Crystalline field effects on magnetic and thermodynamic properties of a ferrimagnetic-centered rectangular structure

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Received: 24 March 2022 / Accepted: 16 August 2022 / Published online: 4 September 2022

Abstract: The phase diagrams and the magnetic properties of the mixed-spin Ising model, with spins $S = 1$ and $\sigma = 1/2$ on a centered rectangular structure, have been investigated using Monte Carlo simulations based on the Metropolis algorithm. Every spin at one lattice site has four nearest-neighbor spins of the same type and four of the other type. We assumed ferromagnetic interaction between the same spins type and antiferromagnetic for different spin types. An additional single-site crystal field term on the $S = 1$ site was considered. We have shown that the crystal field enhances the existence of the compensation behavior of the system. In addition, the effects of the crystal field and exchange coupling on the system’s magnetic properties and phase diagrams have been studied. Finally, the magnetic hysteresis cycles of the system for several values of the crystal field have been found.

Keywords: Crystal field; Mixed-spin Ising model; Monte Carlo simulation; Rectangular lattice; Critical temperature; Compensation temperature

1. Introduction

The topic of mixed spins with different orders is the subject of many areas in physics. For instance, the mixed-spin magnetic systems have been studied vigorously in the last few years by applying different models, such as the Heisenberg model [1], XY-model [2], and Ising model [3], to predict their magnetic and thermodynamic properties. In particular, the mixed-spin Ising model has been used as the simplest model of ferrimagnetic materials. The most crucial property of ferrimagnetic materials is the so-called compensation temperature ($T_{\text{comp}}$) appearance. These non-critical points have zero total magnetization. In contrast, sublattices of the system retain their magnetization against extrinsic effects such as temperature [4]. This phenomenon, in which the total magnetization is zero, can be observed experimentally by tuning the temperature below the critical temperature ($T_c$). Such compensation points have many technological applications, such as thermomagnetic recording media, dynamic and random-access memories, and magneto-optical recording media devices [5–9]. Theoretically, many methods have been used to study these systems based on statistical mechanics, such as renormalization group [10–12], low- and high-temperature series expansion [13–16], finite cluster approximation [17], mean-field theory [18–20], effective field theory [21–23], and Monte Carlo simulations [24–30].

Monte Carlo simulations may be the most reliable method for studying various real/artificial ferrimagnetic material structures in two and three dimensions with various exchange interactions and spins. Numerous studies have examined the crystal field effect on magnetic properties using various spin types [31–38], although many significant structures have not yet undergone detailed investigation.

This paper extends our previous work [24] to include the effects of single-ion anisotropy and applied magnetic fields on magnetization behaviors and compensation points. Monte Carlo techniques will be applied to study the magnetic properties of the magnetic atoms arranged in a 2-D centered rectangular structure. The structure consists of two sublattices: sublattice-A of spin $S = 1$ and sublattice-B of spin $\sigma = 1/2$. Each sublattice has a rectangular structure.

The centered rectangular structure consisting of two sublattices with different coupling strengths (in our case, five different coupling strengths) might be one of the essential structures since this structure can be looked at differently. For example, instead of looking at the structure...
as a two-dimensional structure, one might look at it as a bilayer structure, with one layer consisting of one type of atom arranged in a rectangular sheet. The vertex of a second similar structure layer lies above the center of the first and has a different type of atom. Adding extra bilayers to the structure allows us to study different structures such as bcc and tetragonal structures. Currently, we are in the process of calculating the coupling strengths of FePt, FeNi, FePd and of CoPt, NiPt, CoNiPt2, and of FePt3, CoPt3, NiPt3, and of Fe3Pt, Ni3Pt, Co3Pt using the density functional theory, then applying the Monte Carlo simulations to study the different thermodynamic and magnetic properties of these structures.

