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Noncollinear magnetism and exchange interaction in spin-spiral structures of thin film Fe(110)

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Abstract

Spin-spiral structures in a free-standing Fe(110) monolayer are determined by the first-principles film full-potential linearized augmented plane wave method with intra-atomic noncollinear magnetism. The results obtained predict that the spin-spiral structures are energetically favourable over the collinear ferromagnetic state. The interatomic exchange parameters, which are evaluated from the formation energy of the spin-spiral structures, indicate that a competition between the nearest-neighbour ferromagnetic interaction and the long-distant antiferromagnetic interactions leads to the stabilization of the spin-spiral structures. In addition, the spin–orbit coupling is found to play an important role in determining the magnetic ground state.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Noncollinear magnetism in spin-spiral structures, in which the magnetization is rotated along a certain direction in a crystal, has received much attention in fundamental and applied physics, and so far theoretical progress within the spin-density-functional theory has succeeded in describing spin-spiral structures in itinerant materials such as bulk γ-Fe and U compounds [1–4]. Now, interest in the noncollinear magnetism in thin films has increased because of their potential technological importance, 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 the bulk [5–7]. Little is known quantitatively, however, about the detailed complexity of the spin-spiral structures in thin films. Therefore, it is strongly desirable to understand it from highly precise first-principles calculations.

In order to investigate such complex noncollinear magnetism, we have implemented the film full-potential linearized augmented plane wave (FLAPW) method [8, 9] including intra-atomic noncollinear magnetism, i.e., with no shape approximations of the magnetization [10, 11], which now applies the generalized Bloch theorem [1, 12] to treat incommensurate spin-spiral structures. Here, we apply this approach to determine the spin-spiral structures in a free-standing Fe(110) monolayer. The results obtained predict that

the spin-spiral structures are energetically favourable over the collinear ferromagnetic (FM) state, which is consistent with that calculated with very long supercells for simulating commensurate spin-spiral structures. We also find that a competition between the nearest-neighbour ferromagnetic interaction and the long-distant antiferromagnetic interactions leads to the stabilization of the spin-spiral structures. In addition, the SOC is found to play an important role in determining the magnetic ground state.

2. Model and method

We employed a free-standing Fe(110) monolayer slab with wavevectors, $\mathbf{q}_{001}$, in the [001] direction, and performed self-consistent total energy calculations, assuming a lattice constant matching that of bulk bcc Fe (2.87 Å). The calculations were carried out based on the local spin-density approximation (LSDA) using the von Barth–Hedin exchange–correlation [13] in the scalar relativistic approximation for the conduction electrons, i.e., without the SOC, and fully relativistically for the core electrons. Also, the LSDA calculations for the bulk Fe were performed.

To treat spin-spiral structures, we here applied the generalized Bloch theorem [12, 1] in the film FLAPW method [8, 9] with intra-atomic noncollinear magnetism [10, 11], in which the eigenstate at $\mathbf{k}$ in the first Brillouin zone defined by a chemical unit cell is in the form

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} \begin{pmatrix} C_{\mathbf{k}+\mathbf{G}-\mathbf{q}_\parallel/2,\chi_\uparrow} \exp\left(-\mathrm{i}\frac{\mathbf{q}_\parallel}{2}\cdot\mathbf{r}\right)\psi_{\mathbf{k}+\mathbf{G},\chi_\uparrow}(\mathbf{r}) \\ C_{\mathbf{k}+\mathbf{G}+\mathbf{q}_\parallel/2,\chi_\downarrow} \exp\left(+\mathrm{i}\frac{\mathbf{q}_\parallel}{2}\cdot\mathbf{r}\right)\psi_{\mathbf{k}+\mathbf{G},\chi_\downarrow}(\mathbf{r}) \end{pmatrix},$$

where $\mathbf{q}_\parallel$ is a two-dimensional wavevector of the spin-spiral structure, and $\exp(\mp\mathrm{i}\mathbf{q}_\parallel/2\cdot\mathbf{r})\psi_{\mathbf{k}+\mathbf{G},\chi_\pm}(\mathbf{r})$ is described using the spin-independent LAPW basis [11]. The LAPW basis with a cut-off of $|\mathbf{k}+\mathbf{G}\mp\mathbf{q}_\parallel/2| \leqslant 3.6$ au^{-1} and muffin-tin (MT) sphere radius of 2.3 au is used; lattice harmonics with angular momenta up to $\ell = 8$ are employed to expand the charge and magnetization density, the vector potential, and eigenvectors. In the present method, since the density and potentials are represented by the plane wave description, which must have a translational invariance with a periodicity of the chemical unit cell [3], we introduced two quantities, $u(\mathbf{r}) = \mathrm{e}^{-\mathrm{i}\mathbf{q}_\parallel\cdot\mathbf{r}}[\rho_x(\mathbf{r}) + \mathrm{i}\rho_y(\mathbf{r})]$ and $h(\mathbf{r}) = \mathrm{e}^{-\mathrm{i}\mathbf{q}_\parallel\cdot\mathbf{r}}[v_x(\mathbf{r}) + \mathrm{i}v_y(\mathbf{r})]$, for the density and potentials, respectively.

