RESEARCH ON THE CURIE TEMPERATURE OF FERROMAGNETIC SYSTEM BY MONTE-CARLO ALGORITHM

by

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Original scientific paper
https://doi.org/10.2298/TSCI2203619D

The Monte-Carlo algorithm is an effective method to study the Curie temperature of a ferromagnetic system related to its exchange constant, magnetic moment, and co-ordination number. Curie temperatures of the three types of ferromagnetic systems are calculated, e.g., the hexagonal crystal system, the tetragonal system, and the orthorhombic system. In order to make the calculated magnetic moment--temperature curve fit a steep slope, the size of the supercell of the ferromagnetic system is selected as small as possible, and Monte-Carlo steps are performed 5000000 times at each temperature. The calculation reveals a significant result: the Curie temperature scales with the exchange constant and the square of the magnetic moment.

Key words: *Monte-Carlo, Curie temperature, exchange constant, magnetic moment*

Introduction

The diluted magnetic semiconductor is a new type of semiconductor formed by doping magnetic atoms into non-magnetic semiconductor materials. It possesses two properties, including both charge and spin. Therefore, the dilute magnetic semiconductor combines the characteristics of both semiconductor and magnetism, which has set off a research boom of dilute magnetic semiconductors [1]. Ohno [2] systematically studied the preparation technology, magnetic properties, and magnetic testing techniques of dilute magnetic semiconductors. Dietl *et al.* [3] showed that magnetism originated from holes, and they used the Zener model to predict the Curie temperature of some dilute magnetic semiconductors and found AlMnP, GaMnN, ZnMnO had higher Curie temperature. Sato *et al.* [4] proposed the calculation formula of Curie temperature based on the Heisenberg model as $K_B T_c = 2\Delta E/3c$, where K_B is the Boltzmann constant, T_c – the Curie temperature, c – the doping concentration of the magnetic ions, and ΔE – the energy difference between the antiferromagnetic state and the ferromagnetic state calculated by the First Principle. This is a new method to calculate the Curie temperature by the First Principle. The Heisenberg model has shown great success in calculating the Curie temperature of dilute magnetic and semi-metallic ferromagnetic materials [5-10]. In recent years, ferromagnetism has been found not only in single-layer materials [11-15], but also in multi-layer materials [16]. Since the Curie temperature is lower than room temperature (300 K), the practical application of magnetic devices will be limited. Therefore, increasing the Curie temperature of ferromagnetic materials has become a very important re-

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search focus. Although the Heisenberg model was very successful in calculating the Curie temperature, the calculated Curie temperature was always higher than the experimental value. In order to solve the problem, Duan *et al.* [17] constructed three antiferromagnetic states to calculate Curie temperature of materials. Misirlioglu *et al.* [18] used Ising model to calculate Curie temperature of materials, and a large number of researchers used Monte-Carlo algorithm to calculate Curie temperature of materials [11, 12, 14]. Among these calculation methods, the Curie temperature calculated by the Monte-Carlo algorithm is closest to the experimental value. To calculate Curie temperature, T_c, by Monte-Carlo algorithm, the authors need to obtain the ferromagnetic exchange constant, J, co-ordination number, Z, and spin magnetic moment, S, at each position of the magnetic system. Therefore, the quantitative relationship between T_c, and J, Z, and S is studied in detail in this paper.

Computational methods

Monte-Carlo algorithm

The Monte-Carlo algorithm is essentially a kind of stochastic simulation, which transforms a probability problem into a statistical problem to make an analysis. For a 2-D hexagonal system in which the supercell is $L \times L$ with periodic boundary condition, as shown in fig. 1(a), the lattice constant $a = b$, $\gamma = 60°$, and the co-ordination number $Z = 6$. The Hamiltonian describing the system is [12, 19-21]:

$$H = -\sum_{i,j=1}^{L} JS_{i,j}(S_{i,j-1} + S_{i,j+1} + S_{i-1,j-1} + S_{i-1,j} + S_{i+1,j} + S_{i+1,j+1}) \tag{1}$$

where J is the exchange constant of spin at the nearest neighbor position and S – the spin magnetic moment at each position. If $J > 0$, the ground state of the system is ferromagnetic, if $J < 0$, the ground state of the system is anti-ferromagnetic.

