Magnetization switching in nanoscale ferromagnetic grains: simulations with heterogeneous nucleation

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We present results obtained with various types of heterogeneous nucleation in a kinetic Ising model of magnetization switching in single-domain ferromagnetic nanoparticles. We investigate the effect of the presence of the system boundary and make comparison with simulations on periodic lattices. We also study systems with bulk disorder and compare how different types of disorder influence the switching behavior.

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This work is devoted to computer simulation of magnetization switching in single-domain ferromagnetic nanoparticles. For highly anisotropic systems, simple kinetic Ising models can qualitatively explain many experimental observations. However, to obtain more realistic results additional physical effects must be included in the model. An important aspect of real samples is heterogeneous droplet nucleation due to the presence of the system boundary and due to bulk disorder.

The model used in our study is a square-lattice nearest-neighbor kinetic Ising ferromagnet with random updates using either Glauber or Metropolis single-spin-flip Monte Carlo dynamics. We first investigate systems with boundaries (but without disorder), then we consider disordered systems with periodic boundary conditions. We concentrate on two quantities: the lifetime and the switching field.

To determine the metastable lifetime, we start the simulations with all spins +1 and impose a negative magnetic field. Then we measure (in Monte Carlo Steps per Spin, MCSS) the mean time the sample needs to reach zero magnetization. Having measured this “lifetime” $\tau$ for several values of the magnetic field, one can extract from the data the switching field $H_{sw}$, which is defined as the field that produces a given lifetime. This quantity is often measured in experiments.

We performed Monte Carlo simulation studies of the switching dynamics of a kinetic Ising model defined on circular lattices (which we define as subsets of a square lattice, contained within a circle of given diameter $L$). The Hamiltonian is

$$H = -J \sum_{<ij>} \sigma_i \sigma_j - H \sum_i \sigma_i - H_\Sigma \sum_{i \in \Omega} \sigma_i , \quad (1)$$

where the first two terms represent the standard spin-spin interaction with positive $J$ and the coupling to the external field $H$, respectively. The last term, in which the summation runs only over the sites on the boundary of the lattice $\Omega$, is included to model the effect of the system boundary on nucleating droplets of the stable phase. For $H_\Sigma = 0$ one has a free boundary, whereas positive (negative) $H_\Sigma$ mimic a boundary which effectively repels (attracts) the droplets.

Figure 1 shows the switching fields for a fixed waiting time $\tau$ versus the diameter $L$ of the circular lattice. For the smallest systems, $H_{sw}$ is zero; for slightly larger systems, $H_{sw}$ increases sharply with $L$. This is the coexistence region, in which the stable and metastable phases practically coexist. For larger systems, the behavior depends strongly on the affinity of the boundary for droplets of the equilibrium phase, which here is modeled by different values of $H_\Sigma$; and also on the waiting time $\tau$. In general, the increase in the coexistence region is followed by a decrease of the switching field in the single-droplet region (where switching is triggered by a single critical droplet). This results in a
maximum located at the crossover between the coexistence and single-droplet regions. Similar switching-field peaks are observed in certain experiments on nanoscale ferromagnets. For larger systems, more than one droplet nucleates during the switching process, and the system is in the multidroplet region. There, the switching field becomes asymptotically independent of the system size.

For larger systems, more than one droplet nucleates during the switching process, and the system is in the multidroplet region. There, the switching field becomes asymptotically independent of the system size. Just as in periodic systems, this behavior can be clearly observed in samples in which the boundaries repel droplets of the stable phase (positive $H_S$). For neutral boundaries ($H_S = 0$) the maximum in the switching field can be much less pronounced or it can disappear completely, depending on the waiting time. For example, with $\tau = 1000$, the maximum of $H_{sw}$ completely disappears for $H_S = 0$. In general, to observe the maximum, one needs a longer waiting time. Note that a long waiting time probably corresponds better to most real experimental situations. For theoretical considerations concerning magnetization switching in kinetic Ising systems without disorder, see Refs. 1 and 6.

To study effects of disorder, we simulated the above Ising model on periodic square lattices using Glauber dynamics. The first type of disorder we investigate is produced by defects generated by randomly deleting bonds of the lattice with concentration $c$. Another interesting property of the typical critical droplet is its defect content: the number of deleted bonds associated with the droplet. It can be deduced from Fig. 3, as well as from direct measurements, that the effective concentration of defects within the droplets is considerably larger than the global concentration. This is caused by the fact that the droplets are preferentially located at the crossover between the coexistence and single-droplet regions. Similar switching-field peaks are observed in certain experiments on nanoscale ferromagnets.
nucleated in the vicinity of the defects.

In Fig. 3 we show the effect of the disorder on the switching field. Whereas the switching field is decreased by the disorder, its shape as a function of the system size remains approximately independent of $c$.

Thus, in the intermediate-temperature region studied here, the switching dynamics of the kinetic Ising model on a bond-diluted lattice is essentially the same as in systems without disorder, although the metastable lifetimes and switching fields are considerably reduced by the disorder. The effect of the disorder can be approximately described in terms of an effective medium which affects the growing droplets of the stable phase. Details will be given in a future paper.

Another type of disordered kinetic Ising model is defined by the Hamiltonian $\mathcal{H} = -J \sum_{<ij>} a_i a_j \sigma_i \sigma_j - H \sum_i a_i \sigma_i$, where the amplitudes $a_i$ represent random local magnetic moments. Here, we take them uncorrelated with a “box” distribution of width $W$, centered around unity. The switching dynamics with this type of disorder differs from the one discussed above in several respects. First, the approach in terms of “average” nucleating droplets is not useful because the interesting quantities have broad distributions. Second, there is a lack of self-averaging, even in the intermediate-temperature region studied here. This is demonstrated in Fig. 4 where we show how the mean lifetime is reduced by the disorder. At the same time, the relative width of the probability distribution of the mean individual-sample lifetimes increases. Whereas switching of a sample with a particular realization of the disorder is more deterministic than in a pure system, an ensemble of disordered systems exhibits a wide distribution of lifetimes and, consequently, of switching fields. The mechanism leading to this behavior is that the size of a critical droplet is different in different parts of the disordered lattice.

In summary, we have studied magnetization switching in systems in which heterogeneous nucleation of the equilibrium phase may occur on the system boundary or be associated with bulk impurities.

The presence of the system boundary strongly affects the magnetization switching in small systems since the critical fluctuations of the stable phase tend to nucleate in its vicinity. This considerably decreases the metastable lifetime as well as the switching field, compared to periodic systems. However, the basic features, such as the crossover from the coexistence region to a single-droplet region, and then to a multidroplet region with increasing $L$, can still be observed in systems with a boundary. The switching field as a function of the system size becomes less peaked, but a maximum, located near the crossover between the coexistence and the single-droplet regions, can still be observed if the waiting time is sufficiently long.

We have studied two different types of disordered systems. Diluted-bond disorder can be a toy model for samples with impurities, whereas the model with random magnetic moments could represent films with fluctuating thickness. Our results show that whereas these types of bulk disorder result in shorter metastable lifetimes in general, the details of the magnetization switching can differ considerably for different types of disorder.

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