Monte Carlo study of the possibility of two compensation points in a ferrimagnetic core/shell nanoparticle Ising model

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Abstract: Monte Carlo simulation has been used to study the magnetic properties and the critical behaviors of a single spherical nanoparticle, consisting of a ferromagnetic core of spin-1/2 surrounded by a ferromagnetic shell of spin-3/2 with antiferromagnetic interface coupling, located on a simple cubic lattice. We find a number of characteristic phenomena. In particular, the effects of the shell coupling and the interface coupling on both the critical and compensation temperatures are investigated. We have found that, for appropriate values of the system parameters, two compensation temperatures may occur in the present system.

Keyword: Nanoparticles, Compensation point, Ising model, Monte Carlo simulations.
PACS : 75.50.Tt, 75.40.Mg, 75.75.+a, 05.10.Ln

I. Introduction

Magnetic nanoparticle systems have been receiving considerable attention by both experimental and theoretical researchers [1-6]. A driving motivation in this research is the interest in industrial applications of the emerging nanotechnologies, mainly in the area of information storage [7], sensors [8], permanent magnets [9] and medical applications [10]. These systems have been studied by a variety of techniques, including Monte Carlo simulation [11], variational cumulant expansion method (VCE) [12], mean-field approximation and effective-field theory [13], Green's function technique [14] and differential operator technique with the approximated Van der Wearden identity [15].

Ferrimagnetic materials are currently the subject of a great deal of interest due to their potential technological applications. The occurence of a compensation point has great technological importance, since at this point only a small driving field is required to change the sign of the resultant magnetization. At the compensation temperature, the coercivity of the material increases dramatically facilitating the process of writing and erasing in magneto-optical media [16]. Many efforts have been devoted to study the magnetic properties of ferrimagnetic systems. Based on classical Heisenberg model, Iglesias et al. studied the spherical maghemite ferrimagnetic nanoparticles by using Monte Carlo simulation. They found that the strong surface anisotropy is responsible for a change in the magnetization reversal mechanism of the particle and may lead to the spin configuration in the particle forming a hedgehog-like structure [17]. In order to study the magnetization behavior of a nanoparticle, spherical core-shell model with ferromagnetic core surrounded by a disordered ferrimagnetic surface shell is proposed, it is shown that dynamical effects have a sizeable influence on the exchange bias (EB) properties provided that a strong shell random anisotropy is assumed [18]. Leite et al. [19] have studied the compensation behaviour of a ferrimagnetic small particle on an hexagonal substrate, and they have shown that the particle exhibits one compensation point. In a recent work [20], we have investigated the critical and compensation phenomena of a ferromagnetic core/shell nanocube using Monte Carlo simulation. We have shown that

the compensation temperature exists only below critical values of the shell J_{sh}/J_c and interface $|J_{Int}|/J_c$ interactions and that it increases when J_{sh}/J_c or $|J_{Int}|/J_c$ increases.

The aim of this paper is the study the effects of the shell coupling, the antiferromagnetic interface coupling and the crystal field on the behaviour of the critical temperature and the compensation temperature of an Ising ferrimagnetic core/shell nanoparticle, using Monte Carlo simulations. The outline of this paper is as follows: In Section 2, we give the model and the formalism. In Section 3 we present the results and discussions, while section 4 is devoted to a brief conclusion.

II. Model and formalism

We consider an Ising ferrimagnetic core/shell nanoparticle model with spherical shape of radius R, located on a simple cubic lattice. Three regions are

distinguished inside the particle: a ferromagnetic core with radius Rc, a ferromagnetic shell of thickness Rsh=R-Rc and the ferrimagnetic core/shell interface that is formed by the core (shell) spins having nearest neighbors on the shell (core). The sites of the core are occupied by spins σi, which take the spin values ±1/2, while those of the shell are occupied by spin Sk, which takes the spin values ±3/2 and ±1/2. In the Monte Carlo simulation based on the heat-bath algorithm [21], we apply free boundary conditions in all directions.

The Ising Hamiltonian can be expressed as

$$H = -J_c \sum_{\langle ij \rangle} \sigma_i \sigma_j - J_{sh} \sum_{\langle kl \rangle} S_k S_l - J_{Int} \sum_{\langle ik \rangle} \sigma_i S_k - D \sum_k S_k^2 \qquad (1)$$

The first sum runs over pairs neighboring in the core, the second sum runs over pairs in the shell, and the third sum runs over pairs which interact across the interface between the core and the shell of the particle. Jc, Jsh and JInt are the exchange interactions between nearest-neighbors magnetic atoms in the core, shell of the particle and between nearest-neighbors spins across the core-shell interface of the nanoparticle (JInt<0). D represents the crystal field interaction. At each temperature, typically between 2×104 and 5×104 Monte Carlo steps per spin (MCS) were used for computing averages of thermodynamic quantities after 104 initial MSC has been discarded for equilibration.

