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The Influence Study of Crystal and External Magnetic Fields on the Compensation Temperatures in a Decorated Mixed Spin Ferrimagnet

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Abstract:

It has been dealt with the framework of developed mean-field theory for a decorated ferrimagnet of two sublattices by using Blume-Capel Ising model. Based on particular variations of the spin crystal fields for both interpenetrated lattices, new features of long-range orders have been obtained in this research. For a decorated square lattice consists of spin-3/2 and decorating spin-5/2 ions on the bonds, it has been observed characteristic results. Multicompensation temperatures were induced for the present system. It is worth to note that the contribution of total magnetization to the superparamagnetism phenomenon production of the decorated mixed spin ferrimagnet with $J_1 = -0.5$, $J_2 = -1.0$, has been indicated as well. So, characteristic total magnetization behaviors in the $(M, D_B / |J_2|)$ space has not previously been considered.

Keywords: Decorated mixed-spin model; Developed mean field theory; Spin crystal fields; Ferrimagnetic compensation temperatures; Superparamagnetism.

1. Introduction

Material sciences and engineering have been guided during the last decades to synthesize and to apprehend the novel materials which enable a precise understanding of ordered phenomena in magnetic solids[1,2]. Mixed spin magnetic models have been examined for studying molecular magnetic materials used in the applications of thermo-magneto recording. Recently, smart magnetic systems are investigated for important applications in diverse research fields on the critical behaviors show a compensation phenomenon[3-5]. Low-dimensional molecular ferrimagnets have been attracting much experimental and theoretical interest, such as bimetallic chains of $ACu(pbatOH)3n(H_2O)$ with $A = Ni, Co, Fe$ and Mn [6,7]. Besides, experimental evidence shows that the magnets $AFe^{II}Fe^{III}(C_2O_4)_3$ have a layered

honeycomb structure in which two kinds of magnetic atoms (Fe^{II} and Fe^{III}) alternate regularly, and they show characteristic ferrimagnetic properties[8-12]. R. Masrour et al. [8] used Monte-Carlo simulation to research a mixed spin-3/2 and spin-5/2 ferrimagnetic models. The researchers studied the magnetic properties for decorated square and triangular lattices, respectively, testing the effect of exchange interactions and crystal field on the magnetization of the considered systems. However, A. Jabar and R. Masrour[7] determined the ground state phase diagrams and examined the magnetic properties of mixed spin-5/2 and spin-2 Ising models on a decorated square lattice. The authors found important that the systems exhibit the superparamagnetism behavior. It is worthy note that this paper is a continued work of the obtained results by R. Masrour et al.[8], and outstanding researchers as indicated in Refs.[13-16], respectively. Here, we have discussed within the developed mean field theory(DMFT) a decorated ferrimagnetic Blume-Capel system with finite anisotropic and external field interaction taking into consideration the influence of nodal or decorating ions for obtaining spin compensation temperatures. The effect of anisotropic domains on the compensation temperatures is the pivot of this correspondence. In return, characteristic phenomena observed in the proposed mixed ferrimagnetic models exhibit the superparamagnetism behavior. The magnetic compensation behaviors of our model may be investigated to clarify the characteristic behaviour of the molecule-based magnetic material $Cs_2Mn^{II}[V^{II}(CN)_6]$ is prepared by the addition of manganese(II)($S_B = 5/2$) triflate to aqueous solutions of the hexacyanovanadate(II)($S_A = 3/2$) ion at $0^\circ C$ [1]. The research paper comprises, in Sections 2, a formalism of the Hamiltonian operator and its developed mean field method. For Section 3, it has been studied the possibility of induction of a compensation behavior for the present system under the influence of specific negative values of the spin crystal fields. Besides, we have examined the variations of the global magnetizations against the nodal and decorating crystal anisotropies at $T = 0.5, 0.75, 1.0, 1.5, 1.75 K^\circ$, respectively.

2. Model and Formalism

It is well-known that the cooperative phenomena is a main basis in the study of the assembling interaction influence to describe a mean field proportional to the average moment of a magnetic model. It is important to study a decorated mixed spin ferrimagnetic Blume-Capel system is parted into two sublattices L_1 and L_2 , as shown in Fig.1. Every point of L_1 is taken by an A atom with the fixed spin $\sigma_A = \frac{3}{2}$ that of L_2 , composed of singular decorating point on each point bond of L_1 , is occupied by a B atom with a static spin $\sigma_B = \frac{5}{2}$. The exchange interaction between A and B atom is presumed to

be antiferromagnetic. Besides, one can propose that there exists an antiferromagnetic exchange interaction between every bordering neighbour pairs of atoms. However, the system is designated, in the presence of an external magnetic field h , by the Hamiltonian operator[16,17,18], as follows:

