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Magnetic pattern formation on the nanoscale due to relativistic exchange interactions

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Abstract

We present a multiscale study of the formation of magnetic patterns in Mn monolayers deposited on W(0 0 1) and W(1 1 0) surfaces. We derive the parameters of an extended classical Heisenberg Hamiltonian from relativistic spin-polarized first principle calculations. By using these parameters we perform Monte Carlo simulations to explore the low-temperature spin structures. We find that the antisymmetric Dzyaloshinskii–Moriya interactions induce spin-spirals propagating along an in-plane axis with a wavelength of about 2.2 and 7.2 nm, respectively.
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1. Introduction

The development of magnetic imaging techniques, in particular, spin-polarized scanning tunneling microscopy (SP-STM) permits a resolution of sub-nanometer magnetic patterns such as antiferromagnetic domain walls in ultrathin magnetic films [1]. It is well known that thin films may exhibit large magnetic anisotropy, while it has also been recently shown [2] that the antisymmetric exchange interactions first predicted by Dzyaloshinskii [3] and Moriya [4] can be especially strong at magnetic surfaces. The interplay of different anisotropic exchange interactions and the on-site anisotropy can influence the formation of thin domain walls and give rise to nanometer sized magnetic patterns.

In the present paper the low temperature spin-structures of a Mn monolayer on W(0 0 1) and W(1 1 0) surfaces are studied by means of Monte Carlo (MC) simulations. The parameters appearing in a model Hamiltonian are determined by first principles calculations.

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2. Multiscale modeling

We deal with a classical spin system described by a generalized Heisenberg Hamiltonian

$$H = \frac{1}{2}\sum_{i\neq j}\sigma_i \mathcal{J}_{ij}\sigma_j + \sum_i (K_x\sigma_{ix}^2 + K_y\sigma_{iy}^2), \quad (1)$$

where σ_i is a unit vector parallel to the magnetic moment of an Mn atom at site i, $\mathcal{J}_{ij}$ denote tensorial exchange interactions, K_x and K_y are (bi-axial) on-site anisotropy constants. Quite clearly, for a bcc(0 0 1) surface $K_x = K_y$. In the case of a bcc(1 1 0) surface the x and y in-plane directions correspond to the $(1\,\bar{1}\,0)$ and the (0 0 1) crystal axes and, in general, $K_x \neq K_y$.

We calculated the parameters entering the Hamiltonian (1) in terms of the relativistic spin-polarized Screened Korringa–Kohn–Rostoker (SKKR) method [5]. In particular, $\mathcal{J}_{ij}$ have been derived by using a relativistic extension of the torque method [6]. From a decomposition of the tensorial exchange [6] it turned out that the most relevant parts are the isotropic exchange interactions, J_{ij}, and the antisymmetric exchange interactions, $\mathbf{D}_{ij}[\sigma_i \times \sigma_j]$, with $\mathbf{D}_{ij}$ being the Dzyaloshinskii–Moriya (DM) vectors. It

has to be noted that DM interactions tend to lower the energy of the system upon inducing a non-collinear spin-structure.

By using the Hamiltonian (1) we performed MC simulations on a 32×32 two-dimensional lattice with periodic boundary conditions. The low-temperature spin-state of the system has been searched in terms of simulated annealing starting from the completely disordered state at high temperatures.

3. Results

Subsequent to a self-consistent determination of the effective potentials and exchange fields we calculated the exchange interactions for a large number of atomic pairs of the Mn monolayer. The experimental lattice constant of bcc W was used with no attempts to account for lattice relaxations. Note that the first nearest neighbor (1NN) distance of the Mn atoms is 0.32 nm. The isotropic exchange interactions and the lengths of DM vectors for the first few NNs are listed in Table 1. Excluding the effect of the DM interactions, due to the dominating negative 1NN exchange interactions, the ground state of Mn/W(0 0 1) is ferromagnetic, see also Eq. (1). Because of the positive on-site anisotropy constant, $K_x = K_y = 0.047$ mRyd, we obtained the magnetic moments in this state are aligned normal-to-plane for Mn/W(0 0 1). In the case of Mn/W(1 1 0), the strong antiferromagnetic 1NN interactions give rise to a checkerboard c(2×2) antiferromagnetic structure and the calculated anisotropy constants, $K_x = -0.047$ mRyd and $K_y = 0.037$ mRyd, imply that the magnetic moments are parallel to the $(1\,\bar{1}\,0)$ axis.

Inferring Table 1 it is obvious that some of the DM vectors are almost by an order of magnitude larger than the corresponding anisotropy energies and only by an order of magnitude smaller than the largest isotropic exchange interactions. This is, however, not surprising since in terms of perturbation theory the DM interactions and the uniaxial anisotropy appear in first and second order of the spin–orbit coupling strength, respectively.

The DM vectors, all being parallel to the plane, are depicted in Fig. 1. As it is obvious, in case of Mn/W(0 0 1) DM vectors referring to atomic pairs along a given direction ($\pm x$ or $\pm y$) are parallel to each together, thus their effect to misalign the spins is strengthened. On the contrary, due to the reduced symmetry the DM vectors exhibit a higher complexity for Mn/W(1 1 0) as their spatial distribution shows an apparent asymmetry.

Table 1
Calculated isotropic exchange interactions, J_{ij}, and magnitudes of the DM vectors, D_{ij} (all in mRyd) for the first few nearest neighbors (NN) in a Mn monolayer on W(0 0 1) and on W(1 1 0).