The magnetization per spin in the core and the shell are defined by:

$$m_c = \frac{1}{N_c} \sum_{i=1}^{N_c} \sigma_i \qquad (2)$$

and

$$m_{sh} = \frac{1}{N_{sh}} \sum_{k=1}^{N_{sh}} S_k, \qquad (3)$$

and the total magnetization per site is,

$$M_T = \frac{m_c + m_{sh}}{2} \qquad (4)$$

The total susceptibility □T is defined by

$$\chi_T = \beta N(\langle M_T^2 \rangle - \langle M_T \rangle^2, \qquad (5)$$

with □□1/kBT, N=Nc+Nsh

At the compensation point the total magnetization must vanishes. Then, the compensation temperature can be determined by the crossing point between the absolute values of the magnetizations msh and mc. Therefore, at the compensation point, we must have

|msh(Tcomp)|=|mc(Tcomp)|, (6)

and

sign[msh(Tcomp)]=-sign[mc(Tcomp)]. (7)

The critical temperature are determined from the maxima of the susceptibility curves.

III. Results and discussions

In this section, we study the effect of the antiferromagnetic interface coupling on the compensation temperature of an Ising ferrimagnetic spherical nanoparticle model with core/shell morphology using the Monte Carlo simulation technique. In figure 1, we present the phase diagrams of the particle in the (T/Jc, |JInt|/Jc) plane with Jsh/Jc=0.1, Rc=9, Rsh=3 and for different values of the anisotropy D/Jc. We note that, there exists a critical value (|JInt|/Jc)c of the ratio |JInt|/Jc below which the critical temperature remains constant, and then increases with |JInt|/Jc. Concerning the compensation behavior, we can see that the system presents a compensation temperature for a given range of |JInt|/Jc, which increases when D/Jc is decreased. We can also see that the system can presents two compensation points for a certain range of |JInt|/Jc, this range increases when we decrease D/Jc.

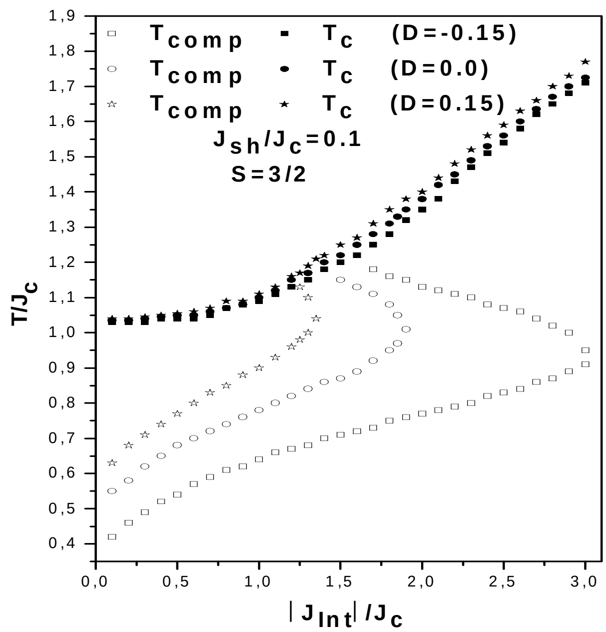

FIG. 1: The phase diagram in (T/J_c, J_{Int}/J_c) plane for J_{sh}/J_c=0.1 and for different value of D/J_c.

To investigate the influence of the crystal field D/Jc on the behavior of the compensation temperature of the particle, we have presented the phase diagrams in the (T/Jc, D/Jc) plane for Jsh/Jc=0.1, Rc=9, Rsh=3 and JInt/Jc=-1 in figure 2 and JInt/Jc=-1.7 in figure 3. The filled and open symbols denote the transition temperature Tc and compensation temperature Tcomp, respectively. It is clear that for JInt/Jc=-1 (fig. 2) the system may present only one compensation temperature. It is also clear that the compensation temperature increases with D/Jc and disappears when D/Jc>0.32. In figure. 3 (JInt/Jc=-1.7), we can remark that the system exhibits two compensation points for -.225≤D/Jc≤0.025. When D/Jc>0.025 there is no compensation point, whereas for D/Jc<-0.225, only one compensation point exists. We can observe that in both figures, the transition temperature is nearly constant.