2. Model and formalism

2.1. Lattice structure and Hamiltonian

The rectangular structure adopted here is the same as in [24]. It consists of two sublattices-A and B: sublattice-A is composed of S-type of spins-1, whereas sublattice-B is composed of \( \sigma \)-type of spins-1/2 (see Fig. 1). The coordination number of each site is 8. The Hamiltonian of the magnetic structure includes nearest-neighbor interactions; the external magnetic field and the crystal field are given as:

\[
H = -J_1 \sum_{\langle ij \rangle} S_i S_j - J_2 \sum_{\langle lm \rangle} \sigma_i \sigma_m - J_3 \sum_{\langle ik \rangle} S_i S_k - J_4 \sum_{\langle ln \rangle} \sigma_i \sigma_n
- J_{12} \sum_{ij} S_i \sigma_i - B \sum_{ij} (S_i + \sigma_i) - H'
\]

where \( H' \) is defined as follows:

\[
H' = D \sum_i S_i^2
\]

\( H' \) represents the crystal field interaction with sublattice-A. In our simulations, the spin moments of each spin are \( S = 1 \) and \( \sigma = 1/2 \). Hence, we associate the \((2S + 1)\) and \((2\sigma + 1)\) possible spin projections \((-1, 0, 1)\) and \((-\frac{1}{2}, \frac{1}{2})\), respectively. The other possible five interactions in \( H \) are, namely, along [10] direction, \( J_1 \) is the \( S - S \) exchange interaction, \( J_2 \) is the \( \sigma - \sigma \) exchange interaction. Along [01] direction, \( J_3 \) is the \( S - S \) interaction, \( J_4 \) is the \( \sigma - \sigma \) interaction. Diagonally \( J_{12} \) is the \( S - \sigma \) antiferromagnetic interaction. The summation indices \( \langle ij \rangle \) and \( \langle lm \rangle \) represent the sums of all nearest-neighbor spins along [10] direction. The summation indices \( \langle ik \rangle \) and \( \langle ln \rangle \) represent the sums of all nearest-neighbor spins along [01] direction. We have taken \( J_1, J_2, J_3, \) and \( J_{12} \) positive to ensure ferromagnetic interaction and \( J_{12} \) negative to ensure antiferromagnetic interaction. \( D \) can have positive or negative values. In this work, the different values of the exchange parameters are kept the same for all simulations presented here. Those parameters are chosen such that \( T_{comp} \) and \( T_c \) exist and taken from our previous work where the crystalline fields effect is ignored [24].

2.2. Monte Carlo simulation and calculations

The Monte Carlo simulation technique and periodic boundary conditions were applied in the x and y directions. A single spin flip is used to generate new configurations, and each flip is accepted or rejected according to the metropolis algorithm [39]. The total number of spins in our simulation is \( N_{tot} = 2450 \), which contains \( N_A = 35 \times 35 \) spins of the \( S \)-type in sublattice-A and \( N_B = 35 \times 35 \) spins of the \( \sigma \)-type in sublattice-B. No significant differences in the results presented here were found by increasing the number of atoms in one direction L to 50 or 100. Calculation of the error is based on the method of blocks [40]. In this paper, the system’s temperature is measured in units of energy.

The sublattice-A and B magnetization per site can be calculated as

Fig. 1 Centered rectangular structure schematic representation. The filled circles represent sublattice-A with spin 1, and the open circles represent sublattice-B with spin 1/2.
\[ M_A = \frac{1}{N_A} \left( \sum_{i=1}^{N_A} S_i \right) \]
\[ M_B = \frac{1}{N_B} \left( \sum_{i=1}^{N_B} \sigma_i \right) \]
\[ M_{\text{tot}} = \frac{N_A M_A + N_B M_B}{N_A + N_B} \]

The sublattice magnetic susceptibilities are given by
\[ \chi_A = N_A \beta \left( \langle M_A^2 \rangle - \langle M_A \rangle^2 \right) \]
\[ \chi_B = N_B \beta \left( \langle M_B^2 \rangle - \langle M_B \rangle^2 \right) \]
\[ \chi_{\text{tot}} = \frac{N_A \chi_A + N_B \chi_B}{N_A + N_B} \]

where \( \beta = \frac{1}{k_B T} \) is the absolute temperature, and \( k_B \) is the Boltzmann factor. For all numerical calculations, we set the Boltzmann factor to one.

Finally, the specific heat of the system is calculated as:
\[ C_v = \frac{k_B}{N_{\text{tot}}} \left( \langle H^2 \rangle - \langle H \rangle^2 \right) \]

At the compensation temperature, \( T_{\text{comp}} \), the sublattice magnetizations are opposite to each other and equal in magnitude. Hence, we determine \( T_{\text{comp}} \) from the computed magnetization data under the following condition:
\[ |M_A(T_{\text{comp}})| = |M_B(T_{\text{comp}})| \]
\[ \text{sign}(M_A(T_{\text{comp}})) = -\text{sign}(M_B(T_{\text{comp}})) \]

with \( T_{\text{comp}} < T_C \) where \( T_C \) is the critical temperature. In this paper, \( T_C \) is determined from the maximum of the susceptibility curves.

