Journal of Magnetism and Magnetic Materials 417 (2016) 30–36

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Critical and compensation points of a mixed spin-2-spin-5/2 Ising ferrimagnetic system with crystal field and nearest and next-nearest neighbors interactions

N. De La Espriella [a,b], C.A. Mercado [b], G.M. Buendía [c,*]

[a] Department of Physics, Universidad de Córdoba, Córdoba 230002, Colombia
[b] Grupo Avanzado de Materiales y Sistemas Complejos (GAMASCO), Colombia
[c] Department of Physics, Universidad Simón Bolívar, Caracas 1080, Venezuela

ARTICLE INFO

Article history:
Received 4 February 2016
Received in revised form
3 May 2016
Accepted 14 May 2016
Available online 18 May 2016

Keywords:
Mixed Ising models
Square lattice
Compensation temperature
Critical temperature

ABSTRACT

We perform Monte Carlo simulations to analyze the magnetic properties of a mixed Ising model, where spins S that can take 5 values , 0, $\pm$ 1, $\pm$ 2, alternate on a square lattice with spins σ that can take 6 values, $\pm 5/2$, $\pm$ 3/2, $\pm$ 1/2. The Hamiltonian of the model includes an antiferromagnetic interaction between the S and σ spins, nearest-neighbors on the lattice, a ferromagnetic interaction between the S spins, next-nearest neighbors on the lattice, and a crystal field. We found that the system presents compensation temperatures in a wide range of the parameters. At the compensation temperature the total magnetization is zero but, contrary to what happens at the critical temperature, the system remains ordered. These temperatures have important technological applications, particularly in the field of thermo-magnetical recording. We calculate the finite-temperature phase diagram of the model. We found that the presence of the compensation temperature is strongly dependent on the next-nearest neighbor interaction term between the S spins, while its value can be calibrated by changing the crystal field.

1. Introduction

Mixed Ising models can be a good starting point to understand some aspects of the thermo-magnetic behavior of complex structures such as molecular magnetic materials. Mixed systems of higher spins located on alternating sites of a lattice have a rich critical behavior that can include interesting magnetic properties, such as first order phase transitions [1], giant magnetoresistance [2], enhanced surface magnetic moment [3], surface magnetic anisotropy [4], re-entrant behavior [5,6], hysteresis loops [7,8] and dynamic compensation behavior [5,9,10], among others. At the compensation point, T_{comp}, the total magnetization vanishes but the system has not yet reached the critical temperature, T_c. This effect is due to the different temperature dependences of the sublattices magnetizations that are antiferromagnetically coupled. At T_{comp}, the coercivity of the material depends strongly on the temperature [11–14], and only a small driving field is required to reverse the sign of the magnetization of a locally heated magnetic domain by using a focused laser beam [15–18]. This behavior has applications in the process of writing and erasing in high density magneto-optical devices [19–22]. Mixed Ising systems have been successfully used to explain the qualitative behavior of the compensation phenomenon and other properties of molecular materials characterized by the mixing of high spin compounds [23–26].

Mixed Ising systems also play a role in the understanding of nanomagnetic structures [27,28]. Nanotubes [29–31], nanorods [32–34], nanofilms [35–37], nanowires [38,39], nanoparticles [40,41], and nanobelts [42,43] are magnetic nanomaterials that can be characterized magnetically through mixed configurations of spins, and whose properties are quite different than those of the bulk materials [44,45]. These structures have applications in such diverse fields as information storage devices [46,**?**], permanent magnets [47], environmental remediation [48] and biomedical applications [49]. Some nanomaterials have been experimentally synthesized and their magnetic behavior has been studied, as is the case of magnetic nanowires Co–Cu [50], $Ga_{1-x}Cu_xN$ [51] and Fe_3O_4 [52]. For the latter system, Chern et al. reported experimental measurements of compensation temperatures [53]. Multilayer systems, such as magnetic thin films, can be adequately simulated by layered mixed spin Ising systems [54,55]. Multilayer spin systems, such as magnetic thin films, have been studied experimentally, presenting interesting properties such as surface magnetoelastic coupling, and surface magnetic anisotropy [4,56,57].

* Corresponding author.
E-mail address: ndelaespriella@correo.unicordoba.edu.co (N. De La Espriella).

http://dx.doi.org/10.1016/j.jmmm.2016.05.046
0304-8853/

To describe complex molecular magnetic materials, several mixed Ising models have been proposed, with lattices of different topologies, diverse couplings, and several approximation methods. Previous work includes spin configurations in square lattices with next and next-nearest-neighbor interactions, crystalline, and external fields [58–62]. In this work, we analyze an Ising ferrimagnet with spins $S=2$ alternating with spins $\sigma = 5/2$ on a square lattice. Besides the antiferromagnetic coupling between the S and the σ spins, we include a ferromagnetic coupling between spins of type S, next-nearest-neighbors on the lattice, and a crystal field. Previous studies in different spin systems, indicate that compensation temperatures are possible when ferromagnetic exchange interactions between next-nearest-neighbors are included [63–67,58].

