Spin-spiral and domain wall structures in monolayer Fe/W(110)

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Abstract

The stability of spin-spiral and domain wall structures in an Fe monolayer on a W(110) substrate is theoretically investigated. By analyzing the exchange parameters obtained from first principles total energy calculations, we find that a competition between the nearest-neighbor ferromagnetic and long-distant antiferromagnetic exchange interactions leads to a stabilization of the spin-spiral structures. When the strong magnetocrystalline anisotropy (MCA) arising from the Fe/W(110) interface is introduced, however, the formation of the spin-spiral structures is suppressed and the ground state appears to be the ferromagnetic state - as observed in experiments. In addition, the strong MCA is found to play a key role in determining the domain wall structures.

Key words: spin-spiral structures, domain wall structures, monolayer Fe/W(110), first principles calculations
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1. Introduction

Noncollinear magnetism in spin-spiral and domain wall structures, in which the magnetization is rotated along a certain direction in a crystal, has received much attention in fundamental and applied physics. Now, interest in the noncollinear magnetism has increased in ultra-thin film systems, in which a breaking of symmetry and an enhanced spin-orbit coupling (SOC) arising from a reduced dimensionality would give rise to new and exotic features differing from those of bulk.[1,2]

To date, magnetism in an Fe monolayer on a W(110) substrate with a ferromagnetic (FM) order are extensively investigated from both experimental and theoretical points of view.[3–7] Recently, however, spin-polarized scanning tunneling microscopy (SP-STM) experiments surprisingly revealed the narrow domain wall with a width of approximately 6 Å in the monolayer Fe/W(110),[8] which is in very contrast to that in the bulk where a stable domain wall width is predicted on the order of 100 Å.[9,10] Moreover, the first principles calculations in the scalar relativistic approximation (SRA), i.e., without SOC, based on the local spin density approximation (LSDA), predicted that the spin-spiral structures are energetically favorable over the FM state by only about 1 meV/atom. The magnetism in the monolayer Fe/W(110) is not, therefore, understood well.

In order to investigate and understand the mag-

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netism in the monolayer Fe/W(110), here, we calculate the formation energy of the spin-spiral structures by means of the film full-potential linearized augmented plane-wave (film FLAPW) method[11,12] that incorporates intra-atomic noncollinear magnetism.[13,14] Then, we determine the exchange parameters within the one-dimensional effective Heisenberg model, and discuss the stability of the spin-spiral and domain wall structures. Indeed, we find that the strong magnetocrystalline anisotropy (MCA) arising from the Fe/W(110) interface plays a key role in determining the spin-spiral and domain wall structures.

2. Model and method

As a model of the monolayer Fe/W(110), a single slab consisting of five layers of W(110) and an Fe(110) monolayer on each side is employed. Although the magnetic properties such as the exchange parameters and the MCA might be sensitive to the lattice parameters, we here assume the experimental values of the lattice constant of bulk W (a=3.16 Å) and of the Fe-W interlayer distance ($d_{\mathrm{Fe-W}}$=1.94 Å)[15]. The magnetization in the spin-spiral structures is assumed to lie on a plane parallel to the surface, since the magnetic easy axis is along the in-plane $[1\bar{1}0]$ direction with a large MCA energy of about 3 meV/atom.[16]

Calculations are carried out in the SRA (without SOC) for the valence electrons and fully relativistically for the core electrons, based on the LSDA using the von Barth-Hedin exchange-correlation,[17] in which the spin-spiral structures are treated by applying the generalized Bloch theorem[18,19] into the film FLAPW method.[11–14] The LAPW basis with a cutoff of $|\mathbf{k}+\mathbf{G}\mp\mathbf{q}/2| \leq 3.6$ a.u.$^{-1}$ and muffin-tin (MT) sphere radii of 2.3 a.u. for the Fe and 2.43 a.u. for the W is used; lattice harmonics with angular momenta up to $\ell = 8$ are employed to expand the charge and spin density, the vector potential, and eigenvectors.

The exchange parameters are determined by the back Fourier transformation for the formation energy of the spin-spiral states, based on the one-dimensional effective Heisenberg model, $H_{\mathrm{eff}} = -\sum_{ij} J_{ij}\mathbf{e}_i\cdot\mathbf{e}_j$, where, $\mathbf{e}_i$ is the unit vector of magnetic moments on the i-th atomic row and J_{ij} is the exchange parameter between the i and j-th rows.

