Journal of Magnetism and Magnetic Materials 432 (2017) 239–244

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

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

Thermal and magnetic phase transition properties of a binary alloy spherical nanoparticle: A Monte Carlo simulation study

Z.D. Vatansever *, E. Vatansever

Department of Physics, Dokuz Eylül University, Tr-35160 İzmir, Turkey

ARTICLE INFO

Article history:
Received 8 September 2016
Received in revised form 9 December 2016
Accepted 27 January 2017
Available online 3 February 2017

Keywords:
Binary alloy systems
Magnetic nanoparticles
Monte Carlo simulation

ABSTRACT

We have used the Monte Carlo (MC) simulation method with Metropolis algorithm to study the finite temperature phase transition properties of a binary alloy spherical nanoparticle with radius r of the type A_pB_{1-p}. The system consists of two different species of magnetic components, namely, A and B with spins $\sigma = 1/2$ and $S = 1$, respectively. A complete picture of phase diagrams, total magnetizations and susceptibilities in related planes have been presented, and the main roles of the radius of nanoparticle, active concentration value of type-A atoms as well as other system parameters on the thermal and magnetic phase transition features of the considered system have been discussed in detail. Our MC investigations clearly show that it is possible to control the critical characteristic behaviors of the system with the help of adjustable Hamiltonian parameters.

1. Introduction

When the physical size of a magnetic system is reduced to a characteristic length, the system has a bigger surface area to volume ratio giving rise to a great many unusual thermal and magnetic properties different from the conventional bulk systems [1]. For instance, according to the experimental and theoretical observations, the metallic nanocrystals have enhanced specific heat in comparison with macro crystals [2,3]. In recent years, there has been active research on small-size nanoparticles both experimentally and theoretically because of their technological [4–6] and biomedical applications [7–11]. For example, from the experimental point of view, the multi-functionality nanowires with an iron core and an iron oxide shell have been synthesized by a facile low-cost fabrication process in Ref. [11]. Here, Ivanov and co-workers report that a multi-domain state at remanence can be obtained, which is an attractive feature for the biomedical applications. Magnetic proximity effect in ferrimagnetic/ferromagnetic core/shell Prussian blue analogues molecular magnet has been found by Bhatt and co-workers in Ref. [12]. They synthesize a ferrimagnetic core of $Mn_{1.5}[Cr(CN)_6] \cdot 7.5H_2O$ surrounded by a ferromagnetic shell of $Ni_{1.5}[Cr(CN)_6] \cdot 7.5H_2O$, and note that such a process allows us to enhance the transition temperature of the core/shell nanoparticle system, compared to the bare-core and bare-shell transition temperatures.

On the other hand, from the theoretical point of view, a great deal of studies have been devoted to investigate the thermal and magnetic features of nanoparticles such as nanocube, nanosphere, nanorod, nanotube as well as nanowire by means of several types of methods for instance mean-field theory (MFT) [13–15], Green function formalism (GF) [16], cluster variation method (CVM) [17], effective-field theory (EFT) with single-site correlations [18–24] and MC simulation technique [13,25–35]. Vasilakaki and co-workers have been studied the thermal and magnetic phase transition properties of antiferromagnetic/ferrimagnetic core/shell nanoparticles in detail by making use of MC simulation technique with Metropolis algorithm [27]. It has been reported that the coercivity and loop shift show a non-monotonic dependence with the core diameter and shell thickness, in agreement with the experimental data. Magnetic phase transitions and hysteretic features of a graphyne core/shell nanoparticles have been investigated in Ref. [28] based on MC simulation method. It has been found that the considered system exhibits a number of unusual and characteristic treatments such as the occurrence of one and two compensation temperatures. Moreover, magnetic phase transition properties of a single spherical core/shell nanoparticle, consisting of a ferromagnetic core surrounded by a ferromagnetic shell with antiferromagnetic interface coupling have been realized within the framework of MC simulation scheme [29]. It is underlined that for appropriate values of the system parameters, multiple compensation points may emerge in the system. They also analyzed the core radius and shell thickness dependencies of the critical behavior of the system, and they found that the values of compensation

* Corresponding author.
E-mail address: zeynep.demir@deu.edu.tr (Z.D. Vatansever).

http://dx.doi.org/10.1016/j.jmmm.2017.01.079
0304-8853/

and transition temperatures vary with changing value of the particle size.

Furthermore, determination of equilibrium phase transition properties of binary alloy systems containing disorder effects problems which may be arisen from a random distributions of the magnetic components or random exchange interactions between the magnetic components in the material has a long history. Many studies have been performed regarding the physical properties of quenched disordered binary magnetic materials based on a variety of techniques such as MFT [36–39], EFT [40–44] as well as MC [45–48], in the context of bulk materials. We learned from these works that the quenched disordered binary alloy systems with different signs and unequal magnitudes of the spin–spin interactions and single ion-anisotropy exhibit unusual and interesting thermal and magnetic behaviors such as presence of a reentrant type character in the magnetization versus temperature profile, compensation and also spin-glass behaviors. Keeping the discussions mentioned above in mind, we intend to elucidate the finite temperature phase transitions and critical properties of a binary alloy spherical nanoparticle with radius r of the type A_pB_{1-p} in this study. The system consists of two different species of magnetic spin components, A with spin $\sigma = 1/2$ and B with spin $S = 1$. In the system, there aren't any un-occupied lattice sites and each lattice site is occupied by type-A or $-B$ atom, depending on the active concentration value of type-A components, p. We perform MC simulation, using Metropolis algorithm and determine the effects of p, the radius of spherical nanoparticle as well as other system parameters on the phase transition features of the considered system. To the best our knowledge, there are no works regarding the thermal phase transition properties of binary alloy type spherical nanoparticle systems, except from Ref. [31] where compensation behavior of a ferrimagnetic spherical nanoparticle system with binary alloy shell is studied by means of MC simulation method. It has been stated that the system exhibits one, two or even three compensation points, depending on the system parameters. We should note that our model is completely different from the system studied in Ref. [31]. That is to say, the magnetic components A and B can locate any place of the nanoparticle, whereas they can only locate the shell part of the particle, in the mentioned work.