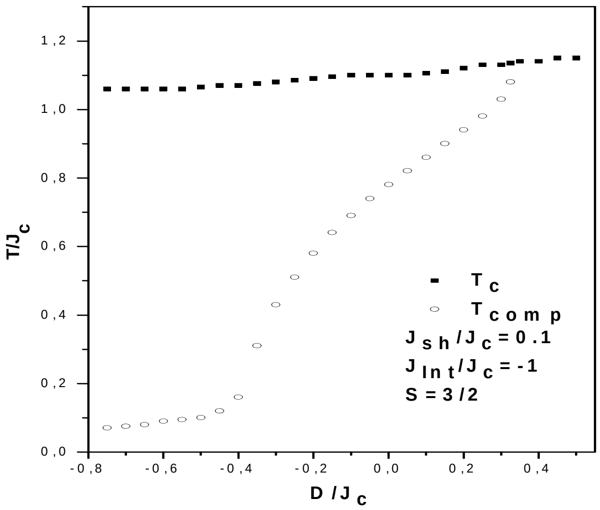

FIG. 2: *The phase diagram in (T/J_c, D/J_c) plane for J_{sh}/J_c=0.1 and for J_{Int}/J_c=-1.*

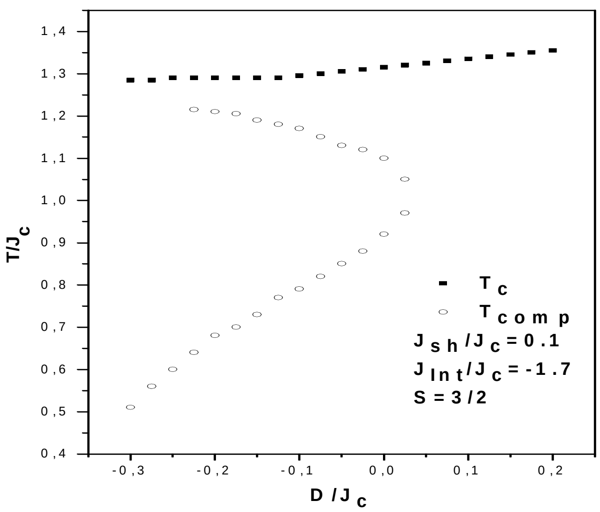

FIG. 3*: The phase diagram in (T/J_c, D/J_c) plane for J_{sh}/J_c=0.1 and for J_{Int}/J_c=-1.7.*

In order to show the effect of the parameter Jsh/Jc on both the compensation and the critical temperatures. We have presented in figure 4 the critical temperature (filled symbols) and compensation temperature (open symbols) versus Jsh/Jc with JInt/Jc=-0.25 and for different values of D/Jc. From this figure, we find a critical value (Jsh/Jc)c of the ratio of the shell coupling to the core one Jsh/Jc which depends on the value of D/Jc (for example for D/Jc=-0.3, (Jsh/Jc)c=0.24). We remark that when Jsh/Jc is less than the critical value (Jsh/Jc)c, Tc is constant and is independent of D/Jc. When Jsh/Jc is greater than (Jsh/Jc)c, Tc increases linearly with Jsh/Jc and depends on D/Jc. On the other hand, the variations of the compensation temperature is very influenced by the variations of Jsh/Jc and D/Jc. It is seen that the compensation temperature increases linearly with Jsh/Jc for Jsh/Jc< (Jsh/Jc)c and disappears when Jsh/Jc is greater than (Jsh/Jc)c.

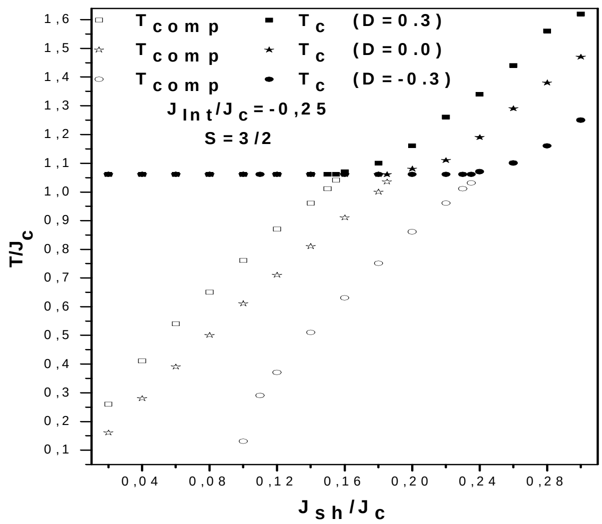

FIG. 4 : *The phase diagram in (T/J_c, J_{sh}/J_c) plane for J_{Int}/J_c=-0.25 and for different value of D/J_c*