$$H = -J_1 \sum_{i,j} \sigma_i^A \sigma_j^B - J_2 \sum_{i,j} \sigma_j^B \sigma_j^B - D_A \sum_i (\sigma_i^A)^2 - D_B \sum_j (\sigma_j^B)^2 - h \left(\sum_i \sigma_i^A + \sum_j \sigma_j^B \right) \quad (1)$$

where the spins $\sigma_i = \pm \frac{1}{2}, \pm \frac{3}{2}$, and $\sigma_j = \pm \frac{1}{2}, \pm \frac{3}{2}, \pm \frac{5}{2}$, are localized in sublattices L_1 and L_2 , respectively. $J_1 (J_1 < 0)$ and $J_2 (J_2 < 0)$ are the exchange interactions. D_A , and D_B are the spin crystal fields and the summations are achieved precisely over nearest-neighbours pairs of spins. The Hamiltonian equation, i.e., Eq.(1) may be rewritten as,

$$H = H_A + H_B \quad (2)$$

that,

$$H_A = -J_1 \sum_{i,j} \sigma_i^A \sigma_j^B - D_A \sum_i (\sigma_i^A)^2 - h \sum_i \sigma_i^A \quad (3)$$

and,

$$H_B = -J_1 \sum_{i,j} \sigma_i^A \sigma_j^B - J_2 \sum_{i,j} \sigma_j^B \sigma_j^B - D_B \sum_j (\sigma_j^B)^2 - h \sum_j \sigma_j^B$$

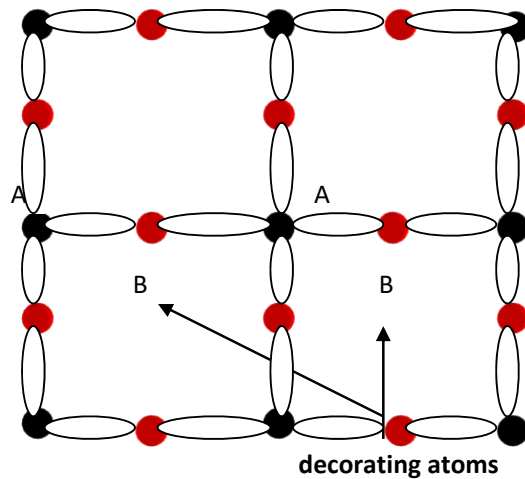


Fig.1. A two-dimensional decorated spin system consisting of two magnetic atoms A(L1) and B(L2), with spins values of 3/2(black balls) and spin=5/2(red balls), respectively.

Now we consider a decorated lattice consisting of N sites. At each site there is an atom or ion has a spin taking two orientations. These cases are described by state variables σ_i , for the spins at the sites i^{th} , which are $\pm\frac{3}{2}, \pm\frac{1}{2}$. In contrast, for state variables σ_j , the spins at the sites j^{th} are $\pm\frac{5}{2}, \pm\frac{3}{2}, \pm\frac{1}{2}$, respectively.

From Eqs.(3), (4), it yields, respectively, using Maxwell-Boltzmann distribution[17,19, 20], that,

$$m_A = \frac{3 \sinh(\frac{3}{2} \beta J_1 z_1 m_B + \frac{3}{2} \beta h) + e^{-2\beta D_A} \sinh(\frac{1}{2} \beta J_1 z_1 m_B + \frac{1}{2} \beta h)}{2 \cosh(\frac{3}{2} \beta J_1 z_1 m_B + \frac{3}{2} \beta h) + 2e^{-2\beta D_A} \cosh(\frac{1}{2} \beta J_1 z_1 m_B + \frac{1}{2} \beta h)} \quad (5)$$

and,

$$m_B = \frac{5 \sinh(\frac{5}{2} \beta K + \frac{5}{2} \beta h) + 3e^{-4\beta D_A} \sinh(\frac{3}{2} \beta K + \frac{3}{2} \beta h) + e^{-6\beta D_A} \sinh(\frac{1}{2} \beta K + \frac{1}{2} \beta h)}{2 \cosh(\frac{5}{2} \beta K + \frac{5}{2} \beta h) + 2e^{-4\beta D_A} \cosh(\frac{3}{2} \beta K + \frac{3}{2} \beta h) + 2e^{-6\beta D_A} \cosh(\frac{1}{2} \beta K + \frac{1}{2} \beta h)} \quad (6)$$

where $K = J_1 z_2 m_A + J_2 z_1 m_B$; and, $\beta = \frac{1}{K_B T}$; z_2, z_1 , are the coordination numbers of the B atoms and the nearest neighbors of the A sublattice, respectively.

