

**Modification of magnetic ordering in ultrathin films using vacancy arrays: Monte Carlo results**

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Monte Carlo simulations are used to investigate the modification of magnetic ordering in ultrathin films by the introduction of a regular array of vacancies. The magnetic moments are coupled by a dipolar interaction and are assumed to form a square lattice. The simulations demonstrate the variations in magnetic ordering with temperature and vacancy concentration for a variety of vacancy configurations.

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**I. INTRODUCTION**

Ultrathin magnetic films have been extensively studied using both experimental and theoretical methods.<sup>1,2</sup> The high level of interest in these systems is generated, in part, by the wide range of ordering phenomena that they demonstrate and, in part, by their potential technological uses.<sup>2,3</sup>

In theory, modifying the magnetic parameters or randomly changing the structure may be used to modify the magnetic properties of the film, however, in practice it may be difficult to achieve precise control of the properties. For example, for systems with both dipolar and exchange interactions, it has recently been demonstrated that the strength of the antiferromagnetic exchange interaction affects the nature of the magnetic ordering.<sup>4-6</sup> While the exchange interaction in a manufactured film may be controlled somewhat by the choice of film and substrate materials, and similar surface science techniques, precise manipulation of the exchange interaction to obtain desired ordering properties may be difficult. Simulation studies have also been used to investigate the effect of randomly distributed vacancies on in plane ordering in ultrathin magnetic films.<sup>7</sup> At the very low densities of vacancies investigated these studies are consistent with earlier predictions,<sup>8,9</sup> however, they also provide some evidence that even at quite low densities a multitude of nearly degenerate low energy states exists and the system may relax to any of these states.<sup>7</sup>

The use of regular arrays of holes (antidots) in ultrathin films has been discussed as a way of controlling the properties of the film.<sup>2</sup> It has the advantage that the connectivity of the film is preserved and so the modification of the interaction is smaller than in, say, an array of magnetic nanodots (that is the interaction between the dots). Moreover, for films which are of the order of nanometers in diameter there is a wide range of possible spacings for the holes and hence the possibility of rather precise control of the effected magnetic properties of the film.

In addition to the possible technological implications of being able to vary the properties of a film in a controlled way, considering systems with regular arrays of vacancies also provides insight into the interplay between magnetic structure and system structure in systems demonstrating order from disorder phenomena. In particular, the introduction of thermal disorder into a system of dipoles confined to the

film plane results in a reduction in symmetry from the continuous symmetry of the ground state to a fourfold discrete symmetry.<sup>8-11</sup> The introduction of random vacancies modifies the discrete fourfold symmetric states selected (at sufficiently low temperature).<sup>7-9</sup> As demonstrated in the work reported here, introducing a regular array of vacancies allows a similar modification of the selected states, however, the manner in which the ground states vary with increasing vacancy concentration may be systematically controlled and studied.

Our simulation results predict the temperature-concentration phase diagrams of materials with vacancies arranged in a regular array. Experimentally the phase transition lines predicted can be located by the measurement of macroscopic quantities such as the magnetic specific heat. However, our simulation results also describe the variation in magnetic structure at the atomic level with vacancy concentration and temperature. There is the fascinating possibility of experimentally probing this variation through direct imaging using techniques that allow atomic resolution of antiferromagnetic structures. In particular, spin-polarized scanning tunneling microscopy is capable of such resolution and can be used to image antiferromagnetic structures in films with in-plane moments by using Fe coated probe tips.<sup>12</sup>

**II. MODEL AND MONTE CARLO SIMULATION METHOD**

In this study a square lattice of magnetic moments interacting through a dipolar interaction was used to model the ultrathin film. The moments are confined to the plane of the lattice and the Hamiltonian of the system is taken to be

$$\mathcal{H} = g \sum_{ij} \left( \frac{\vec{\sigma}_i \cdot \vec{\sigma}_j}{r_{ij}^3} - 3 \frac{\vec{\sigma}_i \cdot \vec{r}_{ij} \vec{\sigma}_j \cdot \vec{r}_{ij}}{r_{ij}^5} \right). \quad (1)$$

As in previous work we simulate an ideal system without a boundary by assuming that the infinite space is tiled with replicas of the basic simulation cell and using Ewald sum techniques to calculate the corresponding modified interactions.<sup>1</sup> The simulations may be thought of as representing a film of atomic moments which interact through a dipolar interaction only; in this case, the vacancies represent the removal of individual atoms. However, the simulations

may also be thought of as representing a regular array of uniform magnetic nanodots which interact through the dipolar interactions between the net moments of the dots; in this case the vacancies represent the removal of nanodots. We choose units such that the dipolar interaction parameter  $g = 1.0$ . Accordingly the temperature scale may be rescaled appropriately to compare with experimental results from either films with atomic vacancies or arrays of antidots.

A variety of system sizes, and vacancy concentrations and configurations have been considered. Results are summarized in the following sections. In almost all cases the simulations were started with the system in a disordered state well above the temperature at which the system without vacancies is known to order<sup>10</sup> and the system is cooled slowly. At  $T = 0.05$  the temperature step was reduced from  $-0.05$  to  $-0.005$  until a temperature of  $T = 0$  was reached. The system temperature was then set to zero and the system allowed us to further relax using the Monte Carlo simulation (i.e., only energy decreasing moves allowed) in order to ensure that the local energy minimum had been reached. In a few cases the system was initiated in an ordered state at zero temperature and slowly raised to a temperature well above the transition temperature. These warming simulations were used to check for consistency and for evidence of metastability effects.

Previously Monte Carlo simulations have been used to demonstrate the ordering of a square lattice of magnetic moments coupled by a dipolar interaction only.<sup>10</sup> This ordering occurs despite the continuous degeneracy of the ground state of the system<sup>10,11</sup> and is associated with the appearance of an effective anisotropy (and an associated gap in the spin wave spectrum) at finite temperatures. The effective anisotropy generated by the thermal fluctuations is such that the ordering tends to be along the axial directions of the lattice. When only the dipolar interaction is present (i.e., no exchange interaction) the low temperature state consists of lines of parallel moments with moments in adjacent lines antiparallel. We refer to this as the colinear ordered state. Adding random impurities<sup>7</sup> or, under certain conditions, an antiferromagnetic exchange interaction<sup>4-6</sup> results in a change to an ordered state in which the moments are at  $45^\circ$  to the axial directions. We refer to this as the microvortex state.

The degree of ordering corresponding to the (zero vacancy) dipolar ground state manifold is measured by calculating the order parameter  $\vec{\Psi}$  with components<sup>4</sup>

$$\Psi^x = \left\langle \frac{1}{N} \sum_i s_i^x \right\rangle; \Psi^y = \left\langle \frac{1}{N} \sum_i s_i^y \right\rangle, \quad (2)$$

where the sum is over all sites on the lattice. The ‘‘gauge transformed’’ spins  $\vec{s}$  have a one-to-one correspondence with the original dipole moments through the transform

$$\vec{s}_i = (s_i^x, s_i^y) = (\epsilon_\alpha^x \sigma_{\alpha,j}^x, \epsilon_\alpha^y \sigma_{\alpha,j}^y) \quad (3)$$

and a ferromagnetic ground state. The label  $j$  in Eq. (3) indicates a distinct four spin plaquette on the square lattice and the label  $\alpha$  indicates one of four sublattice positions within the plaquette. The four-dimensional vectors used to construct the transformation are  $\vec{e}^x = (1, -1, -1, 1)$  and  $\vec{e}^y = (1, 1, -1, -1)$ .

