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Interfacial Dzyaloshinskii-Moriya interaction and orbital magnetic moments of metallic multilayer films

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Dzyaloshinskii-Moriya interaction (DMI) at metallic multilayer interfaces of Co thin films and heavy-metals X (X=Ir, Pt) was investigated from first principles calculations that treat spin-spirals with the spin-orbit coupling. The results predict that the sign of the DMI parameters depends on the heavy-metals at the interfaces, and that the variation of the orbital moments behaves differently depending on the sign of the DMI parameters. [http://dx.doi.org/10.1063/1.4973217]

I. INTRODUCTION

Since the emergence of spintronics around three decades ago, in which both the charge and spin degrees of freedom of electrons are fully utilized, various device applications can be envisaged. A great number of works have since been conducted, ranging from elucidating the basic physical mechanisms to realizing the spintronic phenomena into real working devices.[1] One of the issues challenging the current development of spintronics is the manipulation of homogeneously magnetized regions and/or the magnetic domains. This will allow better ways of transferring magnetic information based on domain-walls (DWs) motion as well designing DWs memory with an unprecedented density and a high energy efficiency.[2] In this respect, understanding magnetism at metallic interfaces between 3*d* transition-metal thin films and heavier-metals has been very important. The net magnetic moments of the transition metals and the strong spin-orbit coupling (SOC) of the heavier metals can be expected to display unique interplays in determining the magnetization textures of the materials.

In such ferromagnetic and heavy nonmagnetic metal interfaces, the Dzyaloshinskii-Moriya interaction (DMI),[3,4] which arises from an asymmetric interface stacking and the strong SOC, plays a key role that may give rise to particular magnetic textures. More specifically, the DMI is essential to stabilize the DWs in a Néel configuration with a given chirality, allowing their first motion by spin Hall effect in a direction fixed by this chirality. Measurement techniques of interfacial DMI have largely developed in the past few years, ranging from visualizing the DWs[5,6] using the spin polarized low energy electron microscopy to exploiting spin-wave frequency via the Brillouin Light Scattering[7–9] or all electrical propagating spin-wave spectroscopy[10] measurements. Such improvements have opened new possibilities to obtain deeper understanding on the origin of the DMI and its relation with the details of the electronic and atomic structures of the materials. It has been known for instance that while the DMI strength is attributed to the SOC at the interfaces, recent observations indicate that the sign of DMI strongly depends on the details of (multi)layer structures.[5,11] Among the most notable cases are the prototypical interfaces of Co and heavier transition metals, where the DMI sign of Co/Ir compared to that of Co/Pt remains a controversy.[5]

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We report in this article systematic electronic structure investigation on the interfacial DMI between Co thin films and heavy-metals of X (X=Ir, Pt). Our results show that the calculated DMI parameters are related to the orbital moments of the heavy metal elements, which is induced by the magnetic moments of the Co atoms. Moreover, different signs of the DMI parameters can be explained by the behaviors of the induced orbital moments of the different heavy metal atom species.

II. MODELS AND METHODS

Self-consistent calculations were performed based on the generalized gradient approximation (GGA)[12] in the scalar relativistic approximation (SRA), i.e. without SOC, by using the full-potential linearized augmented plane-wave (FLAPW) method[13–15] that treats a film geometry by including fully additional (non-periodic) vacuum regions outside of a single slab. We consider a single slab of Co atoms on top of three-atomic layers of X (X=Ir, Pt) assuming a (111) interface. A plane-wave cut-off $|\mathbf{k}+\mathbf{G}|$ of 3.9 a.u.$^{-1}$ has been chosen, and suitable muffin-tin radii for each considered atomic species have been used; 2.4 bohr for Pt and Ir, and 2.2 bohr for Co.

The computation of the DMI was carried out by including the SOC via the second variational method[16,17] using the SRA eigenfunction of spin spiral structure. To describe the latter spin structure, the basis function was reconstructed by introducing the generalized Bloch theorem[18,19] for the spin spiral structure for a large unit cell (supercell) with lattice constant corresponding to wavelength of commensurate spin-spiral structure.[20,21] The magnetization vectors in the spin-spiral structures with the Néel type out-of-plane rotation, as depicted in Fig. 1, are assumed to lie on a plane parallel to the spin-spiral wavevector, q, and perpendicular to the film-plane. We have considered 3600 special k-points (in chemical BZ) in our calculations that include SOC in order to reduce the numerical errors.

III. RESULTS AND DISCUSSION

It is first desirable to check the dependence of the stacking (fcc and hcp) sites of the Co atoms. For this purpose, we compare the total energies of the Co/Pt films with different stacking structures, the results of which are summarized in Table I. In all considered structures, the most stable arrangements at the Co/Pt interfaces are always those with fcc stackings. However, when the Co layer thickness is increased, the hcp stacking of Co on the other Co layer becomes more energetically favorable.