3. Results and discussion

Figure 1 shows the calculated formation energy, ΔE, for the monolayer Fe/W(110) as a function of a wave vector, $\mathbf{q}_{001}$, where $\mathbf{q}_{001}$=0 and 1 indicate the FM and antiferromagnetic (AFM) states, respectively. The figure also presents the ΔE of a bulk bcc Fe with the experimental lattice constant. In the bulk, the ΔE increases with increasing $\mathbf{q}_{001}$, where the spin-spiral states are always less favorable over the FM state. In contrast, the spin-spiral structures in the monolayer Fe/W(110) are energetically stable when $\mathbf{q}_{001}$ is less than about 0.1. The energy minimum appears to be around $\mathbf{q}_{001}$=0.05∼0.1, corresponding to a wavelength of about $10a \sim 20a$, and is only about 1 meV/atom lower in energy than the FM state. This indicates a negative or very weak exchange stiffness. Furthermore, the $\mathbf{q}$ dependence of the ΔE for $\mathbf{q}_{001} < 0.3$ significantly differs from that for $\mathbf{q}_{001} > 0.3$ due to the complex noncollinear magnetism in the W substrate, as pointed out previously.[16]

The calculated exchange parameters for the Fe(110) monolayer and the bulk Fe are shown in Fig. 2. In the bulk, the nearest-neighbor exchange parameter has a large positive value leading to a strong stabilization of the FM state, while those in the second and third neighbors are antiferromagnetic with one or two order of magnitude smaller than that of the nearest-neighbor. For the monolayer Fe/W(110), however, the nearest-neighbor exchange parameter is significantly reduced over that in the bulk, by a factor of three.

Moreover, the exchange interactions in the long-distant neighbors over the fourth neighbor are antiferromagnetic with a magnitude of 1 meV/atom. When the formation energy is calculated by omitting the long-distant exchange interactions (i.e., by using the exchange parameters up to the third neighbor), no spin-spiral state is found to be stable. Thus, a competition between the nearest-neighbor ferromagnetic and long-distant antiferromagnetic

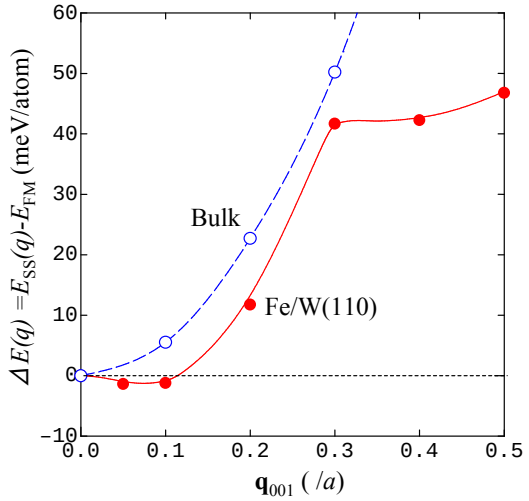

Fig. 1. Calculated formation energy of spin-spiral structures as a function of a wave vector, $\mathbf{q}_{001}$, for monolayer Fe/W(110) (closed circles) and bulk Fe (open circles). $\mathbf{q}_{001}$=0 and 1 indicate the FM and AFM states, respectively. The reference energy ($\Delta E = 0$) places the total energy of the FM state.

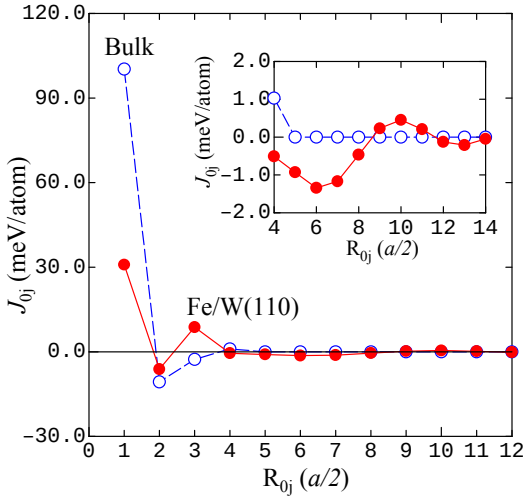

Fig. 2. Calculated exchange parameters for monolayer Fe/W(110) (closed circles) and bulk Fe (open circles) as a function of a distance, R_{0j}, which are obtained by mapping into the one-dimensional effective Heisenberg model, $H_{\rm eff} = -\sum J_{ij} e_i \cdot e_j$.

exchange interactions leads to the stabilization of the spin-spiral structures.

