Antiferromagnetic domains in a two-dimensional Heisenberg square lattice

D. S. Deng and X. F. Jin
State Key Laboratory of Applied Surface Physics, Fudan University, Shanghai 200433, China

Ruibao Tao*
Department of Physics, Fudan University, Shanghai 200433, China

(Received 12 November 2001; published 19 March 2002)

An intrinsic mechanism for the antiferromagnetic domain formation has been proposed in a two-dimensional Heisenberg square lattice. The results indicate that the competition between the magnetic anisotropy and the dipole-dipole interaction can indeed yield both the Bloch type and Néel type domain structures. Using a spin dynamics calculation with fast Fourier transformation, we further show some representative antiferromagnetic domain patterns and their phase diagram as a function of the competition.

DOI: 10.1103/PhysRevB.65.132406 PACS number(s): 75.50.Ee, 75.25.+z, 75.30.−m, 75.70.Kw

The unidirectional magnetic anisotropy in a ferromagnet (FM)/antiferromagnet (AFM) system, an effect discovered in 1956 and referred as exchange bias,[1] has currently received much attention because of its importance in the magnetic storage industry.[2–4]. To understand the exchange bias observed in experiments, it is generally believed that a clear picture about the detailed micromagnetic structure is the key issue.[5,6] Using the polarization-dependent x-ray magnetic dichroism spectra microscopy, the antiferromagnetic domains (AFMD) in epitaxial thin films were recently observed,[7,8] meanwhile their correlation to the local exchange bias was established.[9] It is further realized that the AFMD structures are surface and interface dependent as a breaking symmetry effect.[10,11]

Different from the well-understood ferromagnetic domain mechanism promoted by the reduction of magnetostatic energy, the origin of domain formation in an AFM is not straightforward, since the magnetostatic effect is expected to play a less important role for an overall compensated AFM system. In fact, the existence of domain in antiferromagnets was proposed by Néel in 1953, to explain the increase of susceptibility of antiferromagnets with field intensity.[12] Yin-Yuan Li argued that the domain wall would owe its stability to the presence of lattice imperfections.[13] Malozemoff mentioned the AFMD derived from the random exchange interactions similar to random field.[14] However, so far, theoretically AFMD is still only attributed to the extrinsic origins such as defects, meanwhile experimentally AFMD has attracted present efforts in exchange bias system and also been demonstrated clearly.[7–11] Then it is naturally interesting to explore: Does there exist any intrinsic origins of AFMD?

In this paper, we propose that a competition between the dipole-dipole interaction and the magnetic anisotropy may be an intrinsic mechanism for the domain formation in a two-dimensional (2D) Heisenberg antiferromagnet with an in-plane anisotropy. The key point is that these two interactions tend to align the spins perpendicular and parallel to the plane, respectively, in this AFM system. In other words, for an antiferromagnet with the in-plane anisotropy, the dipole-dipole interaction favors the spins standing perpendicular to the plane while the anisotropy prefers them lying down in the plane. Therefore an antiferromagnet with the dipole-dipole interaction alone prefers to align its spins perpendicular to the plane. As the in-plane anisotropy is turned on, the instability of the originally homogenous AFM phase starts to develop and finally leads to the domain formation. The following will indicate that the instability can be monitored by the magnon excitation energy gap.

For a two-dimensional Heisenberg model with square lattice, the Hamiltonian is

$$H = J\sum_{\langle i,j\rangle} S_i \cdot S_j + D\sum_i S_z^2 + U_{\text{dipole}}, \tag{1}$$

$$U_{\text{dipole}} = \frac{1}{2}\sum_{i,j} \Omega_{ij}\left[(S_i \cdot S_j) - \frac{3}{r_{ij}^2}(r \cdot S_i)(r \cdot S_j)\right], \tag{2}$$

where $J>0$ represents the antiferromagnetic ordering, D the anisotropy strength, and U_{dipole} the dipole-dipole interaction, and $\Omega_{ij}=\Omega(r_{ij})^{-3}[\Omega=(gu_B)^2/a^3$, g the Lande factor, u_B the Bohr magneton, a the lattice constant]. After the Holstein-Primakoff (HP) transformation[15] under the harmonic approximation, the Hamiltonian becomes

$$H = U_0 + H_1 + H_2 + H_3, \tag{3}$$

where U_0 is a constant, and H_1, H_2, H_3 represent the exchange, anisotropy, and dipole-dipole interactions, respectively. In dividing the system into two sublattices a and b, we can obtain

$$H_1 = JS\sum_{\langle l,m\rangle} [(a_l^+ a_l + b_m^+ b_m) - (a_l^+ b_m^+ + a_l b_m)], \tag{4}$$

$$H_2 = -(2S-1)D\left(\sum_l a_l^+ a_l + \sum_m b_m^+ b_m\right), \tag{5}$$

where a_l, b_m label the two antiferromagnetic sublattices a and b:

$$H_3 = H_a + H_b + H_{ab}, \tag{6}$$

where H_a, H_b are the dipole-dipole interactions in the a, b sublattices, respectively, while H_{ab} is the dipole-dipole inter-

