Monte Carlo investigation of mixed spin Ising 2D-nanoparticles

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Abstract
The magnetic properties of mixed spin-1/2 and spin-1 Ising 2D-nanoparticles (circle and square) with core–shell structure are examined by the use of the Monte Carlo simulation. The phase diagrams are investigated and show qualitatively interesting features. In particular, three and four physically different phases are identified for the square and circle nanoparticles, respectively. These phases are separated by different transitions that could be called ordinary, core and shell transitions according to the strengths of the exchange interactions.

1. Introduction
In recent years, special attention has been paid to the magnetic properties of the nanomaterials such as nanoparticles, nanorods, nanobelts, nanowires and nanotubes, from both theoretical and experimental points of view. This is due to their promising applications in nanotechnology. They can be used in biomedical applications [1, 2], biosensors [3], nonlinear optics [4], permanent magnets [5], environmental remediation [6] and information storage devices [7, 8]. At present, the scientists arrive to fabricate such kinds of fine nanoscaled materials [9, 10], and the magnetization of certain nanomaterials such as γ-Fe₂O₃ nanoparticles has been experimentally measured [11]. In particular, magnetic nanowires and nanotubes such as ZnO [12], FePt, and Fe₅O₄ [13] can be synthesized by various experimental techniques and they have many application in nanotechnology [14, 15]. They are also utilized as raw materials in fabrication of ultra-high density magnetic recording media [16–18]. On the other hand, the magnetic properties of the nanometric scale materials show some unexpected properties. These latter are strictly related to their sizes and dimensions.

Theoretically, Ising model has been successfully used to explain many characteristic phenomena of nanomagnetic systems using a variety of techniques, including mean field theory [19–21], effective field theory with correlations [22–25], Monte Carlo simulation [26–29], variational cumulant expansion method [30, 31], and Green’s function techniques [32].

Recently, the study of two sublattice mixed spin systems have become one of the actively studied subject in statistical physics. It has also been applied successfully to the investigation of materials with a nanostructure [33–35]. They are of interest for the following main reasons. The first one is that they have less symmetry than their single-spin counterparts. The second one is that they are well adapted to study a certain type of ferrimagnetism [36], and finally many new phenomena are observed in these systems, which cannot be seen in the single-spin Ising model [37].

The magnetic properties in nanoparticles are strongly influenced by the existence of the surface. This is because the finite size effects and the reduced coordination of the surface spins, which are inherent to the nanoparticle, cause a fundamental change in the magnetic order at the surface that produces some effect on the inner spins of the nanoparticle [38, 39]. In fact, due to their reduced coordination number, the shell atoms have less translational symmetry and the exchange interaction between two adjacent shell atoms is different than that of the core atoms. As a consequence of these facts, the shell may exhibit an ordered phase even if the core itself is disordered.

In a very recent work [40], we have studied the magnetic properties of the mixed spin transverse Ising 2D-nanoparticles, using finite cluster approximation. For instance, it has been shown that all sublattice-
magnetizations vanish at a unique transition temperature. Thus the shell and the core undergo an order-disorder transition at the same temperature for any strength of the exchange interactions.

The aim of this paper is to investigate the mixed spin Ising nanoparticles consisting of spin-1/2 and spin-1 for two different shapes (circle and square) by the use of Monte Carlo simulation according to the Metropolis algorithm [41], we study the influence of the various exchange parameters on the phase diagram. In particular, we examine systematically how the core–shell coupling affects the core and shell magnetic behavior.

Our presentation is as follows. In section 2, we briefly present the model and give out the expressions used during the simulation. The numerical results and discussions are arranged in section 3.

2. Model and formulation

We consider two kinds of 2D-nanoparticles (circle and square), as depicted in figure 1. They are described by a mixed spin Ising model consisting of surface shell and core. The sites of the core are occupied by a central spin \( \sigma \) surrounded by spins \( S \), while those of the shell are occupied by spins \( \sigma \).

The Hamiltonian of the system is given by

\[
H = -J_1 \sum_{(i,j)} \sigma_i \sigma_j - J \sum_{(m,n)} S_m S_n - J_1 \sum_{(i,m)} \sigma_i S_m - J_2 \sum_{(k,m)} \sigma_k S_m
\]  

where the summations stand for the nearest neighbours spins. \( J_1 \) is the exchange interaction between two nearest neighbour magnetic atoms at the surface shell. This latter is coupled to the next shell in the core with the exchange interaction \( J_1 \). \( J \) is the exchange interaction between spins \( S_i \) in the core. \( J_2 \) is the exchange interaction between the central site \( \sigma_k \) and the sites \( S_m \) belonging to the first ring.

