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Magnetic structures and out-of-plane magnetic anisotropy at the exchange bias interface: Co/FeMn

Kohji Nakamura* and Tomonori Ito
Department of Physics Engineering, Mie University, Tsu, Mie 514-8507, Japan

A. J. Freeman
Department of Physics and Astronomy, Northwestern University, Evanston, Illinois 60208, USA
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The magnetic structures and anisotropy at the compensated ferromagnetic/antiferromagnetic Co/FeMn interface are investigated by the highly precise first principles full-potential linearized augmented plane-wave method that incorporates intra-atomic noncollinear magnetism in order to understand the magnetic complexity involved in the spin-flop coupling and the presence of intra-atomic noncollinear magnetism. The self-consistent results predict that the Fe moments in the FeMn layer reorient away from their directions in bulk FeMn so as to be parallel to the Co moment direction—a reorientation that induces an out-of-plane magnetic anisotropy. These results appear to support and confirm recent experimental x-ray magnetic circular dichroism findings that rule out spin-flop coupling as the mechanism for exchange bias in this system.

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An important role in accounting for exchange bias is played by local magnetic structures at ferromagnetic (FM)/antiferromagnetic (AFM) interfaces as well as in structures that include domain walls and defects in the FM and AFM volumes.[1–7] One key interest in this phenomenon lies in understanding magnetic structures at a compensated FM/AFM interface where an equal number of positive and negative exchange interactions exist across the interface. Ideally, this compensated AFM interface has no net magnetic moment. Recently, Koon[8] predicted within the Heisenberg model, a perpendicular (spin-flop) coupling at the compensated AFM interface in which the AFM moments at the interface were found to cant to induce a small net moment. Including imperfections at the interface such as defects and roughness, which give a small number of uncompensated spins, Schulthess and Butler[9] demonstrated the exchange bias shift with the correct order of magnitude by using the Landau–Lifshitz–Gilbert equation.

The magnetic structures in bulk FeMn, one of the exchange bias AFM materials, have been intensively investigated both experimentally[10–13] and theoretically.[14–20] The magnetic ground state is agreed to be the 3*Q* noncollinear magnetic structure, in which the magnetic moments align toward the center of the cell of four atoms. It is thus expected that FeMn is an ideal compensated AFM material.

Most recently, however, x-ray magnetic circular dichroism (XMCD) measurements[21–25]observed that the Fe moments at the Co/FeMn interface are aligned parallel to the Co moments. This indicates that spin-flop coupling is not the mechanism for the exchange bias in this system.

From the theoretical point of view, the few calculations performed for the magnetic structures,[26,27] imposed a restraint to consider only collinear magnetic structures; thus the magnetic complexity at the interface is not yet clear. Indeed, intra-atomic noncollinear magnetism was demonstrated to play an important role in determining the magnetic structures in bulk FeMn [20] as well as in the FM/AFM (NiFe/NiMn) interface.[28] Therefore, highly precise predictions with first principles quantum mechanics including intra-atomic noncollinear magnetism are strongly desirable to derive the true magnetic ground state.

Here we present magnetic structures of the Co/FeMn interface as obtained with the full-potential linearized augmented plane-wave (FLAPW) method[29,30] that now incorporates intra-atomic noncollinear magnetism.[28,31] These self-consistent calculations predict that the Fe moments in the FeMn layer reorient away from their bulk directions so as to be parallel to the Co moment direction, and thus appear to support and confirm the recent experimental findings.[21–25] In addition, we find that an out-of-plane magnetic anisotropy is induced at the Co/FeMn interface. These predictions offer possible improvements in understanding the exchange bias in this system and invite further experimental confirmation.

Calculations were carried out based on the local spin density approximation using the von Barth–Hedin exchange correlation[32] and the scalar relativistic approximation without spin-orbit coupling (SOC). To treat the intra-atomic noncollinear magnetism so as to allow its direction to vary continuously all over space,[28,31,33] the electron density and the effective potential are treated with a 2×2 density matrix, and the basis functions are specified with the spin-independent LAPW basis in order to avoid discontinuity in augmentation of the basis functions at the muffin-tin (MT) radius.[28,31] No local orbitals[33] are incorporated since, as previously demonstrated,[31] the spin-independent LAPW basis does not degrade the accuracy when done as in standard FLAPW calculations for 3*d* metals. The LAPW basis with a cutoff of $|\mathbf{k}+\mathbf{G}|<3.6$ a.u.$^{-1}$ and MT sphere radii of 2.3 a.u. for all atoms are used. Lattice harmonics with angular momenta up to $\ell=8$ are employed to expand the charge and magnetization density, the vector potential, and the eigenfunctions.