The free energy of this configuration is calculated from the Hamiltonian as[7,20,21],

$$F \leq \Phi = F_0 + \langle H - H_0 \rangle_0 \quad (7)$$

F_0 is the free energy of a paramagnetic state and H_0 is a trial Hamiltonian operator be contingent on variational parameters, as,

$$H_o = -\sum_i [\lambda_1 \sigma_i^A + D_A (\sigma_i^A)^2 + h \sigma_i^A] - \sum_j [\lambda_2 \sigma_j^B + D_B (\sigma_j^B)^2 + h \sigma_j^B] \quad (8)$$

these parameters are linked to the distinguishable spins and the crystal fields of the two sublattices, λ_1 , λ_2 , and D_A, D_B , respectively. The approximated free energy f can be obtained by minimizing Eq.(7) with λ_1 , and λ_2 , are variational parameters. Thus, Eq.(7) is evaluated as,

$$f \equiv \frac{\Phi}{N} = -\frac{1}{2\beta} \{ \ln(K_1 + K_2) + \ln(K_3 + K_4 + K_5) \} - \frac{1}{2} (J_1 z_1 m_A m_B + J_2 z_1 m_B^2 - \lambda_1 m_A - \lambda_2 m_B) \quad (9)$$

where,

$$K_1 = 2e^{\frac{9}{4}\beta D_A} \cosh(\frac{3}{2} \beta \lambda_1 + \frac{3}{2} \beta h); \quad K_2 = 2e^{\frac{1}{4}\beta D_A} \cosh(\frac{1}{2} \beta \lambda_1 + \frac{1}{2} \beta h);$$

$$K_3 = 2e^{\frac{25}{4}\beta D_B} \cosh\left(\frac{5}{2}\beta\lambda_2 + \frac{5}{2}\beta h\right); K_4 = 2e^{\frac{9}{4}\beta D_B} \cosh\left(\frac{3}{2}\beta\lambda_2 + \frac{3}{2}\beta h\right);$$

$$K_5 = 2e^{\frac{1}{4}\beta D_B} \cosh\left(\frac{1}{2}\beta\lambda_2 + \frac{1}{2}\beta h\right)$$

and,

$$\lambda_1 = J_1 z_1 m_B ; \lambda_2 = J_1 z_1 m_A + 2J_2 z_1 m_B$$

The ferrimagnetic state displays different signs of sublattices magnetizations, and there can be a point of compensation ($T_{Comp} < T_C$), where T_C is the Curie temperature, that the total magnetization is vanished [10,11, 23,24,25], as,

$$M = \frac{m_A + 2m_B}{3} \tag{10}$$

with the condition, $sign|m_A(T_{Comp})| = -sign|m_B(T_{Comp})|$; $T_{Comp} < T_C$

3. Results and discussion

The developed mean field approximation (DMFA) is used for obtaining characteristic features of a decorated mixed spin-3/2 and spin-5/2 square Blume-Capel Ising model has numerically processed. The proposed model is treated by minimizing Gibbs-Bogoliubov free energy function (Eq.(9)). The work essence is the influence study of spin crystal fields and external magnetic fields on the compensation temperatures. The actions of low temperatures, and magnetic crystal fields, i.e., ferrimagnetic anisotropies, on the curves of magnetization have been applied, one can observe Fig.2. It is worthy note a sublattice magnetization either falls to zero or to another point resulting in a first-order phase transition [10,26]. Whereas, the sublattice magnetization is fast altered that it does go to zero, because the configuration goes through two phases separating the ferrimagnetic or antiferromagnetic phase from the paramagnetic one, so this phenomenon is defined as the second-order phase transition or the Curie transition [27,28]. As shown in Figs.2,3, interesting features have been examined in the $(m_A, T), (m_B, T)$ planes, with $J_1 = -0.5, J_2 = -1.0$, when the values of spin crystal field, $D_B / |J_2|$ are changed. Particularly, in the ranges $-1.25 \leq D_B / |J_2| \leq -0.25$, $-3.5 \leq D_B / |J_2| \leq -2.0$, with fixed values of decorated or nodal fields $D_A / |J_2| = -2.5$, and $D_A / |J_2| = 1.0$, respectively. From the figures, it is shown that the magnetization happens at a temperature in which the magnetizations change discontinuously. That is to say the system experiences a jump which corresponds to the first-order

transition to induce new phases are (2.5,-1.0), (1,-1.5), when $-1.0 \leq D_B / |J_2| \leq -0.25$, $D_B / |J_2| = -2.25$, for $D_A / |J_2| = -2.5$, and $D_A / |J_2| = 1.0$, respectively.

