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Dynamic phenomena in magnetic ternary alloys

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ABSTRACT

We apply Monte Carlo simulation with local spin update Metropolis algorithm to investigate dynamic critical phenomena in a magnetic ternary alloy system with the chemical formula AB_pC_{1-p} comprising ferromagnetic and antiferromagnetic exchange interactions simultaneously. We perform a detailed investigation of the critical behavior of the system by presenting the phase diagrams in various planes and corresponding thermal and magnetic features as functions of several adjustable parameters, such as the temperature, mixing ratio p and external field amplitude h_0. We also revisit the equilibrium critical phenomena of the system which were previously handled by several theoretical tools and we re-examine former, widely studied properties. It is a fact that magnetic ternary alloy system has a special point at which the phase transition temperature of the system becomes independent of mixing ratio of ions B and C in equilibrium. However, our detailed results explicitly show that when a magnetic ternary alloy system is subject to a periodically driven time-dependent magnetic field, special point character of system tends to disappear, and hereby dynamic phase transition characteristics of the system begin to depend on the active concentrations of magnetic components.

1. Introduction

Control of thermal and magnetic properties of magnetic materials is one of the most challenging but also most difficult issues in the field of magnetism. A typical magnetic material presents monotonic increases in the magnetization value when the temperature decreases below its critical temperature. Contrary to the ordinary magnets, Prussian blue analogs constituting an important class of molecular based magnets exhibit unusual thermal and magnetic behaviors. These magnetic structures can be regarded as a composition of three different spin sources originating from the presence of metallic ions in the form AB_pC_{1-p}. For example, the magnet $(Fe^{II}_pMn^{II}_{1-p})_{1.5}Cr^{III}(CN)_6$ containing both ferromagnetic ($J_{Fe-Cr} > 0$) and antiferromagnetic ($J_{Mn-Cr} < 0$) superexchange interactions displays the photoinduced magnetic pole inversion [1]. Based on Mean-Field Theory (MFT) calculations of $(Ni^{II}_{0.22}Mn^{II}_{0.60}Fe^{II}_{0.18})_{1.5}[Cr^{III}(CN)_6]\cdot 7.6H_2O$, Ohkoshi and co-workers design a magnet which shows two compensation temperatures (at which the resultant magnetization vanishes) below its critical temperature [2]. We note that such a point has a technological importance in the field of magneto-optic recording, because at this point only a small driving field is required to change the sign of the resultant magnetization [3,4].

From the theoretical point of view, a number of studies regarding the equilibrium critical and compensation treatments in a mixed-spin ternary alloy system have been realized by means of MFT [5–14], Effective-Field Theory (EFT) with single-site correlations [15–17], Bethe-Lattice Approximation (BA) [18], Green Function Formalism (GFF) [19], and Monte-Carlo simulation (MC) [13,14,20–27]. In some of these studies, the location of R_C (here $R = |J_{AC}|/J_{AB}$ superexchange interactions ratio, and at this critical value of R the transition temperature of the system becomes independent of the mixing ratio of B and C ions) has been examined as a function of several physical factors, such as lattice dimensionality, lattice stoichiometry, and anisotropy in the exchange interactions, etc. For instance, by comparing the results for square [23] and simple cubic [25] lattices, former predictions suggest a reduction of R_C for higher lattice dimensions. However, based on our results which will be discussed in the following, this is a contradictory prediction, since the value of R_C for a square lattice is found to be almost identical to that obtained for a simple cubic lattice [25]. Apart from these, according to MFT analysis performed by Bobák and co-workers [5], R_C was found to be independent of lattice coordination number (and consequently dimensionality) whereas based on the BA [18] it was

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reported that R_C increases with increasing coordination number. At this point, it would not be an improper statement to underline that in light of the evidences provided by former MFT [5] and recent MC analysis [25], R_C is a critical property of a ternary alloy model which may be independent of lattice dimensionality. Based on the lattice stoichiometry, it was also previously reported by Žukovič and Bobák [25] that the lattice stoichiometry has no significant effect on R_C. However, an anisotropy in the exchange interaction causes a prominent increment of R_C. Namely, a three dimensional Heisenberg ternary alloy (represents isotropic case) exhibits $R_C = 0.4$ [28] whereas for the Ising system (represents highly anisotropic case) we have $R_C = 0.47$ [25].

All of these evidences point out that despite the presence of certain discrepancies, the variation of R_C in equilibrium systems has been studied in detail, however whether the value of R_C is affected in the presence of periodically oscillating magnetic fields or not remains as an important question to be answered, and it provides an open issue for debate. Hence, in the following we will discuss for the first time the non-equilibrium behavior of the system due to the externally applied periodic fields. Since the previously published pioneering works based on MFT and MC simulations [29–31], it is now well established that in the presence of periodic magnetic field oscillations, a magnetic material may undergo a dynamic phase transition from dynamically paramagnetic to dynamically ferromagnetic state with increasing temperature, due to the manifestation of dynamic symmetry breaking phenomena. More specifically, whether a magnetic system exhibits a dynamic phase transition or not strictly depends on the two characteristic time scales, namely the relaxation time τ' of the magnetic system, and the oscillation period τ of the external field. In the case of $\tau' > \tau$, the system cannot relax within a complete cycle of the magnetic field, hence can not follow the external field, but oscillates around a non-zero value which means that the system is in dynamically ferromagnetic phase whereas for $\tau' < \tau$, the magnetization can follow the external field but with some delay which corresponds to the dynamic paramagnetic phase. Indeed, the dynamic state of the system (para- or ferro-) can be controlled via changing at least one of the adjustable physical quantities such as the amplitude and frequency of the external field, or the temperature of the system. Keeping the discussions mentioned above in mind, we motivate ourselves to revisit the equilibrium critical phenomena of the system which were previously handled by several theoretical tools, additionally, to determine the time-dependent magnetic field effects on the dynamic phase transition features of magnetic ternary alloy system.

