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A simulation study on the magnetic ordering in an artificial geometrically frustrated lattice

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ABSTRACT

A Monte Carlo simulation on the magnetic ordering of the artificial geometrically frustrated square lattice shows that the system exhibits the spin ice state and the disorder state for strong and weak dipolar interactions. We demonstrate that the long-range dipolar interactions are significant for the short-range spin ice state.

1. Introduction

Frustration is a universal phenomenon which arises in both the disorder and well-ordered systems when all the pairwise interactions in these systems cannot be minimized simultaneously [1–3]. The frustration which arises from the topology of a well-ordered structure rather than from disorder is often known as geometrical frustration [4]. A simple geometrically frustrated model is the triangular lattice with nearest neighboring spins coupled antiferromagnetically [5]. The simple triangular lattice is currently very important as the basic building block of many real frustrated magnets typically such as the two-dimensional (2D) kagomé lattice consisting of vertex-sharing triangles [6–8], and the 3D pyrochlore structure of vertex-sharing tetrahedra [9–13]. The discovery of real geometrically frustrated magnets stimulates a great deal of interest in exploring the physics of frustration. On the other hand, however, owing to the difficulty of probing the individual spin moment in the atomic spin magnets, it is not easy for us to gain a deep understanding of how the spins locally accommodate the frustration of spin–spin interactions. An artificial geometrically frustrated lattice can provide an alternative means to study the geometrically frustrated magnetism and is also exciting for opening novel electronic devices [14].

Wang et al. first realized an artificial geometrically frustrated magnet composed of an array of lithographically fabricated single-domain ferromagnetic islands [15]. They observed that for the closely-spaced islands a short-range order exists and that for the widely-spaced islands the magnetic moments of islands become completely disorder. Libál et al. investigated numerically the ice state in two artificial geometrically frustrated systems composed of charged colloids in optical traps [18] and nanostructured superconductors [19]. They found that both systems obey the ice rules and that in the colloid system a long-range ordered ground state appears for strong colloid–colloid interactions. Recently, the magnetic configurations in an artificial geometrically frustrated lattice analogous to the lattice proposed by Wang et al. were further investigated in the presence of applied field by Remhof et al. [20]. Apart from the frustrated square lattices mentioned above, the artificial geometrically frustrated triangular and kagomé lattices had also been extensively studied both experimentally and theoretically [21–24].

Motivated by the experimental results reported by Wang et al. [15], in the present work we aim to investigate theoretically the role of dipolar interactions for the magnetic ordering of artificial geometrically frustrated square lattices using a Monte Carlo technique. Our results demonstrate that the dipolar interactions play an essential role for determining the magnetic ordering or spin ice behavior of the geometrically frustrated system. When the dipolar interaction is very strong, the short-range order exists, that is, the spin ice rules are well obeyed, and for the weak interactions the disorder state appears. Additionally, a long-range ordered state is found within an intermediate regime of dipolar coupling strength in our results.

2. Model and method

The advancement in lithographic patterning techniques makes it possible to fabricate the ordered nanostructured magnetic ma-

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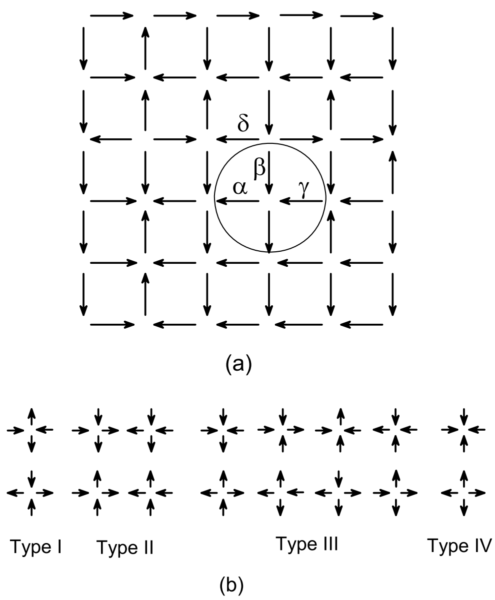

Fig. 1. (a) A schematic of the artificial frustrated square lattice on which the Greek symbols label spins for later use in correlation calculation. (b) Four types of vertices, including 16 possible magnetic configurations.

