Magnetic correlations beyond the Heisenberg model in an Fe monolayer on Rh(0 0 1)

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Abstract

Motivated by a recent experimental observation of a complex magnetic structure (Takada *et al* 2013 *J. Magn. Magn. Mater.* **329** 95) we present a theoretical study of the magnetic structure of an Fe monolayer deposited on Rh(0 0 1). We use a classical spin Hamiltonian with parameters obtained from *ab initio* calculations and go beyond the usual anisotropic Heisenberg model by including isotropic biquadratic interactions. Zero-temperature Landau–Lifshitz–Gilbert spin dynamics simulations lead to a complex collinear spin configuration that, however, contradicts experimental findings. We thus conclude that higher order multi-spin interactions are likely needed to account for the magnetic ordering of the system.

Keywords: spin-correlations, spin-dynamics, magnetic ground state, biquadratic and multi-spin interactions, Fe monolayer, DFT

(Some figures may appear in colour only in the online journal)

1. Introduction

Magnetism on the nanoscale has become a central aspect of modern technology, with nanostructures being employed in a multitude of industrial applications. For the ongoing development of technology and our basic understanding of the behaviour of novel materials, experimental and theoretical studies have to be used in concert. Advancements in experimental techniques, and in particular the development of spin-polarized scanning tunneling microscopy (SP-STM) [1], has allowed the direct observation of the magnetic structure of various nanosystems at the atomic scale.

Ab initio calculations can greatly help in understanding the underlying physics behind observed phenomena, and can hint towards hitherto unnoticed features or direct attention to specific systems. By growing Fe thin films epitaxially on various transition metal surfaces the effective Fe lattice constant and the hybridization with the substrate can be tuned, providing in-depth insight into the relationship between electronic and magnetic structure [2, 3]. Using Ir or Rh as a substrate [4–9] is especially interesting, as their in-plane lattice constant is in-between that of bcc-Fe and fcc-Fe.

Recent experimental findings by Takada *et al* [9] employing SP-STM measurements show that the ground state spin configuration of the Fe_1/Rh(0 0 1) thin film is a complex noncollinear structure with a 4×3 magnetic unit cell. A closer inspection of the spin structure proposed by Takada *et al* [9] reveals that it is not a conventional spin spiral, since the spins follow a fanning path rather than a spiral along crystallographic directions.

Earlier first-principles investigations of the same system were based on total energy calculations, and considered only a few simple magnetic configurations [7, 8]. *Ab initio* methods demand huge computational effort and many aspects of noncollinear magnetism as well as finite temperature behaviour are too difficult to manage. By matching first-principles

calculations to classical spin models a less fundamental, yet more tractable and more flexible description of magnetic systems may be given. Kudrnovský *et al* [5] used an isotropic Heisenberg model to predict the magnetic ordering in this system, and suggested some antiferromagnetic or spin spiral ground state.

In this work we investigate the $Fe_1/Rh(0\,0\,1)$ thin film in terms of a spin model consisting of tensorial Heisenberg couplings, as well as higher order two-spin interactions, namely isotropic biquadratic terms. This research is a natural follow-up to our earlier study of the closely related $Fe/Ir(0\,0\,1)$ thin films [6]. We use the spin-cluster expansion (SCE) combined with the relativistic disordered local moment (RDLM) theory [10] to obtain model parameters. We also study the effect of layer relaxations on the magnetic interactions. The theoretical spin configuration is derived by solving the Landau–Lifshitz–Gilbert (LLG) equations at zero temperature. The highly collinear spin structure obtained due to very strong biquadratic interactions allows us to conclude that higher order multi-spin interactions are needed to describe properly the magnetism of this system.

2. Methods and computational details

Computations to obtain the magnetic structure of itinerant systems from first principles usually involve the adiabatic approximation, assuming a separation of time scales between fast (electronic) and slow (spin) degrees of freedom. In terms of the rigid spin approximation the orientational state of the spin system is specified by a set $\{e\}$ of unit vectors e_i describing the orientation of the magnetization at site i.