The Co/FeMn(001) interface is modeled with three-layer Co and seven-layer FeMn superlattice structures, in which an

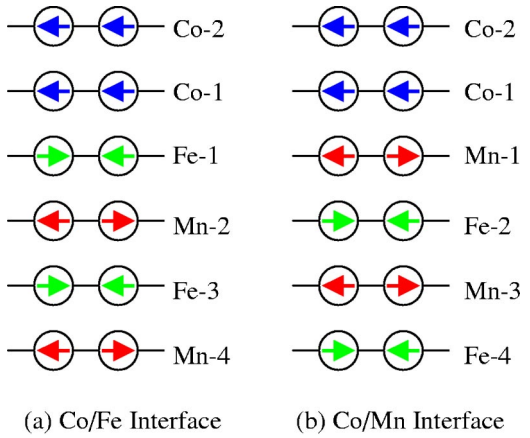

FIG. 1. (Color online) Model and notation for Co and FeMn interfaces, which consist of three-layer Co and seven-layer FeMn superlattice structures. (a) and (b) show the Co/Fe and Co/Mn interface structures, respectively.

$L1_0$ atomic ordering in the FeMn layers is assumed. We consider two atomic interface structures, Co/Fe and Co/Mn, as sketched in Fig. 1(a) and 1(b), respectively. The lattice parameter of the FeMn layer is assumed to be that of its bulk, and for the Co layer the basal plane is assumed to match that of the FeMn layer with the c/a ratio chosen to preserve the experimental atomic volume of hcp Co.

The self-consistent calculations were started with three kinds of symmetries for the three initial magnetic structures, type I, II, and III, depicted in Fig. 2, in which their moments lie on the planes parallel to the interface. For the type I (II) structure, the Fe(Mn) moment axis in the FeMn layer is perpendicular to the Co moment direction while the Mn(Fe) moments orient parallel and antiparallel to the Co direction. The type III structure has the same symmetry as type II, but the Fe moments in the FeMn layer are ferromagnetically aligned.

The calculated moments in the MT spheres along their average moment directions for the Co/Fe and Co/Mn interface structures are summarized in Tables I and II. We could not obtain self-consistent solutions of the type II structure for both interfaces due to their apparent convergence to the type III structure. The tables also give the angles $\phi_{\mathrm{Fe(Mn)}}$ between the two Fe(Mn) moment directions illustrated in Fig. 1 and the induced net moments, M_{FM}, along the Co moment direction.

For both Co/Fe and Co/Mn interfaces in the type I structure, the magnitude of the Mn moments with opposite directions are different since the Co moments break the symmetry

TABLE I. Calculated magnetic moments for the type I and III Co/Fe interface structures. $|M|$ (in μ_{B}) is the magnitude of the moment in the MT sphere along the average moment direction. $\phi_{\mathrm{Fe(Mn)}}$(in degrees) and M_{FM}(in μ_{B}) indicate the angle between two Fe(Mn) moment directions illustrated in Fig. 1 and the induced net moment along the Co moment direction.

	Type I			Type III		
	$\lvert M\rvert$	ϕ_{Fe}	M_{FM}	$\lvert M\rvert$	ϕ_{Mn}	M_{FM}
Co-2	1.71		1.71	1.71		1.71
Co-1	1.53(1.50)		1.52	1.54		1.54
Fe-1	1.89	24	1.85	1.91		1.91
Mn-2	1.46(2.31)		−0.85	2.15	127	−0.99
Fe-3	1.39	118	0.72	1.35		1.35
Mn-4	1.84(2.22)		−0.38	2.19	143	−0.70

of the two Mn sublattice sites as seen in Fig. 2(a), which induces a net Mn moment; the net Fe moment is induced by the canting of the Fe moments. In the type III structure, the Fe moments are parallel to the Co moment direction and the net Mn moment is induced by the canting. In both cases, we observe that the large net Fe moment aligns parallel to the Co moments but the small net Mn moment has the opposite orientation. Also, when moving to the interface the magnitude of the Co moments decreases while those of Fe and Mn increase at the interface, indicating changes in the electronic band structures at the interfaces.