We follow earlier work<sup>10</sup> by calculating

$$P = \left\langle \frac{1}{N} \sum_i (s_i^x)^4 + (s_i^y)^4 \right\rangle \quad (4)$$

to distinguish between the colinear and microvortex phases. This has the value  $P = 1$  in the pure colinear phase,  $P = 0.5$  in the pure microvortex phase, and  $P = 0.75$  in a system with zero effective anisotropy. However, we note that  $P$  is actually a measure of the degree of alignment with the axial or diagonal directions of the square lattice rather than an order parameter for the colinear or microvortex states. Consequently, as discussed below, some care is required in interpreting the calculated values of  $P$ .

Systems of various sizes ( $N = 30 \times 30$  to  $N = 70 \times 70$ ) with various concentrations of vacancies were simulated. We found no evidence of significant finite size effects except as discussed below in Sec. IV. In most cases vacancy concentrations were chosen such that the vacancy array is commensurate with the basic Monte Carlo cell size. However, in order to provide more data points at intermediate concentrations, incommensurate structures were also used. To the accuracy of the simulations we found no systematic differences between the results from the commensurate and incommensurate structures.

### III. MODIFICATION OF THE LOW TEMPERATURE STATES

#### A. Square lattice of vacancies

The variation of the low temperature states with changing concentration of vacancies is indicated by the configurations shown in Fig. 1, for a system with a square array of vacancies. These low temperature states are obtained by simulated cooling of the system from a high temperature to zero temperature by the Monte Carlo method described above. The figure shows the configuration in the gauge transformed system  $\{\vec{s}_i\}$ .

In the absence of vacancies the low temperature state is that of an ordered system with the moments aligned parallel to the axis of the underlying square lattice. Addition of vacancies modifies the zero temperature state obtained. At the lowest concentrations of vacancies considered, the state of the system obtained by cooling to zero temperature shows the moments rotated by  $\pi/4$  relative to the lattice axes with some further slight modification of the angle apparent for moments in the immediate vicinity of the vacancies. This is consistent with a similar observation of a rotation by  $\pi/4$  of the moments in systems with random distributions of low concentrations of vacancies (the microvortex phase).

As the concentration of vacancies is increased the further modification of the zero temperature state by the vacancies is apparent as a further partial rotation of the moments particularly along the lattice lines which connect adjacent vacancies. Hence with increasing concentration of vacancies the system deviates from a homogenous system but remains ordered and the ordered state has the symmetry of the vacancy lattice.

As the vacancy concentration is increased the tendency of the system to form multiple domain states as the system is



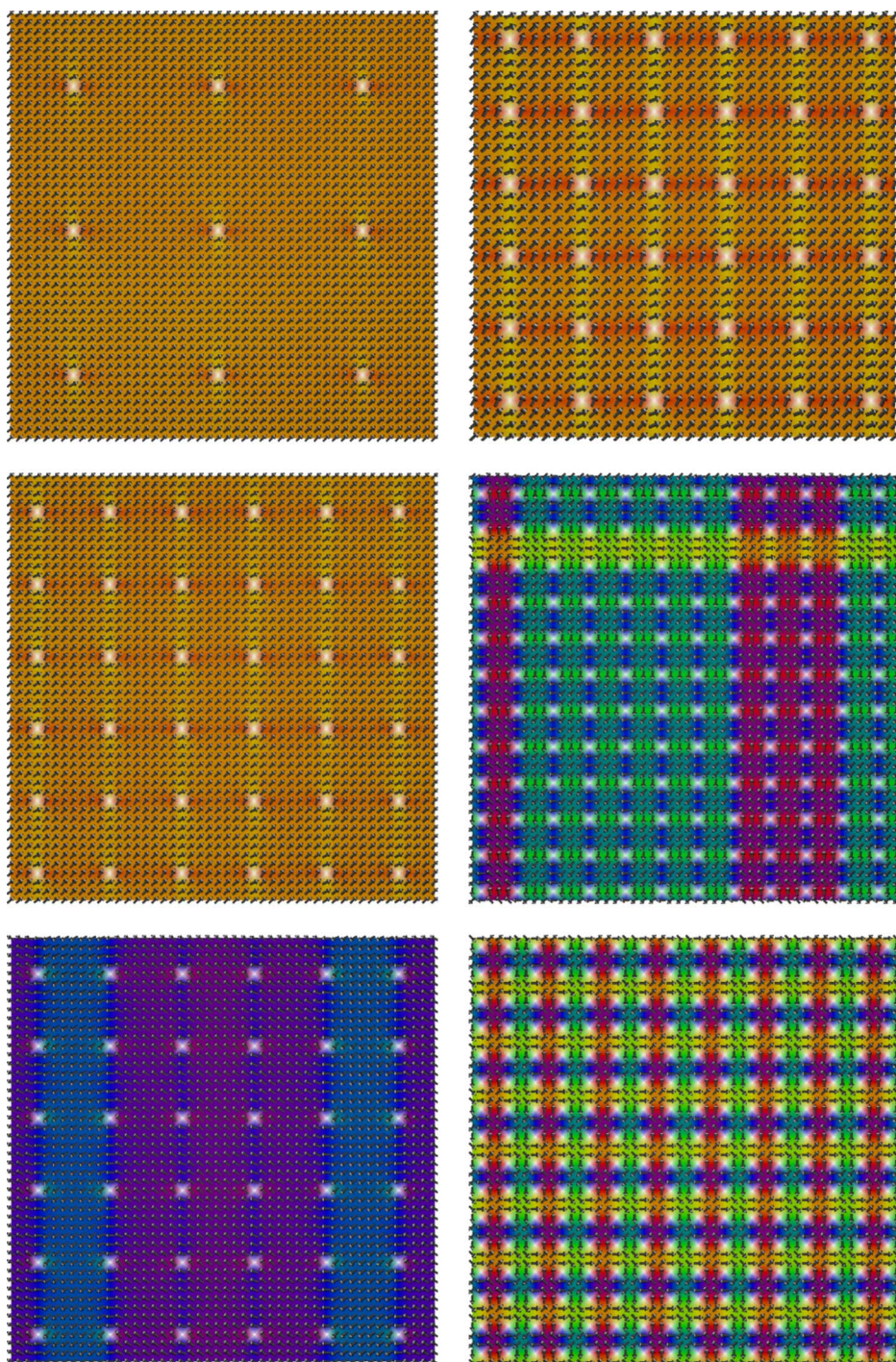


FIG. 1. (Color online) Zero temperature (gauge transformed) configurations obtained by cooling the system with a square array of vacancies and vacancy concentrations of (top left to bottom right)  $c=0.0039$ ,  $0.0156$ ,  $0.0156$  (with domains),  $0.0278$ ,  $0.0625$ , and  $0.111$ . Colors are generated by a color wheel representing the orientation of the moments.

