Study of Mixed Spin (1, 3/2) in Ferrimagnetic Ising Nanowire

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Abstract

A ferrimagnetic mixed spin square Blume-Capel Ising nanowire system depend of spin-1 core and spin-3/2 outer shell have been investigated. The general formula for the temperature dependence of the equilibrium magnetization of the system is presented. The ferrimagnetic core-shell nanosystem shows a compensation point when the exchange interactions are changed at various values of the single-ion anisotropies of shell sublattices and core ones, respectively. So, one can examine interesting phenomena are compensation behaviors and the free energy of the nanosystem, where these phenomena found that the mixed-spin square Blume-Capel Ising nanosystem which is being considered has two spin compensation temperatures in the range of $-0.8 \le D_B |J_1| \le -0.4$, when $J_3 = -0.7$, for two different values of core anisotropy for sublattices of atoms A, $D_A |J_1| = 0$, and $D_A |J_1| = 1.0$, respectively.

Keywords: Magnetization , Ising Model , Compensation point , Crystal field , Square lattice.

1.Introduction

Recently, I drew a lot of attention towards understanding the magnetization processes and related applications. Thus, magnetic wires have provided ground very successful test to understand the microscopic mechanisms that determine the important parameters ostensibly in different applications [A.K. Srivastava and A.DakhamaN]. It revealed the development of nanowire arrays of tiny magnetic different extraordinary properties relevant applications in data storage devices and in highdensity bio-engineering applications [E. Vatansever]. B. Deviren and Y. Sener studied magnetic properties of nanoparticles mixed Ising spin with the basic structure / shell using the effective field with links theory. The researchers found that the system gives new behaviors under the domain crystal effect, core and shell interactions and coupling interface on phase diagrams. In this paper we have investigated the magnetic properties of a ferrimagnetic mixed spin-1 and spin-3/2 square Blume-Capel Ising nanowire system, for a series of molecular based magnets, which is numerically solved by using the mean-field approximation(MFA), in order to clarify the physical background for the characteristic phenomena observed in the ferrimagnetic mixed nanowire models. It is contained in the work as follows. In Section 2, we offer briefly the basic framework of the theory of the average field and give Hamilton of mixed ferrimagnetic spin-(1,3/2) square Blume-Capel Ising nanowire system. In Section 3, numerical results for phase diagrams, the study of the magnetization of the system in detail. Finally, the conclusion is offered in Section 4.

2. Model and Formalism

The proposed model contains of a ferrimagnetic square nanowire consists of the spin-1 core for atoms A and spin-3/2 outer shell for atoms B, respectively, as shown in Figure(1):



Figure1: Square Blume-Capel Ising nanowire with core-shell structure. Each square represents a plaquette consisting of one core spin and four shell spins.

The Hamiltonian of the nanosystem, in the absence of external magnetic field, is written as [4]

$$H = -J_1 \sum S_i^A S_j^B - J_2 \sum S_i^A S_i^A - J_3 \sum S_j^B S_j^B - D_A \sum S_i^{A^2} - D_B \sum S_j^{B^2}$$
(1)

where (S_i^A, S_j^B) takes the values $(\pm 1, \pm \frac{3}{2})$; and D_A is a magnetic anisotropy acting on A-atoms(core anisotropy), D_B is a magnetic anisotropy acting on B-atoms (shell anisotropy). J_1 is the near neighbor exchange parameter between magnetic atoms across the core and the outer shell. J_2 is the nearest neighbor exchange parameter between magnetic atoms in the core. J_3 is the exchange interaction at the outer shell.

The free energy of the nanosystem is obtained from a mean field calculation of the Hamiltonian based on the Bogoliubov inequality [D. J. Sellmyer5]:

$$A \le \Phi = A_0 + \langle H - H_0 \rangle_0 \tag{2}$$

where A is the Gibbs free energy of H given by relation (1), that:

$$A = -k_B T \ln Z \tag{3}$$

 A_0 is the Gibbs free energy of a paramagnetic phase and H_0 a trial Hamiltonian depend on variation parameters, that:

$$A_0 = -k_B T \ln Z_0 \tag{4}$$

 Z, Z_0 are the true partition function and trial one respectively.