IV. Conclusion

In summary, we have studied the magnetic properties and the compensation behaviors of a spherical ferrimagnetic core/shell nanoparticle on an Ising model, located on a simple cubic lattice, where we have taken a coupling constants Jc and Jsh for the core and the shell respectively, and an interface coupling constant JInt between nearest-neighbors spin across the core-shell with JInt<0. Using Monte Carlo techniques we have discussed the influence of the shell coupling, the interface coupling and the crystal field on the critical and compensation temperatures. We have shown that depending on the values of the parameters Jsh/Jc, JInt/Jc and D/Jc the system can exhibit one or even two compensation temperatures.

Acknowledgement : This research is a part of the "Programme Thématique d'appui à la Recherche Scientifique" PROTARS III D12/08. The authors would like to thank the support of CNRST and all the organizations.

V. References

[1] V. Skumryev, S. Stoyanov, Y. Zhang, G.C. Hadjipanayis, D. Givord, J. Nogués, Nature **423**, 850 (2003).
[2] C. Frandsen, C.W. Ostenfeld, M. Xu, C.S. Jacobsen, L. Keller, K. Lefmann, S. Morup, Phys. Rev. B **70**, 134416 (2004).
[3] J. Nogués, J. Sort, V. Langlais, S. Doppiu, B. Dieny, J.S. Munoz, S. Surinach, M.D. Baro, S. Stoyanov, Y. Zhang, Int. J. Nanotechnology **2**, 23 (2005).
[4] H. Kachkachi, J. Magn. Magn. Mater. **316**, 248 (2007).
[5] J. Bansmann, S. H. Baker, C. Binns, J.A. Blackman, J.-P. Bucher, J. Dorantes-Davila, V. Dupuis, L. Favre, D. Kechrakos, A. Kleibert, K.-H. Meiwes-Broer, G.M. Pastor, A. Perez, O. Toulemonde, K.N. Trohidou, J. Tuaillon, Y. Xie, Surface Science Reports **56**, 189 (2005).
[6] D. Kechrakos, K. N. Trohidou, J. Magn. Magn. Mater. **226**, 261 (2004).
[7] R.H. Kodama, J. Magn. Magn. Mater. **200**, 359 (1999).
[8] G. V. Kurlyandskaya, M. L. Sanchez, B. Hernando, V. M. Prida, P. Gorria, and M. Tejedor, Appl. Phys. Lett. **82**, 3053 (2003).
[9] H. Zeng, J. Li, J. P. Liu, Z. L. Wang, and S. Sun, Nature (London) **420**, 395 (2002).
[10] C. Alexiou, A. Schmidt, R. Klein, P. Hulin, C. Bergemann, and W. Arnold, J. Magn. Magn. Mater. **252**, 363 (2002).
[11] M. Vasilakaki and K. N. Trohodou, J. Phys. D: Appl. Phys. **41**, 134006 (2008).
[12] H. -Y. Wang, Y. -S Zhou, E. Wang, D. L. Lin, Chin. J. Phys. **39**, 85 (2001).
[13] T. Kaneyoshi, Phys. Stat. Sol. (b) **242**, 2938 (2005).
[14] D. A. Garanin, H. Kachkachi, Phys. Rev. Lett. **90**, 65504 (2003).
[15] A. F. Bakuzis, P. C. Morais, J. Magn. Magn. Mater. **272**, e1161 (2004).
[16] H. P. D. Shieh and M. H. Kryder, Appl. Phys. Let. **49**, 473 (1986).
[17] O. Iglesias, A. Labarta, Physica B **343**, 286 (2004).
[18] K.N. Trohidou, M. Vasilakaki, L. Del Bianco, D. Fiorani, A.M. Testa, J. Magn. Magn. Mater. **316**, 82 (2007).
[19] V. S. Leite, M. Godoy and W. Figueiredo, Phys. Rev. B **71**, 094427 (2005).
[20] A. Zaim, M. Kerouad and Y. El Amraoui, J. Magn. Magn. Mater. **321**, 1077 (2009).
[21] M.E.J. Newman and G.T. Barkema, Monte Carlo Methods in Statical Physics (Clarendon Press, Oxford, 1999).