Interface disorder and layer transitions in Ising thin films

L. Bahmad, and A. Benyoussef
Laboratoire de Magnétisme et de la Physique des Hautes Energies
Université Mohammed V, Faculté des Sciences, Avenue Ibn Batouta,
Rabat B.P. 1014, Morocco

Abstract

The disorder and layer transitions in the interface between an Ising spin-1/2 film denoted \((n)\), and an Ising spin-1 film denoted \((m)\), are studied using Monte Carlo simulations. The effects of both an external magnetic field, acting only on the spin-1/2 film, and a crystal magnetic field acting only on the spin-1 film, are studied for a fixed temperature and selected values of the coupling constant \(J_p\) between the two films. It is found that for large values of the constant \(J_p\), the layers of the film \((n)\), as well as those of the film \((m)\), undergo a first order layering transition. On the other hand, the only disordered layer of the film \((n)\) is that one belonging to the interface films \((n)/(m)\), for any values of the crystal field \(\Delta\). We show the existence of a critical value of the crystal field \(\Delta_c\), above which this particular layer of the film \((n)\) is disordered. We found that \(\Delta_c\) depends on the values of the constant coupling \(J_p\) between the two films.

Keywords: Interface; Monte Carlo; magnetic thin film; disorder; Layering transitions.

(*) Corresponding author: bahmad@fsr.ac.ma

1 Introduction

Layered structures consisting of alternating magnetic materials, have been subject of many experimental study. These experimental studies have shown that the magnetisation enhancement exists in multilayered films consisting of magnetic layers. The most commonly studied magnetic multilayers are those of ferromagnetic transition metal such as Co or Ni. Several experiments have shown that the magnetisation enhancement exists in multilayered films consisting of magnetic layers. It was found that ferromagnetic coupling can exist between magnetic layers. From the theoretical point of view, great interest has been paid to spin wave excitations as well as critical phenomena [1-3]. The study of thin films is partly motivated by the development of new growth and characterisation techniques, but perhaps more so by the discovery of many exciting new properties, some quite unanticipated. These include, more recently, the discovery of enormous values of magnetoresistance in magnetic multilayers far exceeding those found in single layer films and the discovery of oscillatory interlayer coupling in transition metal...
multilayers. These experimental studies have motivated much theoretical work. Indeed, several methods have been used to study the layering transitions in Ising magnetic films. Benyoussef and Ez-Zahraouy have studied these layering transitions using a real space renormalization group [4], and transfer matrix methods [5]. Using the mean field theory, Hong [6], have found that depending on the values of the exchange integrals near the surface region, the film critical temperature may be lower, higher than, or equal to that of the bulk. Using the perturbative theory, Harris [7] have showed the existence of layering transitions at $T = 0$ in the presence of a transverse magnetic field. The effect of finite size on such transitions has been studied, in a thin film confined between parallel plates or walls by Bruno et al. [8] taking into account the capillary condensation effect. By applying Monte Carlo simulations on thin Ising films with competing walls, Binder et al. [9], found that occurring phase transitions belong to the universality class of the two-dimensional Ising model and found that the transition is shifted to a temperature just below the wetting transition of a semi-infinite fluid [10,11]. Hanke et al. [12] showed that symmetry breaking fields give rise to nontrivial and long-ranged order parameter profiles for critical systems such as fluids, alloys, or magnets confined to wedges.

We showed in one of our earlier works [13] the existence of layering transitions under the effect of a variable surface coupling. Moreover, for an Ising film with a wedge, we found in Ref. [14] the intra-layering transitions under the geometry effect consisting on the existence a wedge. When the film is subject to a random transverse magnetic field [15], we found the layer-by-layer transitions when increasing the concentration $p$ above a critical value $p_c(k)$ for each layer $k$. The aim of this work is to study the interface disorder coupled to layering transitions in a spin$-\frac{1}{2}$ film in interaction with a spin$-1$ film, using Monte Carlo simulations. The paper is organised as follows. In section 2, we give the model and the method used. In section 3 we present results and discussions.