The paper is organized as follows: in Section 2, we briefly introduce our model and MC simulation procedure. The results and related discussions are presented in Section 3, and finally, Section 4 includes our conclusions.

2. Formulation

We consider a ternary alloy system of the type AB_pC_{1-p} under the presence of an oscillating magnetic field. The considered system consists of two interpenetrating square sublattices, each one containing $L^2/2$ sites, and one of the sublattices only have spins S_A=±3/2,±½ while the other sublattice have spins S_B=±1,0 or S_C=±5/2,±3/2,±½. This selection of spin magnitudes mimics the ternary molecular magnet $(Ni^{II}_pMn^{II}_{1-p})_{1.5}[Cr^{III}(CN)_6\cdot zH_2O]$ where $A = Cr$ with $S_{Cr} = 3/2$; $B = Ni$ with $S_{Ni} = 1$ and $C = Mn$ with $S_{Mn} = 5/2$ [23,32]. In this context, it was reported that $J_{Ni-Cr} > 0$ and $J_{Mn-Cr} < 0$. Moreover, in order to simulate a ternary alloy which simultaneously comprises ferromagnetic (FM) and antiferromagnetic (AFM) exchange interactions, it is necessary and sufficient to consider the exchange interactions between the nearest neighbor ions, and contributions from the second nearest neighbor sites can be neglected [32,33]. Under these assumptions, the Hamiltonian can be written in the following form,

$$\widehat{\mathscr{H}} = -J_{AB}\sum_{\langle i,j\rangle} S_i^A S_j^B \delta_j - J_{AC}\sum_{\langle i,j\rangle} S_i^A S_j^C (1-\delta_j) - H(t)\sum_i S_i^A - H(t)\sum_j \left[S_j^B \delta_j + S_j^C (1-\delta_j)\right], \quad (1)$$

where $J_{AB} > 0$ and $J_{AC} < 0$ are ferromagnetic and antiferromagnetic spin-spin exchange interaction terms between different types of magnetic components located on sublattices (see Fig. 1). δ_j is a random variable which can take value of unity or zero depending on whether the site-j is occupied by an ion B or C, respectively. The first and second summations in Eq. (1) are over the pairs of the nearest-neighbor sites while the last two terms are taken over all lattice sites. $H(t)$ refers to a time dependent external magnetic field which is defined as $H(t)=h_0\cos(\omega t)$ where t is the time and h_0 and ω are the amplitude and angular frequency of the magnetic field, respectively. The period of the oscillating magnetic field is given by $\tau=2\pi/\omega$, and it is fixed as $\tau=100$ throughout the study.

In order to elucidate the dynamic phase transition properties of the present many-body spin system, we use the MC simulation technique. We simulate the system on a $L \times L$ square lattice with $L = 128$ under periodic boundary conditions applied in all directions by making use of single-spin flip Metropolis algorithm [34,35]. Thermal variations of the various thermodynamic variables are generated over 50 independent sample realizations. In each MC experiment, the first 10^4 MC steps have been discarded, and the numerical data were collected over the next 10^4 MC steps. We note that this amount of transient steps is found to be sufficient for thermalization for the whole range of the parameter sets.

Our program calculates the instantaneous values of the magnetizations $M_A(t)$, $M_B(t)$, $M_C(t)$ and also the total magnetization $M_T(t)$ at time t as follows:

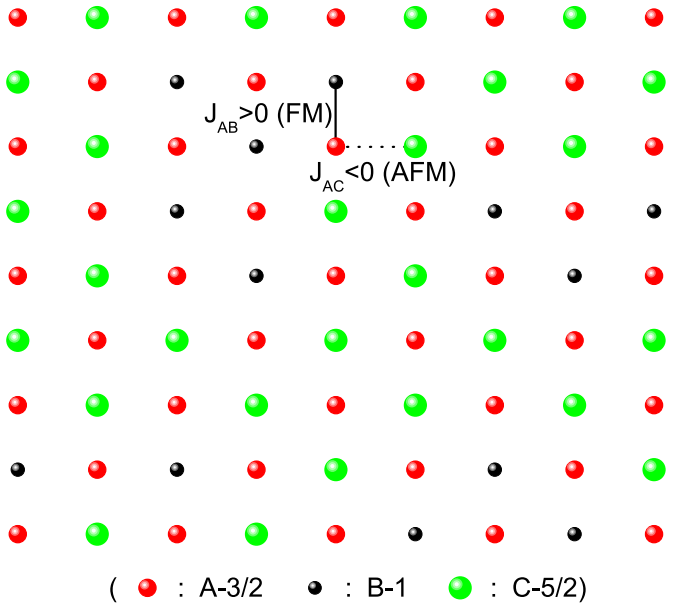

Fig. 1. (Color Online) Schematic representation of ternary alloy spin model defined on a square lattice. The model simultaneously includes ferromagnetic and antiferromagnetic exchange interactions.