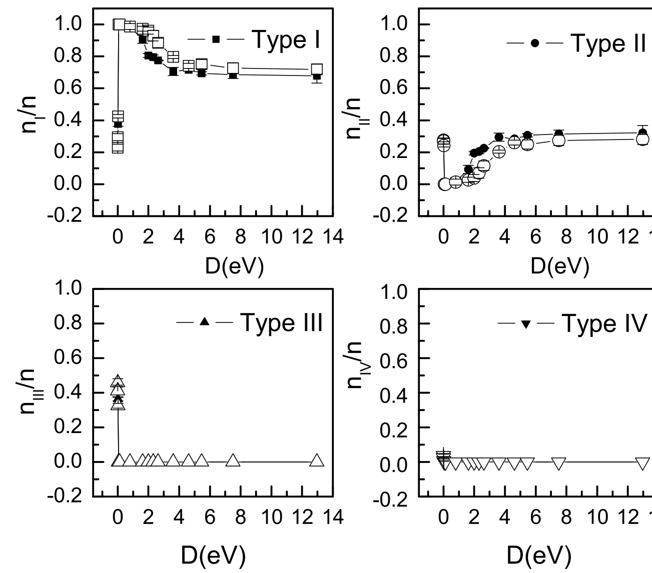

Fig. 2. The fractional populations of type I, type II, type III, and type IV as a function of the strength of dipolar coupling. In each plot the solid symbol indicates the results from all long-range dipolar interactions without cutoff, and the open symbol from the first three nearest neighboring dipolar energies. Error bars are the statistical standard deviation of the populations averaged for 10 independent sample runs.

terials with different topologies [25]. We consider an artificial geometrically frustrated square lattices shown in Fig. 1, which has been realized by an array of single-domain ferromagnetic nanoscale islands in experiment [15]. In this frustrated lattice, the nearest four islands form a vertex where six pairwise island–island interactions cannot be simultaneously satisfied, as depicted by the circle of Fig. 1(a). Here every island can be effectively treated as a giant Ising-like spin due to its single-domain character and moment pointing along its long axis, as pointed in Ref. [15]. Each spin aligns along the horizontal or vertical direction, depending on its position, and is coupled to other spins by dipolar interactions. For the lattice, constituted by two sublattices perpendicular to each other, the exchange coupling between two nearest spins is zero, and the next nearest exchange couplings can be ignored because they are much smaller compared to the nearest dipolar interactions. Thus, the model Hamiltonian of the frustrated lattice can be written by

$$\mathcal{H} = D\sum_{i,j}\left[\frac{\vec{s}_i\cdot\vec{s}_j}{|\vec{r}_{ij}|^3} - \frac{3(\vec{s}_i\cdot\vec{r}_{ij})(\vec{s}_j\cdot\vec{r}_{ij})}{|\vec{r}_{ij}|^5}\right] \tag{1}$$

where $\vec{s}_i$ is a unit vector spin, i.e., $\vec{s}_i = \sigma_i\vec{e}_i$ with $\sigma_i = \pm 1$ and $\vec{e}_i$ defining the long axis of islands, $D = \frac{\mu_0\mu^2}{4\pi d^3}$ is the dipolar coupling parameter with μ_0 the permeability of the vacuum, μ the magnetic moment of each spin and d the distance between two nearest spins along the vertical or horizontal direction, and the sum runs over all spin pairs i and j defining the vector $\vec{r}_{ij}$, measured in unit of d.

According to the experiment [15], the islands possess a large magnetic moment of approximately $3 \times 10^7\mu_B$ and thus the strength of dipolar interactions at nearest neighboring distances can reach the order of magnitude 10^4 K, depending on the lattice spacing. In our simulation, we take the values of dipolar coupling parameter D ranging from 6 meV to 13 eV, i.e., about 100 K to 10^5 K, which is approximately equivalent to the lattice spacing ranging from 310 to 4000 nm in experiment [15].