cooled, increases. Such domain states have been observed at vacancy concentrations as low as 1% ( $c=0.01$ ). In all cases where domains are observed, the domain boundaries are located on the lines of the vacancy lattice. Moreover, the moments located on these domain boundaries tend to be further rotated (in relation to the micro-vortex phase orientation) relative to those on similar vacancy lattice lines which are not on a domain boundary. At the higher concentrations considered, the formation of multiple domain states is almost always observed. This indicates that the introduction of a domain wall has only a small energy penalty thus resulting in a very large number of multiple domain states which are

almost degenerate. [For example, the energy difference per spin between the single domain phase shown in Fig. 1(b) and the multiple domain phase shown in Fig. 1(c) is only  $0.0008g$ ]. These multiple domain states include “plaid” states with both horizontal and vertical domain walls, such as that shown at a vacancy concentration of 6.25% ( $c=0.0625$ ) in Fig. 1.

### B. Face centered square lattice of vacancies

The gross features of systems with vacancies arranged in a face centered square (FCSq) array are similar to those



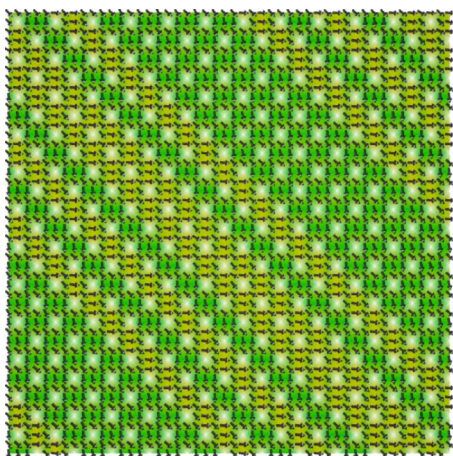


FIG. 2. (Color online) A typical zero temperature configuration obtained by cooling a system with a FCSq arrangement of vacancies ( $c=0.125$ ). The orientation of the domain boundaries relative to the underlying square lattice is typical of domain formation with the FCSq arrangement of vacancies.

found in systems with a square array of vacancies, however, there are some significant differences in the details of the arrangements. Introduction of a small concentration of vacancies again results in a zero temperature phase which is close to the microvortex phase with distortions of that phase close to the vacancy locations. Domain formation is observed at relatively low concentrations of vacancies (3.2%). As in the case of a square array of vacancies, domain walls are aligned with the nearest neighbor edges of the vacancy lattice and, therefore, in this case are rotated by  $\pi/4$  relative to the underlying spin lattice (see Fig. 2).

Once a concentration of 50% of vacancies in a FCSq arrangement is reached, the remaining dipoles form a square lattice oriented at  $\pi/4$  with respect to the  $c=0$  lattice of dipoles. As this is indistinguishable from a square lattice with a lattice spacing expanded by a factor of  $1/\sqrt{2}$ , the low temperature state is the colinear state on the “new” lattice. This low temperature state is shown in Fig. 3 and we note that it does not correspond to a microvortex state on the original lattice. We return to this special case to provide some useful results for finite temperature systems below.

#### IV. VARIATION WITH TEMPERATURE

##### A. Order and anisotropy parameters

The order parameter [defined in Eq. (2)] as a function of temperature is summarized in Fig. 4 and the variation of  $P$  [Eq. (4)] with temperature is summarized in Fig. 5, for a system with a square array of vacancies at various values of vacancy concentration,  $c$ .

At sufficiently low concentrations of vacancies ( $c \leq 2.0\%$ ) the variation in  $P$  and  $\psi = |\tilde{\psi}|$  with temperature is very similar to that observed in the zero vacancy case.<sup>10</sup> Initially as the temperature continues to decrease below the critical temperature for ordering,  $P$  increases above its value in the disordered system indicating that the ordering is essentially of the colinear type. However, at very low tempera-

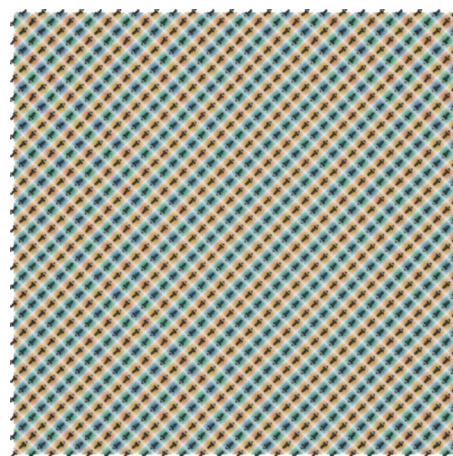


FIG. 3. (Color online) A typical zero temperature configuration obtained by cooling a system with a FCSq arrangement of vacancies ( $c=0.50$ ).

tures there is a rapid decrease in  $P$  and at very low concentrations of vacancies  $P \approx 0.5$  at  $T=0$ . At slightly higher values of concentration the same rapid decrease in  $P$  is observed but the final value is noticeably above 0.5. The initial increase in  $P$  followed by a rapid decrease at a vacancy concentration dependent critical temperature is consistent with an initial ordering transition to a colinear phase followed by a subsequent transition to the microvortex state as the temperature continues to decrease. This phase behavior is similar to that observed in systems with random vacancies at low concentrations of vacancies.<sup>7</sup> At higher concentrations of vacancies ( $2.8 \leq c \leq 11.1\%$ ),  $P$  never reaches a value above 0.75, apparently indicating that the microvortex state is the only ordered state observed; however, as we shall show below, a more subtle analysis of the phase behavior is required to correctly determine the properties of the system at these higher concentrations of vacancies. Notice that at the highest concentration of vacancies considered here ( $c=0.25$ ), the final value of  $P$  is  $P \approx 0.80$  (i.e.,  $P > 0.75$ ) indicating that the distortion of the microvortex state, generated by the vacancies, results in many of the moments lying along or close to the axial directions.

##### B. Dynamical behavior in finite systems

As noted above, for sufficiently high values of the vacancy concentration  $c$  a value of  $P > 0.75$  is not observed in our simulations. We also note that even for low concentrations or zero concentration of vacancies, there is a temperature interval immediately below the ordering temperature where the anisotropy parameter  $P$  is essentially indistinguishable from its isotropic value,  $P=0.75$ . A simple interpretation of these results would lead one to believe that at sufficiently high vacancy concentrations the colinear phase does not occur and that even at lower concentrations of vacancies the colinear phase does not occur until one lowers the temperature somewhat below the ordering temperature. This might be explained by assuming that the anisotropy induced by the thermal fluctuations is insufficient to overcome rotations due to thermal excitations.