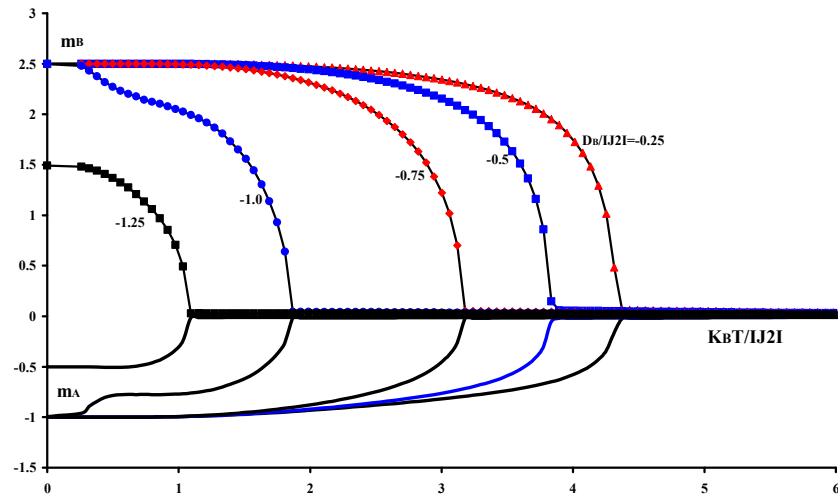


Fig.2. Temperature dependences of the sublattices magnetizations for a decorated ferrimagnetic mixed-spin square system at different values of $D_B / |J_2|$, with fixed value of $D_A / |J_2| = -2.5$, and $J_1 = -0.5, J_2 = -1$.

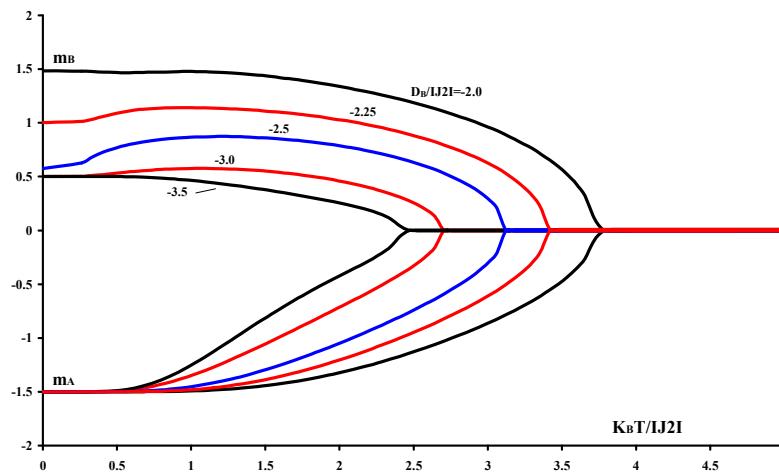


Fig.3. Temperature dependences of the sublattices magnetizations for a decorated ferrimagnetic mixed-spin square system at different values of $D_B / |J_2|$, with fixed value of $D_A / |J_2| = 1.0$, and $J_1 = -0.5, J_2 = -1$.

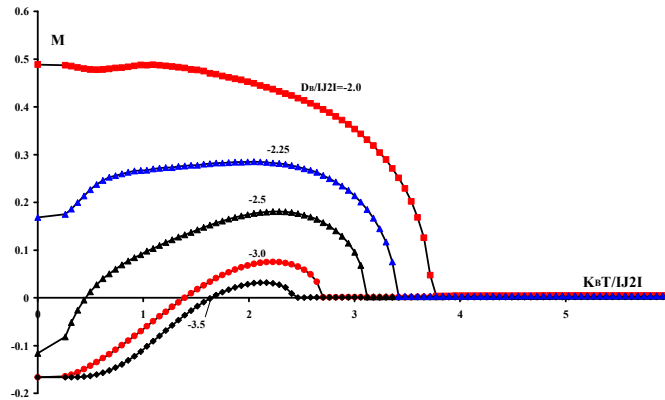


Fig.4. Temperature dependences of the global magnetizations M for a decorated ferrimagnetic mixed spin square system at different values of $D_B / |J_2|$, with fixed value $D_A / |J_2| = 1.0$, and $J_1 = -0.5, J_2 = -1.0$.