In this research we consider one of the possible choices of H_0 , namely:

$$H_{o} = -\sum_{i} [\lambda_{1} s_{i}^{A} + \gamma_{A} (s_{i}^{A})^{2}] - \sum_{j} [\lambda_{2} s_{j}^{B} + \gamma_{B} (s_{j}^{B})^{2}]$$
(5)

 S_i^A taking the values of spins for core-atoms, and S_j^B taking the values of spins for shell-atoms. Whereas λ_1 , λ_2 , γ_A , and γ_B are the variational parameters related to the different spins and the anisotropies of the two sublattices proposed(i.e., the core and shell anisotropies), respectively. Then, the approximated free energy can be obtained by minimizing the right side of equation (2) with respect to variational parameters mentioned above. Thus, Eq.(2) can be expressed as,

$$f \equiv \frac{\Phi}{N} = -\frac{1}{\beta} \{\ln(a+1) + 4\ln b\} + J_1 z_1 m_A m_B + J_2 z_2 m_A^2 + 4J_3 z_3 m_B^2$$

(6)

with,

$$a = 2e^{\beta D_A} \cosh \beta \lambda_1$$
; $\lambda_1 = J_1 z m_B + 2J_2 z m_A$; $z_1 = z_2 = z_3 = z$

and,

$$b = 2e^{\frac{9}{4}\beta D_B} \cosh\frac{3}{2}\beta \lambda_2 + 2e^{\frac{1}{4}\beta D_B} \cosh\frac{1}{2}\beta \lambda_2 ; \quad \lambda_2 = \frac{1}{4}J_1 z m_A + 2J_3 z m_B$$

with,

$$m_{A} = \frac{2\sinh\{t_{1}z_{1}m_{B} + t_{2}z_{2}m_{A}\}}{2\cosh\{t_{1}z_{1}m_{B} + t_{2}z_{2}m_{A}\} + 2e^{-\beta D_{A}}}$$
(7)

$$m_{B} = \frac{1}{2} \frac{3\sinh\{\frac{3}{2}t_{1}z_{1}m_{A} + \frac{3}{2}t_{3}z_{3}m_{B}\} + e^{-2\beta D_{B}}\sinh\{\frac{1}{2}t_{1}z_{1}m_{A} + \frac{1}{2}t_{3}z_{3}m_{B}\}}{\cosh\{\frac{3}{2}t_{1}z_{1}m_{A} + \frac{3}{2}t_{3}z_{3}m_{B}\} + e^{-2\beta D_{B}}\cosh\{\frac{1}{2}t_{1}z_{1}m_{A} + \frac{1}{2}t_{3}z_{3}m_{B}\}}$$
(8)

where, $\beta = \frac{1}{K_B T}$, z is the coordination number of the lattice.

It is worth mentioning that the case ferrimagnetic shows that signs magnetizations different sublattice, and there can be a point of compensation, which total longitudinal magnetization of each site is equal to zero [Fathi Abubrig].

3. Results and discussion

The magnetic phase transitions has been investigated numerically by the use of mean-field approximation (MFA), in order to clarify the physical background for the characteristic phenomena observed in the ferrimagnetic mixed nanowire models. The effect of single-ion anisotropies (i.e., crystal fields) on the compensation phenomenon have been taken into consideration. Besides, we have shown the effect of exchange interactions on the magnetization curves and the phase transition of these systems. Let us consider the thermal variation dependence of the total magnetization for a mixed spin-1 and spin-3/2 square Blume-Capel Ising nanowire as shown in Figure2, Figure3, respectively.

We found some compensation behaviors for square-type nanowire, at different values of $D_A|J_1|$ and $D_B|J_1|$, when $J_1 = -1, J_2 = -1, J_3 = -0.75$, respectively. Fig. 2. reveals interesting phenomena regards compensation temperatures in the range of $0 \le D_A|J_1| \le 3$, for different values of

 $D_B / |J_1| = -1.0, -0.9, -0.8, -0.7, -0.6, -0.5$. One can observe, Fig.2, when $1 \le D_A |J_1| \le 3$, shows a multi-compensation behavior for different $D_B / |J_1| = -1.0, -0.9, -0.8, -0.7, -0.6, -0.5$, respectively. It is worth to note that the compensation point caused by the presence of magnetic variation of atom- B, it is only possible is in the magnetic phase. This magnetizations sublattice undergo to cancel but it is still incomplete so there is spontaneous magnetization of the remaining in the system(M \neq 0), this is evidence to the antiferromagnetic near neighbor interactions[T. Kaneyoshi].



