First publ. in: Journal of Applied Physics 76 (1994), 10, pp. 6341-6343

Monte Carlo simulation of Ising models with dipole interaction

U. Nowak and A. Hucht
Theoretische Tieftemperaturphysik, Universität Duisburg, 47048 Duisburg, Germany

Recently, a new memory effect was found in the metamagnetic domain structure of the diluted Ising antiferromagnet $Fe_xMg_{1-x}Cl_2$ by domain imaging with Faraday contrast. Essential for this effect is the dipole interaction. We use a Monte Carlo method to simulate the low-temperature behavior of diluted Ising antiferromagnets in an external magnetic field. The metamagnetic domain structure occurring due to the dipole interaction is investigated by graphical representation. In the model considered, the antiferromagnetic state is stable for an external magnetic field smaller than a lower boundary B_{c1} while for fields larger than an upper boundary B_{c2} the system is in the saturated paramagnetic phase, where the spins are ferromagnetically polarized. For magnetic fields in between these two boundaries a mixed phase occurs consisting of ferromagnetic domains in an antiferromagnetic background. The position of these ferromagnetic domains is stored in the system: after a cycle in which the field is first removed and afterwards applied again the domains reappear at their original positions. The reason for this effect can be found in the frozen antiferromagnetic domain state which occurs after removing the field at those areas which have been ferromagnetic in the mixed phase.

The three-dimensional Ising model with an antiferromagnetic exchange interaction undergoes a first-order phase transition from an antiferromagnetic to a paramagnetic saturated phase for low temperatures during an increase of the homogeneous external magnetic field. Because of demagnetizing field effects in experimental systems like $FeCl_2$ there occurs a mixed phase for external fields $B_{c1} \leqslant B \leqslant B_{c2}$.[1] In theoretical considerations the existence of a mixed phase is often neglected since dipole interactions have to be considered in order to investigate the mixed phase. Especially in Monte Carlo simulations, the dipole interaction can hardly be taken into account for lattices large enough to investigate domain structures due to its long-range nature: for each spin flip the number of operations to calculate the change in energy scales with the number of spins in the system. However, we used a specially adjusted algorithm to do these calculations efficiently. The details of our method will be published elsewhere.

In this paper, we perform simulations in order to get a deeper understanding of a new memory effect that was found recently in the mixed-phase domain structure of the diluted Ising antiferromagnet $Fe_xMg_{1-x}Cl_2$ by domain imaging with Faraday contrast.[2] The position and shape of paramagnetic saturated domains which grow within the antiferromagnetic state while the field is increasing, is stored in the sense that the domains reappear even after a cycle in which the field is first removed and afterwards again applied. Essential for an investigation of this effect is obviously the dipole interaction, since it is this long-range interaction which is responsible for the occurrence of a mixed phase.

The diluted Ising antiferromagnet in an external magnetic field (DAFF) is an ideal system to study random field behavior theoretically as well as experimentally since it is believed to be in the same universality class as the random field Ising model (RFIM).[3] A well-known feature of the DAFF is the formation of a domain state with extremely long relaxation times (for an overview see Ref. 4). This domain state is frozen even for zero field and it is obtained by either cooling the system in an external field from the paramagnetic high-temperature phase or by decreasing the field correspondingly. The mechanisms which are responsible for the hysteretic properties of the DAFF have been investigated experimentally,[5,6] theoretically,[7] and in computer simulations.[8–11] In the following, we will show that the understanding of the hysteretic behavior of the DAFF is essential for an understanding of the memory effect.

The Hamiltonian of an Ising model with dipole interaction in units of the coupling constant reads

$$H=\sum_{\langle i,j\rangle} \epsilon_i\epsilon_j\sigma_i\sigma_j - B\sum_i \epsilon_i\sigma_i + d\sum_{i,j} \frac{\epsilon_i\epsilon_j\sigma_i\sigma_j}{r^3_{i,j}}(1-3\cos^2\theta_{i,j})$$

where $\sigma_i = \pm 1$ are the spins and the $\epsilon_i = 0,1$ represent the dilution $p = 5\%$. In the first sum $\langle i,j\rangle$ means all combinations of spins which are nearest neighbors. The exchange interaction favoring antiferromagnetic alignment of spins is set equal to one. The second sum represents the interaction with the external magnetic field B. The third sum is over all combinations of spins and d represents the strength of the dipole interaction ($d = 0.5$ in this case). $r_{i,j}$ is the distance between two spins on sites i and j and θ is the angle between the z axis (the direction of the external field) and the distance vector $\mathbf{r}$. In order to simplify the model we restrict ourselves to a two-dimensional system with open boundary conditions representing one plane of the experimental system. As we will see the qualitative behavior of the experimental system is well described by our model as far as the domain structure is concerned, which is responsible for the memory effect.

We use an antiferromagnetic long-range ordered system as the initial spin configuration. The simulation is done at very low temperature, $T = 0.1$. The system builds up a saturated-domain state for a field of $B = 2.65$ which is within the mixed phase, then we investigate the development of this domain state during a field cycle to zero field, $B = 0$, and

FIG. 1. Spin configuration and column magnetization of the simulated system as explained in the text: a metamagnetic domain configuration in the mixed phase.

FIG. 3. Spin configuration and column magnetization of the simulated system: the metamagnetic domain configuration after applying the field again.

then back to the mixed phase, $B=2.65$. The time that is needed to equilibrate the system is a few hundreds of Monte Carlo steps per spin.