The plan of the remainder parts of the paper is as follows: In Section 2, we present our model. The results and discussions are given in Section 3, and finally Section 4 contains our conclusions.

2. Formulation

We consider a binary alloy spherical nanoparticle system of the type A_pB_{1-p} with total radius r, which is schematically shown in Fig. 1. The lattice sites are randomly occupied by two different species of magnetic components A and B with the concentration p and $1-p$, respectively. The Hamiltonian describing our model of magnetic system is given by:

$$\widehat{H} = -J\sum_{\langle i,j\rangle}\delta_{iA}\delta_{jA}\sigma_i\sigma_j + \delta_{iB}\delta_{jB}S_iS_j + \delta_{iA}\delta_{jB}\sigma_iS_j + \delta_{iB}\delta_{jA}S_i\sigma_j - \Delta\sum_i \delta_{iB}S_i^2, \tag{1}$$

here $J > 0$ denotes the ferromagnetic spin–spin interaction term between nearest neighbor spins while Δ refers to the single-ion anisotropy term. The σ and S are Ising spin variables which can take values of $\sigma = \pm 1/2$ and $S = \pm 1, 0$ for the magnetic components-A and $-B$ of the system, respectively. The symbol $\delta_{i\alpha} = 1$ ($\alpha = A$ or B) if site i is occupied by type-α atom and 0 otherwise. The first summation in Eq. (1) is over the nearest neighbor pairs while the second one is over all lattice sites occupied by type-B atoms.

In order to investigate the thermal and magnetic phase transition properties of the binary alloy type spherical nanoparticle system, we use the MC simulation technique with local spin update Metropolis algorithm [49,50]. We simulate the system with radius r up to 18, located on a simple cubic lattice, under free boundary conditions applied in all directions. We can summarize the simulation procedure as follows. First, the simulation starts at a high temperature value using random initial condition, and then the system is slowly cooled down with a reduced temperature step $k_B\Delta T/J = 2\times 10^{-2}$, where k_B and T are Boltzmann constant and absolute temperature, respectively. The spin configurations are generated by selecting the sites sequentially through the binary alloy type nanoparticle system, and making single-spin flip attempts, which are accepted/rejected according to the Metropolis algorithm. Thermal variations of various thermodynamic quantities are generated over 50 independent computer experiments. In each computer experiment, the first 10^4 MC steps have been discarded for thermalization process, and the numerical data are collected over the next 4×10^4 MC steps. Based on our test investigations, we note that this amount of transient steps are found to be sufficient for thermalization for the whole range of the parameter sets. The site randomness in binary alloy systems can be considered as quenched or annealed. We consider only quenched site-disordered binary alloy nanoparticle for which the magnetic components are distributed completely at random throughout the lattice and they are fixed at their positions in one physical realization of the system. In every computer experiment, we choose a new random arrangement of magnetic components by generating different random number sequences. We mention that when dealing with systems of quenched randomness, both thermal and disordered average of any physical quantity should be considered [49]. The thermal averages are carried out by Metropolis algorithm and the disorder averages are performed by simple sampling over 50 independent computer experiments in this study.

Our program calculates the instantaneous values of the magnetizations as follows:

$$\begin{aligned} M_A &= \tfrac{1}{N_A}\sum_{i=1}^{N_A}\sigma_i, \\ M_B &= \tfrac{1}{N_B}\sum_{i=1}^{N_B}S_i, \\ M_T &= \tfrac{N_AM_A+N_BM_B}{N_A+N_B} \end{aligned} \tag{2}$$

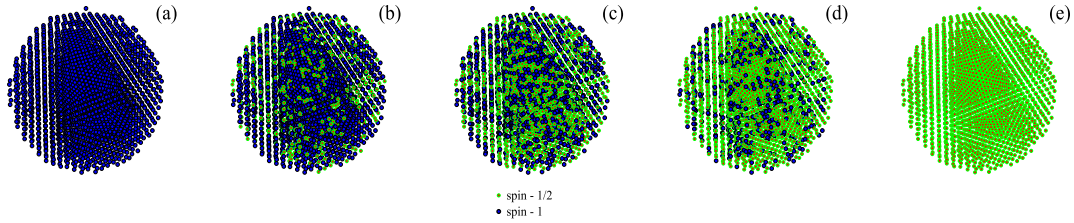

Fig. 1. Schematic representations of the binary alloy spherical nanoparticle of the type A_pB_{1-p} for five selected active concentration values of magnetic components, namely (a) $p = 0$, (b) $p = 0.25$, (c) $p = 0.5$, (d) $p = 0.75$ and (e) $p = 1$.