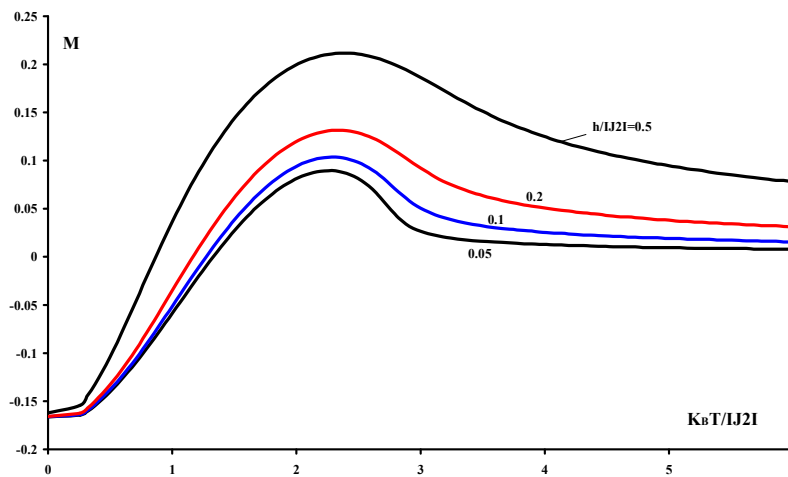


Fig.5. Temperature dependences of the global magnetizations M for a decorated ferrimagnetic mixed spin square system at different values of $h / |J_2|$, with fixed values of $D_A / |J_2| = 1.0$, $D_B / |J_2| = -3.0$ and $J_1 = -0.5, J_2 = -1.0$.

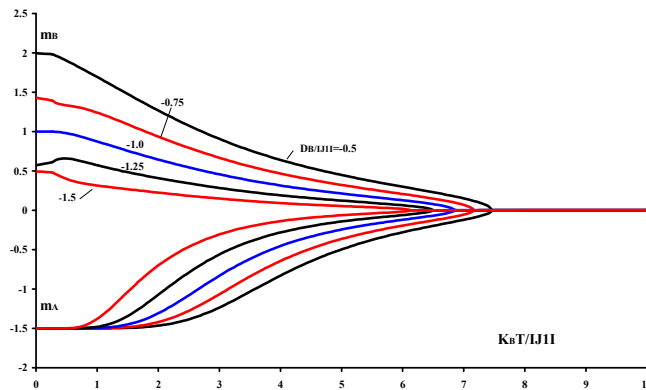


Fig.6. Temperature dependences of the sublattices magnetizations for a decorated ferrimagnetic mixed-spin square system at different values of $D_B/|J_1|$, with fixed value of $D_A/|J_1|=1.0$, and $J_1 = -1.0, J_2 = -0.5$.

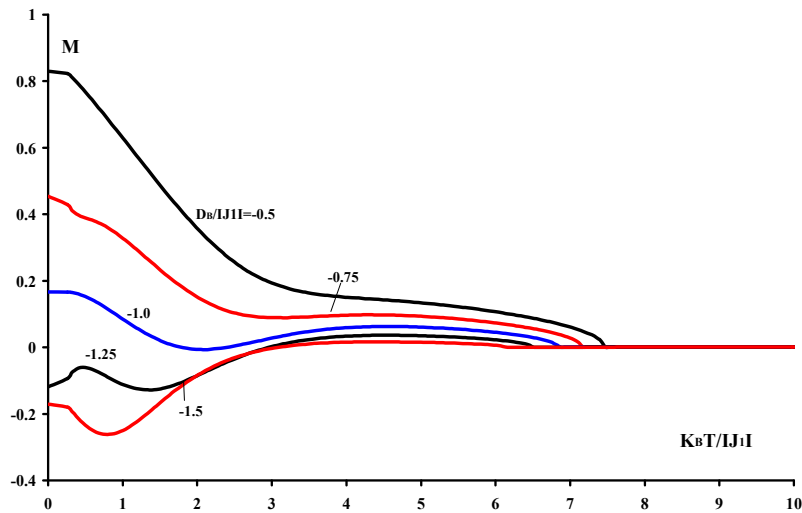


Fig.7. Temperature dependences of the global magnetizations M for a decorated ferrimagnetic mixed spin square system at different values of $D_B/|J_1|$, with fixed value $D_A/|J_1|=1.0$, and $J_1 = -1.0, J_2 = -0.5$.

