ФИЗИКА

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STABILITY OF SKYRMIONS IN THE FRUSTRATED ANTIFERROMAGNETIC/FERROELECTRIC BILAYERS WITH THE TRIANGULAR LATTICE

© I.F. Sharafullin, A.R. Yuldasheva, N.M. Nugaeva and H.T. Diep

The formation and conditions of stability of a skyrmions at the interface between a ferroelectric layer and antiferromagnetic layer with triangilar lattice and its phase transition are studied. All interactions between spins and polarizations are limited to nearest neighbors (NN). The antiferromagnetic exchange interaction among the spins inside antiferromagnetic layer will compete with the perpendicular interface interaction between adjacent layers. The ground state spin configuration at zero temperature is calculated by using the numerical high performance steepest descent method. The resulting configuration is non-collinear. Small values of external field yields small values of angles between spins in the xy plane so that the ground state configurations have antiferromagnetic and non collinear domains. We observe the creation of single spin vortices. We noted that for zero applied magnetic field the skyrmions in the antiferromagnetic/ferroelectric bilayers with triangular lattice can be created in the region of interface magnetoelectric interaction value between 0.85 and 1.95. The strong external magnetic field applied perpendicular to the interface with non-collinear Dzyaloshinskiy-Morya-like magnetoelectric interaction at the interface leads to remove the skyrmion phase and magnetic phase transitions. With increasing the interface magnetoelectric coupling, the skyrmion lattice disappear. We found the formation perfect skyrmion structure at non-zero external magnetic field and moderate values of magnetoelectric interaction. The skyrmions structure is stable in a large region of the interface magnetoelectric interaction between antiferromagnetic and ferroelectric films. The results of Monte Carlo simulations that we carried out confirm that observed skyrmions are stable up to a finite temperature.

Index Term: magnetoelectric interaction, skyrmions, steepest descent method, bilayers, ground state spin configuration, triangular lattice, frustration systems.

Introduction. Surface engineering is a promising method to trigger rich spin constructions such as spin vortexes or fascinating spin textures with topological protection – skyrmions. Magnetic skyrmions – nanoscale topologically protected vortices of spin – have been investigated as potential information carriers in spintronics devices [1–3]. Skyrmions usually form under the influence of an external magnetic field in noncentrosymmetric nanofilms or at interfaces in bilayers and interfacial symmetry-breaking heterostructures [4–6]. We can note, that the magnetic frustration present in this material by nature helped stabilize the phase with skyrmion lattice, which was detected by experimental measurement. Sufficiently strong Dzyaloshinskii-Moriya interaction can then lead to the formation of isolated skyrmions and the perfect skyrmion cristall [7–8]. The magnetic ground state and the phase diagram investigated for systems with antiferromagnet triangular lattice by using first-principles density functional calculations [9]. Without external magnetic field spirals are the most stable textures, and showed the possibility of stabilizing antiferromagnetic skyrmion lattices in such system under the influence of an external magnetic field [9]. From a microscopic approach, Dzyaloshinskii-Moriya (DM) interaction can incerase when the interaction of two magnetic atoms is mediated by a non-magnetic atom via the exchange interaction, and the parameter of DM interaction is proportional to the spin-orbit interaction, which can be quite large in superlattices at interfaces between magnetic films and non-magnetic films [10]. The superstructures naturally lead to the interaction of skyrmions on different interfaces, which has unique dynamics compared to

SHARAFULLIN Ildus Fanisovich – PhD, Bashkir State University, e-mail: Sharafullinif@yandex.ru
YULDASHEVA Alina Rifovna, Bashkir State University, e-mail: alina.yuldasheva.92@mail.ru
NUGAEVA Nuria Mazitovna, Bashkir State University, e-mail: nughaieva97@mail.ru
DIEP The Hung, Laboratoire de Physique Théorique et Modélisation, Université Cergy-Paris, e-mail: diep@cyu.fr

the interaction of the same-interface skyrmions elements [11]. Note that in Ref. [12], we investigated the effects of Dzyaloshinskii-Moriya (DM) magneto-ferroelectric interaction in a "unfrustrated" ferromagnetic/ferroelectric superlattice. In a zero external magnetic field, we showed that the ground state spin configuration is periodically non-collinear. Through the use of a two-times Green's functions, we calculated the spin wave spectrum in a ferromagnet monolayer and in a bilayer sandwiched between ferroelectric films. We showed that when magnetic field is applied in the direction perpendicular to the plane of layers, the skyrmions are arranged to form a crystalline structure at the interface.