3. Results and discussion

This section will present the magnetic and thermodynamic properties of the mixed-spin ferrimagnetic-centered rectangular structure. The influence of the single-ion crystal field and the external magnetic field on phase diagrams, magnetization, specific heat, and system susceptibility will be discussed. Finally, hysteresis loops will be obtained. Note that the error bars are smaller than the point markers for all figures and do not appear.

3.1. Phase diagrams

Figure 2 illustrates the phase diagram in the \((T, J_1)\) plane for different values of the crystalline field, keeping \(J_2, J_3, J_4, J_{12} \) and \( B \) constant. The figure shows a gradual increase in the critical temperature value while the compensation temperature increases linearly as the value of the exchange coupling \( J_1 \) increases. Furthermore, we have noticed that for any value of the exchange coupling \( J_1 \) the compensation temperature of the system increases as the crystalline field increases. More atoms of sublattice-A prefer to stay in the spin -1 state for positive values of \( D \) and in the spin +1 state for negative values of \( D \) as the temperature increases. It is worth mentioning that for \( J_1 < 0.25 \) the compensation temperature appears only for the easy axis anisotropy case. Furthermore, for \( J_1 \geq 2.5 \), the compensation temperature appears only for the hard axis anisotropy case.

Figure 3 shows a phase diagram of the system in the \((T, D)\) plane at \( J_1 = 4.5, J_3 = 0.1, J_4 = 4.0, J_{12} = -0.1, B = 0 \) and for different values of the crystalline field.
field. The critical temperature of the system stays constant, with the crystal field varying. The figure shows that for $D = 0$, the system exhibits critical and compensation temperatures, which can also be confirmed in Fig. 4. On the other hand, when decreasing the negative value of the crystal field, the compensation temperature decreases. This is because introducing a hard axis anisotropy into the system means a very low temperature is needed to ensure a perfectly ordered sublattice-A. Hence, the crossing point of sublattice-A and B magnetization absolute value decreases, thereby the compensation temperature of the system decreases. Increasing the positive value of the crystalline field results in increasing the system’s compensation temperature, which is due to introducing the easy axis anisotropy in the system, suggesting that a higher temperature is needed to disorder sublattice-A by forming magnetic domains inside it. Hence, the crossing point of sublattice-A and B magnetizations’ absolute value increases, increasing the system’s compensation temperature.

3.2. Magnetic properties

In this subsection, we will present the general trend of the magnetization behavior, specific heat, and the system’s susceptibility as a function of temperature for selected values of the system parameters.

To illustrate the influence of the crystalline field on the specific heat, we have plotted in Fig. 4a the specific heat of the system as a function of temperature in the absence of the external magnetic field for different values of the crystalline field. Increasing the temperature results in increasing the internal energy of the system. At higher temperatures, the internal energy curves approach a point at which the concavity of the curve changes. This point corresponds to the critical temperature at which a second-order phase transition to a paramagnetic phase occurs. Hence, this explains the appearance of the second peak in the specific heat curves at higher temperatures.

On the other hand, decreasing the temperature decreases the internal energy of the system. At lower temperatures, the internal energy curves approach a second point at which the concavity of the curves changes again because of the abrupt drop in the magnetization of sublattice-A due to weak exchange couplings $J_1$ and $J_3$. The concavity change in the internal energy curves at lower temperatures coincides with the compensation temperature location. Hence, this explains the existence of the first peak in the specific heat curves at lower temperatures. It is worth mentioning that the concavity change in the internal energy curves at lower temperatures is a non-critical point, i.e., no phase transition occurs at this point.
In Fig. 4b, we have plotted the system’s specific heat as a function of temperature with an external applied field $B = 0.1$ and the same exchange interaction parameters as in Fig. 4a. Again, one can remark that the location of the critical temperature shifted slightly to the right, which suggests that the critical temperature increases as the value of the external magnetic field increases. For both figures, the value of $D$ does not affect the position of the second peak. However, it affects the position of the first peak. The double-peak phenomenon in specific heat and susceptibility curves has been observed in many systems, such as ferrimagnetic mixed-spin ($5/2, 2$) on a bipartite square lattice [41], triple layer spin ($1$–$1/2$–$1$) cubic system [42], ferrimagnetic mixed-spin ($1, 3/2$) Ising nanowire with a hexagonal core–shell structure [43], and ferrimagnetic mixed-spin ($3/2, 5/2$) in a graphene layer [44].