Figure2: The temperature dependences of the total magnetization *M* for a ferrimagnetic mixed-spin square Ising nanowire with, $J_1 = -1$, $J_2 = -1$,

$$J_3 = -0.75$$

This interaction tends to align the spins adjacent in opposite directions as the rising temperature of the system, and therefore the direction of this residual magnetization can switch because of the thermal excitation. The compensation



Figure 3: The temperature dependences of the total magnetization *M* for a ferrimagnetic mixed-spin square Ising nanowire at different values of D_A and, D_B when $J_1 = -1$, $J_2 = -1$, $J_3 = -0.75$.

behaviors shown in Figuress.(2,3) indicate the crossing points between the magnitudes of m_A and m_B which prove the eligibility of Eqs.(7) and (8).

B. Boughazi et al studied a hexagonal nanowire consisting of a ferromagnetic spin-1/2 core and spin-3/2 outer shell coupled with ferrimagnetic interlayer coupling by the use of Monte Carlo simulation. The authors draw a total magnetization versus temperature for some specific values of $R_s(J_s/J)(0,0.05,and0.10)$, respectively. As is clear from these criteria that the system displays the temperature and one compensation. One can compare our results interesting with those [T. Kaneyoshi].

On the other hand, Figure 3, shows the temperature dependence of the total magnetization M for a ferrimagnetic mixed spin Ising nanowire system, with $J_1 = -1$, $J_2 = -1$, $J_3 = -0.75$. One can be observe that nanosystem has two compensation points when $D_A|J_1|=1.0$, and $D_B|J_1|=-0.8$, for $J_1 = -1$, $J_2 = -1$, $J_3 = -0.75$. This is in good agreement with the possibility of compensation in the other two points of

nanosystem that have been discussed in the reference.[T. Kaneyoshi and V. F. Puntes].

Now let us discuss the temperature dependence of the total magnetization M for the mixed spin Ising nanowire ferrimagnetic system with , $J_1=-1$, $J_2=-1$, for $J_3=-1.0$, and $J_3=-0.7$, respectively. In Fig.4, that the system has two compensation points at a fixed value of $D_A|J_1|=0$ and different values of $D_B|J|$, in particular for $J_3=-0.7$. This is in good agreement with the possibility of compensation in the other two points nanosystem that are discussed as in reference.[V. F. Puntes].

From the two figures(5,6), one can found interesting features, i.e., the possibility of multicompensation temperatures are particularly induced, when $D_A |J_1| = 0$, $J_3 = -0.7$, in the range of $-0.8 \le D_B |J_1| \le -0.6$, respectively.



Figure 4 :The temperature dependences of the total magnetization M at constant values of $D_A = 0$ and different values of D_B for $J_1 = -1$, $J_2 = -1$

Conclusions

We have investigated a ferrimagnetic mixed spin-(1,3/2) square Blume-Capel Ising nanowire system by using the mean-field treatment. The effect of single-ion anisotropies(i.e., crystal fields) on the compensation phenomenon have



Figure5: The temperature dependences of the total magnetization m at constant values of $D_A = 0$ and different values of D_B , when $J_2 = -1$, for $J_3 = -0.8, -0.75, -0.7$, respectively.