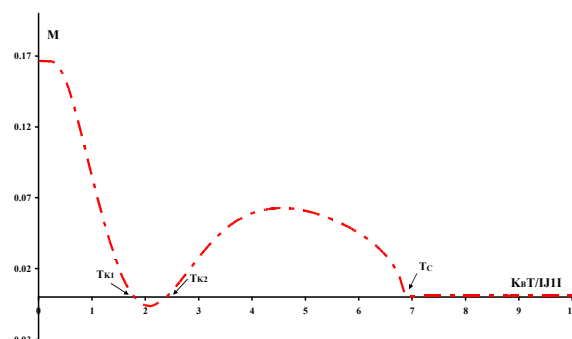


Fig.8. A close view of the temperature dependences of the total magnetization M for the decorated mixed spin square ferrimagnet at a value of $D_B / |J_1| = -1.0$, with fixed values $D_A / |J_1| = 1.0$,

$$h / |J_1| = 0, \text{ and } J_1 = -1.0, J_2 = -0.5.$$

Now let us check Fig.4, which shows the total magnetization versus the absolute temperature for different values of $D_B / |J_2|$ with a fixed value of $D_A / |J_2| = 1.0$. From the figure, one finds that the proposed system may exhibit one spin compensation point $T \neq 0K^\circ$, in the temperature dependence of the magnetization depending on the values of crystal field, i.e., magnetic anisotropies $D_B / |J_2|$ of the sites occupied by B atoms for a particular value of $D_A / |J_2|$. However, in the presence of external magnetic field, the system may induce one compensation point, as well. In this respect, it is numerically obtained a compensation temperature by calculating the coupled equations(i.e., Eqs.(5),(6)) for m_A and m_B , depending on the values of the external magnetic fields $h / |J_2|$, in the range of interesting values of magnetic fields, $0.05 \leq h / |J_2| \leq 0.5$, with fixed values of spin crystal fields $D_A / |J_2| = 1.0$, and $D_B / |J_2| = -3.0$ of the sites occupied by nodal and decorating atoms, respectively(see Fig.5). On the other hand, we have investigated the magnetic properties of the system for a new model, with $J_1 = -1.0$, $J_2 = -0.5$, for different values of $D_B / |J_1|$, at a fixed value of $D_A / |J_1|$. Encouraged results have been obtained in the $(m_{A/B}, T)$, and (M, T) spaces for a decorated ferrimagnetic mixed spin square model, when the values of crystal fields $D_B / |J_1|$ are modified, as shown in Figs.6,7, respectively. Particularly, in the range $-1.5 \leq D_B / |J_1| \leq -0.5$, with fixed values of decorated atoms $D_A / |J_1| = 1.0$, the sublattices magnetizations show characteristic behaviors, as is seen in Fig.6. From the figure, namely, at $T = 0K^\circ$, the sublattices magnetizations m_B , and m_A depend on the negative values of decorating crystal field $D_B / |J_1|$; that is m_B twitches from its maximum values 2.0, 1.0, 1.5, and 0.5, while m_A begins from its

lowest value -1.5, respectively. Since the temperature is increased, so the magnetizations behaviors are strongly subjected to the positive values of $D_A/|J_1|$; for $D_B/|J_1| = -0.5, -0.75, -1.0, -1.25, -1.5$, that the magnetizations tend to be uninterruptedly zero. Fig.7, shows one and two compensation points for different or fixed magnitudes of decorated magnetic anisotropies with the values of $J_1 = -1.0$, $J_2 = -0.5$, respectively. However, as shown from the figure, when $D_B/|J_1| \geq -0.75$, and $D_A/|J_1| = 1.0$, the proposed system has no spin compensation point[18,26]. Fig.8, expresses a close view of the system induction in the plane of temperature dependences of the total magnetization at different values of $D_B/|J_1|$, with fixed value $D_A/|J_1| = 1.0$, and $J_1 = -1.0$, $J_2 = -0.5$, this phenomenon induced in the proposed model, not predicted in the Ne'el theory of ferrimagnetism[28,29].

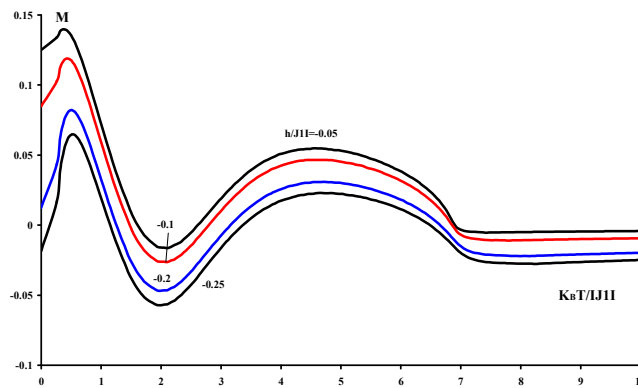


Fig. 9. Thermal variations of the total magnetization M for a decorated mixed-spinsquare ferrimagnet for $D_A/|J_1| = 1.0$, $D_B/|J_1| = -1.0$, and $J_1 = -1.0$, $J_2 = -0.5$ with various values of $h/|J_1|$