2 Model and Monte Carlo simulations

We are studying two coupled magnetic films: a spin-$\frac{1}{2}$ film denoted $(n)$ formed with $n$ square ferromagnetic layers; and a spin$-1$ film denoted $(m)$ formed with $m$ square ferromagnetic layers, Fig. 1. Each layer is a square of dimension $N_x \times N_y = 64 \times 64$ spins. $N_x$ and $N_y$ being the number of spins in the $x$ and $y$ directions, respectively. The juxtaposed plans of the two films are coupled ferromagnetically via a constant $J_p$, so that the Hamiltonian governing the system is given by:

\[ H = -J \sum_{<i,j>_{(n)}} S_i S_j - H \sum_i S_i - J \sum_{<i,j>_{(m)}} \sigma_i \sigma_j - J_p \sum_{i<} \sum_{j>_{(m)}} S_i \sigma_j + \Delta \sum_{j>_{(m)}} \sigma_j^2 \quad (1) \]

where, $S_i(l = i, j) = -1, +1$ are the spin variables in the film $(n)$ and $\sigma_k(k = i, j) = 0, \pm 1$ are the spin variables in the film $(m)$. The spins of the film $(n)$ are subject to an external magnetic field $H$, whereas $\Delta$ is the crystal field acting only on spins of the film $(m)$. The sum $\sum_{<i,j>_{(n)}}$ (resp. $\sum_{<i,j>_{(m)}}$) is performed on nearest neighbour spins of the film $(n)$ (resp. of the film $(m)$). The interaction $J$ between the spins of the film $(n)$ as well as between the spins of the film $(m)$, is assumed to be constant. Values of the interface coupling constant $J_p$ will be discussed in all the following. A preliminary study showed that, when performing Monte Carlo simulations under the Metropolis algorithm, the relevant calculated quantities did not change appreciably for the film thickness: $n, m = 3, 4, 5$ and 8 layers; and when varying the number of spins of
each layer from \( N_x = N_y = 32 \) to 128. Where \( N_x \) and \( N_y \) are the number of spins, of each layer, in the \( x \) and \( y \)-directions, respectively. Taking into account the above considerations, in all the following we will give numerical results for a film thickness \( n = m = 5 \) layers, and \( N_x = N_y = 64 \) spins for each layer.

3 Results and discussion

The geometry of the system we are studying is summarised in Fig. 1, where the two films are coupled via the constant \( J_p \). Each layer of the film \( (n) \) is subject to the external magnetic field \( H \); whereas the layers of the film \( (m) \) are under the crystal field \( \Delta \). Although the model and established equations are valid for arbitrary values number of layers \( n \) and \( m \), numerical results will be given in this work for \( n = m = 5 \) layers. Also the temperature fluctuations will not be taken into account and will be fixed at the value \( T = 3.0 \) in all the following.

In order to outline the effect of the external magnetic field, we plot in Figs. 2a and 2b the layer magnetisation behaviour in each film: \( n \) and \( m \) for a fixed crystal field \( \Delta = 2.0 \). The former figure, plotted for a small coupling constant value \( J_p = 0.5 \), shows that only the layers of film \( (n) \) (spin \( -1/2 \)) transit when increasing the external magnetic field, including the interface layer \( n(1) \). Hence for small values of the parameter \( J_p \) the layering transitions are absent in the film \( (m) \) (spin \( -1 \)) for all values of the external magnetic field. But for higher values of the coupling constant \( J_p \) the layering transitions begin to occur in the film \( (m) \), as it is shown in Fig. 2b for \( J_p = 9.0 \). When increasing the amplitude of \( J_p \) more and more all the layers of the film \( (m) \) transit, following the layering transitions present in the film \( (n) \). This means that for sufficiently large values of the coupling constant \( J_p \), the effect of the magnetic field \( H \) acting on the film \( (n) \) is propagated to the film \( (m) \) layers.

On the other hand, one can ask if the crystal field \( \Delta \), applied on the film \( (m) \) and disordering its layers, can affect the layers of the film \( n \). To answer this question, we plot in Figs. 3a and 3b the layer magnetisation behaviour in each film as a function of the crystal field \( \Delta \) for a fixed value of the external magnetic field \( H = 0.20 \) and two values of the coupling constant \( J_p \). Indeed, the only disordering layer of the film \( (n) \) is that one belonging to the interface: \( n(5) \). The disorder of this specific layer is affected neither by small values of the coupling constant: \( J_p = 0.5 \) in Fig. 3a; nor by higher values: \( J_p = 9.0 \) in Fig. 3b. Hence, the disorder of the film \( (m) \) does not affect the layers of the film \( (n) \) except the special layer directly connected to the interface between the two films.