The method that we adopt in the study of the mixed spin nanoparticles (circle and square) consisting of spin-1/2 and spin-1 described by the Hamiltonian (1) is the Monte Carlo simulation (MC) with the use of a standard importance sampling method. The spin configurations were generated by sequentially traversing the lattice and making single-spin flip attempt, which are accepted or rejected according to the Metropolis algorithm. Data are generated with \( 5 \times 10^4 \) Monte Carlo steps per spin after discarding the first \( 10^4 \) steps per spin.

Our system consists of three shells, namely one shell of the surface and two shells in the core. The surface shell contains \( N_{\text{shell}} \) spins-1/2. The outer boundary of the core contains \( N_S \) spins-1 and \( N_{\text{center}} = 1 \) concerning the central site of the core with spin-1/2. Thus the core contains \( N_{\text{core}} \) spins (\( N_{\text{core}} = N_S + N_{\text{center}} \)). The total number of spins is \( N_T = N_{\text{shell}} + N_{\text{core}} \).

- \((N_{\text{shell}} = 12, N_S = 6, N_{\text{center}} = 1)\) and \((N_{\text{shell}} = 16, N_S = 8, N_{\text{center}} = 1)\) are respectively, the spin numbers of circle and square 2D-nanoparticles.

The magnetization \( M \) of a configuration is defined by the sum over all the spin values of the lattice sites. The order-disorder transition temperature is determined from the peak of the susceptibility.

The magnetizations per site are calculated from

\[
M_{\text{shell}} = \frac{1}{N_{\text{shell}}} \sum_{i=1}^{N_{\text{shell}}} \sigma_i
\]
The total magnetization per site is defined by

\[ M_{\text{core}} = \frac{1}{N_{\text{core}}} \left( \sum_{i=1}^{N} S_i + \sigma_i \right) \]  

(3)

The shell and core susceptibilities per site are calculated from

\[ \chi_{\text{shell}} = \beta N_{\text{shell}} (M_{\text{shell}} - \langle M_{\text{shell}} \rangle^2) \]  

(5)

\[ \chi_{\text{core}} = \beta N_{\text{core}} (M_{\text{core}}^2 - \langle M_{\text{core}} \rangle^2) \]  

(6)

with \( \beta = 1/K_B T \) and \( K_B \) is the Boltzmann’s constant and \( T \) denotes the temperature.

In the present work, we consider that the shells at the surface and in the core interact with each other via the same coupling \( (J_1 = J_2) \), and all interactions as well as the temperature are normalized with the exchange interaction \( J_2 \).

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**Figure 2.** Phase diagrams in \((T/J_1, J/J_2)\) plane, of the (a) square and (b) circle nanoparticles.
3. Results and discussion

We have performed our calculations, to study the magnetism of both nanoparticles, in $J/J_z - T/J_z$ parameter plane. We are first concerned with the evaluation of the order-disorder transition temperatures for the shell and core orderings. These transitions $T_c$(shell) and $T_c$(core) are determined from the maximum of the shell and core magnetic susceptibilities, respectively.