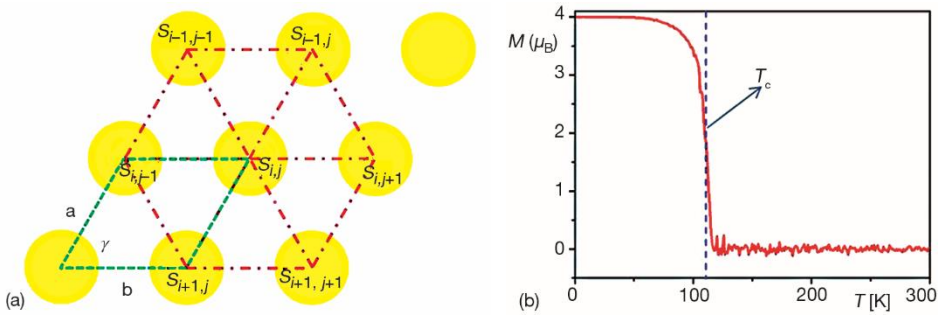

Figure 1. (a) The 2-D hexagonal system, $a = b$, $\gamma = 60°$ and $Z = 6$, (b) the M-T curve of the ferromagnetic system, the temperature corresponding to the inflection point defined as the Curie temperature

Monte-Carlo algorithm steps:

Step 1: At any temperature, T, suppose that the system is in the ferromagnetic ground state and all spins up.

Step 2: Generate a pair of random numbers (i, j), $1 \le i, j \le L$.

Step 3: According to eq. (1), calculate the energy:

$$E_1 = JS_{i,j}(S_{i,j-1} + S_{i,j+1} + S_{i-1,j-1} + S_{i-1,j} + S_{i+1,j} + S_{i+1,j+1})$$

and

$$E_2 = -JS_{i,j}(S_{i,j-1} + S_{i,j+1} + S_{i-1,j-1} + S_{i-1,j} + S_{i+1,j} + S_{i+1,j+1})$$

Step 4: Generate a random number r with a uniform distribution between (0, 1). When $r \leq \exp[-(E_2 - E_1)/(4k_BT)]$, $S_{i,j}$ will turn over once, that is, $S_{i,j} = -S_{i,j}$. When $r > \exp[-(E_2 - E_1)/(4k_BT)]$, $S_{i,j}$ will not turn over and keep the original state.

Step 5: Steps 2-4 are called a complete Monte-Carlo step. Repeat steps 2-4, and the system enters a stable state after enough Monte-Carlo steps.

Step 6: In stable state, calculate the magnetic moment:

$$M = \frac{\sum_{i,j=1}^{L} S_{i,j}}{L \times L}$$

Step 7: Select a wide enough temperature range, calculate M at each temperature, and draw M-T curve, as shown in fig. 1(b), the temperature corresponding to the inflection point of the curve is defined as the Curie temperature of the ferromagnetic system.

Selection of calculation parameters

The Monte-Carlo algorithm, described in section *Monte-Carlo algorithm*, is essentially a probability problem, so theoretically, the larger the parameter L and Monte-Carlo steps, the better the simulation effect. However, too large L and Monte-Carlo steps will greatly reduce the computational efficiency. In order to obtain good calculation results with high efficiency, parameter L and Monte-Carlo steps were calculated and tested to select appropriate L and Monte-Carlo steps.

Firstly, the parameter L was tested. When testing, take $J = 0.638$ meV, $S = 4\mu_B$, steps = 10000, and the M-T curve of the system were drawn when L = 50, 100, 150, 200, 250, and 300, respectively. As shown in fig. 2(a), the larger the parameter L, the smoother the curve. Considering the calculation efficiency and results, L was selected as 200.

Secondly, the parameters Monte-Carlo steps were tested. When testing, take $J = 0.638$ meV, $S = 4\mu_B$, $L = 200$, and the M-T curves of the system were drawn when steps = 1×10^4, 1×10^5, 1×10^6, 3×10^6, and 5×10^6, respectively. As shown in fig. 2(b), the larger the steps, the sharper the inflection point of M-T curve, and the more accurate the simulated T_c. Therefore, steps = 5×10^6 was selected.