System	Mn/W(0 0 1)			Mn/W(1 1 0)				
NN	1	2	3	1	2	3	4	5
J_{ij}	−3.91	1.10	0.12	7.30	−3.84	−0.85	2.17	−1.38
D_{ij}	0.57	0.04	0.24	0.09	0.22	0.03	0.23	0.20

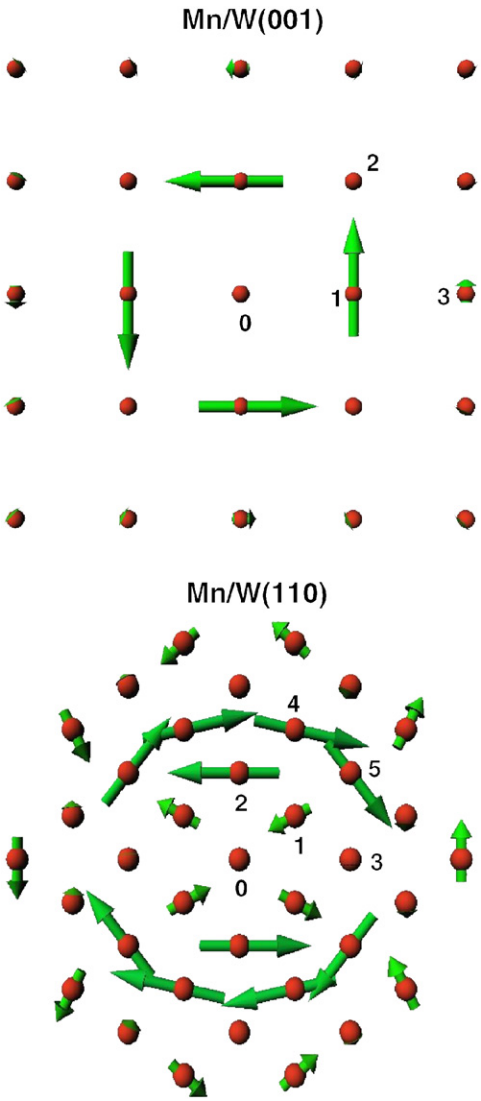

Fig. 1. Sketch of the Dzaloshinskii–Moriya vectors (green arrows) corresponding to a central atom (labelled by 0) and its nearest neighbors. Selected nearest neighbors are labelled by the same numbers as in Table 1.

By using the above parameters, including also the antisymmetric DM interactions in Hamiltonian (1), we performed MC simulations for both systems. The magnetic patterns we obtained for a sufficiently low temperature, $k_B T = 0.02|J|$ ($J = \sum_j J_{ij}$), are shown in Fig. 2. In the case of Mn/W(0 0 1) we find that the ferromagnetic order is nearly maintained along the (1 1 0) direction, whereas a spin-spiral propagating along the $(1\,\bar{1}\,0)$ direction evolves with a wavelength of about 2.2 nm. The formation of this spin-spiral is the consequence of the large and competing DM vectors between NNs along the x and y axes.

In the case of Mn/W(1 1 0), the large asymmetry of the DM interactions seen in Fig. 1 gives rise to a cycloidal spin-spiral along the $(1\,\bar{1}\,0)$ direction that modulates the

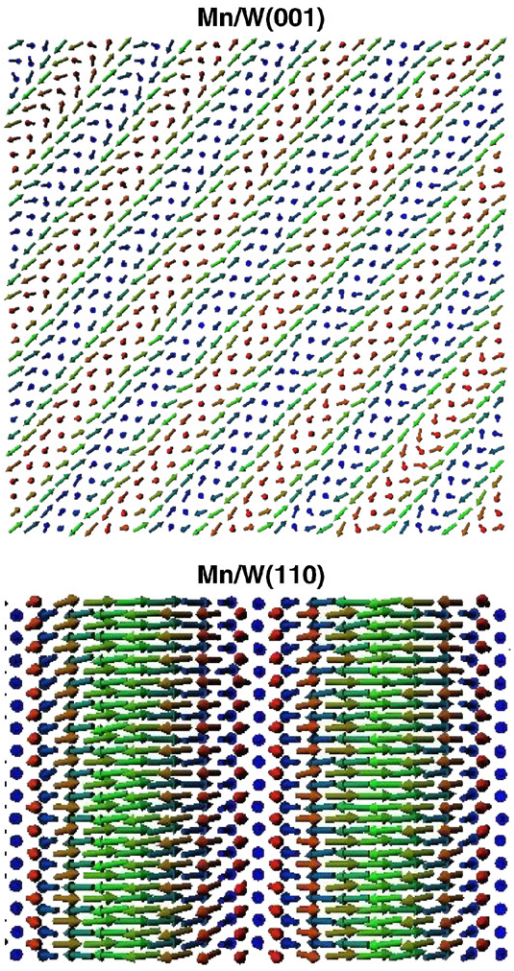

Fig. 2. Schematic view of the low-temperature spin structures of Mn/W(0 0 1) and Mn/W(1 1 0) as obtained from the MC simulations. Blue, green and red arrows denote spins pointing downwards, in-plane and upwards, respectively.

underlying antiferromagnetic arrangement. The estimated wavelength of this spin-spiral is about 7.2 nm. Although one-half of this wavelength should be compared with the periodicity of about 6 nm seen recently for the same monolayer system in SP-STM images [2], the agreement between our simulations and the experiment is satisfactory. In addition, a different theoretical approach used in Ref. [2] predicted a wavelength for this spin-spiral close to our value (8 nm).

In this paper we have shown that relativistic effects, in particular, D–M interactions can be strong enough to induce non-collinear spin-structures in thin magnetic films. It is tempting that such effects play a crucial role in forming different types of magnetic structures also in finite nanoparticles.

Acknowledgments

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