We study magnetic thin film systems in terms of an extended tensorial Heisenberg model of the form:

$$\mathcal{H}(\{e\}) = \sum_i e_i \underline{\underline{K}}_i e_i - \frac{1}{2}\sum_{i \neq j} e_i \underline{\underline{J}}_{ij} e_j - \frac{1}{2}\sum_{i \neq j} B_{ij} \left(e_i \cdot e_j\right)^2 .$$
(1)

The traceless symmetric matrices $\underline{\underline{K}}_i$ describe the on-site anisotropy energy, whereas the exchange tensors $\underline{\underline{J}}_{ij}$ can be decomposed as:

$$\underline{\underline{J}}_{ij} = J_{ij}^{\mathrm{I}} \underline{\underline{I}} + \underline{\underline{J}}_{ij}^{\mathrm{A}} + \underline{\underline{J}}_{ij}^{\mathrm{S}},$$
(2)

where $\underline{I}$ denotes the unit matrix. These contributions can be easily interpreted, since J_{ij}^{I} is the isotropic Heisenberg interaction (note that according to equation (1) a positive Heisenberg coupling is ferromagnetic, i.e. it favours the parallel alignment of the interacting spins), the antisymmetric matrix $\underline{\underline{J}}_{ij}^{\mathrm{A}} = \frac{1}{2}(\underline{\underline{J}}_{ij} - \underline{\underline{J}}_{ij}^T)$ corresponds to the Dzyaloshinskii–Moriya (DM) interaction [12, 13], and $\underline{\underline{J}}_{ij}^{\mathrm{S}} = \frac{1}{2}(\underline{\underline{J}}_{ij} + \underline{\underline{J}}_{ij}^T - \frac{2}{3}(\mathrm{Tr}\,\underline{\underline{J}}_{ij}) \cdot \underline{\underline{I}})$ describes the second order two-site anisotropy. The last term in equation (1) describes the isotropic biquadratic interaction, with a positive coupling preferring collinear (either parallel or antiparallel) orientation.

We use the SCE introduced originally by Drautz and Fähnle [14, 15] combined with the RDLM method [16–18] implemented within the framework of the screened Korringa–Kohn–Rostoker (SKKR) multiple scattering theory [11] to

obtain parameters for the spin model from first principles. The SCE allows one to systematically expand the adiabatic magnetic energy surface of a spin system over a set of basis functions constructed from spherical harmonics, leading to a generalized spin model of the form [14, 15]:

$$\mathcal{H}(\{e\}) = \mathcal{H}_0 + \sum_i \sum_{L \neq (0,0)} \widetilde{J}_i^L Y_L(e_i)$$
$$+ \frac{1}{2}\sum_{i \neq j} \sum_{L \neq (0,0)} \sum_{L' \neq (0,0)} \widetilde{J}_{ij}^{LL'} Y_L(e_i) Y_{L'}(e_j) + \dots,$$
(3)

where Y_L are real spherical harmonics and the summations exclude the constant spherical harmonic of composite quantum number $L = (\ell, m) = (0, 0)$.

On the one hand, the coefficients of the SCE spin model in equation (3) can be related to those of the conventional spin Hamiltonian in equation (1). For instance, the $\ell, \ell' = 1$ components of $\widetilde{J}_{ij}^{LL'}$ can be directly related to the $\underline{\underline{J}}_{ij}$ tensor, and the isotropic biquadratic coupling can be expressed as [6]:

$$B_{ij} = -\frac{3}{8\pi}\sum_{m=-2}^2 \widetilde{J}_{ij}^{(2,m)(2,m)}.$$
(4)

On the other hand, the orthonormality of the spherical harmonics implies that the function defined by equation (3) can be projected to obtain the SCE coefficients, for example:

$$\widetilde{J}_{ij}^{LL'} = \int \mathrm{d}^2 e_i \int \mathrm{d}^2 e_j \langle \mathcal{H} \rangle_{e_i, e_j} Y_L(e_i) Y_{L'}(e_j),$$
(5)

where $\langle \mathcal{H} \rangle_{e_i, e_j}$ denotes the partial average of $\mathcal{H}(\{e\})$ with fixed spin directions at sites i and j. Associating these averages of the spin model with the partially averaged *ab initio* grand potential allows us to extract interaction parameters from the electronic structure. The SCE method is especially useful combined with RDLM theory, wherein the partial averages of the grand potential can be directly calculated as opposed to using a huge number of individual electronic structure calculations to obtain the averages [6, 10]. While the method can be formulated to include multi-spin interactions with ease, the computation of these terms is currently beyond the capabilities of our computer code.