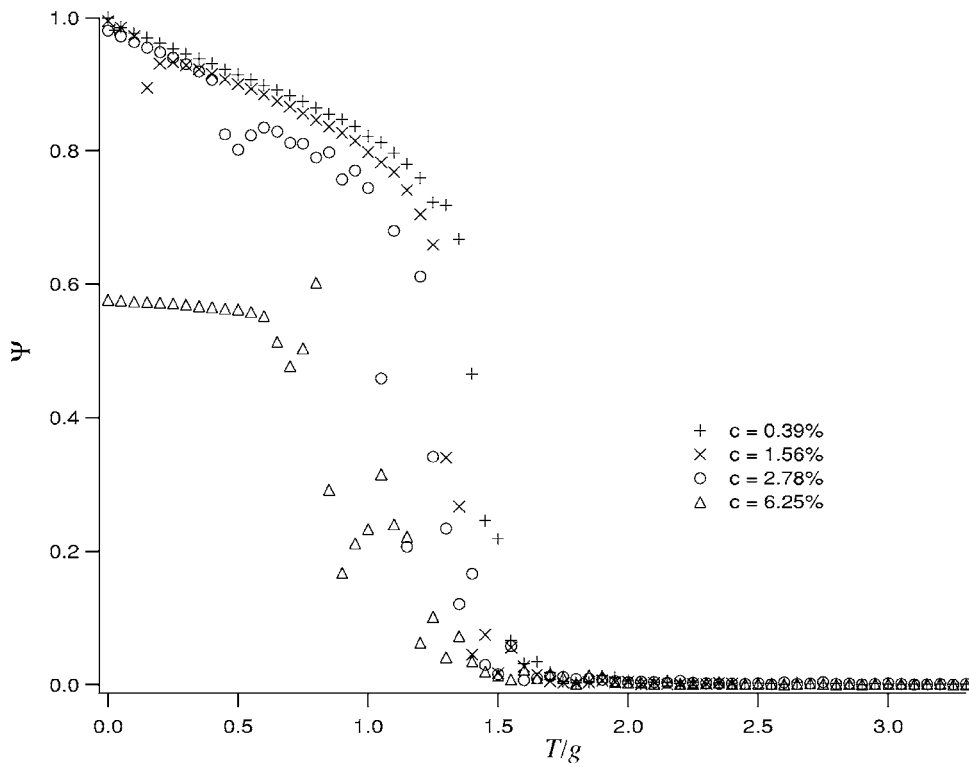


FIG. 4. Variation of the order parameter with temperature in a system with a square array of vacancies at concentrations of  $c=0.0039(+)$ ,  $0.0156(x)$ ,  $0.0278(o)$ , and  $0.0625(\Delta)$ .

This appears to be confirmed by plotting the average value of  $s_x$  and  $s_y$  as a function of temperature (Fig. 6). For a range of values immediately below the ordering temperature the values of  $\langle s_x \rangle$  and  $\langle s_y \rangle$  are scattered with no obvious systematic variation. At higher concentrations of vacancies this region of temperature continues until the onset of the microvortex state at which point both  $\langle s_x \rangle$  and  $\langle s_y \rangle$  stabilize at values characteristic of the microvortex phase ( $|s_x| \approx |s_y|$

$\approx 1/\sqrt{2}$ ). At lower values of vacancy concentration, the values of  $\langle s_x \rangle$  and  $\langle s_y \rangle$  stabilize at values characteristic of a colinear phase, this is usually preceded by temperature intervals in which  $\langle s_x \rangle$  and  $\langle s_y \rangle$  are stable but where the orientation changes as one continues to lower the temperature.

Both the low and high vacancy concentration behavior in these ranges can be explained as a dynamical effect in which the thermal excitations cause the order parameter to fluctuate

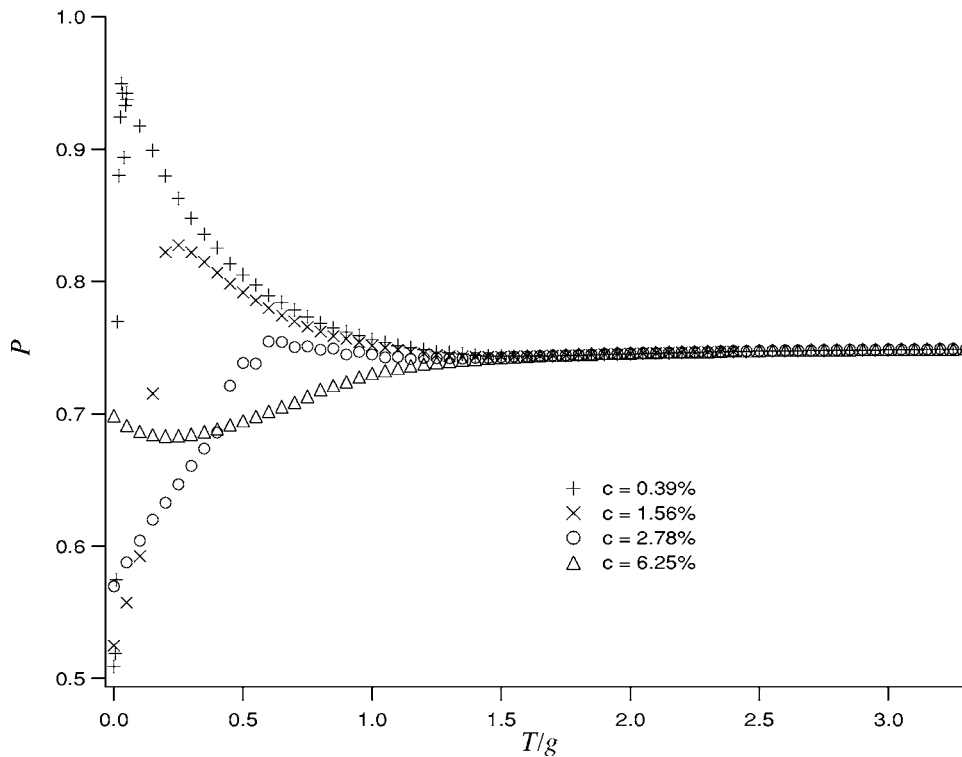


FIG. 5. Variation of the anisotropy parameter,  $P$ , with temperature in a system with a square array of vacancies at concentrations of  $c=0.0039(+)$ ,  $0.0156(x)$ ,  $0.0278(o)$ , and  $0.0625(\Delta)$ .

