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Magnetic stripe domain pinning and reduction of in-plane magnet order due to periodic defects in thin magnetic films

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ABSTRACT

In thin magnetic films with strong perpendicular anisotropy and strong demagnetizing field two ordered phases are possible. At low temperatures, perpendicularly oriented magnetic domains form a striped pattern. As temperature is increased the system can undergo a spin reorientation transition into a state with in-plane magnetization. Here we present Monte Carlo simulations of such a magnetic film containing a periodic array of non-magnetic vacancies. We find that the defects produce two effects. At low temperatures the vacancies can take the place of a high energy spin and lower the energy of a domain boundary. This results in pinning of the domain boundaries, which stabilizes parallel orientation of stripes against thermal fluctuations. At higher temperatures, when spins are canted, we find that vacancies produce a dilution effect arising from the reduced demagnetizing field. The defects favor perpendicular spin alignment and disrupt long range ordering of spin components parallel to the sample. This increases cone angle and reduces in-plane correlations, leading to a reduction in the spontaneous magnetization.

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1. Introduction

Quasi-two dimensional ultra thin magnetic films engender a large area of theoretical and technical interest, due in part to the large variety of magnetic properties that can be produced [\[1,2\]](#page--1-0) and their applications in data storage [\[3,4\]](#page--1-0). For a sufficiently high ratio of dipole to exchange coupling strengths, the ground state of thin magnetic films can consist of magnetic stripe domains [\[5](#page--1-0)–[7](#page--1-0)]. For films with a strong perpendicular anisotropy a second phase transition is possible, in which spins reorient, resulting in a non-zero magnetization parallel to the sample plane [\[8](#page--1-0)–[10\]](#page--1-0).

There are a number of lithographic techniques that can be used to create nanometer scale magnetic structures [\[11](#page--1-0)–[19\]](#page--1-0). When compared with isotropic films, periodic magnetic nano structures have been shown to significantly alter macroscopic properties such as anisotropy [\[20,21](#page--1-0)], magneto-resistance [\[20\],](#page--1-0) coercive field [\[22](#page--1-0)–[24\]](#page--1-0) and spin reorientation temperature [\[25](#page--1-0),[26](#page--1-0)].

On the micro scale, magnetic stripe domains can appear with long range orientational order [\[7,6,27](#page--1-0)] or forming complex patterns [\[28,6](#page--1-0)]. Nano scale patterning has been used to create pinning sites for domain walls [\[29](#page--1-0)–[33](#page--1-0),[25](#page--1-0)]. When the period of pinning cites is comparable to the natural stripe width, long range orientational order can be stabilized [\[34,26](#page--1-0)].

Theoretically these quasi-two dimensional systems have been studied with a variety of methods. For two dimensional isotropic systems the problem of melting is reasonably well understood [\[35\],](#page--1-0) in particular the spin reorientation transition (SRT) and stripe melting have been studied analytically [\[36](#page--1-0)–[39\]](#page--1-0) and with computer simulation [\[40](#page--1-0)–[42\]](#page--1-0). Theoretically the problem of melting in two dimensional systems has been considered for the case of particles with a periodic potential [\[43\]](#page--1-0). The pinning of domain walls has been explored for both random [\[44\]](#page--1-0) and periodic defects [\[45\]](#page--1-0). Recently micro-magnetic computer simulations have explored the contribution of periodic defects and edge effects to magnetic reversal and hysteresis [\[46\].](#page--1-0) Here we perform Monte Carlo simulations on a stripe forming magnetic system in order to understand the effect of periodic non-magnetic defects on the thermally driven spin reorientation and stripe melting transitions. At low temperatures these defects result in pinning of the domain boundaries stabilizing parallel orientation of stripes against thermal fluctuations. At higher temperatures, when spins are canted the defects produce a dilution effect arising from the reduced demagnetizing field, leading to a reduction in the spontaneous magnetization.

