Journal of Magnetism and Magnetic Materials 321 (2009) 3193–3197

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

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

Dependence on dilution of critical and compensation temperatures of a two-dimensional mixed spin-1/2 and spin-1 system

Ekrem Aydiner [a,*], Yusuf Yüksel [b], Ebru Kis-Cam [b], Hamza Polat [b]

[a] Department of Physics, Istanbul University, Tr-34134 Istanbul, Turkey
[b] Department of Physics, Dokuz Eylül University, Tr-35160 Izmir, Turkey

ARTICLE INFO

Article history:
Received 17 February 2009
Received in revised form
15 May 2009
Available online 29 May 2009

PACS:
75.50.Gg
05.10.Ln

Keywords:
Compensation temperature
Ferrimagnetic
Monte Carlo simulation

ABSTRACT

In this study, dependence on site dilution of critical and compensation temperatures of a two-dimensional mixed spin-1/2 and spin-1 system has been investigated with Monte Carlo simulation. The dependence of the thermal and magnetic behaviors on dilution of mixed spin system has been discussed. We have shown that the critical and compensation temperatures of diluted mixed spin system linearly decrease with increasing number of diluted sites.

1. Introduction

Ferrimagnetic systems i.e., materials have got considerable attention due to their technological applications. These systems consist of different spin sublattices and therefore they are also called as mixed spin systems. One of the most important properties of these systems is that they have a compensation temperature. In a ferrimagnetic spin system, sublattices have inequivalent moments interacting antiferromagnetically. At low temperatures, even though inequivalent moments of sublattices are antiparallel, they may not cancel each other owing to different temperature dependencies of the sublattice magnetizations. Fortunately, sublattices of a ferrimagnetic system compensate each other completely at $T = T_{comp}$ below the Néel temperature [1]. This critical point value is called as compensation temperature or compensation point of ferrimagnetic spin system. At the compensation point, the total magnetization of ferrimagnetic system vanishes and only a small driving field is required to reverse the sign of magnetization of a locally heated magnetic domain by using a focused laser beam. Hence, writing and erasing processes can be achieved at this point. This kind of ferrimagnetic systems are known as magneto-optic materials.

In technological applications, it is important to produce the material i.e., spin system which has a desired compensation temperature. In recent studies, it has been shown that dilution plays a role on the compensation point of a ferrimagnetic mixed spin system. Therefore, the effects of dilution on the compensation temperature of mixed spin systems have been studied and interesting phenomenon have been found. For example, Bobák and Jaščur [2] and Xin et al. [3–5] investigated the thermal and magnetic properties of a mixed spin-1/2 and spin-1 ferrimagnetic system on square and honeycomb lattices within the framework of an effective-field theory with correlations. They obtained a number of interesting phenomena, such as possibility of two compensation points in the total magnetization curve. They also discussed the influence of the crystal field interaction and concentration of the non-magnetic atoms on the magnetic and thermal properties of the system and observed the tricritical point, reentrant phenomena and two compensation points. Bobák and Jurčišin [6] and Kaneyoshi et al. [7] investigated a diluted Ising ferrimagnetic system by using an effective-field approximation and showed that the system exhibits two or three compensation points in certain concentration ranges of magnetic atoms and crystal field for spin-$(1, 3/2)$ and spin-$(2, 5/2)$ systems, respectively. Spin-1/2 and spin-1 ferrimagnetic model on a hexagonal lattice was studied by Godoy et al. [8] by employing mean-field calculations and Monte Carlo simulations. They showed that the phase diagram in the plane magnitude of spin-1 exchange interactions versus crystal field intensity exhibits a

* Corresponding author. Fax: +90 212 455 5855.
E-mail address: ekrem.aydiner@istanbul.edu.tr (E. Aydiner).

0304-8853/$ - see front matter © 2009 Elsevier B.V. All rights reserved.
doi:10.1016/j.jmmm.2009.05.042

very narrow region of compensation points. In addition, the influence of a transverse field on the compensation point was examined on honeycomb and square lattices [9–11].

As it can be seen from previous studies dilution effects on the thermal and magnetic behavior of the ferrimagnetic mixed systems have been investigated in detail. However, dependence of the critical and compensation temperatures on dilution has never been taken into account up to now. Therefore, this point still deserves particular attention for mixed spin systems. In this paper, we discuss dependence of the critical and compensation temperatures on dilution in a two-dimensional mixed spin-1/2 and spin-1 system with Monte Carlo simulation method. We find that the critical and compensation temperatures linearly decrease as the number of diluted sites increases in two-dimensional mixed spin-1/2 and spin-1 system.

2. The model and simulation technique

In order to investigate the effect of dilution on the critical and compensation temperatures and on the other physical quantities, we consider antiferromagnetically interacting two-dimensional mixed spin (1/2, 1) system with Hamiltonian

$$H = -J_1 \sum_{\langle nn \rangle} \sigma_i S_j - J_4 \sum_{\langle nnn \rangle} \sigma_i \sigma_k + D \sum_j S_j^2 \quad (1)$$

where $\sigma = \pm 1/2$ and $S = \pm 1, 0$. The first sum in Eq. (1) is over the nearest-neighbor and the second one is over the next-nearest-neighbor spins. J_1 ($J_1 < 0$) and J_4 parameters define exchange interactions between the neighbor spins, and D is the crystal field.