Figure 5 shows the system’s total magnetization as a temperature function for selected values of the system parameters. In Fig. 5a, we varied the crystalline field for $J_1 = 0.3, J_2 = 4.5, J_3 = 0.1, J_4 = 4.0, J_{12} = -0.1,$ and $B = 0.$ The figure shows L-type magnetization. We observe two magnetization zero points corresponding to the compensation and critical temperatures in the magnetization curves. Note that the first magnetization zero point of each magnetization curve moves left for negative values of the crystalline field, which suggests that the compensation temperature decreases as the negative value of the crystal field increases. On the other hand, increasing the crystalline field’s positive value increases the compensation temperature. The second magnetization zero point corresponds to the critical temperature at which a second-order phase transition to the paramagnetic phase occurs. One can note that by using large negative values of the crystal field, more magnetic domains inside sublattice-A appear even at low temperatures, decreasing the value of the total magnetization. Comparable comportment of the magnetization as a function of temperature has been confirmed in two-dimensional mixed-spin ($1, 1/2$) graphene-like Ising nanoparticles [45], a ferrimagnetic mixed-spin ($2, 5/2$) Ising system on a layered honeycomb lattice [46], and a ferrimagnetic mixed-spin ($2, 5/2$) system on a bipartite square lattice [41].

In Fig. 5b, we have used the same system parameters as in Fig. 5a but at $B = 0.1.$ Again, we have noticed that both critical and compensation temperatures have increased because the applied field tends to orient the spin in its direction.

To see the effect of the crystalline field $D$ on the total magnetization $M$ at a certain temperature $T$, we plot in Fig. 6 the $(M$ vs. $D)$ curve at $T = 1.$ The total
magnetization approaches zero as the crystalline field increases. This increase is attributed to the fact that using large positive values of the crystalline field makes it harder to flip the spin in sublattice-A, decreasing the value of the total magnetization. On the other hand, the absolute value of the total magnetization increases as the hard axis crystalline field increases. The figure also shows the effect of the externally applied field. It shifts the magnetization value to be smaller. This result agreed with that found in Fig. 5.

The magnetic susceptibility $\chi$ versus $T$ at different values of $D$ is shown in Fig. 7a for $B = 0$ and Fig. 7b for $B = 0.1$. The figure shows double peaks where the lower peak indicates the position of $T_{\text{comp}}$ and the higher peak indicates the position of $T_C$. The crystal field effect gives higher susceptibility values at $B = 0$. The results here confirm the magnetization behavior in Fig. 5. Note that the location of the double peaks shifted slightly to the right in the presence of the external magnetic field. Hence, the critical and compensation temperatures increase as the strength of the magnetic field increases. The inset shows the location of the first peak of the susceptibility curves at which the compensation temperature occurs.

Figure 8 shows the hysteresis loops at $T = 1$ for different values of $D$. The figure shows that the magnetization curves reach the saturation value $|M|= 0.75$ faster for the easy axis anisotropy than for the hard axis anisotropy. Simultaneously, remanence magnetization and coercivity increase as $D$ decreases. Furthermore, it is worth mentioning that for the hard axis anisotropy, $D < 0$, more work is needed to reverse the direction of the magnetization. Hence, the area of the loop increases. On the other hand, for the easy axis anisotropy, $D > 0$, less work is needed to reverse the magnetization direction. Hence, the area of the loop decreases.