From total energy calculations, the type III structure is found to be energetically favored compared to type I, by 46 and 24 meV/cell for the Co/Fe and Co/Mn interface structures, respectively. Thus, the Fe moments align parallel to the Co moments. These results are consistent with the recent XMCD experimental observations.[21–25] For a more quantitative comparison it is, of course, necessary to include the effects of atomic disordering in the FeMn. Very recently, however, low energy electron diffraction and Auger spectroscopy experiments[34] have pointed out a segregation of the Fe atoms at the surface for the disordered FeMn alloys. This segregation would provide an Fe-rich composition at the interface, which may be close to our Co/Fe interface model of Fig. 1(a).

The calculated magnetic structure of the FeMn layer in the type III structure is similar to the one theoretically proposed by Spišák and Hafner [Table 1(h) in Ref. 18] for bulk $L1_0$ FeMn, namely, parallel Fe moments and canted Mn moments opposite to the Fe moment direction but with $\phi_{\mathrm{Mn}}=128°$. In case of the bulk, although Spišák and Hafner's

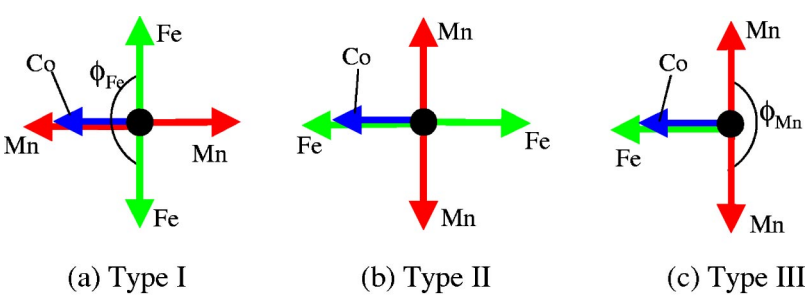

FIG. 2. (Color online) Three kinds of symmetries for initial magnetic structures, type I, II, and III. Arrows represent the average moment directions of Co (blue), Fe (green), and Mn (red). Angles $\phi_{\mathrm{Fe(Mn)}}$ between two Fe(Mn) atoms on (001) planes are defined.

TABLE II. Calculated magnetic moments for the type I and III Co/Mn interface structures. The notations are same as in Table I.

	Type I			Type III		
	$\|M\|$	ϕ_{Fe}	M_{FM}	$\|M\|$	ϕ_{Mn}	M_{FM}
Co-2	1.70(1.64)		1.67	1.62		1.62
Co-1	1.16		1.16	1.11		1.11
Mn-1	1.90(2.32)		−0.42	2.25	148	−0.62
Fe-2	1.39	148	0.38	1.31		1.31
Mn-3	1.89(2.13)		−0.24	2.17	142	−0.71
Fe-4	1.50	139	0.52	1.39		1.39

structure is energetically less favorable than the ground state of the 3Q noncollinear magnetic structure,[20] the calculated energy difference is very small, only 0.11 meV/atom. Therefore, the magnetic interaction across the Co/FeMn interface will easily overcome the small energy increase due to the reorientation of the Fe moments in the FeMn layer.

Furthermore, we find that, compared to the bulk FeMn case,[20] the intra-atomic noncollinear magnetism in the FeMn interface is strongly suppressed by the contact with the Co. Figure 3 shows the spatial distribution of the calculated magnetization $\mathbf{m}(\mathbf{r})$ on the (001) planes for the type III Co/Fe interface structure. At Fe-3, which is far away from the interface, the magnetization density has a complicated pattern with the moment direction varying continuously on a smaller length scale inside the atoms as seen in bulk FeMn.[20] At Fe-1 of the interface, however, the moments inside the atom lie almost collinear. We estimated the moments away from the average direction by calculating $\int_{\mathrm{MT}}|\mathbf{m}_{\perp}(\mathbf{r})|d\mathbf{r}$, where $\mathbf{m}_{\perp}(\mathbf{r})$ is the perpendicular component of the magnetization. These result in 0.11 and 0.24 μ_B for Fe-1 and Fe-3, respectively, corresponding to about 6% and 18 % of their total moments. It is striking that the intra-atomic noncollinearity at the Fe-1 is considerably reduced compared to that of Fe-3.