In ref. [13] the effect of the frustration in a superlattice composed of alternating frustrated magnetic and ferroelectric films, both with simple cubic lattice was investigated. We showed that frustration gives rise to an enhancement of skyrmions created by the DM interaction at the magnetoelectric interface in applied external magnetic field.

Model and skyrmions. The frustrated antiferromagnetic/ferroelectric bilayers with the triangular lattice that we study here is composed of magnetic and ferroelectric films. All interactions between spins and polarizations are limited to nearest neighbors (NN). The full Hamiltonian is expressed as:

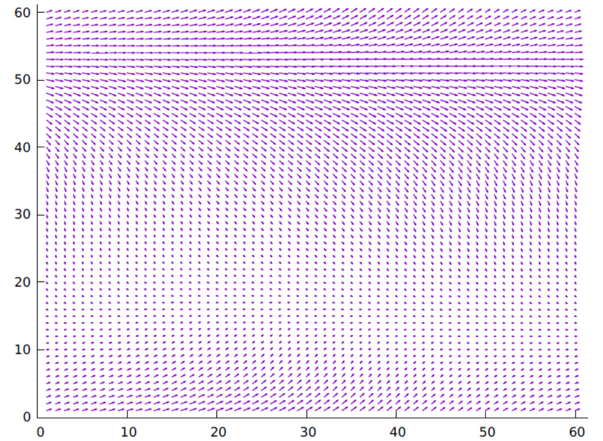
$$H = -\sum_{i,j} J_{ij}^m \vec{S}_i \cdot \vec{S}_j - \sum_{i,j} J_{ij}^f \vec{P}_i \cdot \vec{P}_j - - \sum_{i,j,k} J^{mf} \vec{P}_k \cdot [\vec{S}_i \times \vec{S}_j] - \sum_{\langle i \rangle} \vec{H} \cdot \vec{S}_i \quad (1)$$

where $\vec{S}_i$ is the spin on the i-th site, $J_{ij}^m < 0$ the antiferromagnetic interaction parameter between a spin and its nearest neighbors and the sum is taken over NN spin pairs. We suppose that $J_{ij}^m = J^m$ for Heisenberg spins everywhere in the magnetic film. The external magnetic field $\vec{H}$ is applied along the z-axis which is perpendicular to the plane of the layers. $\vec{P}_i$ is the polarization on the i −th lattice site, J_{ij}^f the interaction parameter between NN polarisations. Interface coupling we consider $J^{mf} > 0$.

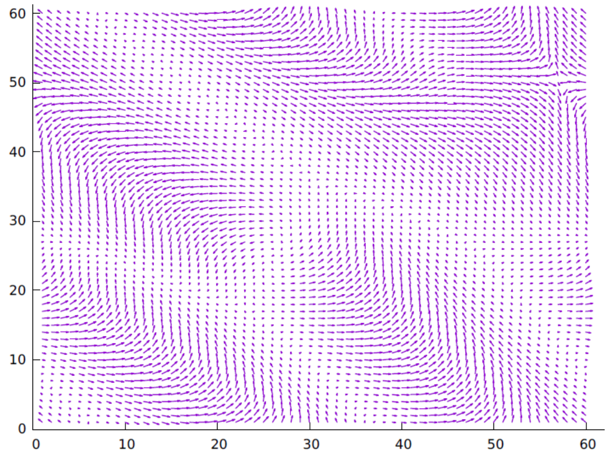
Let us determine the ground state spin configurations in magnetic monolayer, sandwiched between two ferroelectric layers. The antiferromagnetic exchange interaction among the spins will compete with the perpendicular interface interaction, namely $\vec{P}_k \cdot [\vec{S}_i \times \vec{S}_j]$ term. The resulting configuration is non-collinear.