Once a set of model parameters is obtained, these may be used to determine the ground state magnetic configuration. To assess the magnetic ordering we use zero-temperature (deterministic) Landau–Lifshitz–Gilbert spin dynamics simulations as a means for energy minimization using the code developed by our group and employed already in [6] (and extended to stochastic LLG simulations in [19]). The LLG equation describes the motion of magnetic moments $M_i = M_i e_i$,

$$\frac{\partial M_i}{\partial t} = -\gamma' M_i \times H_i^{\mathrm{eff}} - \frac{\alpha \gamma'}{M_i} M_i \times \left(M_i \times H_i^{\mathrm{eff}}\right),$$
(6)

where α is the phenomenological Gilbert damping parameter, $\gamma' = \frac{\gamma}{1+\alpha^2}$ and γ is the gyromagnetic ratio of the electron. The

effective magnetic fields are given by:

$$
\begin{aligned}
\boldsymbol{H}_i^{\text{eff}} &= -\frac{1}{M_i} \nabla_{e_i} \mathcal{H}(\{e\}) \\
&= -\frac{2}{M_i} \underline{\underline{K}}_i \, e_i + \frac{1}{M_i} \sum_{j(\neq i)} \underline{\underline{J}}_{ij} \, e_j \\
&\quad + \frac{2}{M_i} \sum_{j(\neq i)} B_{ij} \left(e_i \cdot e_j \right) e_j.
\end{aligned}
\tag{7}
$$

The various terms of the spin model can be easily manipulated in these simulations, in particular to examine how the biquadratic couplings affect the ground state spin structure.

In our calculations the geometry consisted of a single layer of Fe on a semi-infinite Rh fcc-(0 0 1) substrate with a semi-infinite vacuum region on top, with an in-plane lattice constant of 2.6898 Å corresponding to the experimental value for bulk Rh. Layer relaxations were taken into account by varying the distance of the Fe layer from the substrate. The local spin density approximation (LSDA) of density functional theory was used according to the parametrization of Vosko, Wilk and Nusair [20]. The atomic sphere approximation was employed with an angular momentum cutoff of $\ell_{\max} = 2$. For the computation of interaction parameters Brillouin zone (BZ) integrations were carried out with up to 2485 points in the irreducible wedge of the BZ to ensure numerical precision. In spin dynamics simulations the initial state was random, and lattices consisting of 64×64 sites were used with free boundary conditions, or 128×128 in cases where the wavelength of the expected ground state (based on the Heisenberg interaction) was comparable to the smaller system size.

3. Results

3.1. Spin model parameters

We performed self-consistent-field calculations for the Fe monolayer on Rh(0 0 1) for several values of the (inward) layer relaxation of the Fe layer between 0% and −15%, −9% being the experimental value [21]. The Fe local spin moment changes moderately from 2.93 μ_B to 2.84 μ_B in this relaxation range, with 2.87 μ_B for the experimental geometry. We found that in every case the on-site anisotropy is much smaller than the two-site contribution, and that the Fe–Fe interaction parameters show strong dependence on the layer relaxation, similar to our previous findings in Fe$_1$/Ir(0 0 1) [6]. Moreover, due to the smaller atomic number of Rh with respect to Ir, the relativistic interaction terms in the present system are smaller relative to the isotropic Heisenberg couplings than in the case of Ir substrate.

For a quantitative comparison of energy scales, the dominant value of each component of the Heisenberg tensor is collected in table 1 for a few Fe layer relaxations. For 0%, −5% and −9% relaxation the components of the first nearest neighbour (NN) are shown, while for −15% relaxation those of the second NN exchange tensor are shown, with the exception of the DM interaction magnitudes, which are maximal for second NN's in every case. The isotropic Heisenberg interaction clearly dominates among the bilinear terms, while

Table 1. Comparison of the dominant energy scales of the bilinear interactions in Fe$_1$/Rh(0 0 1) for a few values of the Fe layer relaxation, obtained with the SCE method in a DLM reference state. J^{I}, D and $J_{zz} - J_{xx}$ stand for the isotropic Heisenberg interaction, the magnitude of the DM vector and the two-site anisotropy, respectively. Note the difference in units used.