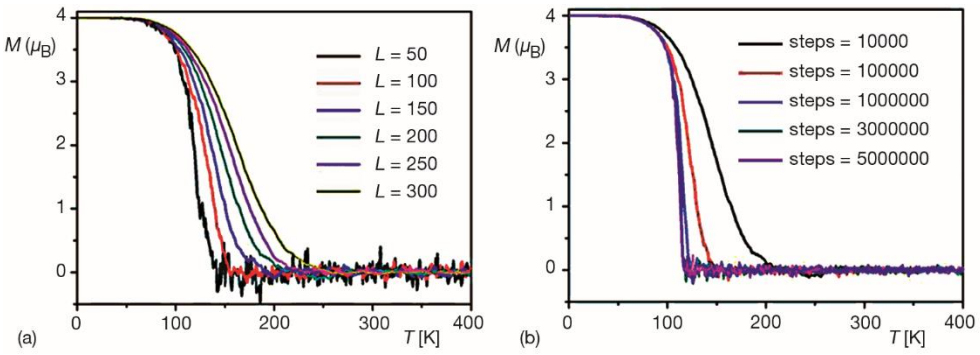

Figure 2. (a) The *M*-*T* curve when *L* takes different values and (b) the *M*-*T* curve when steps takes different values (*for color image see journal web site*)

By testing L and steps, when J = 0.638 meV, $S = 4\mu_B$, L = 200, steps = 5×10^6, the Curie temperature obtained was 109 K, which is completely consistent with the Curie temperature in reference [12]. This proves that the calculation parameters in this paper are reasonable, so it is finally determined that L = 200, steps = 5×10^6. These two parameters will be used in the following calculations.

Results and discussion

This section mainly describes the relationship between Curie temperature and exchange constant, J, magnetic moment, S, and co-ordination number, Z. According to the different co-ordination number, 2-D hexagonal system (Z = 6), tetragonal system (Z = 4), and orthogonal system (Z = 2) were researched and discussed, respectively.

Results and discussion of 2-D hexagonal systems

The supercell structure of the 2-D hexagonal system is shown in fig. 3(a), the lattice constant $a = b$, $\gamma = 60°$, and there are six atoms adjacent to $S_{i,j}$, so the co-ordination number Z = 6, the system Hamiltonian is:

$$H = -\sum_{i,j=1}^{L} JS_{i,j}(S_{i,j-1} + S_{i,j+1} + S_{i-1,j-1} + S_{i-1,j} + S_{i+1,j} + S_{i+1,j+1}) \tag{2}$$

According to the Monte-Carlo algorithm in section *Selection of calculation parameters*, the supercell with L = 200 is selected, and the Monte-Carlo steps = 5×10^6. The Curie temperatures of S = 1, 2, 3, $4\mu_B$, J = 0.5, 1, 1.5, 2, 2.5, 3 meV were calculated, respectively.

As shown in fig. 3(b), there is a linear relationship between Curie temperature, T_c, and exchange constant, J, that is $T_c = k\times J$, where k = 107.14, 60.70, 27.30, and 6.64, respectively.

As shown in fig. 3(c), there is a quadratic relationship between Curie temperature, T_c, and magnetic moment, S, that is $T_c = k\times S^2$, where k = 32.27, 26.84, 21.48, 16.08, 10.80, and 5.44, respectively.

Through further mathematical analysis, the relationship between the Curie temperature T_c, J, and S was obtained:

$$T_c = 10.748JS^2 \tag{3}$$

Results and discussion of the 2-D tetragonal system

The supercell structure of the 2-D tetragonal system is shown in Fig. 4.a, the lattice constant $a = b$, $\gamma = 90°$, and there are four atoms adjacent to $S_{i,j}$, so the co-ordination number Z = 4, the system Hamiltonian is:

$$H = -\sum_{i,j=1}^{L} JS_{i,j}(S_{i,j-1} + S_{i,j+1} + S_{i-1,j} + S_{i+1,j}) \tag{4}$$

As shown in fig. 4(b), there is a linear relationship between Curie temperature, T_c, and exchange constant, J, that is $T_c = k\times J$, where k = 107.14, 60.70, 27.30, and 6.64, respectively.