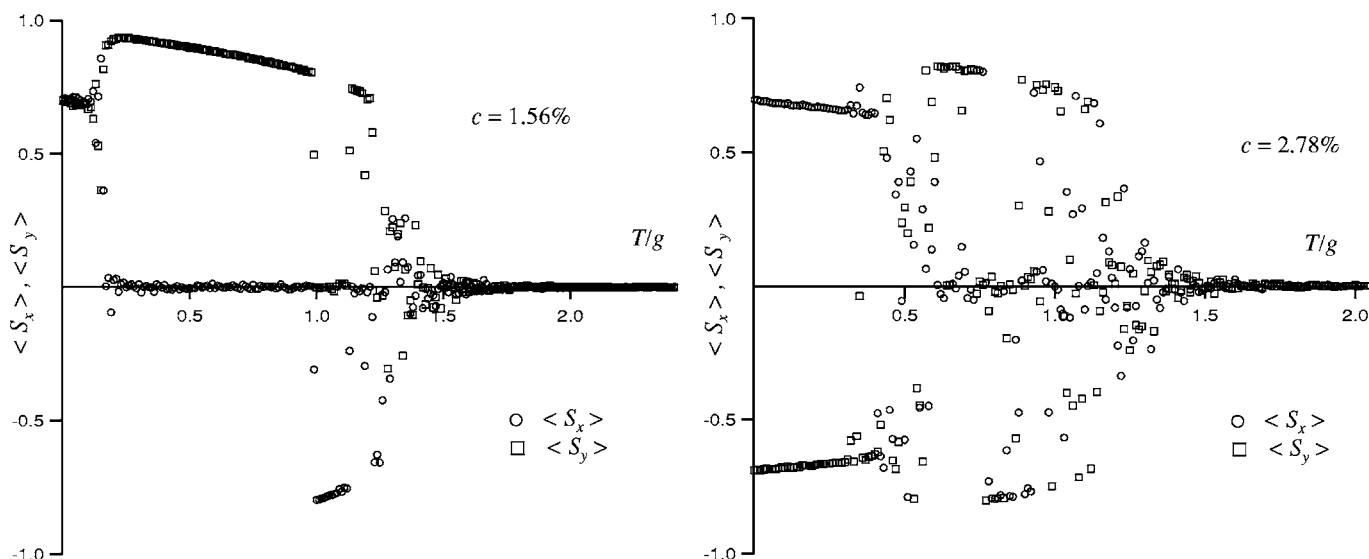


FIG. 6. Averages of the  $x$  and  $y$  spin components as functions of temperature for systems with a square array of vacancies at concentrations of (a)  $c=0.0156$  and (b)  $c=0.0278$ .

between the free energy minima. If the temperature is sufficiently high the typical thermal excitation energy is comparable to the energy barrier and the moments will rotate between the axial directions easily. As the temperature is lowered the thermal energy becomes comparable with the energy barrier due to the anisotropy which is in turn generated by the thermal excitations; the rate of fluctuations of the order parameter becomes comparable with the time spent at each temperature in the simulations. Finally at sufficiently low temperature the probability of an excitation over the energy barrier is negligible and the particular ordered phase becomes stable (at least on times probed in these simulations).

A more detailed analysis of this dynamical behaviour was obtained by plotting  $\langle s_x \rangle$  and  $\langle s_y \rangle$  as a function of time for fixed temperature and vacancy concentration. We then plot the self-correlation function,  $\gamma(t)$ , defined by

$$\rho(t) = \langle \vec{s}_i(t) \cdot \vec{s}_i(0) \rangle - \langle \vec{s}_i(t) \rangle \langle \vec{s}_i(0) \rangle, \quad (5)$$

$$\gamma(t) = \frac{\rho(t)}{\rho(0)}, \quad (6)$$

and assume that a relaxation time  $\tau$  may be defined by fitting the data to the form

$$\gamma(t) = \exp(-t/\tau). \quad (7)$$

In Figure 7 we show the typical variation of  $\tau$  with temperature. The smooth behavior of the curve in the temperature interval from the ordering temperature to the microvortex transition temperature implies that there is only a single phase in this region but the relaxation time is (relatively) very short just below the ordering transition temperature. However, the relaxation time increases rapidly as the microvortex transition is approached. At higher concentrations of vacancies the short relaxation time persists almost all the way to the microvortex transition and therefore a stable

single colinear phase is not observed. These dynamical effects account for the absence of a value of  $P > 0.75$  even though the system may be said to be in a colinear phase. At vacancy concentrations of  $c > 0.04$  anomalous behavior of  $\tau$  with temperature was sometimes observed, however, we concluded that this was primarily an artifact of domain formation.

A finite size analysis of this dynamical behavior was then carried out by defining a temperature  $T_s(c, L)$  for given vacancy concentration,  $c$ , and linear system size,  $L$ , as the temperature at which a stable single colinear phase appears in our simulation. For the smaller system sizes used,  $T_s$  is well below the ordering temperature, however, it rises relatively rapidly with system size when the larger system sizes are included. Extrapolating to  $1/L \rightarrow 0$  indicates that it approaches the ordering transition temperature in this limit. Thus the destabilizing of the single colinear phase by these dynamical effects is a finite system effect.

## V. PHASE DIAGRAMS

### A. Square lattice of vacancies

While the concentration of vacancies cannot be continuously varied if the nature of a chosen vacancy lattice is to be maintained, we can nonetheless plot the points  $(T_c, c)$  and  $(T_{mv}, c)$ , corresponding to the ordering and microvortex transitions, respectively, on a temperature-concentration phase diagram for those values of  $c$  corresponding to a chosen lattice type for the vacancy array. Figure 8 is the phase diagram for a system with a square lattice of vacancies, produced in this way. While it is possible to identify both  $T_c$  and  $T_{mv}$  from the simulations reported here at all of the values of  $c$  considered, some caution is needed. As we noted above, domain formation is a characteristic feature of the low temperature behavior of these systems for all but the very lowest of vacancy concentrations considered. In a finite system, there is always one dominant phase so the system can be said

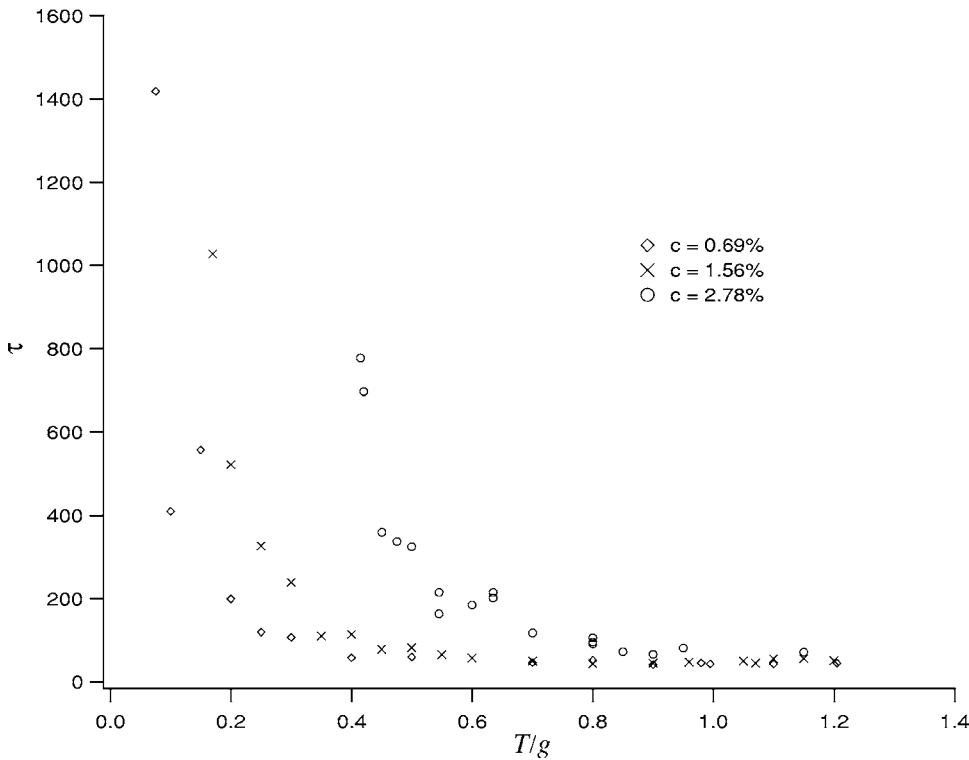


FIG. 7. Relaxation time,  $\tau$ , as a function of temperature for systems with a square array of vacancies at concentrations of  $c=0.0069(\diamond)$ ,  $0.0156(\times)$ , and  $0.0278(\circ)$ .