3. Results and discussion

Figure 1 shows the calculated formation energy, ΔE, for the Fe(110) monolayer as a function of the $\mathbf{q}_{001}$, where $\mathbf{q}_{001} = 0$ and 1 indicate the FM and antiferromagnetic (AFM) states, respectively. The figure also gives that for the bulk Fe. In contrast to results for the bulk where the spin-spiral structures are less favourable over the FM state, the spin-spiral structures in the Fe(110) monolayer are energetically favourable when the $\mathbf{q}_{001}$ is less than about 0.22. The energy minimum appears to be around $\mathbf{q}_{001} = 0.15$, corresponding to a wavelength of about $7a$, and is about 4 meV/atom lower in energy than the FM state. The present results (closed marks in figure 1) are consistent to those (open marks) calculated with very long supercells corresponding to the commensurate spin-spiral structures, i.e., with no application of the generalized Bloch theorem.

In order to further gain insight into magnetism in the spin-spiral structures, we estimated interatomic exchange parameters within the one-dimensional effective Heisenberg model, $\mathcal{H}_{\mathrm{eff}} = -\sum_{\langle ij\rangle} J_{ij}\mathbf{e}_i\cdot\mathbf{e}_j$, where $\mathbf{e}_i$ is the unit vector of magnetic moments on the ith atomic row and J_{ij} is the exchange parameter for the i and jth atomic rows, by carrying out a Fourier back-transformation [14, 15] for ΔE. The calculated exchange parameters for the

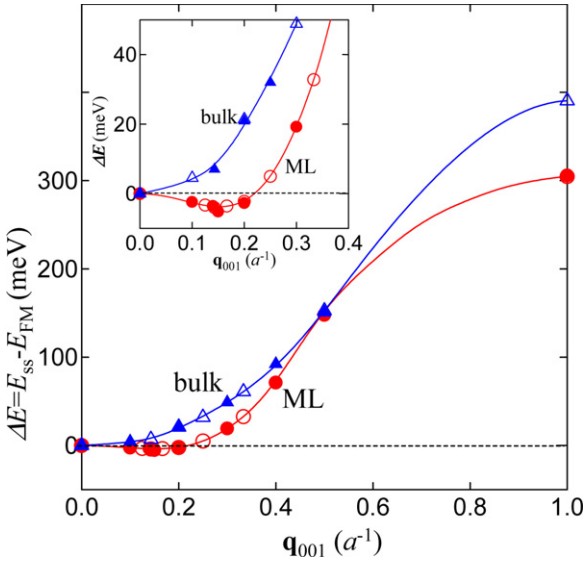

Figure 1. Formation energies of spin-spiral structures as a function of wavevector, $\mathbf{q}_{001}$, for Fe(110) monolayer (closed circles) and bulk Fe (closed triangles). Open marks represent results for commensurate spin-spiral structures calculated with long supercells.

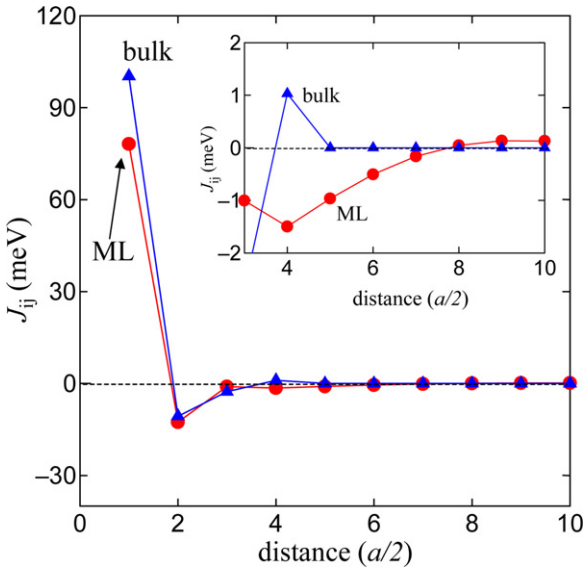

Figure 2. Calculated exchange parameters for Fe(110) monolayer (closed circle) and bulk Fe (closed triangles), mapped to the one-dimensional effective Heisenberg model, $\mathcal{H}_{\text{eff}} = -\sum J_{ij}\, e_i \cdot e_j$.