To determine the ground state, we minimize the energy of each spin by using the numerical minimization "steepest descent method". At each spin, we calculate numerically its local field components acting from nearest neighbors and we align the spin in direction of its local field. We consider next spin and repeat the same calculation untill all sites are visited. This realizes one iteration procedure, to determine ground state we repeat ten thousand iterations to have the system energy convergence. We use a sample size $N \times N \times L$. For most calculations, we select $N = 60$ and $L = L_m + L_f = 2$ using the periodic boundary conditions in the xy plane. Exchange parameters between spins and polarizations are taken as $|J^m| = J^f = 1$.

Examples of ground state of the magnetic interface layer are shown in Fig. 1, using small values of interface coupling $J^{mf} = 0.75$ with zero field (Fig. 1*a*) and $H = 0.05$ (Fig. 1*b*).



(a)



(b)

Fig. 1. Three-dimensional (3D) view of the ground state (GS) configuration of the interface for $H = 0$, $J^m = -1$, $J^f = 1$, $J^{mf} = 0.75$ (*a*) and $H = 0.05$ (*b*)

Small values of external field yields small values of angles between spins in the xy plane so that the ground state configurations have ferromagnetic and non collinear domains. And we can see the creation of single spin vortices.

Fig. 2 shows an examples with $J^{mf} = 0.85$ (Fig. 2 (a)) and we observe the beginning of the creation of the skyrmion lattice at antiferromagnetic layer with triangular lattice. Fig. 2 (b) shows an examples with $J^{mf} = 1.00$ we can observe the skyrmions for the surface antimagnetic layer. We noted that skyrmion lattice in a antiferromagnetic/ferroelectric superlattices with triangular lattice can created in region of interface coupling $J^{mf} \in (-1.75, -0.85)$ and applied field $H \in (0.02, 0.1)$ and skyrmions are not formed at any values of applied magnetic field.

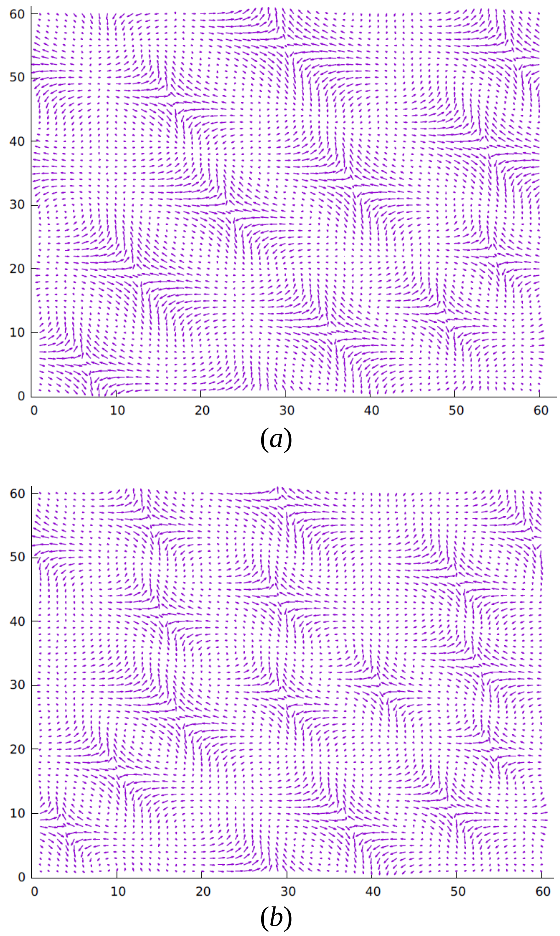


Fig. 2. Three-dimensional (3D) view of the ground state (GS) configuration of the interface for $H = 0, J^m = -1, J^f = 1$, $J^{mf} = 0.85$ (*a*), $H = 0.05$, $J^{mf} = -1.00, H = 0.05$ (*b*)

We apply a magnetic field in z-direction, which is perpendicular to the plane of films. There is a competition between ferromagnetic exchange, magnetoelectric interaction between spins and polarizations at interface layer and the influence of external magnetic field. Let us consider the critical value of the magnetoelectric interaction parameter J^{mf} =1.85, at this value the skyrmion phase collapses at $H = 0.05$ on the triangular lattice. The ground state at $J^m = 1.0$, $J^f = 1.0$, $J^{mf} = 1.85$ is very sensitive to the applied magnetic field – a clear and periodic skyrmion structure is formed for small magnitude of H^z.