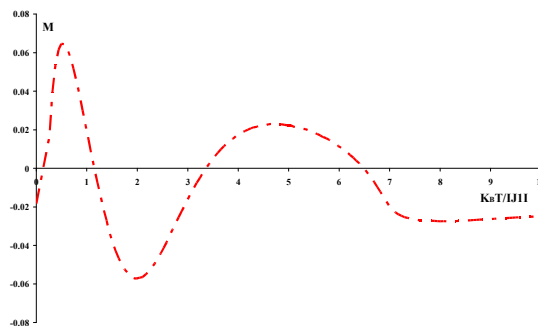


Fig.10. A close view of the temperature dependences of the total magnetization M for the decorated mixed spin square ferrimagnet at a value of $D_B/|J_1| = -1.0$, with fixed values $D_A/|J_1| = 1.0$, $h/|J_1| = -0.25$ and $J_1 = -1.0$, $J_2 = -0.5$.

Once again, in the presence of longitudinal fields, it is found the proposed system has a very interesting feature in the thermal variation of the decorated system magnetization under the influence of an external magnetic field, at a particular value of $D_B/|J_1| = -1.0$, with fixed values of $D_A/|J_1| = 1.0$, $h/|J_1| = -0.25$, and $J_1 = -1.0$, $J_2 = -0.5$, one can observe Fig.10. Our present system may induce more than three compensation points are found easily comparing to the previous works that have been published in Refs.[23,30]. It is worth to note that, the obtained results exhibit an interesting feature of critical temperatures T_K for selective values of negative magnetic fields, in the range $-0.25 \leq h/|J_1| \leq -0.05$ (Fig.9).

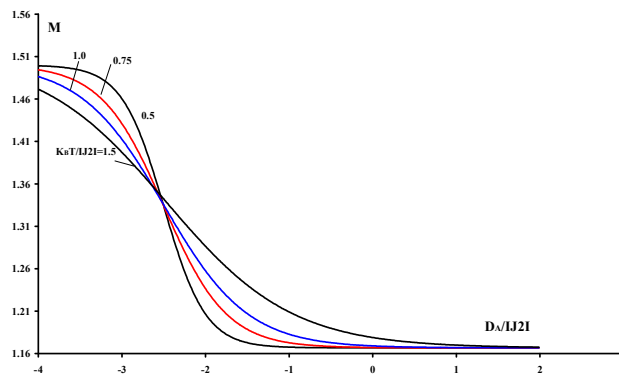


Fig.11. The variations of the global magnetization M versus the crystal field $D_A/|J_2|$ for a decorated ferrimagnetic mixed-spin square system at fixed value of $D_B/|J_2| = 1.0$, with $J_1 = -0.5$, $J_2 = -1.0$.

Fig.11 shows the remanences of the total magnetization as a function of the magnetic anisotropy of a decorated sublattice, i.e., a nodal sublattice, $D_A/|J_2|$, at fixed value of $D_B/|J_2| = 1.0$, with $J_1 = -0.5$, $J_2 = -1.0$. for $T = 0.5, 0.75, 1.0, 1.5 K^\circ$, respectively. As $D_A/|J_2|$ is increased, so the total magnetization is decreasingly changed, namely, when $D_A/|J_2| > -4.0$, i.e., this decrease contributes to the variation of the total magnetization for a decorated ferrimagnet which is being considered. However, the residual magnetization refers to the decorated ferrimagnet is spontaneously magnetized ($M \neq 0$) [26,28]. On the other hand, Fig.12 illustrates with $D_B/|J_2|$ increasing, the total magnetization is slightly changeable at first and then increases when $D_B/|J_2| > -4.0$, i.e., the total magnetization is increased when $D_{BC}/|J_2| \geq -2.14$. So, the magnetization increases quickly to reach saturation value which depends somewhat on the absolute temperature. One compares our results with those of authors [8] who presented comparable studies of magnetic properties of decorated ferrimagnetic mixed spin-3/2 and spin-5/2

Ising systems using the Monte-Carlo simulations. Besides, our present system undergoes the superparamagnetism behavior for a crystal field $D_B/|J_2| = -4.0$, and for this value the total magnetization equals zero[14]. It is found, from Fig.12, that with $D_B/|J_2| = -4.0$, at the absolute temperature $T = 1.75K^\circ$, the system becomes a superparamagnetism. It is clearly Fig.13 shows that our decorated system produces superparamagnetic phenomenon at $T = 1.5K^\circ$, and $1.75K^\circ$ for $D_A/|J_2| = 0.5, 1.0$, with $J_1 = -0.5$, $J_2 = -1.0$, respectively. The examined results are in good agreement with those ones examined by A. Jabar, and R. Masrour[14]. However, the researchers found the total magnetization increases with increasing the crystal field for several values of exchange interactions between nodal and decorating ions and between decorating ones of a square lattice, respectively.