The system has a size of 190×50 ($x\times z$), i.e., 190 columns and 50 rows. The figures show spin configurations of the simulated system as well as the mean magnetization of the columns of the system. The external magnetic field is aligned with the easy axis of the spins, the z direction. Each site of the two-dimensional square lattice is represented by a square, the vacancies of the system are shown as black, upspins as grey and downspins as white squares. The mixed phase (Fig. 1) consists of antiferromagnetic domains (checkerboardlike) and paramagnetic saturated (ferromagnetic) domains (grey, "spinup"). In the latter domains the spins are aligned with the field. The domains have the form of stripes. This follows directly from the nature of the dipole interaction which favors those spins to order ferromagnetically which are on lattice sites placed along the direction of the easy axis leading to the development of ferromagnetically ordered columns. Also shown in the upper part of Fig. 1 is the column magnetization, i.e., the mean magnetization of each column of the system. This quantity corresponds to the Faraday contrast that is observed in experiments. Since the domains are striped there is a sharp contrast between antiferromagnetic domains (magnetization≈0) and paramagnetic saturated domains (magnetization≈1/per spin).

Lowering the field to zero the saturated domains vanish (Fig. 2) and the magnetization decreases to nearly zero. However, an accurate analysis of this zero-field spin configuration shows that it is not completely antiferromagnetically long-range ordered. Instead, those regions of the system which have been paramagnetic saturated in the field now consist of an antiferromagnetic domain structure corresponding to the domain state of a DAFF after field decreasing. Why does this happen?

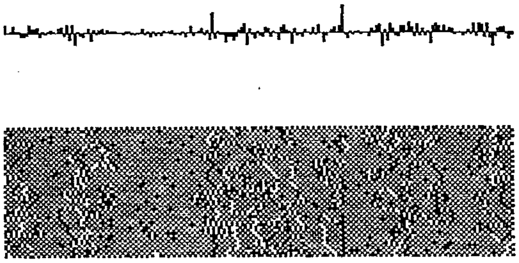

FIG. 2. Spin configuration and column magnetization of the simulated system: an antiferromagnetic domain configuration after removing the field.

In a field-decreasing procedure the antiferromagnetic–paramagnetic phase boundary is crossed in a direction from the paramagnetic to the antiferromagnetic phase. In this case, due to the unconventional dynamics of the DAFF which follows from random-field pinning, the system cannot develop a long-range ordered state. Instead, it freezes in an antiferromagnetic domain state. This effect is the reason for the unconventional structure of the system after removing the external field. In regions of the system which have been paramagnetic saturated in the mixed phase, a frozen antiferromagnetic domain state develops while in the regions of the system which have been antiferromagnetic nothing changes, the long-range order persists. The nonexponential dynamics of antiferromagnetic domains in a DAFF after removing the external field has been investigated earlier (see Ref. 12; and references therein). The domains are frozen and remain practically constant on time scales accessible for observation. Note that due to the existence of antiferromagnetic domains and domain walls, respectively, there is a finite column magnetization. This magnetization is small compared to the magnetization of a saturated domain but it is larger than the magnetization of an antiferromagnetic column which is also not exactly zero due to fluctuations of the vacancy distribution in our finite system.

After applying the magnetic field again, once more a configuration of striped antiferromagnetic domains arises (Fig. 3). Comparing this configuration with the original domain configuration (Fig. 1) one finds that the original domain configuration is nearly reproduced, at least in that sense that paramagnetic saturated domains grow first at those places which have been paramagnetic saturated before. This is the memory effect. Its origin is the antiferromagnetic domain configuration of the system after removing the field (Fig. 2). The regions which consist of an antiferromagnetic domain state are less stable than the long-range ordered regions since the first contain domain walls. These regions are the first in which saturated domains during an increase of the external field occur, restoring the original metamagnetic domain configuration.

This work was supported by the Deutsche Forschungsgemeinschaft through Sonderforschungsbereich 166.

[1] J. F. Dillon, Jr., E. Yi. Chen, and H. J. Guggenheim, Phys. Rev. B **18**, 377 (1978).

[2] J. Mattsson, J. Kushauer, D. Bertrand, J. Ferré, and W. Kleemann, J. Mag. Mag. Mater. **130**, 216 (1994).

[3] S. Fishman and A. Aharony, J. Phys. C **12**, L729 (1979).

[4] D. P. Belanger and A. P. Young, J. Mag. Mag. Mater. **100**, 272 (1991).

[5] R. J. Birgeneau, R. A. Cowley, G. Shirane, and H. Yoshizawa, J. Stat. Phys. **34**, 817 (1984); D. P. Belanger, S. M. Rezende, A. R. King, and V. Jaccarino, J. Appl. Phys. **57**, 3294 (1985).

[6] U. A. Leitão, W. Kleemann, and I. B. Ferreira, Phys. Rev. B **38**, 4765 (1988); P. Pollak, W. Kleemann, and D. P. Belanger, Phys. Rev. B **38**, 4773 (1988).

[7] J. Villain, Phys. Rev. Lett. **52**, 1543 (1984).

[8] G. S. Grest, C. M. Soukoulis, and K. Levin, Phys. Rev. B **33**, 7659 (1986).

[9] U. Nowak and K. D. Usadel, Phys. Rev. B **39**, 2516 (1989).

[10] U. Nowak and K. D. Usadel, Phys. Rev. B **44**, 7426 (1991).

[11] U. Nowak and K. D. Usadel, Phys. Rev. B **46**, 8329 (1992).

[12] S-J. Han, D. P. Belanger, W. Kleemann, and U. Nowak, Phys. Rev. B **45**, 9728 (1992).