On the other hand, the effect of the interface coupling constant is summarised in Figs. 4a and 4b corresponding to a low crystal field value \( \Delta = 0.5 \) and a higher value \( \Delta = 9.0 \), respectively. It is found that starting from a totally disordered film \( (m) \) for low values of \( \Delta \), when increasing the coupling constant \( J_p \) values, all the layers of the film \( (m) \) undergo non null magnetisations (keeping the sign of the film \( (n) \) layers), see Fig. 4a. While for higher values of the crystal field \( \Delta \), see Fig. 4b , the increasing coupling \( J_p \) values does not affect, neither disorder of the film \( (m) \) layers, nor the layer magnetisations of the film \( (n) \). Indeed, the special layer \( n(5) \) disordered for the high crystal field value \( \Delta = 9.0 \) at low values of the coupling \( J_p \), is not affected by increasing the coupling \( J_p \) between the two films.

In the following we will focus our interest on the particular layers of the interface of the films: \( n(5) \) belonging to the spin-1/2 film \( (n) \), and \( m(1) \) belonging to the spin-1 film \( (m) \). Indeed, concerning the transition of the layers \( n(5) \) for a fixed crystal field value \( \Delta = 1.0 \) we show in
Fig. 5a the effect of increasing coupling $J_p$ on this layer. It is shown that the transition of the layer $n(5)$ inside the film $(n)$ is not affected by increasing the coupling $J_p$ from low values 0.1, 1.0 to a higher value 9.0. Whereas, under the same conditions, the transition of the layer $m(1)$ is strongly affected by increasing the coupling $J_p$, See Fig. 5b. This layer does not transit for $J_p = 0.1$ and any value of the external magnetic field $H$.

On the other hand, the layer $n(5)$ disorders for $\Delta \geq 9.0$, see Fig. 6a, for any coupling $J_p$ value; whereas the layer $m(1)$ disorders for $J_p = 0.1$ at $\Delta \approx 2.0$, for $J_p = 1.0$ at $\Delta \approx 6.0$ and for $J_p = 9.0$ at $\Delta \geq 10.0$, Fig. 6b. This means that the crystal field needed to disorder these layers depends on the coupling $J_p$ of the interface between the two films. A scenario of this dependence is plotted in Fig. 7 for the layer $n(5)$ and a fixed external magnetic field $H = 0.20$. It is seen, from this figure, that to disorder the layer $n(5)$ for low values of the coupling $J_p$, small values of the crystal field are needed. When increasing the coupling $J_p$, the crystal field $\Delta_c$ undergoes a maximum value at $\approx 9.0$, and decreases when increasing the coupling $J_p$ more and more.

4 Conclusion

The disorder and transitions of the interface between an Ising spin-1/2 film denoted $(n)$, and an Ising spin-1 film denoted $(m)$, has been studied using Monte Carlo simulations. The effects of both an external magnetic field, responsible on the interface transition, and a crystal magnetic field needed to disorder the interface are studied for a fixed temperature. It is found that for low values of the coupling $J_p$, the layers of the film $(n)$ undergo a first order layering transition. These transitions are also found in the film $(m)$, for higher values of the coupling $J_p$ between the two films. On the other hand, the layers of the film $(m)$ disorder when increasing the crystal magnetic field for any coupling $J_p$ value, but the only disordering layer of the film $(n)$ is that one belonging to the interface between the films $(n)/(m)$.

On the other hand, we show the existence of a critical value of the crystal field $\Delta_c$, above which this particular layer of the film $(n)$ is disordered at given values of the interface coupling $J_p$.

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Figure Captions

Figure 1:
Geometry of the system formed with two films coupled via the constant $J_p$. Each layer of the film $(n)$ is subject the external magnetic field $H$; whereas the crystal field $\Delta$ is acting only on the layers of the film $(m)$. The films $(n)$ and $(m)$ are formed with the same number of layers, $N = 5$.

Figure 2:
The external magnetic field effect on the layer magnetisation in each film, for a fixed crystal field $\Delta = 2.0$. (a) For a small coupling constant value $J_p = 0.5$, only the layers of film $(n)$ transit when increasing the external magnetic field, including the interface layer $n(5)$. The layering transitions are absent in the film $(m)$ for this small value of the coupling constant. (b) For a higher value of the coupling constant $J_p = 9.0$ the layering transitions begin to occur in the film $(m)$ following the layering transitions present in the film $(n)$.