2. Method

The system is modeled as a two dimensional square array of Heisenberg spins $s_i \in \mathbb{S}^2$, with lattice spacing α

$$
H = \frac{J}{2} \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} \mathbf{s}_{\mathbf{i}} \cdot \mathbf{s}_{\mathbf{j}} + K \sum_{\mathbf{i}} (s_{\mathbf{i}}^z)^2 + \frac{C_D}{2} \sum_{\mathbf{i}, \mathbf{j}} \frac{1}{r_{\mathbf{ij}}^3} (\mathbf{s}_{\mathbf{i}} \cdot \mathbf{s}_{\mathbf{j}} - 3\mathbf{s}_{\mathbf{i}} \cdot \hat{\mathbf{r}}_{\mathbf{ij}} \mathbf{s}_{\mathbf{j}} \cdot \hat{\mathbf{r}}_{\mathbf{ij}})
$$
(1)

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where *i* and *j* represent two dimensional indexes, $\mathbf{i} = (i_x, i_y)$, $s_i^z = s_i \cdot \hat{z}$ and $\langle ... \rangle$ indicates the sum extends only over nearest neighbors. J, K and C_D represent the strength of the exchange coupling, perpendicular anisotropy and dipole coupling respectively. In order to introduce non-magnetic defects, some lattice sites are left empty. These defects are arranged as a regular square array with spacing w_d . The system is evaluated with Metropolis algorithm Monte Carlo. In order to remove edge effects, periodic boundary conditions are introduced. After the change of co-ordinates $\mathbf{r}_{nm} = \mathbf{G} + \rho_{\mathbf{n}'\mathbf{m}'}$, where $\rho_{\mathbf{n}'\mathbf{m}'} = (\rho_x, \rho_y)$ and $\rho_x, \rho_y \in [0, L]$, dipole coupling is calculated over a series of replicas of the original system [\[47,48](#page--1-0)] the dipole interaction and Monte Carlo steps are parallelized on a GPU using the stream processing method described in [\[42\]](#page--1-0). Non-magnetic sites $s_i = 0$ are not updated.

3. Results

In order to create a periodic array of defects we select a system size of $L = 64\alpha$ and defect spacing $w_d = 8\alpha$. In real systems the width of stripes is of order tens of nanometers (or more) and so our parameter choice inherently involves some degree of course graining. Here we select our parameters in order to simulate three distinct phases. With increasing temperature we simulate a low temperature perpendicular striped phase, a canted phase with a net in plane magnetization and the high temperature paramagnetic phase, an example of such a system is found in Pt/Co/Pt thin films [\[26\].](#page--1-0) The ratio of exchange to dipole coupling is selected to be $\mathcal{J} = J/C_D = 8.9$ giving a stripe width of $w_s = 8\alpha$. In the absence of defects, the two dimensional Hamiltonian described in Eq. [\(1\)](#page-0-0) has been studied previously by Whitehead et al. [\[41\]](#page--1-0) for varying K. In these simulations it was shown that varying the ratio $K = K/C_D$ determines the sequence of phases observed with increasing temperature. For $K < 12$ the system has saturated in-plane magnetization at zero temperature and only a single phase transition can be observed (the paramagnetic transition at the Curie point). For intermediate values $12 < K < 14$, the system forms stripes as the ground state where the spins are canted near the domain boundaries leading to finite magnetization at zero temperature. Here we wish to examine a sequence of phases where the parallel magnetization is not present at low temperature. For this reason we select $K = 15$ ensuring that the ground state is not canted $(s_i \cdot \hat{z} = \pm 1)$.

At $T=0$, when the system is ordered, we find that for the choice of parameters above, the lowest energy occurs when domain boundaries pass through magnetic defects (this minimizes the energy by replacing a high energy spin with a defect). The system is initiated in the ground state and Monte Carlo ensembles are generated disregarding initial states to allow the system to equilibrate. We find that the equilibrium is generally quite rapid (of order $10⁴$ sweeps). However at temperatures where significant magnetic ordering occurs equilibrium is slower. In these cases when the simulation is performed increased equilibrium times of up to 10^5 sweeps are required. A further 5×10^4 steps are taken with states recorded every 50 steps. Previously we determined that 50 steps allowed sufficient independence between ensemble configurations [\[42\]](#page--1-0). In order to examine the effects of the defects results are included from an identical simulation performed on a perfect lattice that we shall refer to as the isotropic case.¹