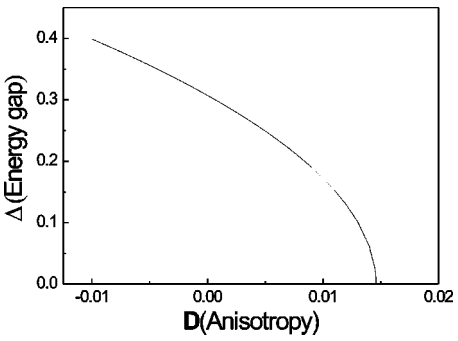

FIG. 1. The magnon excitation energy gap (Δ) as a function of the anisotropy.

action between the two sublattices. Setting $r^+=x+iy, r^-=x-iy$, we can rewrite the forms as

$$H_a=-S\sum_{i,j}\ \Omega_{ij}a_i^+a_i-\frac{1}{2}S\sum_{i,j}\ \Omega_{ij}a_i^+a_j - \frac{3}{4}S\sum_{i,j}\ \Omega_{ij}\left(\frac{r_+^2}{r^2}a_i^+a_j^+ + \frac{r_-^2}{r^2}a_ia_j\right), \tag{7}$$

$$H_b=-S\sum_{i,j}\ \Omega_{ij}b_i^+b_i-\frac{1}{2}S\sum_{i,j}\ \Omega_{ij}b_i^+b_j - \frac{3}{4}S\sum_{i,j}\ \Omega_{ij}\left(\frac{r_+^2}{r^2}b_i^+b_j^+ + \frac{r_-^2}{r^2}b_ib_j\right), \tag{8}$$

$$H_{ab}=\frac{1}{2}S\sum_{l,m}\ \Omega_{lm}(a_l^+a_l+b_m^+b_m) + \frac{1}{4}S\sum_{l,m}\ \Omega_{lm}(a_l^+b_m^+ + a_lb_m) + \frac{3}{4}S\sum_{i,j}\ \Omega_{lm}\left(\frac{r_+^2}{r^2}a_l^+b_m + \frac{r_-^2}{r^2}a_lb_m^+\right). \tag{9}$$

The quantum fluctuation coming from the higher order terms is expected to be suppressed significantly by the anisotropy which can result in gap in excitation energy. Now the Hamiltonian (3) can be diagonalized by the general (U,V) transformations with numerical calculation,[16] so the excitation energy ϵ_n and the magnon energy gap $\Delta=\min[\epsilon_n]$ are obtained. It is obvious that a positive Δ means the state without quantum fluctuation is stable or metastable, otherwise the state will be unstable and turn to an inhomogeneous or domain state.

Figure 1 shows the magnon gap Δ as a function of the anisotropy strength D for 8×8 2D square lattice sites, with parameters. $J=1$, $\Omega=0.01$, and $S=1$ (quantum spin). First of all, it is noticed that there exists a gap $\Delta>0$ for the case with easy axis perpendicular to the plane ($D<0$). This is understandable because both the anisotropy and the dipole-dipole interaction tend to align the spins perpendicular to the plane. Therefore it costs energy $\Delta>0$ for any excited states, or any spin configuration changes. However, for an easy plane anisotropy ($D>0$), the anisotropy tends to align the spins in the plane while the dipole-dipole favors to get the spins out of plane. It is the increasing of the in-plane anisotropy that causes the energy gap Δ decreasing then finally reaching to zero. Once $\Delta=0$ is reached, it means that this homogenous perpendicular ground state becomes unstable and needs to be reconstructed.

To understand what the final state of the system is and how the spin configuration looks, now we will carry out a classical spin dynamics simulation focusing on the case of easy plane anisotropy. We obtain AFMD spin configuration by classical spin dynamics, i.e., the local effective field is determined from the gradient of the energy $\mathbf{H}_i^{\text{eff}}=-\partial H/g u_B\partial\mathbf{S}_i$, and $\{\mathbf{S}_i\}$ is required to satisfy the Laudau-Lifshitz equation of motion EOM with the Gilbert-Kelley form for the damping term $(\partial/\partial t)\mathbf{S}_i=g u_B\mathbf{S}_i\times[\mathbf{H}_i^{\text{eff}}-\eta(\partial)/(\partial t)\mathbf{S}_i]$, where η denotes the damping parameter. This damping term is phenomenological and is included to remove the energy from the system and to ensure that the magnetic system is in a stable or metastable equilibrium after sufficient steps. The fast Fourier transformation (FFT) method[17] which will reduce N^2 algorithm to $N\log_2 N$, has also been accepted in the spin dynamics to calculate the long range dipole-dipole interaction local field with large scale lattice sites.