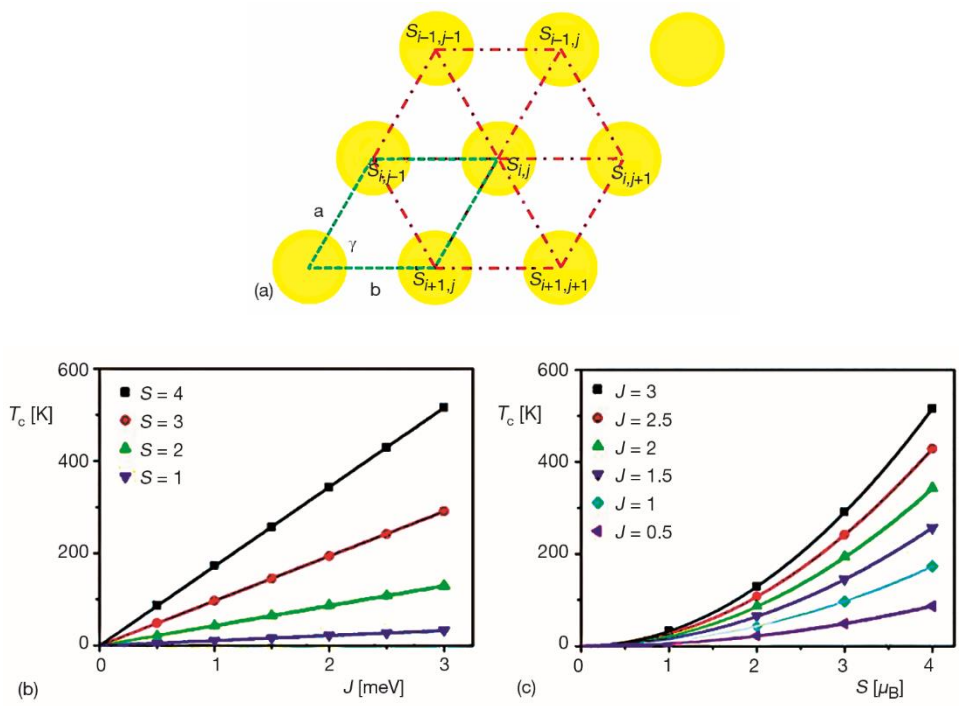

Figure 3. (a) The 2-D hexagonal system, $a = b$, $\gamma = 60°$, $Z = 6$, (b) the curve of T_c and J, and (c) the curve of T_c and S (*for color image see journal web site*)

As shown in fig. 4(c), there is a quadratic relationship between Curie temperature, T_c, and magnetic moment, S, that is $T_c = k \times S^2$, where k = 20.03, 16.84, 13.45, 10.13, 6.75, and 3.38, respectively.

Through further mathematical analysis, the relationship between the Curie temperature, T_c, J, and S was obtained:

$$T_c = 6.713JS^2 \tag{5}$$

Results and discussion of 2-D orthogonal systems

The supercell structure of the 2-D orthogonal system is shown in fig. 5(a), the lattice constant $a > b$, $\gamma = 90°$, and there are two atoms adjacent to $S_{i,j}$, so the co-ordination number $Z = 2$, the system Hamiltonian is:

$$H = -\sum_{i,j=1}^{L} JS_{i,j}(S_{i,j-1} + S_{i,j+1}) \tag{6}$$

According to the Monte-Carlo algorithm in section *Selection of calculation parameters*, the supercell with L = 200 is selected, and the Monte-Carlo steps = 5×10^6. The Curie temperatures of S = 1, 2, 3, 4μ_B, J = 0.5, 1, 1.5, 2, 2.5, 3 meV were calculated, respectively.

As shown in fig. 5(b), there is a linear relationship between Curie temperature, T_c, and exchange constant, J, that is T_c $k \times J$, where k = 22.55, 13.30, 6.44, and 1.67, respectively.