Figure 3:
The layer magnetisation behaviour in each film as a function of the crystal field $\Delta$ for $H = 0.20$. (a) For a small value of the coupling constant: $J_p = 0.5$, when increasing $\Delta$ all the layers of the film $(m)$ are disordered but the only disordering layer of the film $(n)$ is that one belonging to the interface: $n(5)$. (b) For a higher value of the coupling constant: $J_p = 9.0$, the disorder of the film $(m)$ layers does not affect the layers of the film $(n)$ except the special layer $n(5)$ directly connected to the interface between the two films.

Figure 4:
The interface coupling effect on the layer magnetisation behaviour in each film for a constant external magnetic field $H = 0.20$ and two crystal field values: (a) For $\Delta = 0.5$ and starting from a totally disordered film $(m)$ all the layers of the film $(m)$ undergo non null magnetisations when the coupling $J_p$ between the films is increasing. (b) For a higher crystal field value $\Delta = 9.0$, the increasing coupling $J_p$ values does not affect, neither the disorder of the film $(m)$ layers, nor the layer magnetisations of the film $(n)$, except the special layer $n(5)$ belonging to the interface.

Figure 5:
Magnetisation behaviour of the interface layers: $n(5)$ and $m(1)$ for a fixed crystal field value $\Delta = 1.0$ and different values of the coupling constant $J_p = 0.1, 1.0$ and 9.0, as a function of the external magnetic field $H$. (a) The transition of the layer $n(5)$ inside the film $(n)$ is not affected by increasing the coupling constant. (b) The layer $m(1)$ does not transit for low values
of the coupling, e.g. $J_p = 0.1$. The transition of this layer is only seen for large values of the coupling $J_p$.

**Figure 6:**
Magnetisation behaviour of the interface layers: $n(5)$ and $m(1)$ for a fixed external magnetic field value $H = 0.20$ and different values of the coupling constant $J_p = 0.1$, 1.0 and 9.0, as a function of the crystal field $\Delta$. The crystal field needed to disorder the layer $n(5)$ (a) and the layer $m(1)$ (b) depends strongly on the coupling $J_p$ between the two films.

**Figure 7:**
The critical crystal field $\Delta_c$ needed to disorder the layer $n(5)$ as a function of the coupling $J_p$, for a fixed external magnetic field $H = 0.20$. $\Delta_c$ presents a maximum value for a coupling $J_p \approx 12.0$ and decreases when increasing the coupling $J_p$ between the two films.
Fig. 1

n(1)
n(2)
....
....
n(5)

Jp

m(1)
m(2)
....
....
m(5)

H

Δ
\[ \Delta = 2.0 \]
\[ J_p = 0.5 \]

Fig. 2a
Fig. 2b

$\Delta = 2.0$

$J_p = 9.0$

$n(k), m(k)$

$H$
Fig. 3a

H = 0.2

$J_p = 0.5$
Fig. 3b

\[ H = 0.20 \]
\[ J_p = 9.0 \]
Fig. 4a

$H = 0.20$

$\Delta = 0.5$
Fig. 4b

\[ n(5) \]

\[ H = 0.20 \]
\[ \Delta = 9.0 \]
Fig. 5b

![Graph showing the relationship between $m(1)$ and $H$ for different $J_p$ values: $J_p=0.1$, $J_p=1.0$, and $J_p=9.0$. The graph includes data points for each $J_p$ value, with the $m(1)$ values plotted against $H$ on the x-axis and y-axis.](image-url)
Fig. 6b

The diagram illustrates the relationship between $m(1)$ and $\Delta$ for different values of $J_p$. The curves represent:

- $J_p = 0.1$ (squares)
- $J_p = 1.0$ (circles)
- $J_p = 9.0$ (triangles)

As $\Delta$ increases, $m(1)$ decreases for all values of $J_p$. The curves for $J_p = 0.1$ and $J_p = 1.0$ are distinct from the curve for $J_p = 9.0$, indicating a more pronounced decrease in $m(1)$ for smaller values of $J_p$.
Fig. 7

\[ H = 0.20 \]

\[ \Delta c \]

\[ J_p \]