been taken into consideration. It has carefully changed the magnetic anisotropies so that one can study the phenomena of interest are the behaviors of compensation in which these phenomena are found that the mixed-spin square Blume-Capel Ising nanosystem which is being considered has one compensation temperature when the core anisotropy is in the range $1.0 \le D_A / |J_1| \le 5.0$ at $D_B / |J_1| = -0.8$, for $J_1 = -1$, $J_2 = -1$, $J_3 = -0.75$. Besides, our nanosystem has two spin compensation temperatures in the range of $-0.8 \le D_B |J_1| \le -0.4$, when $J_3 = -0.7$, for two different

values of core anisotropy for sublattices of atoms A, $D_A|J_1|=0$, and $D_A|J_1|=1.0$, respectively. It have been shown that the appearance of spin compensation points is independent of D_A ; however D_A influences the magnitudes of these points in the temperature space. On the other hand, from the point of view of the pilot, it was synthesized quasi-one-dimensional heterotrinuclear complex $[NiCr_2(bipy)_2(C_2O_4)_4(H_2O)]H_2O$, which shows a rare case of antiferromagnetism between Ni(II)S = 1 and Cr(III)S = 3/2.



Figure 6: The thermal dependence of the total magnetization m at constant values of D_B =- 0.8and different values of D_A , when $J_2 = -1$, for $J_3 = -0.8, -0.75, -0.7$, respectively.

References

[A] A.K. Srivastava, R.S. Singh, K.E. Sampson, V.P. Singh and R.V. Ramanujan, Metallurgical and Materials Transactions A ,38A, 717. 2007.
[A] A.DakhamaN.Benayad, J.Magn.Magn.Mater,213,117(2000).
[B] B. Boughazi, M. Boughrara, M. Kerouad, Physica A, 465, 628(2017).
[E] E. Vatansever, H. Polat, J.Magn.Magn. Mater.,343,221, 2013.
[D] D. J. Sellmyer, M. Zheng, R. Skomski, J. Phys.: Condens. Matter ,213, ,R433. 2001.

[F] Fathi Abubrig, Open J. Applied Sciences, 3,270. 2013.
[T] T. Kaneyoshi, J. Phys. Chem. Solids, 87, 104(2015).
[T] T. Kaneyoshi, Solid Stat. Commun., 244,51(2016).
[V] V. F. Puntes, K. M. Krishnan and A. P. Alivisatos, Science, 291, ,2001,2115.

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الخلاصة:

تم دراسة نظام ايزنك نانوي فيريمغناطيسي مختلط يتكون من عزوم 1 في النواة وعزوم 3/2 في الغلاف لشبيكة مربعة تخضع لقوانين بوم كايبل. تم تقديم العلاقة الاساسية لتمغنط التوازن المعتمد على درجة الحرارة الخاصة بالنظام. النظام النانوي الفيريمغناطيسي المتكون من نواة-غلاف يظهر نقطة تعادل عندما تكون قيم معامل التفاعل المتبادل متغيرة ولعدة قيم من المجالات البلورية الخاصة بغلاف الشبيكة الفرعية ونواتها. من الممكن ان نلاحظ ظاهرة مهمة سلوك التعادل بالاضافة للطاقة الحرة للنظام النانوي حيث وجدنا ان هذه لظاهرة الموجودة بنظام ايزنك لبرم مختلط والخاضعة لقوانين بلوم كيبل قيد دراسة بحيث يملك نقطتيان تعادلتين لمدى من القيم المجالات البلورية و هي 0.4 مان النانوي حيث وجدنا ان هذه لظاهرة الموجودة بنظام ايزنك لبرم مختلط والخاضعة لقوانين بلوم كيبل قيد دراسة بحيث يملك نقطتيان تعادلتين مدى من القيم المجالات البلورية و هي 0.4 مان النانوي حيث وجدنا ان هذه لظاهرة الموجودة المدى من القيم المجالات البلورية و هي 0.4 مان الناوي الشبيكة الفرعية مان الماني يادما تكون قيم , المدى من القيم المجالات البلورية من المجالات البلورية النام النانوي الم مانيك الفرعية مان القرار الماني الماني المانين المانين المانين المانين المانين المانين المان الناني المانين المان الفري المانين المان التوانين المانين المانية المارة الموجودة إلى المانين المانين المانين المان النانوي حيث وجدنا ان هذه لظاهرة الموجودة الما والمانين المانين المانيان المانين ا

الكلمات المفتاحية: التمغنط نموذج ايزنك درجة حرارة التعادل المجال البلوري الشبيكة المربعة.