The initial spin configuration is set to be random. After the sufficient iterating calculation, the system finally reaches to a stable or a metastable spin configuration. In our simulation, 256×256 lattice sites are considered in the simulation and the parameters in Eq. (1) are $J=1.000$, $\Omega=0.0252$, $S=1$ (classical spin), and D adjustable. In addition we define $f=D/\Omega$, and $M=\langle\Sigma_i|S_i^z|\rangle$. They are used to describe respectively the competition between the anisotropy and the dipole-dipole interaction, and the average spin component out of plane. It is noticed that there exist two types of antiferromagnetic domains, i.e., the Bloch type and Néel type domains, a situation very similar to the ferromagnetic domains in thin film systems.[18] The Néel type antiferromagnetic domains are expected for a larger f, because the strong anisotropy forces the spins almost lying down in the plane. However, the Bloch type antiferromagnetic domains are

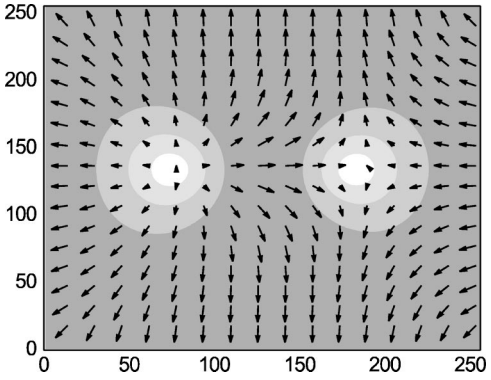

FIG. 2. A representative Bloch type antiferromagnetic domain pattern with a small in-plane anisotropy. Background color from white to gray indicating the different in-plane spin component domain areas.

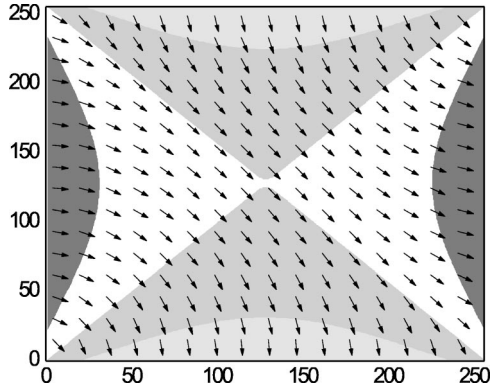

FIG. 3. A representative Néel type antiferromagnetic domain pattern with a large in-plane anisotropy. Background color from light gray to dark gray showing the different spin orientation domain areas.

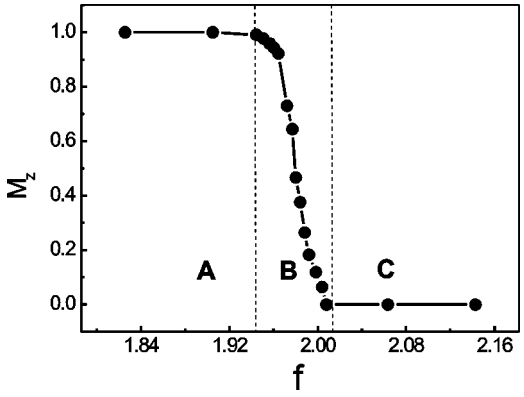

FIG. 4. The phase diagram as a function of $f\,(=D/\Omega)$. In the figure, phase *A*: the homogenous AFM state; phase *B*: the Bloch type domains; phase *C*: the Néel type domains.

more favorable for a smaller *f*, because the week anisotropy allows the spins out of plane with nonzero *M*.

A Bloch type antiferromagnetic domain pattern for $f=1.98$, is shown in Fig. 2. For simplicity in illustration, the spins displayed in this figure are chosen from one of the sublattices, and only those from $S(1)$, $S(17)$, $S(33)$, . . . , in the lattice. The amplitude of the arrows represents the spin component in the plane. The different in-plane spin component domain areas are presented by background color from white to gray in the figure. The spins are twisted three dimensionally.

Figure 3 indicates a Néel type antiferromagnetic domain pattern for a larger $f=2.38$. Again, the spins displayed in this figure are chosen from one of the AFM sublattices, and by every eight sites in the sublattice. The different spin orientation domain areas are shown by background color from light gray to dark gray in the figure.