When describing results we will refer to the normalized temperature $T = k_B T C_D^{-1}$. In [Fig. 1](#page--1-0) sample states are shown for low temperatures near to where orientational order is destroyed. In the absence of defects, as τ is increased, the striped system initially undergoes roughening at the stripe boundaries. The roughened domain boundaries are associated with localized canting of the spins away from perpendicular alignment. As temperature is further increased the system undergoes bridging between stripes that leads to the destruction of long range orientational order. With the inclusion of defects the same general trends occur: stripe roughening followed by bridging and eventual destruction of long range order. However, the presence of defects stabilizes the striped order at higher temperatures. In addition, differences in morphology are observed. In the absence of defects the stripes display long wavelength undulations. In the presence of defects walls are pinned. Instead of long wavelength bending, fluctuations exist as roughening of the sections of wall between defects. Also, in contrast to the isotropic case, we observe that this initial roughening of stripes is not associated with the appearance of canted spins. This reduced canting likely results from the dilution effect discussed below in Section 3.2.

In [Fig. 2](#page--1-0) the behavior of the two systems is shown at temperatures above the loss of orientational order. In both cases the system forms regions with spins canted towards in-plane alignment and the existence of long range order in the in-plane components. While there is clear long range order of the in-plane components we note that the spins do not lie completely in-plane. This is due to the relatively strong anisotropy K required for an Ising like ground state. Although spins do not reorient entirely, this state still has the important feature of interest in real systems; the appearance of finite magnetization above a temperature driven transition out the striped state. For this reason we will refer to this transition as a spin reorientation transition. As temperature is increased the systems become increasing granular before reaching the paramagnetic limit.

3.1. Orientational order parameter

At low temperatures, configurations where domain boundaries include a defect reduce the exchange energy by $\mathcal J$ (since the energetically unfavorable interaction across the domain boundary is removed). This short range effect leads boundaries being locally pinned at defects. In order to analyze the loss of orientational order we locate vertical and horizontal perpendicular domain walls by using n_h^2 and n_v^2 [\[41,49,42\]](#page--1-0)

$$
n_h^z = \frac{1}{2N} \sum_{\mathbf{i}, \mathbf{j}} 1 - \text{sgn}(\mathbf{s}_\mathbf{i} \cdot \hat{\mathbf{z}} \mathbf{s}_\mathbf{j} \cdot \hat{\mathbf{z}})
$$

$$
n_v^z = \frac{1}{2N} \sum_{\mathbf{i}, \mathbf{j}} \sum_{\text{h.n.n}} 1 - \text{sgn}(\mathbf{s}_\mathbf{i} \cdot \hat{\mathbf{z}} \mathbf{s}_\mathbf{j} \cdot \hat{\mathbf{z}})
$$
 (2)

where v.n.n and h.n.n indicate that the sums should be taken over all pairs of spins which are nearest neighbors in the horizontal and vertical directions respectively. The orientational order is given by

$$
\mathcal{O}_z = \langle |\mathbf{n}_h^z - \mathbf{n}_v^z| / (\mathbf{n}_h^z + \mathbf{n}_v^z) \rangle \tag{3}
$$

With the inclusion of defects the sums in Eq. (2) are restricted to run over all pairs that are not defects.

In [Fig. 3](#page--1-0) \mathcal{O}_z is plotted as a function of the normalized temperature T .

At low T both systems display a striped array with smooth boundaries corresponding to $\mathcal{O}_z = 1$. We observe that, while the transition profile is similar, the presence of defects increases the transition temperature by approximately $\Delta T = 1/2$.

3.2. In plane magnetic order

At high temperature when spins are no longer entirely perpendicular the system can display net magnetization parallel to the system plane. Letting $M_x = 1/N\Sigma_i s_i^x$ and $M_y = 1/N\Sigma_i s_i^y$ (with $N = L^2$), the inplane magnetization is

$$
M_{\parallel} = \langle (M_{X}^{2} + M_{y}^{2})^{1/2} \rangle. \tag{4}
$$

¹ Here the term isotropic refers to the virgin film being simulated. Since we have course grained the system into a lattice our model has the lattice translational symmetry.

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