Fig. 3 shows the case $H = 0.05$. At $J^m = -1.0$, $J^f = 1.0$, $J^{mf} = 1.75, H = 0.05$ a skyrmion lattice is formed with perfect lattice. The skyrmion phase for the critical value $J^{mf} = 1.75$ is stable in the region of the external magnetic field (0.01, 0.24). At $H > 0.24$ all the spins are parallel to the $z-$ axis in the case $J^{mf} = 1.75$.

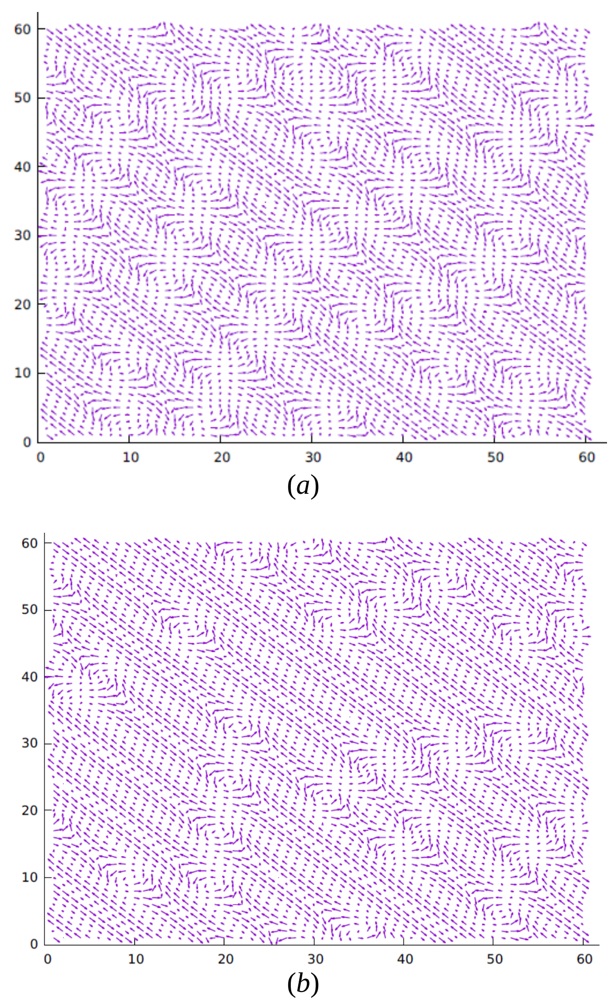


Fig. 3. Three-dimensional (3D) view of the ground state (GS) configuration of the interface for $H = 0, J^m = -1, J^f = 1$, $J^{mf} = 1.75$ (*a*), $H = 0.05$, $J^{mf} = 1.95$ (*b*)

The ground state calculations shown that with increasing the interface magnetoelectric coupling, the skyrmion lattice disappear, for example in the Figure 3b shown the example $J^{mf} = 1.95$. We can see that the number of skyrmions on the surface has sharply decreased with comparing the case $J^{mf} = 1.75$ (See Fig. 3a).

Monte Carlo results. We used the Metropolis algorithm to simulate the system at $T \neq 0$. We performed calculations for systems with different sizes $N \times N \times L$ where N varied from 40 to 1000 and the thickness L varied from 2 to 36. It should be noted that changing the lateral size of N does not affect the results on skyrmions shown in the article. We used $N = 60$ and $L_m = L_f = 2$. With this thickness, skyrmions were observed in the surface antiferromagnetic layer, as seen in the previous section. We discard 10^6 Monte Carlo steps (MCS) per spin in order to equilibrate the system and average energies and order parameters over the next 10^6 MCS/spin. For order parameter of antiferromagnetic layer we compare the actual configuration obtained by slowly heating the selected ground state spin configuration by projecting it on the selected ground state. In our case of skyrmion structure, we have observed the ground state is stable up to a finite T. The order parameter $M_m(n)$ plays the role of the charge number, which evolves with T and goes to zero at the phase transition . In Figures 4–5 one can see the results of Monte Carlo simulations. In Fig 4 we show the energy of antiferromagnetic film versus temperature for $J^{mf} = 0.5, 0.85, J^m = -1$, for different values of the strength of external magnetic field. Here shown also the case of a skyrmion lattice$J^{mf} = 0.85$ – in the presence of more enhanced magnetoelectric interaction at the interface between the antiferromagnetic and ferroelectric films (See Fig. 4 blue line). One can see from this figures that in the case of competition between the antiferromagnetic interaction between the nearest neighboring spins and the stronger magnetoelectric interaction between the nearest neighbors spins and ferroelectric polarizations at the adjacent ferroelectric layer the phase transition occurs at a much lower temperature. This is due to the fact that in the presence of such competition in the external magnetic field, topologically protected structures – skyrmions – appear in the ground state in the antiferromagnetic film. We discussed this phenomenon in detail in the previous chapter. And this phase disappears at a much lower temperature than the temperature at which a phase transition of the order-disorder type occurs.