Our Monte Carlo simulation was carried out on the above frustrated lattice with free boundary condition. In our simulation, the lattice consists of 1800 spins, and a standard single spin flip Metropolis algorithm is used. A Kirkpatrik cooling scheme is used with 190 successive temperature steps from 4000 K to 200 K in the absence of magnetic field [16,17]. At each temperature, the convergence of the relaxation process towards equilibrium has been observed for any initial configuration after 10^4 Monte Carlo steps per spin are performed. Hence, the single-spin-update algorithm is efficient in our case. To reduce boundary effects only the core of the lattice is analyzed.

3. Results and discussions

In the frustrated square lattice, the vertices can be classified into four types in terms of their energy, as illustrated by type I, type II, type III, and type IV in Fig. 1(b). The local magnetostatic energies for four vertex types are $E_{\mathrm{I}} = -1.6216D$, $E_{\mathrm{II}} = -0.5D$, $E_{\mathrm{III}} = 0$, $E_{\mathrm{IV}} = 2.6216D$, respectively, with D being the dipolar coupling parameter in Eq. (1). According to the statistical distribution, the fractional populations of four vertex types should be $n_{\mathrm{I}}/n = 0.125$, $n_{\mathrm{II}}/n = 0.25$, $n_{\mathrm{III}}/n = 0.5$, and $n_{\mathrm{IV}}/n = 0.125$ if the island–island interactions are zero and thus the individual moment orientation is completely random. For real materials, the different dipolar interactions between islands will lead to different distributions of vertex types, depending on the lattice spacing.

Fig. 2 shows the fractional populations of four types of vertices as a function of the strength of dipolar couplings. The data by solid symbols and open symbols represent results from considering all long-range dipolar interactions and only the first three nearest neighboring dipolar interactions, respectively. It can be seen that in the limit of weak dipolar interaction strength, the population of each vertex type is approximately equal to that of an array of isolated islands and that in the limit of strong interaction strength, the population of type I is about 0.7, that of type II is about 0.3, and those of types III and IV are zero, which indicates a spin ice state of "two spins in, two spins out" configurations at the vertices. This result shows a qualitative agreement with those of experiment for extremely large and small lattice spacings [15]. But, on an intermediate dipolar coupling parameter scale, our results show a long-range ordered ground state, in which case only type I exists and other three vertex types disappear, as was predicted previously

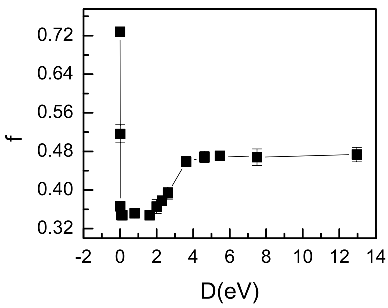

Fig. 3. The local degree of frustration as a function of dipolar interaction strength in the case of considering the first three nearest neighboring dipolar energies.

by the standard model of spin ice [28] and was reported in the colloidal version of artificial frustrated systems for strong colloid–colloid interactions [18]. This dipolar parameter scale on which an ordered ground state appears is from 0.06 to 0.8 eV, which is approximately equivalent to the lattice spacing from 600 to 1700 nm in experiment [15]. The ordered ground state in our results still obeys the spin ice rules, but it was not observed in the experiment. This can be a consequence of the demagnetization effect in experiment, while only the thermal effect is considered in our simulations.

In addition, it is found from Fig. 2 that n_{I}/n is larger and n_{II}/n is smaller for three nearest neighboring distance cutoff than all dipolar interactions, and that the dipolar coupling scale on which the long-range ordered state arises is wider under the same condition as the above one. These results mean that the dipolar interactions can suppress the development of a long-range ordered state. According to the local magnetostatic energy of each vertex type given above, the local energy of type I is lowest. Thus, if only the first nearest neighboring dipolar interactions are considered, an ordered ground state can always be generated by arraying alternatively two kinds of magnetic configurations of type I, independent of the strength of dipolar coupling. In this case, the system is unfrustrated, which is obviously inconsistent with experimental results. Therefore, our results suggest that the larger the nearest neighboring cutoff distance is, the heavier the degree of frustration is, which can give an explanation for a larger ordered state scale for considering three nearest neighboring distance cutoff. Our results demonstrate that the long-range dipolar interactions play an essential role for the magnetic ordering of this frustrated square lattice.