The mixed spin-2 and spin-5/2 Ising ferrimagnet has been used as the prototype of certain molecular-based magnetic materials. For example, the model properly represents the compound $AFe^{II}Fe^{III}(C_2O_4)_3$, $A = N(n - C_nH_{2n+1})_4$, $n=3$–5, where $Fe^{II}=2$ and $Fe^{III}=5/2$ [68]. This model has also proved to be relevant to study a rich variety of thermomagnetic phenomena, such as first-order phase transitions reported on Bethe and honeycomb lattices, and simulated through exact recursion relations and Monte Carlo methods [1,69,70]; tricritic behavior in square, Bethe and honeycomb lattices [60,69,70]. Compensation temperatures were reported when the model was simulated on Bethe, honeycomb and layered honeycomb lattices [6,23,66,71,72]. The existence of hysteresis loops has been reported when the system is under the effect of oscillating and longitudinal magnetic fields, and different anisotropies [10,70]. This model has also been used to study the effects of interlayer coupling, and the crystal field, on the internal energy, the specific heat, and the magnetic susceptibility [73]. The ground-state diagram of the system is quite complex, and has been calculated for different combinations of interactions [74].

The outline of this work is as follows. In section 2 we define the model and present the Monte Carlo method. The effects of the next-nearest-neighbor exchange interaction and the single-ion anisotropy on the phase diagram are discussed in section 3. Finally, in section 4 we present our conclusions.

2. Model and monte carlo simulation

The system is a mixed Ising ferrimagnet were spins S and σ are located on alternating sites of a square lattice of size $L \times L$ with $L=80$. The Hamiltonian of the system is

$$\widehat{H} = -J_1 \sum_{\langle nn \rangle} S_i^A \sigma_j^B - J_2 \sum_{\langle nnn \rangle} S_i^A S_k^A - D \sum_i (S_i^A)^2 - D \sum_j (\sigma_j^B)^2 \tag{1}$$

Where $S^A = \pm 2, \pm 1, 0$ and $\sigma^B = \pm 5/2, \pm 3/2, \pm 1/2$ are the spins on the sites of the interpenetrating sublattices A and B, respectively. J_1 is the nearest-neighbors exchange parameter, J_2 is the next nearest-neighbor exchange parameter, and D is a crystal field, responsible of the anisotropy of the system. The first sum is performed over all pairs of nearest-neighbor spins, i.e. between spins S and σ. The second sum is performed over all pairs of next nearest-neighbors type S spins. The sums over i and j are performed over all sites of the sublattices A and B, respectively. We choose an antiferromagnetic coupling between nearest neighbors, $J_1 < 0$, and a ferromagnetic coupling between next nearest-neighbors, $J_2 > 0$, and take periodic boundary conditions. All the parameters in the Hamiltonian are in units of energy. Throughout the paper we use the notation: $D' = D/|J_1|$, $J_2' = J_2/|J_1|$ and $k_BT' = k_BT/|J_1|$, such that D', J_2' and k_BT', are dimensionless. k_B is the Bolzmann constant. Here for simplicity we assume that D' represents an average crystal field felt by the entire lattice. The effect of different crystal fields in this model, in the absence of the interaction J_2 has been analyzed in [75].

The simulation of the model is carried out by a heat bath Monte Carlo method. The data are obtained with $M = 5 \times 10^4$ Monte Carlo Steps per Site (MCSS), after discarding the first 10^4 steps per site to reach equilibrium. Errors are estimated using the method of blocks, where the sample is divided into b blocks, such that each block has $M_b = M/b$ measurements. When M_b is larger than the correlation length, the averages of the blocks can be considered statistically independent. Thus, errors can be calculated as the standard deviation of the averages of the blocks [76]. In this work $b=10$.

The magnetization per site of the sublattices, M_A,M_B, and the total magnetization per spin, M_T, are defined as:

$$M_A = \frac{2}{L^2}\left\langle \sum_i S_i^A \right\rangle \quad M_B = \frac{2}{L^2}\left\langle \sum_j \sigma_j^B \right\rangle$$
$$M_T = \frac{1}{2}(M_A + M_B) \tag{2}$$

An efficient way to locate the compensation temperatures, T_{comp}, is to find the intersection point of the absolute values of the sublattice magnetizations [63], i.e.

$$|M_A(T_{comp})| = |M_B(T_{comp})| \tag{3}$$

with the conditions:

$$\mathrm{sign}(M_A(T_{comp})) = -\mathrm{sign}(M_B(T_{comp})), \tag{4}$$

$$T_{comp} < T_c \tag{5}$$

where T_c is the critical temperature of the system at which both the total and sublattice magnetizations go to zero. These relations assure that at T_{comp} the total magnetization is zero due to the cancellation of the magnetizations of the sublattices.

Defining $\beta = 1/k_BT$, we calculate the specific heat per site C, and the total magnetic susceptibility per spin χ_T, as:

$$C = \frac{\beta^2}{L^2}\left(\langle H^2\rangle - \langle H\rangle^2\right) \tag{6}$$

$$\chi_T = \frac{\beta}{L^2}\left(\langle M_T^2\rangle - \langle M_T\rangle^2\right) \tag{7}$$

where $\langle H\rangle$ represents the internal energy of the system.

3. Results and discussion

3.1. Ground-state phase diagram

The ground-state diagram for this model has already been published by some of us [74]. In order to understand the behavior of the system as $T \to 0$ we reproduce it in Fig. 1. Due to the existence of the J_2 and D terms in addition to the J_1 interaction, the diagram has a complex structure. At finite temperature there can be tricritical points and first order phase transitions near the coexistence lines between different ground states [77,1,67,78]. The ground-state phase diagram of this model has ten different regions. The spins configurations in each region and the equations of the coexistence lines can be found in ref [74].

3.2. J_2' effects

In order to investigate the effect of the exchange interaction, J_2'