To simulate the system, we initially chose spins S and σ randomly, but with equal number, in a discrete lattice according to Eq. (1). We also set equal number of non-magnetic atoms randomly in each sublattice. Then, we employed Metropolis Monte Carlo simulation algorithm [12] to Eq. (1) on a $L \times L$ square lattice with periodic boundary conditions. Configurations were generated by selecting the sites in sequence through the lattice and making single-spin-flip attempts, which were accepted or rejected according to the Metropolis algorithm. Data were generated over 100 realization for $L = 16, 32$ and 64 with different numbers of non-magnetic atoms by using 25 000 Monte Carlo steps per site after discarding the first 2500 steps. Our program calculates the sublattice magnetizations M_A and M_B, the total magnetization M, the magnetic susceptibility χ and the specific heat C for different densities of diluted sites. These quantities are defined as

$$M_A = \frac{2}{L^2} \left\langle \sum_j S_j \right\rangle \quad (2)$$

$$M_B = \frac{2}{L^2} \left\langle \sum_i \sigma_i \right\rangle \quad (3)$$

$$M = \tfrac{1}{2}(M_A + M_B) \quad (4)$$

$$\chi = \frac{1}{kT}(\langle M^2 \rangle - \langle M \rangle^2) \quad (5)$$

$$C = \frac{1}{kT^2}(\langle E^2 \rangle - \langle E \rangle^2) \quad (6)$$

where T denotes temperature, E is the internal energy of the system, and k is Boltzmann constant (here $k = 1$).

To determine the compensation temperature T_{comp} from the computed magnetization data, the intersection point of the absolute values of the sublattice magnetizations was found using the relations

$$|M_A(T_{comp})| = |M_B(T_{comp})| \quad (7)$$

$$sign(M_A(T_{comp})) = -sign(M_B(T_{comp})) \quad (8)$$

with $T_{comp} < T_c$, where T_c is the critical temperature i.e., Néel temperature. Eqs. (7) and (8) indicate that the sign of the sublattice magnetizations is different, however, absolute values of them are equal to each other at the compensation point.

3. Numerical results and discussion

In order to see the effect of the non-magnetic atoms on the magnetic and thermal behaviors of a two-dimensional mixed spin system defined with Eq. (1), choosing $J_1 = -2, J_4 = 8$ and $D = 2.6$ we give the results of 64×64 square lattice for $N = 0, 64, 256, 512$ in Figs. 1–6. Here we must state that the nearest-neighbor interaction J_1 in Eq. (1) does not play a role on the compensation temperature, whereas observation of the compensation temperature depends on the parameters J_4 and D. This point has been discussed in Refs. [13,14]. Therefore, in this study, we have particularly focused on the effect of the different dilution rates with non-magnetic atoms N for arbitrary fixed J_1, J_4 and D. On the other hand, to analyze the effect of the non-magnetic atoms on the critical and compensation temperatures, for fixed $J_1 = -2$, $J_4 = 8$ and two different crystal field values $D = 1.6$ and 2.6 we give the results of different lattice sizes ($L = 16$, 32, 64) for different densities of diluted sites in Figs. 7 and 8.

In Fig. 1, temperature dependencies of sublattice magnetizations M_A, M_B and susceptibility χ of non-diluted square lattice are given for $J_1 = -2$, $J_4 = 8$ and $D = 2.6$. As expected for chosen parameters, the mixed spin system has a compensation point near $T/|J_1| = 3.6$ and a critical point near $T/|J_1| = 5.3$ as seen from Fig. 1. The results of M_A, M_B and χ for these parameters are in an excellent agreement with the results of Ref. [13].

In Fig. 2, total magnetization versus temperature has been plotted for several numbers of non-magnetic atoms N ($N = 0$, 64, 256, 512) for fixed $J_1 = -2, J_4 = 8$ and $D = 2.6$. In this figure, there are two zeros of magnetization curves for different numbers of non-magnetic atoms. The first zero indicates the temperature value at which total magnetization M is zero which corresponds to the compensation temperature point, and on the other hand,

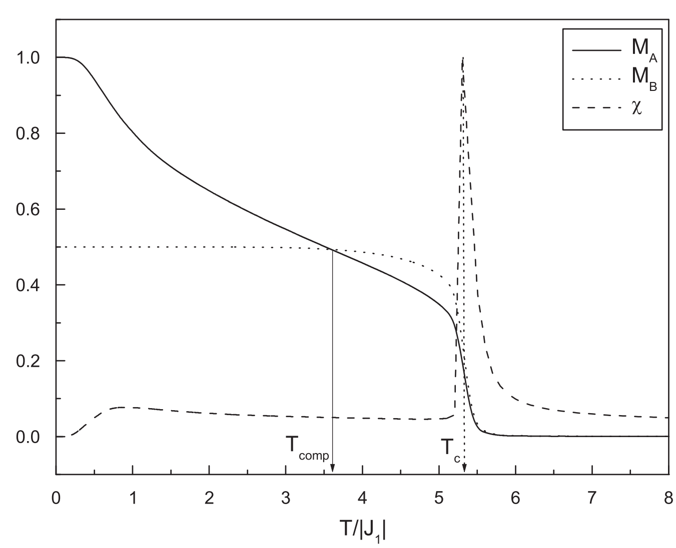

Fig. 1. The temperature dependencies of sublattice magnetizations M_A, M_B and susceptibility χ of non-diluted square lattice for $J_1 = -2, J_4 = 8$ and $D = 2.6$.