Relaxation	J^{I} [mRy]	D [μRy]	$J_{zz} - J_{xx}$ [μRy]
0%	1.90	36.8	8.73
−5%	1.17	63.8	8.04
−9%	0.591	77.6	7.76
−15%	−0.555	79.4	6.44

by increasing the inward relaxation the DM interaction significantly increases. It should be noted, however, that while at smaller layer relaxations the isotropic terms are much larger than the DM interaction, for the experimental geometry and beyond there is only a factor of around 7 between the two contributions, implying that relativistic interactions have to be taken into account for a proper description of the system.

In figure 1 the isotropic Heisenberg interaction, J_{ij}^{I}, and the isotropic biquadratic interaction, B_{ij}, are plotted versus the interatomic distance for various values of the Fe layer relaxation. For ideal (i.e. unrelaxed) geometry there is a strong ferromagnetic (FM) Heisenberg coupling between the first NN's, with weakly antiferromagnetic (AFM) second and third NN couplings. However, as the Fe inward relaxation is increased, an AFM tendency arises in the Heisenberg interactions. The first NN couplings decrease in value and become AFM at high relaxations, while the second and third NN AFM couplings become gradually stronger. In particular at the experimental geometry (−9% Fe relaxation) we can see a weakened first NN FM coupling competing with second and third NN AFM couplings of the same magnitude, leading to a strong frustration of the Heisenberg terms. The same qualitative behaviour was also found in Fe$_1$/Ir(0 0 1) [6], but the AFM tendency is weaker in the present system.

The biquadratic interactions are very strongly localized; only the first nearest neighbour couplings are significant. The first NN values are furthermore only weakly sensitive to the layer relaxation, and their positive value implies that they prefer a collinear arrangement of interacting spins. For small relaxations the Heisenberg terms most likely prefer FM ordering of the spins, which also complies with the weaker biquadratic terms. However, due to the comparative insensitivity of the biquadratic terms to relaxation, the bilinear and biquadratic couplings are of a similar strength near the experimental relaxation. Considering that the spin spiral states preferred by the frustrated Heisenberg terms are incompatible with the biquadratic couplings of positive sign, we anticipate a very strong influence of the biquadratic terms on the ground state spin structure due to this additional frustration, to be verified by spin dynamics simulations.

3.2. Spin dynamics simulations

For ideal geometry the ground state turned out to be indeed FM, with no frustration between the exchange interactions and the biquadratic terms. As the Fe layer relaxation is
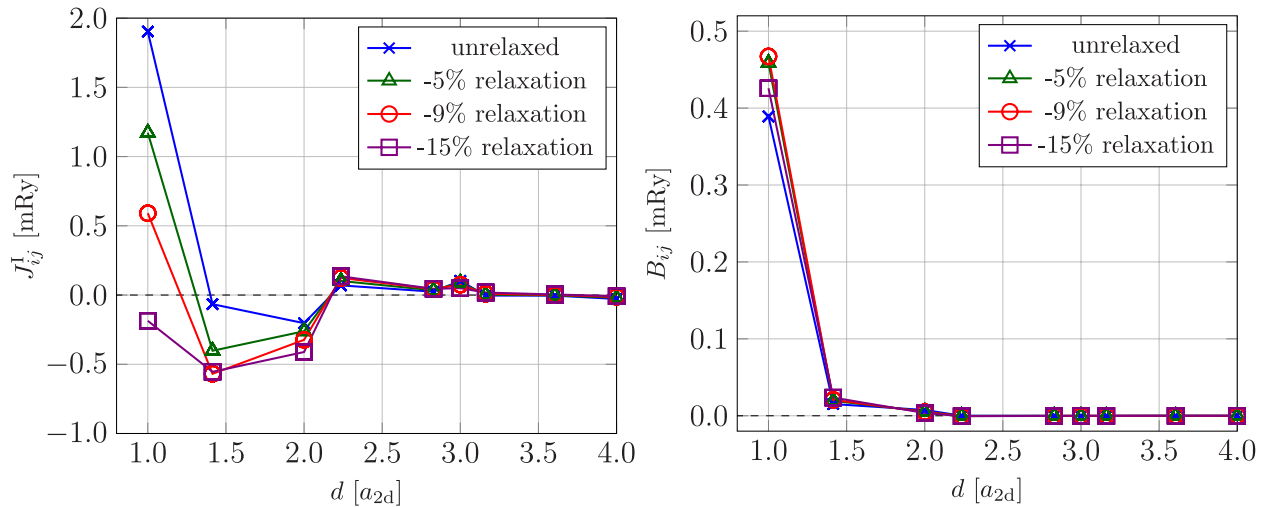
Figure 1. Calculated isotropic Heisenberg (J^{I}_{ij}) and biquadratic (B_{ij}) couplings in geometrically unrelaxed and relaxed Fe$_1$/Rh(0 0 1) thin films versus interatomic distance (d) in units of the in-plane lattice constant (a_{2d}).