As is shown in figure 2, the square and circle nanoparticles have qualitatively different phase diagrams. Indeed, for square nanoparticle, as shown in figure 2(a), three physically different phases are identified. These phases are indicated on the phase diagram by the following symbols: SF, CF (both shell and core are ferromagnetic), SP, CP (both shell and core are paramagnetic), SP, CF (shell paramagnetic and core ferromagnetic). These phases are separated by different transition lines. In order to denote these transitions, we use the following symbols and terminology: (o) ordinary transition, (s) shell transition, and (c) core transition. As is seen from this figure, if the ratio $R = J/J_z$ is less than a critical value $R^o = (J/J_z)^o$, the nanoparticle (shell and core) order at the same transition temperature (for instance, for $J/J_z = 4$, $(J/J_z)^o = 0.900$). This is the ordinary phase transition. If $R$ is larger than $R^o$, the nanoparticle exhibits two successive transitions. First, the core may ferromagnetically order at a temperature $T_c$(core) while the shell is still paramagnetic. Secondly, as the temperature is lowered, the shell orders at a shell transition temperature $T_c$(shell). These two phase transitions are called the core and shell transitions respectively. As can be expected, $(J/J_z)^o$, $T_c$(core) and $T_c$(shell) depend on the value of the shell coupling. For circle nanoparticle, the phase diagrams are shown in figure 2(b). In addition to the three phases SFCF, SPCP, SFCF, a fourth phase is identified namely SFCP (shell ferromagnetic and core paramagnetic). As seen in the figure, the ordinary transition (o) is reduced, for the circle shape, to a single point $(R^c = (J/J_z)^c$, $T_c/J_z)$ in the phase diagram, which depends on shell coupling $J_z$. In addition to this ordinary transition, the circle nanoparticle may exhibit four other types of transitions: two shell transitions and two core transitions. Indeed, for $R > R^o$, the system may exhibit two transitions $(S_1)$ and $(C_1)$ similar to those transitions (S) and (C) found for the square nanoparticle. On the other hand, the non-existence of ordinary transition line gives rise to two transition lines denoted in the phase diagram by $(S_2)$ and $(C_2)$. In fact, for $R < R^o$, the nanoparticle undergoes two successive transitions. First, the shell may ferromagnetically order (SFCP) (second kind of shell transition $(S_3)$) whereas the core is paramagnetic. Secondly, as the temperature is lowered, the core orders (SFCF) (second kind of core transition $(C_2)$). All core and shell transitions are determined from the peaks of core and shell susceptibilities, respectively. As is shown in figure 3, the corresponding peaks are located on different or at the same transition temperature according to the shape of the nanoparticle and the strength of the ratio $J/J_z$ in comparison with the critical value $(J/J_z)^o$.

Since the location of this latter critical ratio depends on the shell coupling, we plot in figure 4 the variation of $R^c$ with $J_z/J_z$. In fact, for the square nanoparticle, the curve presented in figure 4(a) separates the domain where the shell and core order at the same transition temperature $T_c$(core) $= T_c$(shell)) from the domain where $T_c$(core) $> T_c$(shell). Similar curve for the circle nanoparticle is drawn in figure 4(b) indicating the two domains which correspond, respectively, to the cases $T_c$(core) $> T_c$(shell) and $T_c$(core) $< T_c$(shell). As clearly seen from the figures, $(J/J_z)^c$ increases with increasing values of the shell coupling.

Figure 3. Magnetic susceptibilities versus $T/J_z$ for (a) square and (b) circle nanoparticles, with selected values of $J/J_z$ and $J_z/J_z$.
On the other hand, in figures 5(a), (b) we present in \((T_c(\text{core}) / J_2, J / J_2)\) plane the phase diagrams for square and circle nanoparticles for some selected values of the shell coupling \(J_s\). As is clearly shown in these figures, for a fixed value of \(J_s\), the core order-disorder transition temperature increases gradually with the increase of \(J\). We note that for relatively low strength of this interaction, \(T_c(\text{core})\) increases with \(J_s\). This dependence is less and less sensitive for higher values of the core coupling, and the core transition temperature becomes completely independent of \(J_s\) for any strength of the shell coupling \(J_s\). It is worthy to indicating that, in our very recent work [38], we found similar behaviors for 2D-nanoparticle with circle and square shape by the use of the finite cluster approximation.

4. Conclusions

In this work, we have investigated the mixed spin Ising nanoparticles consisting of spin-1/2 and spin-1 for two different shapes (circle and square) by the use of the Monte Carlo method. We have been mainly interested in the calculation of the phase diagram for the both kind of nanoparticles. Their phase diagrams are qualitatively...
different. Indeed, for square nanoparticle, three physically different phases are identified according to the
temperature and the strengths of the exchange interactions: (i) both shell and core are ferromagnetic, (ii) both
shell and core are paramagnetic and (iii) shell paramagnetic and core ferromagnetic. For the circle nanoparticle,
in addition to the above phases, we identified a fourth phase where the shell is ferromagnetic whereas the core is
paramagnetic. All these phases are separated by transition lines that could be called ordinary, core and shell transitions.