Figure 9 shows the phase diagram of the antiferromagnetic coupling interaction $J_{12}$ versus the anisotropy constant $D$. The color gradient shows the value of the compensation temperature, whereas the white color in the background demonstrates the values of $J_{12}$ and $D$ at which the compensation behavior of the system disappears. For positive values of $D$, the compensation temperature increases as $|J_{12}|$ increases meaning that you need to increase the temperature to overcome the exchange interaction and flip the spin. However, for negative values of $D$, the compensation temperature could be decreasing, increasing, or increasing, then decreasing as $|J_{12}|$ increase. For example, a competition between the exchange coupling parameter and the crystal anisotropy constant makes the compensation temperature for $D = -1.5$ start increasing and then decreasing as $|J_{12}|$ increases. The lowest compensation temperature occurs for negative values of $D$, and
for these small values to occur, both values of \( D \) and \( J_{12} \) must be close to zero or at relatively high negative values of \( D \) and \( J_{12} \). Also, it is interesting to know that for \( |J_{12}| \leq 0.6 \) and \( |J_{12}| \geq 0.9 \) the compensation temperature increases as \( D \) increases. However, for \( 0.6 < |J_{12}| < 0.9 \) the compensation temperature decreases and then increases as \( D \) increases.

Figure 10 shows the positive part of the hysteresis loop at \( T = 1 \) and different values of crystal anisotropy constant. A larger external field is needed to achieve the same degree of magnetization, \( |M| = 0.75 \), as the anisotropy constant decreases.

Figure 11 shows the magnetization curves as a function of coupling strength \( J_1 \) between \( S \)-type atoms along [10]

direction at \( T = 1 \) for different values of the crystalline field. The intersection points represent the value of the exchange coupling \( J_1 \) at which a compensation behavior in the system is achieved. For both hard and easy axis anisotropies, the value of \( J_1 \) should be small to obtain compensation behavior in the system. However, as \( D \) increases, a smaller interaction constant \( J_1 \) is needed to flip the spin in sublattice-A. For large values of \( J_1 \) sublattices-A and B are entirely ordered at \( T = 1 \), and both hard and easy axis anisotropies have no effect on the direction of the spins in both sublattices, which explains the behavior of the total magnetization of the system \( |M| = 0.25 \).

Figure 12 shows the total magnetization \( M \) as a function of interaction coupling strength \( J_{12} \) at \( T = 1 \) for different values of the anisotropy constant \( D \). From the figure, we
noticed that for strong antiferromagnetic exchange coupling, $J_{12} < 0$, a magnetization value of 0.25 is achieved because all spins of type $\sigma$ are $-1/2$, and type $S$ are 1, which gives a mean value of 0.25. Decreasing the value of $D$ (hard axis), one must strengthen the coupling interaction to achieve saturation. On the other hand, if the interaction between different types of spins is ferromagnetic ($J_{12} > 1$) a constant magnetization of -0.75 is achieved. In this case, all atoms of $\sigma$ type have a value of $-1/2$, and of $S$ type have -1, which gives a mean value of -0.75. The saturation is faster along the easy axis, and you need to increase the value of $J_{12}$ to reach the saturation for negative crystalline fields. The most intriguing point is when the coupling interaction between different spins is zero. At this value, an absolute magnetization value is 0.25 regardless of the anisotropy constant. The value can be achieved when the spins of different types are opposite, i.e., the system is in a ferrimagnetic phase.

4. Conclusions

Using Monte Carlo simulations, we investigated the effect of the crystal anisotropy $D$ on the compensation temperature. Our results showed that increasing $D$ enhances the compensation temperature, and it appears for a wide range of $J_{12}$ values. The remanence, coercivity, and hysteresis loop area increase as $D$ decreases. Large negative values of the crystal field decrease the total magnetization value as it generates more magnetic domains inside sublattice-A even at low temperatures. The critical temperature and the compensation temperature increase as the applied magnetic field or $J_1$ increases. Our system has compensation temperature for small $J_{12}$ values and the sublattices became ordered for large $J_1$ values.

All magnetization versus temperature curves are of the N-type. However, the magnetization is increased gradually with increasing $D$(see Fig. 6). Moreover, the saturation of magnetization is reached faster with increasing $D$. Finally, our data reveal strong anisotropic behavior with varying $D$.

Author’s contribution All authors contributed to the study’s conception and design. In addition, Rama Abu Haifa and Abdalla Obeidat performed data collection and analysis. Maen Gharaibeh wrote the first draft of the manuscript, and all authors commented on previous versions. Finally, all authors read and approved the final manuscript.

Funding The authors declare that no funds, grants, or other support were received during the preparation of this manuscript.

Declarations

Conflict of interest The authors have no relevant financial or non-financial interests to disclose.

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