increased, however, the competition between these two types of interactions and the frustration of the Heisenberg couplings becomes pronounced, and the ground state is no longer FM. The change from the FM ground state appears quite suddenly. At −7% relaxation the ground state is still FM, while at −8% the spin structure becomes a seemingly random collinear ensemble of up and down spins, indicating that the biquadratic coupling dominates the interaction landscape. Figure 1 suggests that since the magnitude of the biquadratic terms is weakly sensitive to Fe layer relaxation, this rapid onset of a new type of ground state is due to the decrease of the first NN FM and the increase of second and third NN AFM Heisenberg couplings, leading to the frustration of the exchange interactions.

This qualitative picture holds true for larger relaxations including the experimental geometry. The exchange interactions by themselves would prefer some kind of spin spiral due to competing FM and AFM couplings (see figure 1). This frustration allows the comparatively strong first NN biquadratic couplings to overcome the bilinear terms. As the biquadratic couplings with a positive sign prefer a collinear, either parallel or antiparallel, orientation of the interacting spins, for experimental geometry this leads to the collinear spin structure shown in figure 2.

The biquadratic terms themselves do not distinguish between parallel and antiparallel pairs of spins. Omitting bilinear terms, the collinear ground state would be massively degenerate even for a given common axis of orientation, with spins pointing randomly along the common axis. Even though the Heisenberg terms cannot destroy the collinear spin structure preferred by the biquadratic terms, they can lift the aforementioned degeneracy, appearing as a periodic modulation in the random collinear state of spins.

To trace this effect we computed the lattice Fourier transform of the spin structures obtained from simulation,

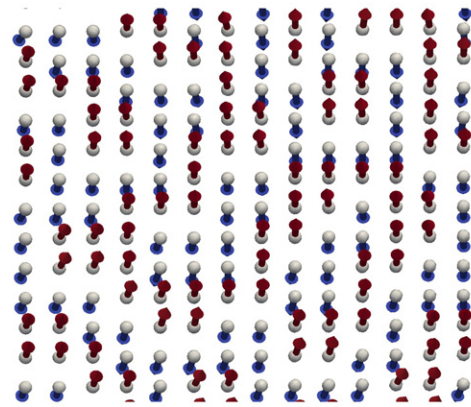$$m(q) = \frac{1}{N} \sum_{j=1}^{N} e^{-iqR_j} e_j, \qquad (8)$$

Figure 2. Approximate ground state spin configuration simulated with spin-model parameters calculated for experimental geometry. The spins are coloured according to the *z* component, with the red colour pointing upward and the blue colour pointing downward.

where N is the number of spins in the sample and e_j is the unit vector describing the direction of the spin at site R_j. The scalar quantity $m(q) = \sqrt{m(q)^* \cdot m(q)}$ then plays the role of an indicator of any modulation with wave vector q in the simulation. In figure 3(*a*) this scalar is plotted in the entire BZ for experimental geometry. While the value of $m(q)$ is overall very small in the sample indicating that there are only weak correlations in the structure, there is a pattern emerging from the near-zero background in the shape of a rotated square. This is the additional modulation arising from the Heisenberg interaction buried in the spin configuration.