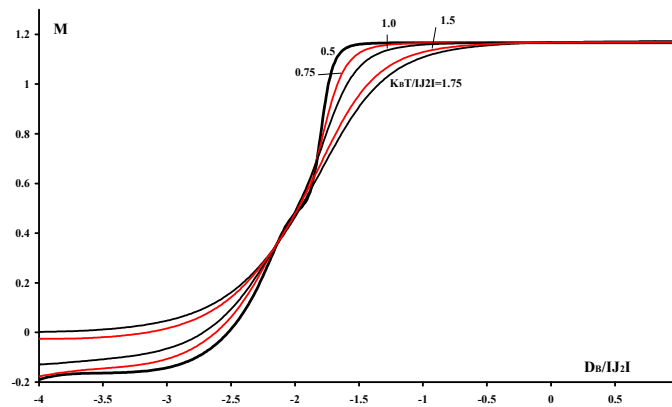


Fig.12. The variations of the global magnetization M versus the crystal field $D_B/|J_2|$ for a decorated ferrimagnetic mixed-spin square system at fixed value of $D_A/|J_2|$, with $J_1 = -0.5$, $J_2 = -1.0$.

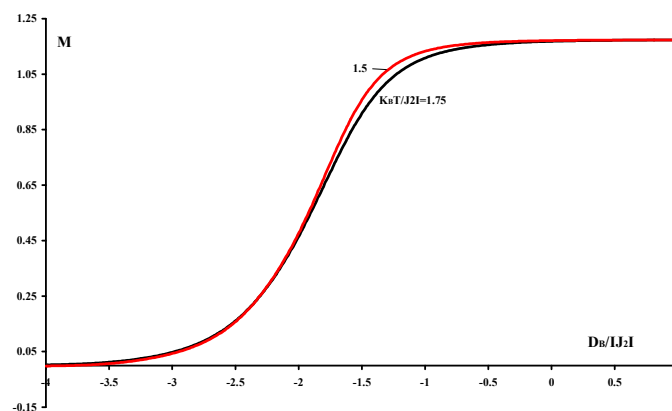


Fig.13. The variations of the global magnetization M versus the crystal field $D_B/|J_2|$ for a decorated ferrimagnetic mixed-spin square system at $D_A/|J_2| = 0.5, 1.0$, and $K_B T/|J_2| = 1.5, 1.75$, with $J_1 = -0.5$, $J_2 = -1.0$, respectively.

4. Conclusions :

In this correspondence the developed mean field theory(DMFT) has been given to induce spin compensation temperatures and to reveal superparamagnetic transition temperatures of a decorated ferrimagnetic mixed-spin(3/2,5/2) square Blume-Capel device. Under the influence of spin crystal fields (i.e., magnetic anisotropies), and external magnetic fields, it has been investigated the proposed system. It is worthy note that the spin crystal fields have been carefully influenced for induction a ferrimagnetic compensation behavior. So, Figs.4,5 illustrate a singular compensation point for specific values of decorating magnetic anisotropies $D_B / |J_2|$ with the values of $J_1 = -0.5$, $J_2 = -1.0$. Furthermore, two or rather more than three compensation temperatures induced in the decorated mixed spin square Blume-Capel system when the decorating crystal fields and magnetic fields are in the ranges $-1.5 \leq D_B / |J_1| \leq -0.5$, or $-0.25 \leq h / |J_1| \leq -0.05$, for $J_1 = -1.0$, $J_2 = -0.5$, one can see Figs.7,9, respectively, giving a new behavior not classified in the Neel theory[29]. The compensation behaviors shown in Figs.4,5,7,8,9 and 10, designate the intersections between the magnitudes of nodal atoms and decorating ones which confirm the suitability of Eqs.(5) and (6), respectively. However, a comparison between our results and with those obtained by M. Boughrara and M. Kerouad, in the decorated Ising film on a cubic lattice structure. The system consists of (1/2,1) ions, in which Monte-Carlo simulation predicts one or two compensation temperatures[30]. As far as we concerned, the magnetization behaviors in the $(M, D_{A/B} / |J_2|)$ planes have not been already considered showing the total magnetization remanence is as a function of crystalline anisotropy(observe Figs.11,12, 13, respectively). It is worthwhile that the novel magnetic behaviors of our proposed model may be examined to clarify the characteristic behavior of the molecule-based magnetic material $Cs_2Mn^{II}[V^{II}(CN)_6]$ is prepared by the addition of manganese(II)($S_B = 5/2$) triflate to aqueous solutions of the hexacyanovanadate(II)($S_A = 3/2$) ion at $0^\circ C$ [1,31].

Conflict of Interest:

It is worthy note the authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this manuscript.

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