probable when this ratio is less than one. The metastable configurations correspond to the points where $s(n)/g(n)=1$ and $\partial_n[s(n)/g(n)]>0$. In this figure we clearly see the shifts in these positions to the right with increasing field. The distances between these points and the subsequent points where $s(n)/g(n)=1$ and $\partial_n[s(n)/g(n)]<0$ are the quantities which interest us most. They are the volumes of the critical fluctuations, or the activation volumes (as indicated by $V_A$ in Fig. 2(b)). Like the waiting times, the activation volumes differ widely. More importantly, they increase with decreasing field. In other words, the activation volumes are not simply related to the size of an island or any other volume directly defined by the lattice morphology. Unfortunately, because of the narrow field region in which our simulations are feasible, it is difficult to say what the functional form of the field dependence is [12].

CONCLUSIONS

Compared to experiment, in computer simulations it is much easier to look at the processes and quantities which govern the dynamics of domain-wall motion in a magnetic medium. We used the novel approach of Ref. [18] to identify the thermally activated fluctuations of domain walls which are responsible for the domain wall motion, and to measure parameters of these fluctuations. In particular, we were able to measure Barkhausen volumes and activation volumes at different locations in the system. We demonstrated that in addition to the disorder-induced distribution of activation volumes, each individual activation volume increases as the strength of the applied field decreases. We emphasize that this effect, mostly neglected in the experimental literature, plays an important role in the field dependence of the domain-wall velocity. Although here we only studied a particular model for iron sesquilayers on tungsten, our observations are expected to apply to other systems in which domain-wall motion is thermally activated.

ACKNOWLEDGMENTS

This research was supported by NSF Grant No. DMR-9520325, FSU-MARTECH and FSU-SCRI (DOE Contract No. DE-FC05-85ER25000).
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