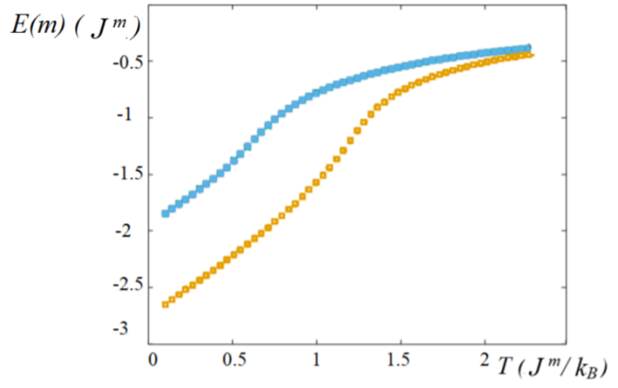


Fig. 4: Energy of antiferromagnetic film versus temperature for $N = 60$ and $L_m = L_f = 2$, $J^{mf} = 0.85$, $J^m = -1.00$. Blue color correspond the case of parameters $J^{mf} = 0.85$, H = 0.05, H = 0.07, H = 0.10 (coincide). Gold color correspond the case $J^{mf} =$ = 0.50, H = 0.04

In Fig. 5 we show the order parameter of antiferromagnetic film versus temperature for $J^m =$ = $-1.0, J^{mf} = 0.5$, $J^{mf} = 0.85$ for different values of the strength of external magnetic field. We emphasize that in the case $J^{mf} = 0.5$ we did not observe skyrmions without and with any values of the external magnetic field. In the case $J^{mf} = 0.85$, we observe the formation of skyrmions at very small value of applied field, and an interesting fact is that they are destroyed at the same critical temperature $T_C = 0.47$ for different values of the external magnetic field. The case of a larger noncollinear magnetoelectric interaction at the interface of two films is shown in Fig. 6.

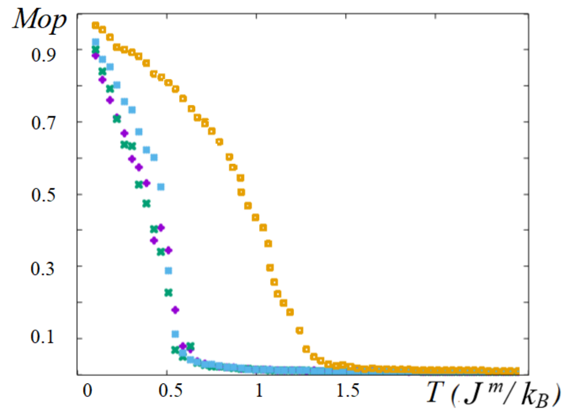


Fig. 5. Order parameter of antiferromagnetic film versus temperature for $N = 60$ and $L_m = L_f = 2$, $J^{mf} = 0.85$, $J^m = -1.00$. Blue color correspond the case of parameters $J^{mf} = 0.85$, $H = 0.05$, violet color correspond to $J^{mf} = 0.85$, $H = 0.07$, green color $J^{mf} = 0.85$, $H = 0.10$. Gold color correspond the case $J^{mf} = 0.5$, $H = 0.5$

We note that the results of Monte-Carlo simulations are shown in the dimensionless unit: energy in the unit of ferromagnetic interaction parameter J^m and T in the unit of J^m/k_B ($k_B -$ the Boltzmann constant). And the results of simulations can be used for superlattices and magnetic nanofilms with different interaction parameter J^m. We can calculate the energy in units of Joules by multiplying the value of energy in Fig. 4 by the value of J^m.