to be ordered (although the saturation value of the order parameter may be reduced), however, in the large system limit we would expect all equivalent phases to be equally represented and therefore while the system would be locally ordered it would not display global order. While such domain phases are metastable the dynamical process for removing topological defects in dipolar systems may be very slow (see, for example, the paper by Bromley *et al.*<sup>13</sup> and references

therein) and, therefore, these states may be very long lived at least on time scales available to current simulations.

We have attempted to determine the limiting slope of the line  $T_{mv}(c)$  as  $c \rightarrow 0$  by forming least-squares fits to the data points then performing a range of fit analysis. Taking the overall error bounds in the data points into account, our estimates are just consistent with the result of Prakash and Henley who obtained a slope of 5.75.<sup>9</sup> However, the error

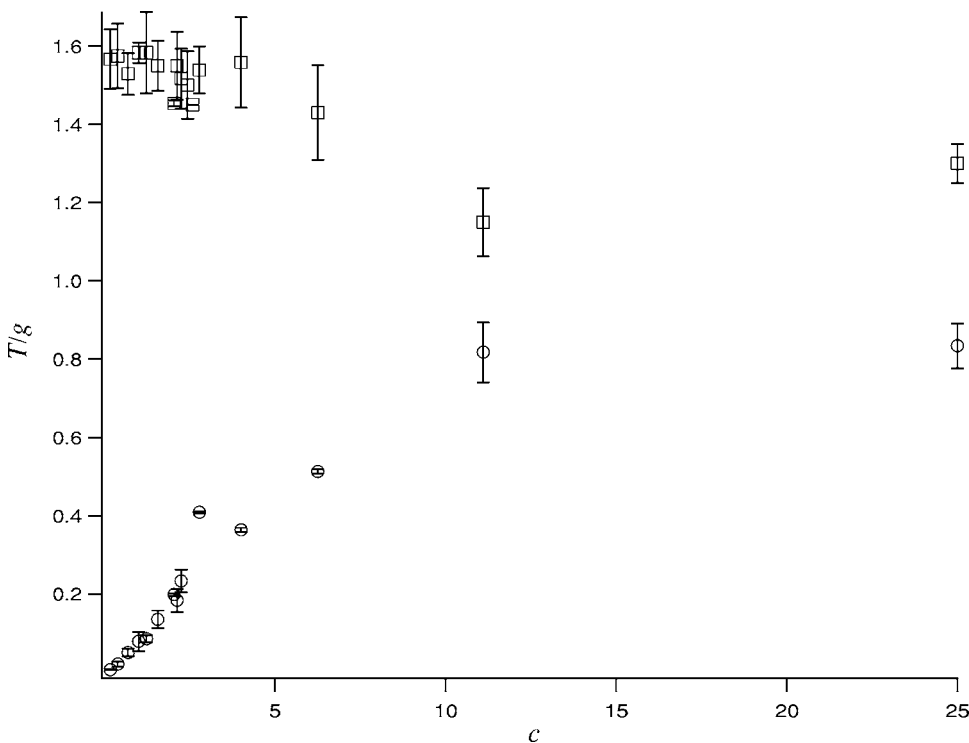


FIG. 8. Phase diagram for a system with a square array of vacancies. Independent simulation runs are performed at each value of  $c$  for which data points are shown (error bounds represent variations over independent simulations at fixed  $c$ ). Each simulation consists either of cooling the temperature from an initial high value or heating from zero temperature with a previously determined low temperature state as the initial state.



bounds on our estimate are fairly wide and the central estimate is lower than the result of Prakash and Henley. Further work is needed to determine if the truncation of the dipolar interaction, used by Prakash and Henley, effects this limiting slope.

### B. Face centered square lattice of vacancies

While the general features of the phase diagram for the FCSq array of vacancies is similar to that for the Sq array described above, consideration of certain special points on the phase diagram is useful in illuminating the general properties of the system and in particular the limit of very sparse systems. As noted above, at a vacancy concentration of 50% with vacancies arranged in a FCSq lattice the remaining dipoles form a square lattice. This is identical to the original ( $c=0$ ) lattice of dipoles except for a rotation by  $\pi/4$  and a dilation such that the lattice spacing is increased by a factor of  $\sqrt{2}$ . Since this “new” square lattice is identical to the original other than the rescaling and rotation, it must exhibit the same magnetic properties including a single ordered phase, i.e., the colinear phase, and a single phase transition, i.e., the order disorder transition. The dipoles in this colinear phase will be aligned parallel to the axis of the “new” square lattice of dipoles and the order-disorder transition temperature will be related to the transition temperature of the original ( $c=0$ ) lattice by  $T_c(c=0.50)=T_c(c=0)/\sqrt{2^3}$ .

This process may be continued by removing 50% of the dipoles on the new lattice again using a FCSq arrangement of vacancies (defined on the “new” lattice). Again this will result in a square lattice of dipoles and the same argument as above shows that at a vacancy concentration of  $c=75\%$  (relative to the original lattice of dipoles) generated by this process there is a single ordered phase with an order-disorder transition temperature related to the  $c=0$  transition temperature by a simple rescaling factor of  $\sqrt{2^6}$ . We may now generate iteratively a sequence of vacancy arrays labeled by  $i$  with vacancy concentrations relative to the original lattice of dipoles of

$$c_i = \sum_{j=1}^i 2^{-j} = 1 - 2^{-i}, \quad (8)$$

at each such concentration on the phase diagram there will be a single, colinear, ordered phase with an order-disorder critical temperature of

$$T_i = \frac{T_0}{\sqrt{2^{3i}}}, \quad (9)$$

where  $T_0$  is the order-disorder critical temperature for the original system with zero vacancies. Moreover, points at other concentrations in the interval  $[c_i, c_{i+1}]$  may be generated by a corresponding rescaling of the concentrations and critical temperatures for data points in the concentration interval  $[0, c_1]$ . In the limit  $c_i \rightarrow 1$  (or equivalently  $i \rightarrow \infty$ ) the values of  $c_i$  become very dense on the  $c$  axis. If  $c_i$  is approximated by a continuous variable  $c$  in this limit, the corresponding critical temperature for the order disorder transition is

$$T_c = T_0(1 - c)^{3/2}. \quad (10)$$

This line approaches the  $c$  axis tangentially as  $c \rightarrow 1$  and we conclude that the dipole system orders at sufficiently low temperature no matter how sparse it is. Figure 9 shows a phase diagram for the system with a FCSq array of vacancies generated by using data points from our simulations in the vacancy concentration interval  $[0, 0.5]$  and the iterative procedure described above to generate points in the interval  $[0.5, 1.0]$ . We note also that, to the accuracy of these simulations, the actual data points for the order-disorder transition temperature of a system with a regular array of vacancies is quite well predicted by this line regardless of which array of vacancies considered here is chosen.

