Continuous spin reorientation in antiferromagnetic films

Juan J. Alonso$^1$ and Julio F. Fernández$^2$  

$^1$Física Aplicada I, Universidad de Málaga, 29071-Málaga, Spain$^3$,  
$^2$ICMA, CSIC and Universidad de Zaragoza, 50009-Zaragoza, Spain$^4$

We study anisotropic antiferromagnetic one-layer films with dipolar and nearest-neighbor exchange interactions. We obtain a unified phase diagram as a function of effective uniaxial $D_e$ and quadrupolar $C$ anisotropy constants. We study in some detail how spins reorient continuously below a temperature $T_s$, as $T$ and $D_e$ vary.

PACS numbers: 75.45.+j, 75.50.Xx  
Keywords: spin reorientation, magnetic films, anisotropy, phase diagram

Considerable attention has been devoted to the magnetic properties of ultrathin magnetic films in the last years. An interesting feature of magnetic films is discontinuous spin reorientation (DSR), i.e., thermally driven switching between perpendicular and in-plane spin alignment at a temperature $T_p$ below the ordering temperature $T_0$. DSR has been studied both experimentally and theoretically. It has been established that DSR depends on the competition between dipolar interactions and uniaxial anisotropy often found in films. Continuous spin reorientation (CSR) is also very interesting. A thermally driven CSR transition was first observed experimentally in bulk systems at some temperature $T_s$ well below $T_0$ [1]. Below $T_s$, all spins rotate continuously as a whole as $T$ is varied in these systems. After these experiments Horner and Varma [2] proposed an early phenomenological model in which higher anisotropies, which compete with the uniaxial anisotropy, were required for obtaining CSR. More recently, CSR has been observed in ferromagnetic thin films [3]. Some nonhomogeneous multilayer models have been proposed to explain CSR [4].

The aim of this paper is to report numerical results on CSR for one-layer antiferromagnetic films. It is important to note that CSR is always associated with a SR phase defined by its own broken symmetries [3, 4]. For instance, the order parameter $m$ may be perpendicular ($\theta = 0$) to the film plane in the $T_s < T < T_0$ range, and tilt away ($0 < \theta < \pi$) from the easy magnetization axis below $T_s$, thus breaking additional symmetries [3]. To our knowledge, such SR magnetic phase has not been observed in numerical simulations of antiferromagnetic films.

We consider a system of classical unit spins $\{S_i\}$ in a square lattice with Hamiltonian $H = H_J + H_d + H_o$ where $H_J$, $H_d$, and $H_o$ are for short range exchange, long range dipolar, and anisotropy interactions, respectively. We use periodic boundary conditions. The exchange and dipolar energy between two antiparallel out of plane nearest neighbors spins is $J < 0$ and $-\varepsilon_d$, respectively. Furthermore, there is site uniaxial $-D(S_i^z)^2$ plus fourfold $-C[(S_i^x)^4 + (S_i^y)^4]$ anisotropy energies. Similar models have been studied for $C = 0$, and some DSR between degenerate in-plane and out-of-plane states have been found as $T$, $J$ and $D$ vary [7]. For ferromagnetic films, on the other hand, Jensen et al. have considered $C \neq 0$ but obtained [8] phase diagrams only for $T = 0$.

Ground state configurations obtained from Monte Carlo simulations are exhibited in Fig. 1. States designated with a $c$, can be defined by $S_i^c = \tau_i^x \cos \theta$, $S_i^y = \tau_i^y \sin \theta \sin \phi$, $S_i^z = \tau_i^z \sin \theta \cos \phi$ where $\tau_i^x = (-1)^{\theta(i)}$, $\tau_i^y = (-1)^{\tau(i+y)}$, and $\tau_i^z = (-1)^{\tau(i)+\theta(i)}$. On the other hand, states designated with a $s$ are defined by $\tau_i^s = \tau_i^y = \tau_i^z = (-1)^{\tau(i)+\theta(i)}$. A suitable order parameter for both $c$ and $s$ is $m^c = N^{-1} \sum_i S_i^c \tau_i^c$.

We calculate energies for these configurations as in Ref. [6], and find a surface anisotropy energy $\Delta$ that behaves as an easy axis anisotropy. We find that $\Delta = 2\varepsilon_d$ for $s$ states and $\Delta = -1.23\varepsilon_d + 2J$ for $c$ states. This suggests we can define an effective anisotropy as $D_e = D + \Delta$ and obtain a unified phase diagram for both $s$ and $c$ states.