Conclusion. In this paper we have studied the phase transition and ground state spin configurations in bilayers formed by alternate antiferromagnetic and ferroelectric layers by the use of Monte Carlo simulation and high performance steepest descent method. Antiferromagnetic films and ferroelectric films were modeled as frustrated magnetic and "unfrustrated" ferroelectric films with triangular lattice. We found the formation of a stable skyrmions in the ground state of antiferromagnetic/ferroelectric bilayers with triangular lattice in a region of $J^{mf} \in (0.85, 1.95)$ at zero values of applied magnetic field. In the case $J^{mf} = 0.85$, we observe the formation of skyrmions at very small value of applied field, and an interesting fact is that they are destroyed at the same critical temperature $T_C = 0.47$ for different values of the external magnetic field. The very strong magnetoelectric interaction at the interface leads to remove the magnetic phase transitions. The existence of skyrmions at the antiferromagnetic-ferroelectric interface in ground state at very weak value of the strength magnetic field is very interesting and may have different applications in digital technologies and spintronics [14, 15]. We found the formation of perfect periodic skyrmions structure at moderate values of interface magnetoelectric coupling.

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УСТОЙЧИВОСТЬ СКИРМИОНОВ В ФРУСТРИРОВАННЫХ АНТИФЕРРОМАГНИТНОМ/СЕГНЕТОЭЛЕКТРИЧЕСКОМ БИСЛОЯХ С ТРЕУГОЛЬНОЙ РЕШЕТКОЙ

© И.Ф. Шарафуллин[1], А.Р. Юлдашева[1], Н.М. Нугаева[1], А.Т. Дьеп[2]

[1] Физико-технический институт, Башкирский государственный университет, Россия, 450076, Республика Башкортостан, г. Уфа, ул. Заки Валиди, 32

[2] Laboratoire de Physique Théorique et Modélisation, Université Cergy-Paris, France, CNRS, UMR 8089, 95302, Cergy-Pontoise

В работе исследованы процесс формирования и условия устойчивости скирмионов на границе раздела сегнетоэлектрического и антиферромагнитного слоя с треугольной решеткой и особенности фазовых переходов, происходящих в системе. Все взаимодействия между спинами и поляризациями ограничены ближайшими соседями (NN). Антиферромагнитное обменное взаимодействие между спинами внутри антиферромагнитного слоя конкурирует с перпендикулярным межфазным взаимодействием между соседними слоями. Спиновая конфигурация в основном состоянии при нулевой температуре определялась с использованием высоко-производительного численного метода наискорейшего спуска. Полученная конфигурация основного состояния неколлинеарна. При малых значениях напряженности внешнего магнитного поля между взаимодействующими спинами формируются малые углы в плоскости *xy*, так что конфигурации основного состояния имеют антиферромагнитные и неколлинеарные домены. Расчеты демонстрируют также формирование одиночных спиновых вихрей. Обнаружено, что при нулевом приложенном магнитном поле скирмионы в бислое антиферромагнетик / сегнетоэлектрик с треугольной решеткой могут образовываться в диапазоне значений межфазного магнитоэлектрического взаимодействия от 0.85 до 1.95. Сильное внешнее магнитное поле, приложенное перпендикулярно границе раздела с неколлинеарным магнитоэлектрическим взаимодействием Дзялошинского–Мория на границе раздела, приводит к исчезновению скирмионной фазы и магнитных фазовых переходов. Обнаружено формирование идеальной скирмионной структуры при ненулевом внешнем магнитном поле и умеренных значениях поверхностного магнитоэлектрического взаимодействия. Скирмионная решетка устойчива в большом диапазоне значений межфазного магнитоэлектрического взаимодействия между антиферромагнитными и сегнетоэлектрическими пленками. Результаты проведенного нами моделирования методом Монте-Карло подтверждают, что наблюдаемые скирмионы стабильны до конечной температуры.

Ключевые слова: магнитоэлектрическое взаимодействие, скирмионы, метод наискорейшего спуска, бислой, спиновая конфигурация основного состояния, треугольная решетка, фрустрированные системы.