Fe(110) monolayer and the bulk Fe are shown in figure 2. In both cases, the exchange parameter of the nearest neighbour has a large positive value of 78 meV/atom for the monolayer and 100 meV/atom for the bulk, which leads to ferromagnetic interaction, while those of the second and third neighbours are antiferromagnetic at one order of magnitude smaller than that for the nearest neighbour. In the Fe(110) monolayer, however, the exchange

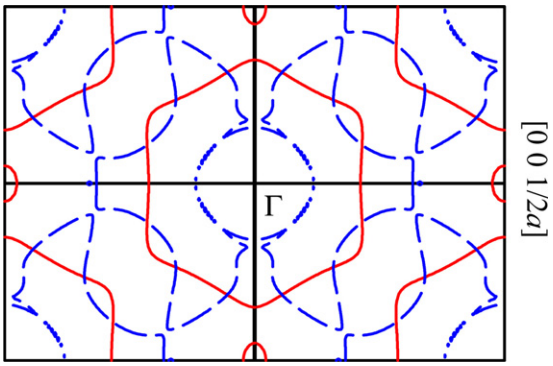

Figure 3. Calculated Fermi surfaces of Fe(110) monolayer assuming a ferromagnetic state. Solid and dashed lines represent majority-spin and minority-spin states, respectively.

interactions of the long-distant neighbours up to seventh neighbours are antiferromagnetic with a magnitude of 0.1–1.5 meV/atom, which is contrast with the bulk case where such long-distant exchange interactions are negligibly small. Thus, a competition between the nearest-neighbour ferromagnetic interaction and the long-distant antiferromagnetic interactions leads to the stabilization of the spin-spiral structures obtained.

Figure 3 shows the calculated two-dimensional Fermi surface of the Fe(110) monolayer assuming the FM state. The Fermi surface between the majority-spin and minority-spin states clearly possesses a nesting feature perpendicular to the [001] direction. The nesting vector connecting majority-spin and minority-spin states in the [001] direction will give rise to singularities in the generalized susceptibility that lead to an instability of the ferromagnetic state against the formation of the spin-spiral structures. Indeed, the nesting vector was estimated to be about 0.2, which corresponds to the wavelength of about the tenth neighbour and roughly to the $\mathbf{q}_{001}$ with the energy minimum in figure 1. Thus, the stability of the spin-spiral structures and the long-range antiferromagnetic exchange interaction in figure 2 may be attributed to the nesting feature in the Fermi surface.

Finally, in order to discuss the SOC effect in the spin-spiral structures of the Fe(110) monolayer, we performed FLAPW calculations including the SOC for the commensurate spin-spiral structure with $\mathbf{q}_{001} = 1/(7a)$ by using the long supercell, and find that the magnetic structure is not changed significantly. In order to further clarify the SOC effects, we multiplied the SOC Hamiltonian with a constant prefactor, λ, and calculated non-self-consistently the formation energy, ΔE_{SOC}, of the spin-spiral structures. The results, shown in figure 4, demonstrate that the ΔE_{SOC} clearly increases as λ increases and the spin-spiral structures will turn out to be less favourable when λ increases by an order of magnitude. Therefore, the magnetic ground state in a system having the strong SOC that leads to a large magnetocrystalline anisotropy (MCA) would be ferromagnetic since the magnetization rotation in the spin-spiral structures, which changes the orientation from the easy axis, increases the total energy.

4. Summary

We investigated the stability of the spin-spiral structures in the Fe(110) monolayer by means of the FLAPW method. The results indicate that the spin-spiral structures are energetically favoured over the collinear FM state. The calculated exchange parameters indicate that the competition between the nearest-neighbour ferromagnetic interaction and the long-distant

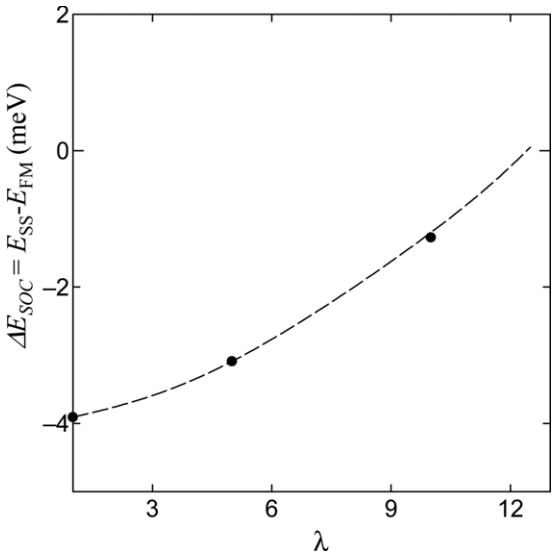

Figure 4. Formation energy of the spin-spiral structure with $\mathbf{q}_{001} = 1/(7a)$ for the Fe(110) monolayer as a function of the SOC prefactor λ.

antiferromagnetic interactions leads to the stabilization of the spin-spiral structures obtained. The spin-spiral structures may be, however, less favourable for the systems having a large MCA arising from the strong SOC at substrate interfaces [16, 17].

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