From above, we know that the dipolar interactions are responsible for the frustration of the system. In order to describe quantitatively the local frustration of the system, we introduce a frustration parameter [26,27]

$$f = \frac{|E_{id}| - |E_i|}{|E_{id}|} \tag{2}$$

where E_{id} is a ground state energy of a relevant unfrustrated spin i and E_i is an actual energy of the spin i. Fig. 3 displays the frustration parameter as a function of the strength of dipolar interaction. In this calculation, we consider the first three nearest neighboring interactions. The degree of local frustration is largest for the arrays of non-interacting islands, $f = 0.73$, and smallest at a long-range ordered ground state of the system, $f = 0.34$, and the frustration parameter reaches a stable value $f = 0.47$ for large dipolar interactions.

Furthermore, to gain a deep insight into the nature of frustration in this frustrated system, we also calculate the pairwise correlation functions between three types of neighboring pairs, i.e., the nearest spin pairs α and β, the next nearest pairs α and γ, and the third nearest pairs α and δ, as labeled in Fig. 1(a). The spin pairs i

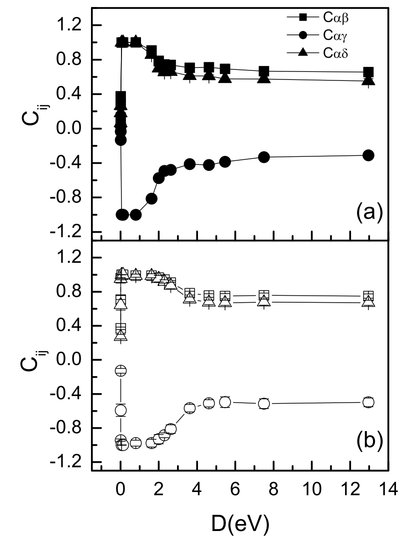

Fig. 4. The pairwise correlation coefficients as a function of the strength of dipolar interactions for three different spin pairs, i.e., α and β, α and γ, and α and δ. The correlation coefficients for long-range dipolar interactions without any cutoff (a) and for dipolar interactions up to the third nearest neighboring distances (b).

and j correlation coefficient is defined by $C_{ij} = 1$ $(i, j = \alpha, \beta, \gamma)$ if two moments s_i and s_j are aligned to minimize the dipole interaction energy, and $C_{ij} = -1$ if two moments are aligned to maximize the dipole energy [15]. Fig. 4 displays the correlation coefficients as a function of strength of dipolar interactions. For very weak dipolar interactions, all spin pairs have a very weak correlation. As the dipolar coupling increases, the correlation for all three spin pairs becomes strong, but the correlation between pairs α and γ is negative. Of all three types of spin pairs, the correlation between pairs α and β is strongest, which should be a result of the strongest dipolar interactions between α and β. The correlation between α and δ is stronger than one between α and γ. With the further increase of dipolar interactions, the correlation coefficients finally approach a stable value for three neighboring spin pairs. The correlations of our results agree qualitatively with those of experiment [15], but the values of correlation coefficients in our simulation are larger than those in experiment. Additionally, it is found that the correlation coefficients obtained from the long-range interactions without any cutoff are relatively smaller than those from three nearest neighboring interactions cutoff, as is shown in Figs. 4(a) and 4(b). This can be a consequence of the suppression of long-range dipolar interactions to the ordered magnetic state.

4. Conclusions

In conclusion, we have studied the effect of dipolar coupling strength on the magnetic ordering in an artificially geometrical frustrated square lattice using the Monte Carlo method. Our simulated results show that for relatively strong dipolar coupling the spin arrangement of the system satisfies the ice rules of two spins in, two spins out magnetic configurations at each vertex, and that for very weak dipolar interactions a disordered state is found. Our results are in qualitative agreement with those of experiments [15, 18]. Additionally, we find a long-range ordered state on certain dipolar coupling strength scales, which was not observed in the experiment [15]. This can be ascribed to the demagnetization effect in experiment but in our simulation the magnetic state is considered in thermal effect. Moreover, it is found that the long-range dipolar interactions play a significant role in determining the spin ice state of the artificial geometrically frustrated square lattice.

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