It is now interesting to discuss the effect of the MCA since the monolayer Fe/W(110) has a large uniaxial MCA arising from the strong SOC at the W interface.[16] We here carry out calculations with the Heisenberg Hamiltonian by adding the MCA contribution, $-\sum_i K\cos^2\theta_i$, where K and θ_i are an uniaxial MCA constant and an angle of the moment direction from the easy magnetization direction, respectively, and analyze the stability of the spin-spiral structures by changing K. The results are shown in Fig. 3 (solid line) with K varying from 0 to 5 meV. The dotted line in the figure represents the calculated energy as a collinear FM state is assumed. When K is less than 2.3 meV, the spin-spiral states are energetically favorable over the FM state. However, the ground state having larger K value than 2.3 meV becomes the FM state, since the magnetization rotation in the spin-spiral structures, which changes the orientation from the easy axis, increases the total energy. Indeed, the predicted MCA energy (3.3 meV/atom) of the monolayer Fe/W(110) from the first principles calculations[16] indicates that the ground state is the FM state - as observed in experiments.[3]

We finally demonstrate the domain wall structures based on the effective Heisenberg model with K=3.3 meV. The results for the angle, θ, of the moment direction in the domain wall are shown in Fig. 4 (closed circles). The moments rotate rapidly within approximately five lattice constants (∼16 Å) without any discontinuous changes. Thus, the results clearly demonstrate the narrow domain wall structure, and are qualitatively consistent with the SP-STM observations.[8]

Furthermore, in order to clarify the effect in the long-distant antiferromagnetic exchange interactions on the domain wall structures, we again carry out calculations by omitting the long-distant exchange interactions, which are also given by open circles in the Fig. 4. Although the wall width slightly increases by reduced the long-distance exchange interaction, both results (closed and open circles) shows almost similar behavior each other, and therefore the narrow domain wall structure is mainly determined by the large MCA.

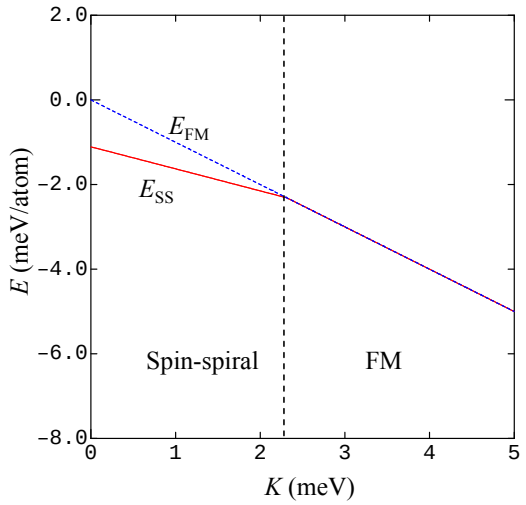

Fig. 3. Calculated energy of spin-spiral structures (solid line) as a function of a uniaxial MCA constant, K, based on the effective Heisenberg model. Dotted line represents results as a collinear FM state is assumed.

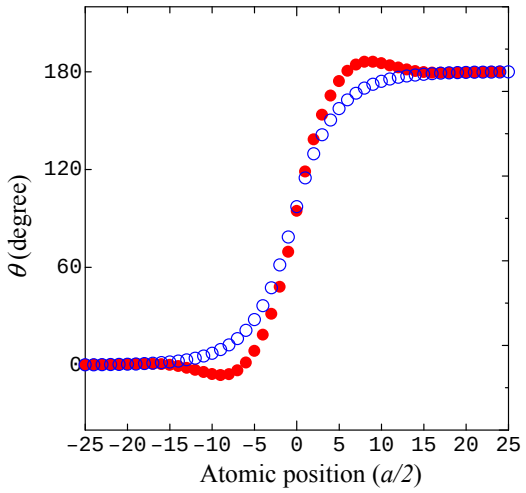

Fig. 4. Angles θ of magnetic moment directions in a domain wall (closed circles), calculated based on the effective Heisenberg model with K=3.3 meV. Open circles represent the results by using the exchange parameters up to the third neighbor.

4. Conclusion

The stability of the spin-spiral structures in the monolayer Fe/W(110) was investigated by means of the FLAPW method, and the exchange interaction within the effective Heisenberg model were determined. Without the MCA contribution, the spin-spiral structures are found to be energetically favored over the FM state due to the long-distant antiferromagnetic exchange interactions. When the strong MCA arising from the Fe/W(110) interface is introduced, however, the formation of the spin-spiral structures is suppressed and the ground state appears to be the FM state - as observed in experiments. We also determined the domain wall structures, where the moments rotate rapidly within approximately five lattice constants, and found that the narrow domain wall structure is mainly determined by the large MCA.

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