To link the pattern seen in figure 3(*a*) to the bilinear couplings we determined the spatial modulation preferred by them. To this end, we used a mean field estimate based on the $\underline{\underline{\chi}}(q)$ paramagnetic spin susceptibility, given by:

$$\underline{\underline{\chi}}(q) = \left[3k_B T \underline{\underline{I}} - \underline{\underline{J}}(q) \right]^{-1}, \qquad (9)$$

where T is the temperature, k_B is the Boltzmann constant and $\underline{\underline{J}}(q)$ is the lattice Fourier transform of the exchange tensor [6].

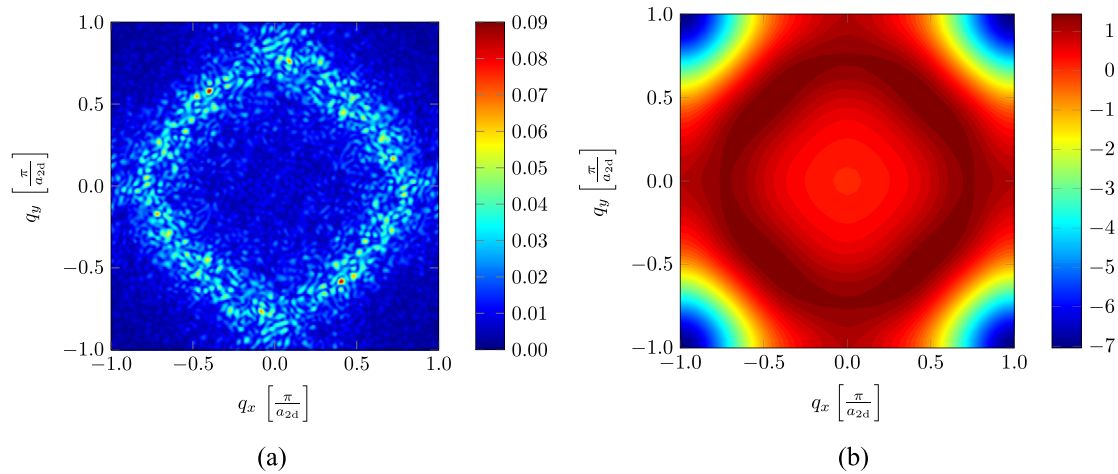**Figure 3.** (*a*) The scalar lattice Fourier transform, $m(q)$, of the obtained spin structure for experimental geometry. (*b*) The maximal eigenvalues, $J(q)$, of the lattice Fourier transform of the calculated exchange tensors for experimental geometry in mRy units.

This formula implies that the highest temperature where the susceptibility is singular and, thus, a mean field estimate for the wave vector of the ordered state to which the paramagnetic state is unstable, is given by the global maximum of the eigenvalues of $\underline{\underline{J}}(q)$ in the BZ. The maximal eigenvalues, $J(q)$, of the $\underline{\underline{J}}(q)$ matrices for experimental geometry are plotted in figure 3(*b*).

The similarity between the two quantities as shown in figure 3 is evident. The $J(q)$ shows a shallow, nearly degenerate maximum line along a rounded square, indicating that the ground state preferred by the Heisenberg terms is somewhere along these q points. It is clear that this maximum line fits perfectly to the Fourier transform of the spin structure in figure 3(*a*), verifying that the random collinear configuration forced by the biquadratic terms is further modulated by the bilinear interactions. The qualitative picture seen in figure 3 is the same for every relaxation equal to or larger than -8%. The sensitivity of the Heisenberg terms to layer relaxation causes the $J(q)$ surfaces to evolve somewhat with increasing inward relaxation, leading to a change in the weak modulation of the $m(q)$ pattern.

We also performed a set of spin dynamics simulations with the biquadratic terms artificially turned off. As expected, for the larger layer relaxation values the simulations evolved into clear single-q helical spin spirals propagating along the $(1, 1)$ direction, with wave vectors agreeing neatly with the numerical maxima of the corresponding $J(q)$ surfaces, being $q = (0.47, 0.47)\frac{\pi}{a_{2d}}$ for experimental geometry. The frustration arising from the competing first and second NN Heisenberg interactions is overall quite similar to what we found for the $Fe_1/Ir(0\,0\,1)$ system [6].

