Monte Carlo simulation of the magnetic ordering in thin films with perpendicular anisotropy

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Abstract

We present a Monte Carlo simulation of a model of a thin film consisting of a two-dimensional square lattice of classical Heisenberg spins with perpendicular anisotropy, short-range exchange and long-range dipolar interactions with the aim to explain the dependence on the magnetic history of the in-plane to out-of-plane reorientation transition observed in experiments. © 1999 Elsevier Science B.V. All rights reserved.

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Magnetic ordering in thin films and nanoscale structures is a subject of current increasing interest because of the wide variety of magnetic patterns that can be stabilized depending on the interplay between the perpendicular induced surface anisotropy, the exchange interaction and the long-range dipolar forces between the microscopic entities. In particular, magnetic force microscopy images obtained in many thin film systems have shown that out-of-plane magnetic order varies from bubble-like patterns [1] to labyrinthian striped domains [2], moreover, Lorentz electron diffraction of similar system indicates that in-plane order consists of vortex-like structures [3]. Of special interest are the reorientation transition from out-of-plane to in-plane magnetization with increasing temperature [4], film thickness [5,6], and magnetic history [1,2]. As an example of the last case, it has been observed that in Co granular alloys [2], the application of a perpendicular demagnetizing magnetic field to an initial in-plane configuration evolves towards a metastable striped domain structure that returns to the initial state in a long time scale.

With the aim to explain the variety of magnetic behaviours of the above experimental results we present a Monte Carlo simulation of a two-dimensional square lattice (lattice spacing \(a\)) of classical Heisenberg spins of magnetic moment \(\mu\), and perpendicular anisotropy \(K\), short-range exchange \(J\) and long-range dipolar interactions with Hamiltonian [4]:

\[
H = -J\sum_{m,n} S_m \cdot S_n - K \sum_m (S_m)^2 + g \sum_{m \neq n} \frac{1}{r_{mn}} \left( S_m \cdot S_n - \frac{3(S_m \cdot r_m \cdot S_n)}{r_{mn}^2} \right),
\]

where \(g = \mu^2/a^3\). Spins may represent either atoms or grains, in which case \(J\) stands for the indirect exchange coupling between grains through the matrix.\(^3\) The ground state energy of this model as a function of parameters \(J/g\) and \(K/g\) defines the phase diagram as shown in Fig. 1 for a 50 \(\times\) 50 system. The system orders out-of-plane while the energy of the limiting Ising model (\(K = \infty\)) is less than that of the limiting planar model (\(K = -\infty\)). In this case, the ground state evolves from antiferromagnetic order towards striped domains of increasing width as \(J/g\) increases. When the ground state

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\(^3\)For simulations of magnetization reversal in thin films modelled by an array of cells and a different treatment of interaction see Ref. [7,8].
Fig. 1. Ground state energy as a function of $J/g$ for the planar model (solid line), the Ising model (solid circles) and the general case for several values of $K/g$ as indicated in the figure (open symbols). Dashed lines correspond to the Ising model plus the anisotropy energy corresponding to the nearest finite $K$ curve.

Fig. 2. Snapshots of the configurations at different stages of the relaxation of an initially saturated sample with $K/g = 3.3$ and $J/g = 1.0$. Images in the right column indicate the out-of-plane component of the magnetization (black for down spins and white for up spins) while the ones in the left column correspond to the in-plane projections of a detail of the $25 \times 25$ region in the upper left corner. The first row shows the equilibrium configuration and the following correspond to the times indicated in Monte Carlo step units.

energy of the planar model is below the Ising one the system orders in-plane forming structures of vortices of increasing diameter as $J/g$ increases and tending to in-plane ferromagnetic (FM) order. Most interestingly, we have observed that for any given value of $K/g$, there is a range of $J/g$ values around the intersection between the planar and Ising ground state lines for which the in and out-of-plane configurations are quasi-degenerated. If the system is in one of these points of the phase diagram and it is perturbed out of the equilibrium configuration by an external force that is subsequently removed, it slowly relaxes towards equilibrium passing through metastable intermediate states that may correspond to a very different kind of ordering than the equilibrium one. As an example of this kind of experiments we have simulated the evolution at zero magnetic field of a system with $K/g = 3.3$ and $J/g = 1.0$ (see Fig. 2) that is initially saturated in the out-of-plane direction. In the first stages of the relaxation the system forms striped out-of-plane structures that slowly evolve towards the equilibrium configuration with spins forming in-plane vortices. It is interesting to note that in real thin film systems defects may exist (as it happens in granular alloys) that act as pinning centers of these intermediate states, this could be the origin of the wide variety of history dependent magnetic configurations observed in experiments.

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References