As previously mentioned, it is confirmed by the simulation of spin dynamics that when the anisotropy becomes too small, the spins are all aligned vertical to the plane and the domains vanish. Therefore it is interesting to establish an overall phase diagram as a function of *f*, i.e., the competition between the anisotropy and the dipole-dipole interaction. Figure 4 shows such a phase diagram with $J=1$, $\Omega=0.0252$. The dash lines divide the phase diagram into three parts. When *f* is small, just the homogenous AFM state, all the spins are perpendicular to the plane and no domains in such a finite lattice are realized. As *f* increases, the spin configuration with Bloch type domains is more favorable in energy. Finally when *f* reaches sufficient large, the spin configuration with Néel type domains becomes more stable.

The above discussions for 2D lattice sites can easily be generalized to an ultrathin film case compared directly with the experiments. It should also be pointed out that 3D AFMD is still an open question. The predicted two types of AFMD still need be verified by further experiments. These AFMD studies might also open the door to the further exchange bias research.

In summary, an intrinsic mechanism for antiferromagnets in a 2D Heisenberg square lattice is proposed to explain the observed AFMD experiments. We suggest that there exist two types of antiferromagnetic domains, and further show their phase diagram as a competition between the dipole-dipole interaction and the anisotropy.

This work was supported by the National Natural Science Foundation of China, Shanghai Research Center of Applied Physics and a research grant for nano materials science, Chinese Science Academy. X.F.J. also acknowledges support from the Cheung Kong Scholars Program, Hong Kong Quishi Science Foundation, Y. D. Fok Education Foundation and International Center for Quantum Structures, CAS.

*Corresponding author. Email address: rbtao@fudan.ac.cn

[1] W.H. Meiklejohn, C.P. Bean, Phys. Rev. **102**, 1413 (1956); **105**, 904 (1957).

[2] B. Dieny, V.S. Speriosu, S.S.P. Parkin, B.A. Gurney, D.R. Wilhoit, and D. Mauri, Phys. Rev. B **43**, 1297 (1991).

[3] C. Tsang, Fontana Re, Lin T, Heim De, Speriosu Vs, Gurney Ba, and Mason Ml, IEEE Trans. Magn. **30**, 3801 (1994).

[4] S.S.P. Parkin, K.P. Roche, M.G. Samant, P.M. Rice, R.B. Beyers, R.E. Scheuerlein, E.J. O'Sullivan, S.L. Brown, J. Bucchigano, D.W. Abraham, Yu Lu, M. Rooks, P.L. Trouilloud, R.A. Wanner, and W.J. Gallagher, J. Appl. Phys. **85**, 5828 (1999).

[5] J. Nogues and I.K. Schuller, J. Magn. Magn. Mater. **192**, 203 (1999).

[6] A.E. Berkowitz and K. Takano, J. Magn. Magn. Mater. **200**, 552 (1999).

[7] J. Stöhr, A. Scholl, S. Anders, J. Lüning, M.R. Scheinfein, H.A. Padmore, and R.L. White, Phys. Rev. Lett. **83**, 1862 (1999).

[8] A. Scholl, J. Stöhr, J. Lüning, J.W. Seo, J. Fompeyrine, H. Siegwart, J.-P. Locquet, F. Nolting, S. Anders, E.E. Fullerton, M.R. Scheinfein, and H.A. Padmore, Science **287**, 1014 (2000).

[9] F. Nolting, A. Scholl, J. Stöhr, J.W. Seo, J. Fompeyrine, H. Siegwart, J.-P. Locquet, S. Anders, J. Lüning, E.E. Fullerton, M.F. Toney, M.R. Scheinfein, and H.A. Padmore, Nature (London) **405**, 767 (2000).

[10] H. Ohldag, A. Scholl, F. Nolting, S. Anders, F.U. Hillebrecht, and J. Stöhr, Phys. Rev. Lett. **86**, 2878 (2001).

[11] F.U. Hillebrecht, H. Ohldag, N.B. Weber, C. Bethke, U. Mick, Phys. Rev. Lett. **86**, 3419 (2001).
[12] L. Néel, *Proceedings of the International Conference on Theoretical Physics*, Kyoto and Tokyo, September, 1953 (Science Council of Japan, Tokyo, 1954), p. 701.
[13] Yin-Yuan Li, Phys. Rev. **101**, 1450 (1956).
[14] A.P. Malozemoff, Phys. Rev. B **35**, 3679 (1987), and references therein.
[15] T. Holstein and H. Primakoff, Phys. Rev. **59**, 1098 (1940).
[16] Lei Zhou, Ruibao Tao, and Yoshiyuki Kawazoe, Phys. Rev. B **54**, 9924 (1996).
[17] See for example, William H. Press *et al.*, *Numerical Recipes in Fortran 77: The Art of Scientific Computing*, Vol. 1 of Fortran Numerical Recipes (University of Cambridge, Cambridge, 1996), Chap. 12.
[18] E.Y. Vedmedenko, H.P. Oepen, A. Ghazali, J.C.S. Levy, and J. Kirschner, Phys. Rev. Lett. **84**, 5884 (2000).