## VI. SUMMARY

In addition to those simulations of dipole systems with square (Sq) and face centered square (FCSq) arrays of vacancies described above, we have also performed Monte Carlo simulations of dipole systems on a square lattice with triangular arrays of vacancies and rectangular arrays of vacancies. Apart from changes in the details of the ordered phases and domain structures which might be predicted based on the results above, the general features of the ordering and structure of the phase diagrams is similar to that discussed above.

The simulation results reported above demonstrate that the introduction of a very small concentration of vacancies generates a new phase at low temperature in addition to the colinear phase. The system initially orders in the colinear phase below the order-disorder critical temperature, however, as the system temperature is further reduced the system undergoes an abrupt transition to the new phase at a finite temperature. At very low concentrations of vacancies this new ordered phase is the microvortex ordered phase (with some distortion centered on the vacancies) that has been discussed in the context of systems with random vacancies<sup>7</sup> and systems with negative exchange interaction.<sup>4,5</sup> Indeed, at very low concentrations of vacancies the behavior of systems with random vacancies and regular arrays of vacancies are very similar. At all but the lowest values of vacancy concentration considered, domain formation plays a significant role in the low temperature properties of the system. In the case of the square array of vacancies, the frequent appearance of domains appears at concentrations of vacancies as low as 1% ( $c=0.01$ ). Domain walls are in almost all cases located on vacancy lattice lines. At the lower vacancy concentrations at which domains occur the domain walls tend to be parallel giving a striped arrangement of domains. However, at higher concentrations of vacancies complex plaid patterns of domains form with intersecting domain walls. While the domain walls retain some structure such as alignment with the vacancy lattice lines, their positioning and, consequently, intersections appears to be quite random in these plaid phases. The observation of these phases implies that the energy cost for domain formation is quite low and that, therefore, the plaid phases will form a system of nearly degenerate states



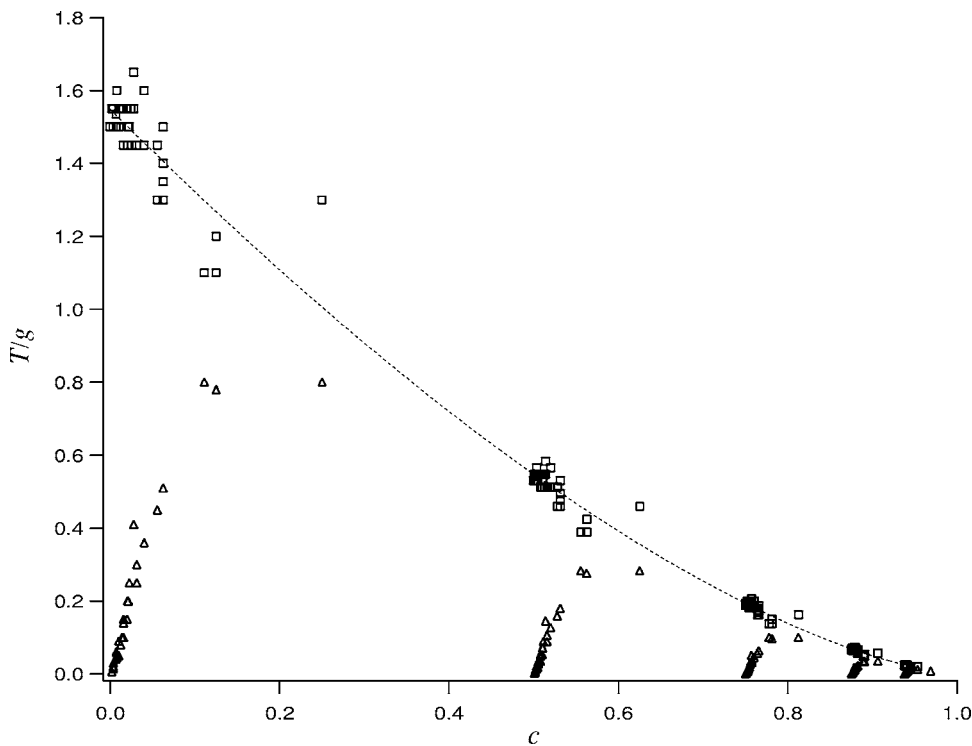


FIG. 9. Phase diagram for a system with a face centered square array of vacancies. Data points for  $c > 0.5$  are generated using the iterative procedure described in the text. The dotted line is the function  $T_c(c) = T_c(0)(1 - c)^{3/2}$ .

with energies just above the single domain state. Moreover, while these states will eventually relax to the single domain states the dynamical process for this is very slow (at least on the scale of times that can be simulated). In this sense these states can be considered to be analogous to glasses; however, as described above, an ordering temperature can still be identified for the systems simulated in this work.

In general, immediately below the critical temperature  $T_c$  the collinear phase is destabilized by thermal fluctuations over a range of temperatures which depends on system size and vacancy concentration. In sufficiently small systems for certain vacancy concentrations this range of temperature extends to the lower critical line. This destabilization, while not significant for typical films of atomic dipoles [ $O(100) - O(1000)$  atoms across], will be significant in small arrays of nanodots. Of course, such small systems would also be affected by edge effects which are not included in this study.

By considering the special case of vacancy arrays generated by an iterative procedure based on FCSq arrays of vacancies we are able to extend our results to vacancy concentrations in the range  $[0.5, 1.0]$  and determine an asymptotic form for the dependence of the order-disorder critical temperature in the limit of vacancy concentration  $c \rightarrow 1.0$ , thus demonstrating that the system orders no matter how sparse it becomes. In their pioneering work on order disorder phenomena in dipolar systems, Prakash and Henley speculated that a “percolation threshold” exists for systems with a random distribution of vacancies. The system considered by Prakash and Henley had a dipolar interaction which was truncated at nearest neighbor distances; such a system obviously has a percolation threshold, however, our present results suggest that no such percolation limit exists for dipolar systems with full long ranged interactions. A further simple argument based on the nature of the dipole interaction itself

also suggests this possibility. Consider a random array of point dipoles distributed on a continuous plane. If the plane is infinite then the only measures of length are those generated by the positioning of the dipoles in the space. For example, the square root of the areal density of dipoles provides such a measure and all lengths scale with this measure. Now if the system is uniformly rescaled so that its areal density changes, the vector which positions any dipole relative to any other dipole changes in length but not its orientation relative to a system of axes with origin at one of these dipoles. Therefore the only change which occurs in the dipole-dipole interaction is simply a rescaling of the factor that multiplies both the isotropic and anisotropic terms of the interaction. Thus if we can find a random array of point dipoles which orders at a finite temperature we can generate an arbitrarily sparse system which also orders at a suitably rescaled but finite transition temperature. (Notice that this result does not hold for other long ranged interactions, such as the RKKY interaction, where a uniform rescaling may change the overall sign as well as the magnitude of the interaction).