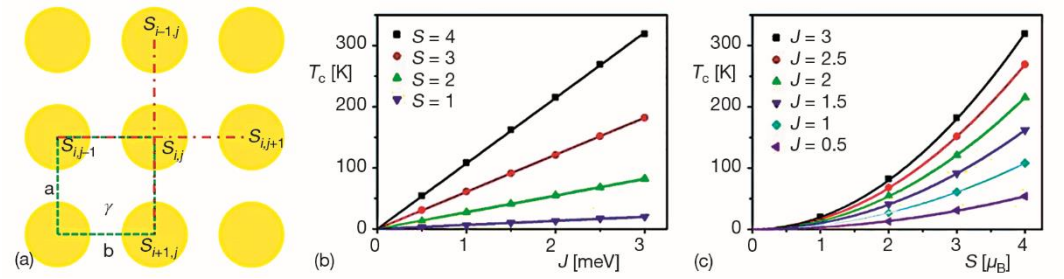

Figure. 4. (a) The 2-D tetragonal system, $a = b$, $\gamma = 90°$, $Z = 4$, (b) the curve of T_c and J, and (c) the curve of T_c and S (*for color image see journal web site*)

As shown in fig. 5(c), there is a quadratic relationship between Curie temperature, T_c, and magnetic moment, S, that is $T_c = k \times S^2$, where k =4.20, 3.56, 2.92, 2.34, 1.53, and 0.80, respectively.

Through further mathematical analysis, the relationship between the Curie temperature, T_c, J, and S was obtained:

$$T_c = 1.435JS^2 \tag{7}$$

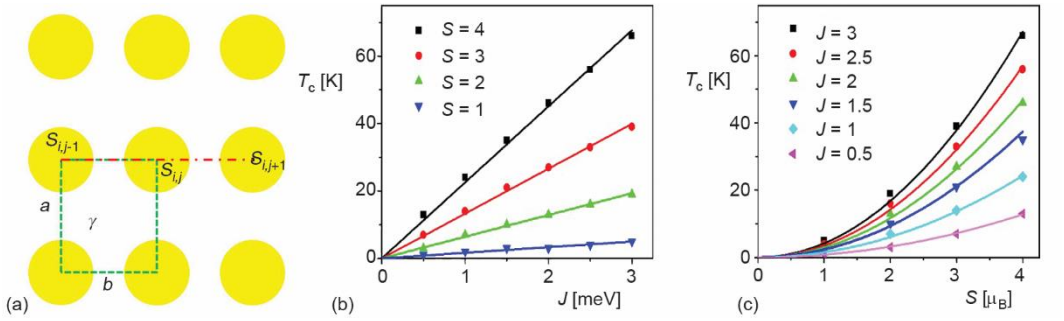

Figure 5. (a) The 2-D orthogonal system, $a > b$, $\gamma = 90°$, $Z = 2$, (b) the curve of T_c and J, and (c) the curve of T_c and S (*for color image see journal web site*)

Conclusions

In this research, Monte-Carlo algorithm was used to calculate the Curie temperature of the ferromagnetic system, and the influence of the size of the supercell, L, and the steps of Monte-Carlo on the M-T curve was focused. Through a series of calculation and testing, it was found that when L = 200 and steps = 5×10^6 a smooth M-T curve with a sharp inflection point was obtained, and whereby an accurate value of the Curie temperature, T_c, could be obtained. Besides, the quantitative relationship between the Curie temperature, T_c, and the ferromagnetic exchange constant, J, and the spin magnetic moment, S, was studied with the different co-ordination numbers (Z = 6, 4, 2), respectively. The results showed that there was a linear relationship between T_c and J, a square relationship between T_c and S, and according to eqs. (3), (5), and (7), the larger the co-ordination number, the higher the Curie temperature.

Acknowledgment

The research work is supported by the National Natural Science Foundation of China (11861049) and the Nature Science Foundation of Inner Mongolia (2017MS0101; 2018MS01027).

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Paper submitted: September 1, 2020
Paper revised: September 1, 2021
Paper accepted: September 1, 2021