![FIG. 1: Magnetic phase diagram for dipolar systems in their ground states for $J \leq 0$. $s$ and $c$ states correspond to exchange dominated systems with $J < -1.61\varepsilon_d$ and dipolar dominated systems with $-1.61\varepsilon_d < J < 0$, respectively. Full and dashed thick lines stand for first- and second-order transitions, respectively. SR stands for the spin reorientation phase, in which $0 < \theta < \pi/2$.]
for $T = 0$, as shown in Fig. 1. $s$ configurations give a lower energy for $J < -1.61 \varepsilon_d$ while $c$ states are more favorable for $-1.61 \varepsilon_d < J < 0$. Interesting experimental realizations of the latter condition could be found in Ref. [9].

In both cases we find a z-collinear phase ($\theta = 0$) if both $D_e > 0$ and $D_e > C$ are fulfilled. In-plane configurations ($\theta = \pi/2$) are prefered for $D_e < C$. More interestingly, we obtain a spin reorientation phase for $C < D_e < 0$ in which $\theta$ covers the $0 < \theta < \pi/2$ range. Minimization of the total energy gives $\tan \theta = \sqrt{D_e/(C - D_e)}$ and therefore spins rotate continuously from $\theta = 0$ to $\pi/2$ as $D_e$ varies from 0 to $C$, as shown in the inset of Fig. 2. Symbols in the same inset correspond to numerical data obtained by cooling from the paramagnetic phase to $T = \varepsilon_d$, $J$ for different values of $D_e/C$.

We have explored temperature driven CSR in the SR phase by MC simulations for both exchange and dipolar dominated systems. For that purpose we calculate the order parameter ($m_x^2, m_y^2, m_z^2$) and the energy as a function of $T$. We find two different regions (see figs. 2 and 3). Upon cooling below $T_0$, in-plane configurations appear for $D_e/C > 0.65$, and spins rotate towards the z axis below a second order transition at $T_s < T_0$. On the other hand, for $D_e/C < 0.65$ spins point out of the plane below $T_0$, and rotate towards the xy plane as $T$ decreases below $T_s$. Finally, we find, that the ratio $T_s/T_0$, as in $d = 3$ systems [3], seems to depend mainly on $D_e/C$ and not on $J$ or $\varepsilon_d$.

---

[1] E. M. Gyorgy, J. P. Remeika and F. B. Hagedorn, J. Appl. Phys. 39, 1369 (1968).
[2] H. Horner and C. M. Varma, Phys. Rev. Lett. 20, 845 (1968).
[3] M. Farle et al., Phys Rev. B 55, 3708 (1997); G. Garreau, E. Beaurepaire, K. Oujnadela and M. Farle, Phys. Rev. B 53, 1083 (1996); R. Sellmann et al., Phys. Rev. Lett. 64, 054418 (2001).
[4] A. Moshel and K. D. Usadel, Phys. Rev. B 51, 16111 (1995); L. Udvardi et al., Philos. Mag. B 81, 613 (2001).
[5] L. D. Landau and E. M. Lifshitz, Electrodynamics of Continuous Media, 2nd ed. (Pergamon, Oxford, 2004), pp. 150-162.
[6] J. F. Fernández and J. J. Alonso, Phys. Rev. B 73, 024412 (2006).
[7] K. De’Bell, A. B. MacIsaac, J. P. Whitehead, Rev. Mod. Phys. 72, 225 (2000) and references therein.
[8] P. J. Jensen and K. H. Bennemann Phys. Rev. 42, 849 (1990).
[9] G. Ahlers, A. Kornblit, and H. J. Guggenheim, Phys. Rev. Lett. 34, 1227 (1975); G. Mennenga, L. J. de Jongh, and W. J. Huiskamp, J. Magn. Magn. Mater. 44, 59 (1984); M. R. Roser and L. R. Corruccini, Phys. Rev. Lett. 65, 1664 (1990); D. Bitko, T. F. Rosenbaum, and G. Aeppli, Phys. Rev. Lett. 77, 940 (1996).
FIG. 3: Phases of pure dipolar \((J = 0)\) films for \(C = -\varepsilon_d\) obtained from MC simulations. \(\circ (\times)\) stand for systems of 16 \(\times\) 16 (32 \(\times\) 32) spins respectively. Transition temperatures have been obtained from peaks observed in the specific heat. Systems have been cooled in \(\Delta T = 0.01\varepsilon_d/k_B\) steps of \(4 \times 10^5\) MC sweeps each. Similar phase diagrams have been obtained for \(J < 0\).