We note also that in the iterative procedure based on FCSq arrays of vacancies there exist “special” values of concentration at which only a single ordered phase exists. Unfortunately, we were not able to extrapolate the data in a sufficiently reliable way to determine where the two phase lines coalesce.

Finally we note that, while we have shown the Sq and FCSq vacancy array data points separately in Figs. 9 and 10, respectively, if the data points are combined on a single phase diagram they lie close to a single line in both the case of the order-disorder transition and the case of the collinear to microvortex transition. Moreover, the line

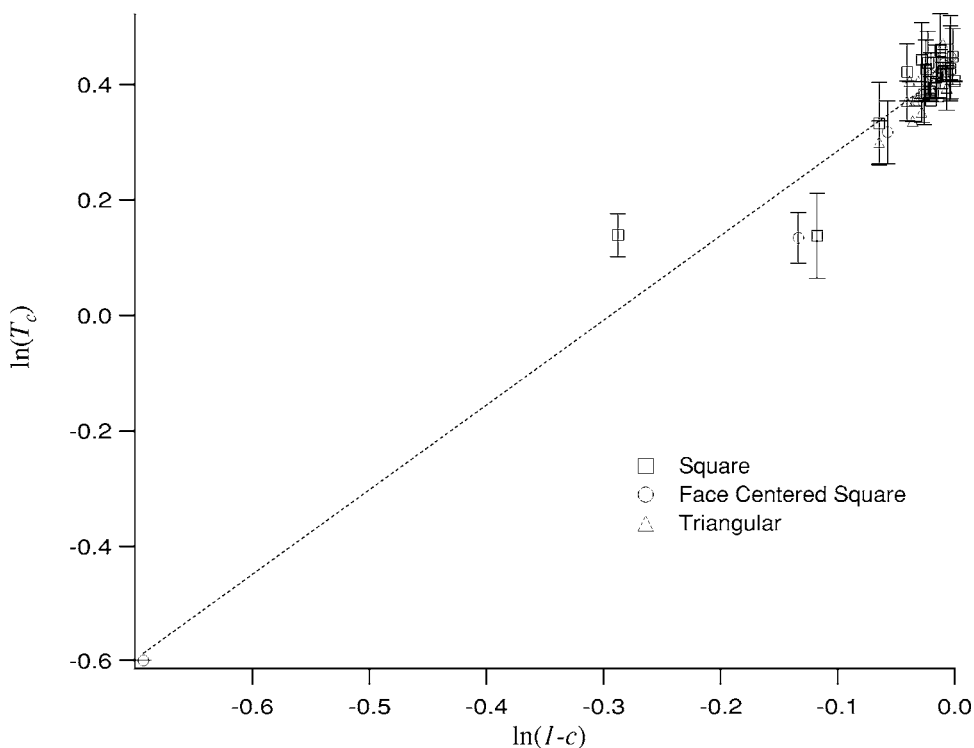


FIG. 10. A plot of  $\ln(T_c)$  vs  $\ln(1-c)$  for various arrays of vacancies (square,  $\bullet$ , face centered square,  $\diamond$ , and triangular,  $\triangle$ ) and vacancy concentration  $c \leq 50\%$ . The slope of the least-squares regression line shown is  $1.44 \pm 0.07$  (one standard error). Excluding the data point from an independent simulation with a face centered square array of vacancies at  $c = 50\%$  results in a regression line slope of  $1.4 \pm 0.2$ .

$$T_c = T_0(1-c)^{3/2}, \quad (11)$$

obtained from our consideration of extending the FCSq data as described above, provides a reasonable estimate of the order disorder transition temperature as a function of the vacancy concentration irrespective of the vacancy array used (again to the accuracy of the present Monte Carlo data). Figure 10 demonstrates this by plotting  $\ln(T_c)$  vs  $\ln(1-c)$  for three different types of vacancy array. The slope of the least-squares regression line for this plot is  $1.44 \pm 0.07$  consistent with the “scaling form” given above. We note that the location of the exact value of  $T_c$  for intermediate values of  $c$  is more uncertain because of the noise in the data at intermediate values of  $c$ . We assume that this additional noise is due to the rather weak nature of the anisotropy and consequent instability of the single collinear phase for  $T \leq T_c$  in systems of the size considered here. To overcome this difficulty data points for intermediate values of  $c$  in Fig. 10 represent averages over several Monte Carlo simulations for a given vacancy array and the error bounds represent the variation in  $T_c$  obtained from those simulations. Due to the spacing of the accessible values of  $c$  the data point at the highest value of  $c$  in Fig. 10 ( $c = 0.50$ ) which is for a FCSq vacancy array might play a strong role in determining the slope of the regression line. We have therefore repeated the fitting procedure with this point removed. The slope of the resulting least-squares regression line ( $1.4 \pm 0.2$ ) while having a wider error bound and slightly lower central estimate remains consistent with the scaling form for  $T_c$  as a function of  $c$ , given above. We conclude that this scaling form is a useful guide to the change in  $T_c$  due to vacancy presence.

The specific results presented here are, of course, dependent on the fact that we have excluded magnetic interactions

other than the dipolar interaction from our model. For example, the introduction of either a positive or negative exchange interaction parameter, in a system with axial anisotropy and a dipolar interaction, results in either a ferromagnetic or simple antiferromagnetic ground state, respectively, for a system with no vacancies, if the magnitude of the exchange interaction exceeds a fairly low threshold.<sup>14</sup> More recent results for systems with no vacancies and no on-site anisotropy have shown that an antiferromagnetic interaction may (depending on magnitude) change the nature of the effective anisotropy associated with the dipolar interaction and consequently change the preferred axes for the order parameter. Preliminary results for this system with the addition of random vacancies indicate that the structure of the phase diagram is quite rich<sup>15</sup> and we are currently investigating how the addition of exchange interactions effect the system studied in this paper. The addition of exchange interactions breaks the self-similarity which we exploited to map the system with a face centered square array of vacancies at a concentration below 50% to the corresponding system with vacancy concentration above 50%. Consequently comparing results for systems with exchange interaction with the “scaling law” relating transition temperature to vacancy concentration obtained in this work will be of some interest. Last we note that the introduction of vacancy arrays can be used to directly modify or control exchange interactions. For example, if the exchange interaction is assumed to be between nearest neighbors only in the original model, introducing the 50% concentration of vacancies in a face centered square array reproduces the original lattice structure but the magnetic system now contains dipolar interactions only. Consequently the introduction of regular arrays of vacancies allows one to move between systems dominated by exchange interactions in their ground state to pure dipole systems.

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