4. Discussion and conclusions

In summary, we found that the (bilinear) exchange interactions in $Fe_1/Rh(0\,0\,1)$ depend strongly on the distance between the Fe overlayer and the substrate, and that their competition leads to strong frustration near the experimental geometry, similar to what was found in $Fe_1/Ir(0\,0\,1)$ [5, 6]. More importantly, we found that biquadratic couplings are comparable to

the Heisenberg terms, and even dominate those near the experimental geometry. Consequently, for Fe layer relaxations between -8% and -15% we obtained a complex collinear ground state spin structure from spin-dynamics simulations. The fact that the 'correction' of the biquadratic terms to the second-order spin model drastically alters the ground state spin configuration implies that the usual anisotropic Heisenberg model is insufficient to describe this system, and one should not even expect to reproduce experimental findings using this approximation.

Although in [9] no structure was observed related to an intermixing or alloying, the question of surface intermixing is still an interesting theoretical prospect. While in bulk FeRh even a small number of Fe anti-site defects unbalances the electronic structure [22], this effect is likely less pronounced in a monolayer geometry and in any way is expected to enhance a FM tendency in the system, which again would be inconsistent with experimental observations. To test this statement we performed SCE-RDLM calculations using the experimental geometry for the cases of 4% and 10% intermixing between the Fe monolayer and the topmost Rh layer. Indeed we found only minor change in the dominating Fe–Fe isotropic exchange and biquadratic couplings, while the changes in the DM interactions by one order less in magnitude were also not significant. In particular, the wave vector of the ground state preferred by the bilinear terms (based on the mean field estimate) did not change due to the intermixing.

It is known that multi-spin interactions in small magnetic clusters can be at an energy scale comparable with the bilinear couplings [23]. Their inclusion in the mapping of *ab initio* total energy might significantly affect the computational estimates for Heisenberg interactions [24]. If strong enough, these terms can even influence the ground state spin configuration of magnetic monolayers [2, 25], in extreme cases leading to the formation of exotic noncollinear spin structures such as nanoskyrmion lattices [26].

From the point of view of the SCE, a complete second-order (four-spin) SU(2)-invariant correction to the Heisenberg

model is given by a general energy term [15]

$$E(2) = \sum_{ij} J_{ij}^{(2)} \left(e_i \cdot e_j \right)^2 + \sum_{ijk} J_{ijk}^{(3)} \left(e_i \cdot e_j \right) \left(e_j \cdot e_k \right)$$
$$+ \sum_{ijkl} J_{ijkl}^{(4)} \left(e_i \cdot e_j \right) \left(e_k \cdot e_l \right), \tag{10}$$

where the summations always run over sets of distinct sites. This would suggest that the biquadratic terms we chose to be included in equation (1) are of the same importance as the three and four-spin interactions. However, within the framework of the SCE-RDLM method two-site interactions describe two electron propagations to lowest order, while three and four-spin interactions need at least three and four propagations, respectively (see equations (26) and (27) in [10]). Due to the decay of the Green's function with distance, this suggests that the biquadratic terms should, in general, be more important than multi-spin interactions, albeit the latter can easily be of the same magnitude as multiple-scattering corrections to the former.

All things considered, the spin structures obtained with our simulations are still very unlikely especially with regard to experiments, suggesting that even with the inclusion of the isotropic biquadratic terms we are far from grasping the true magnetic ground state of the system. As for the spin configuration observed in the experiment, upon closer examination one may realize that the 4×3 period in [9] does not correspond to a single-q spin spiral. A lattice Fourier transform of the proposed configuration seems to show modulations corresponding to three distinct, symmetry unrelated wave vectors, namely $q = (1, 0)\frac{\pi}{a_{2d}}$, $(0, \frac{2}{3})\frac{\pi}{a_{2d}}$ and $(\frac{1}{2}, \frac{1}{3})\frac{\pi}{a_{2d}}$. This fact is in accordance with our findings, in that it seems improbable to be defined by the ground state of a simple Heisenberg model.

Acknowledgments

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