The reorientation of Fe moments in the FeMn layer would be induced mainly at the interface, i.e., close to the Co layer. Indeed, the recent XMCD experiments[24] detected the magnetic domain images of the Fe and Mn due to the existence of their net moments when the FeMn was in contact with the Co layer; the magnetic asymmetry of the Fe displays a strong dependence on the FeMn thickness, presenting a high value for approximately the first 3 ML FeMn, decreasing continuously with increasing FeMn thickness, and reaching an apparently small value above 6 ML. Therefore, the bulk 3Q structure may be recovered continuously when the FeMn thickness increases above 3–6 ML.

It is now interesting to discuss the magnetocrystalline anisotropy (MCA) at the Co/FeMn interface, since the reorientation of the Fe moments at the interface and the induced net moment in the AFM layer changes the spatial magnetic symmetry, which leads to a large change of magnetic properties such as the MCA. In order to determine the MCA, we employed the second variational SOC method[35,36] using the calculated scalar relativistic eigenvectors with 3456 special k points in the Brilliouin zone; this sufficiently suppresses numerical fluctuations to less than 0.03 meV/cell of the MCA

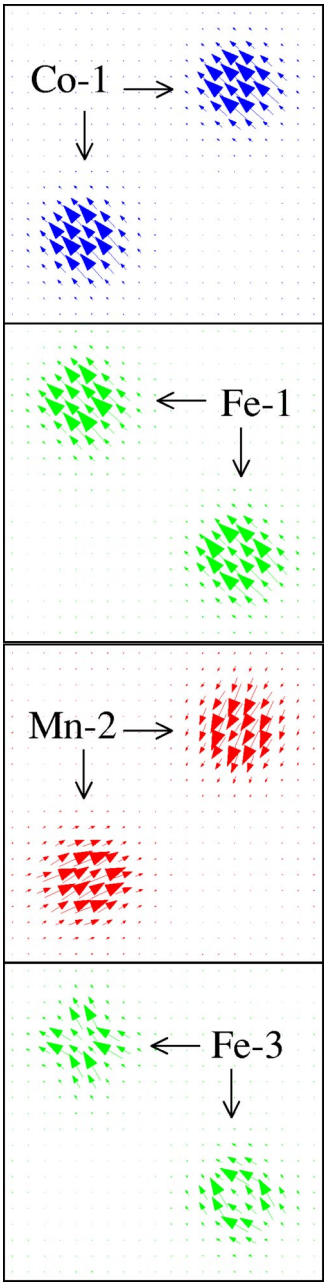

FIG. 3. (Color online) Spatial distribution of the calculated magnetization $\mathbf{m}(\mathbf{r})$ on (001) planes for the type III Co/Fe interface structure. Arrows represent the moment directions and their magnitudes by lengths.

energy (E_{MCA}). Here, the E_{MCA} is obtained as an energy difference for changing the global magnetization orientations as the average Co moment (and therefore the ferromagnetically coupled Fe moment) orients along the [110] (in-plane) and [001] (out-of-plane) directions.

The calculated E_{MCA} is 1.54 and 1.23 meV/cell for the Co/Fe and Co/Mn interface structures, respectively. Thus, energetically the Co (and Fe) moments point along the out-of-plane direction. When considered individually, the MCA for the single Co film is known to have an in-plane MCA,[36] and bulk FeMn with the 3Q noncollinear magnetic structure may have a small MCA due to the symmetry of the magnetic

structure. Assuming Spišák and Hafner's structure (with parallel Fe moments and canted Mn moments for bulk FeMn), we find that the calculated E_{MCA} has a positive value of 0.23 meV/atom, which shows the out-of-plane MCA. Therefore, the out-of-plane MCA in the Co/FeMn case may arise from the reorientation of the Fe moments at the Co/FeMn interface. In support of this, recent experiments reported the out-of-plane exchange bias in CoFe/FeMn and FeNi/FeMn.[40,41] This may indicate that the out-of-plane MCA at the interface is induced by the reorientation of the moments in the FeMn layer as seen in our calculations.

Significantly, an out-of-plane exchange bias has been observed recently in FM Co/Pt multilayers with the out-of-plane MCA when in contact with an AFM layer such as CoO(111) and FeF_2(001) after field cooling along the out-of-plane orientation.[37,38] Also, in the Permalloy(Py)/CoO system even though the Py layer has intrinsic in-plane MCA, the out-of-plane exchange bias was established with decrease of the Py layer thickness.[39] In all these cases, out-of-plane AFM spin components are necessary to obtain the out-of-plane exchange bias.

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*Electronic address: kohji@phen.mie-u.ac.jp

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