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References

[1] Alexiou C, Schmidt A, Klein R, Hullin P, Bergemann C and Arnold W 2002 J. Magn. Magn. Mater. 252 363
[2] Soundarya N and Zhang Y 2008 Rec. Pat. Biomed. Engin. 1 34
[3] Kuryla-Maksakaya G V, Sanchez M L, Hernando B, Frida V M, Gorria P and Tejedor M 2003 Appl. Phys. Lett. 82 3053
[4] Nie S and Emory S R 1997 Science 273 1102
[5] Zeng H, Li J, Liu J P, Wang Z L and Sun S 2002 Nature 420 395
[6] Elliott D W and Zhang W X 2001 Environ. Sci. Technl. 35 4922
[7] Hayashi T, Hirono S, Tomita M and Umemura S 1996 Nature 381 772
[8] Kodama R H, Berkowitz A E, McNiff J E and Foner J S 1996 Phys. Rev. Lett. 77 394
[9] Ruhrig M, Khamshempour B, Kirk K J, Chapman J N, Atchison P, McVitie S and Wilkinson C D W 1996 IEEE Trans. Magn. 32 4452
[10] Scherfl T, Fidler J, Kirk K J and Chapman J N 1997 J. Magn. Magn. Mater. 175 193
[11] Martinez B, Obraadors X, Balcells L, Rouanet A and Monty C 1998 Phys. Rev. Lett. 80 181
[12] Fan Z and Lu J G 2006 Int. J. High-speed Electron. Systems 16 883
[13] Su Y C, Skomski R, Sorge K D and Sellmyer D J 2004 Appl. Phys. Left. 84 1525
[14] Skomski R 2003 J. Phys. Condens. Matter. 15 R841
[15] Schlörb H, Haehnel V, Khatri M S, Srivastav A, Schultz L and Fähler S 2010 J. Magn. Magn. Mater. 322 3014
[16] Wang H, Zhou Y, Lin D L and Wang C 2002 Phys. Status Solidi B 247 2364
[17] Leite V S and Figueiredo W 2005 Physica A 356 379
[18] Kenyoshi T 2009 Phys. Status Solidi B 246 2359
[19] Michael F, Gonzalez C, Mujica V, Marquez M and Ratner A M 2007 Phys. Rev. B 76 224409
[20] Kenyoshi T 2010 J. Magn. Magn. Mater. 322 3014
[21] Canko O, Erdinç A, Taskin F and Atis M 2011 Phys. Lett. A 375 3547
[22] Sarli N and Keskin M 2012 Solid State Commun. 152 354
[23] Boughrara M, Kerouad M and Zaim A 2014 J. Phys.: Condens. Mater. 26 79
[24] Eglesias O, Battle X and Labarta A 2007 J. Phys.: Condens. Matter. 19 406232
[25] Vasilakaki M and Trohidou K N 2009 Phys. Rev. B 79 144402
[26] Vasilakaki M and Trohidou K N 2009 Phys. Rev. B 79 144402
[27] Wang H, Zhou Y, Lin D L and Wang C 2002 Phys. Status Solidi B 232 254
[28] Wang H, Zhou Y, Wang E and Lin D L 2001 Chin. J. Phys. 39 85
[29] Garanin D A and Kachkachi H 2003 Phys. Rev. Lett. 90 65504
[30] Leite V S, Godoy M and Figueiredo W 2005 Phys. Rev. B 71 094427
[31] Zaim A, Kerouad M and El Amraoui Y 2009 J. Magn. Magn. Mater. 321 1077
[32] Canko O, Erdinç A, Taskin F and Tildirim A F 2012 J. Magn. Magn. Mater. 324 508
[33] Néel L 1948 Ann. Phys. (Paris) 3 137
[34] Alba-yarik E and Keskin M 2003 J. Magn. Magn. Mater. 261 196
[35] Kodama R H, Makhlof S A and Berkowitz A E 1997 Phys. Rev. Lett. 79 1393
[36] Makhlof S A, Parker F T, Spada F E and Berkowitz A E 1997 J. Appl. Phys. 81 5561
[37] Mouhib M, Benayad N and Azhari M 2016 J. Magn. Magn. Mater. 419 325
[38] Metropolis N, Rosenbluth A W, Rosenbluth M N, Teller A H and Teller E 1953 J. Chem. Phys. 21 1087
[39] Kantar E, Deviren B and Keskin M 2013 Eur. Phys. J. B 86 233