In the next step, we calculate the energies of the spiral structures for the Co/Pt_3 and Co/Ir_3 as a function of q along the M direction. We consider negative (positive) q values corresponding to magnetization vectors rotating in a left- (right-) handed way. For both Co/Pt_3 and Co/Ir_3 interfaces, in the neighborhood of $q = 0$, the formation energy ΔE_{spiral}, defined as the energy difference between the spiral structure and the collinear ferromagnetic one, increases approximately proportional to the square of q. In addition, we obtain an asymmetry in the ΔE_{spiral} with respect to the left- and right-handedness as a result of the broken inversion-symmetry at the interface, which gives rise to the

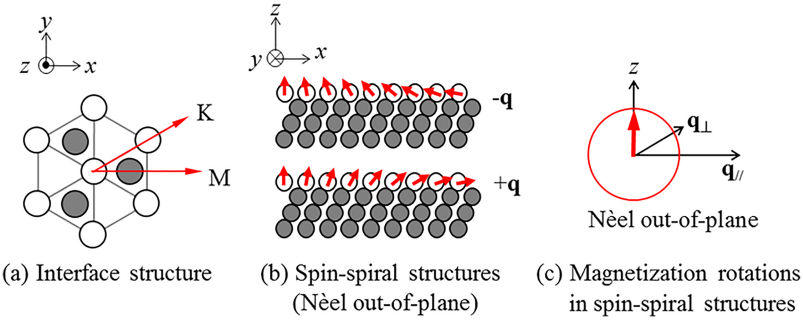

FIG. 1. (a) Interface structure of fcc-stacking, where open and closed circles represent Co and Pt atoms, respectively, at the interface and arrows indicate spin-spiral wave directions along M and K directions. (b) Magnetization vectors in the spin-spiral structures, negative (positive) value of the q means a left- (right-) handed rotation. (c) The Néel type out-of-plane magnetization rotation considered here, assumed a rotation plane to lie parallel to the q and perpendicular to the film-plane.

TABLE I. Total energies of Co/Pt thin films with different (fcc and hcp) stackings and Co layer thicknesses. The reference energy ($\Delta E = 0$) is set to that of the ground state stacking. The fcc stacking of Co on Pt layer at interface always favors energetically over the hcp stacking.

	Co_3	Co_2	Co_1	ΔE (meV)
Co_1/Pt_3	-	-	hcp (h)	73.1
	-	-	fcc (f)	0.0
Co_2/Pt_3	-	h	h	20.1
	-	f	h	99.9
	-	h	f	0.0
	-	f	f	48.3
Co_3/Pt_3	h	h	h	50.7
	f	h	h	86.9
	h	f	h	134.1
	h	h	f	0.0
	f	f	h	164.8
	f	h	f	37.9
	h	f	f	67.6
	f	f	f	100.2

interfacial DMI. The DMI parameters, D, were then estimated by the least square fit of a polynomial function, where the coefficient of the linear term corresponds to these interaction parameters. The results are summarized in Fig. 2.

Now, comparing the obtained DMI parameters for both fcc and bcc stackings, as displayed in Fig. 2(a), reveals that the D parameter for the fcc stacking is larger than that of the hcp one although the sign does not change. The D in the Co/Pt_3 has always a positive value while that in the Co/Ir_3 has a negative one. We have further checked the direction dependence of D by additionally computing spin spiral structures along the K direction, however, no significant difference can be observed. Also, the Co thickness dependence of the D, as shown in Fig. 2(b), was investigated. The D roughly converges to a constant value for each interface although the absolute value of the D decreases when the Co thickness increases, and thus the sign of the D does not alter with the increase of layer thickness. The results of the Co/Pt agree with experiments[10,22,23] and suggest that the DMI originates mainly at the interfaces. In contrast, for the Co/Ir(111), where it is still controversial even in the sign of the D,

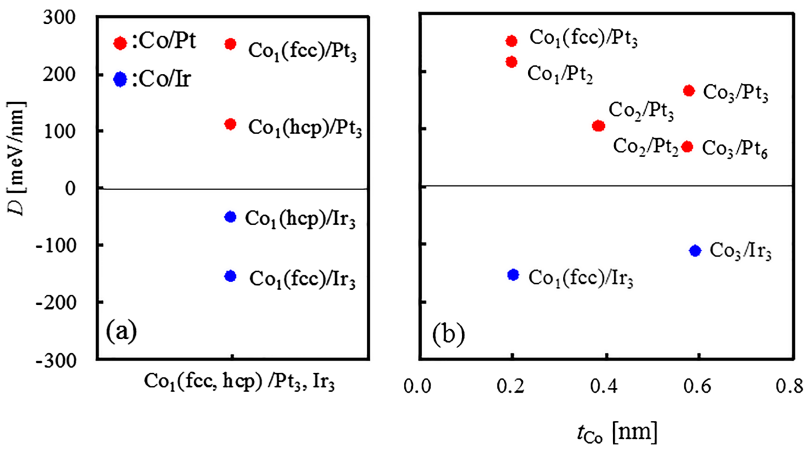

FIG. 2. (a) DMI parameters, D, in Co/Pt_3 and Co/Ir_3 when the Co atom stacks on the fcc and hcp sites of the Pt and Ir layers. Red and blue circles indicate the results for the Co/Pt_3 and Co/Ir_3. (b) DMI parameters, D, for Co/Pt (red circles) and Co/Ir (blue circles) bilayers as a function of the thickness of Co layers.

our calculations rather support the experiments of Hrabec et al.,[24] in which a negative D value was observed by magnetic-field based measurements.

Deeper inspection on the D of the Co/Pt and Co/Ir interfaces shows the opposite sign for both interfaces. To date, there has been no clear explanation on the sign difference between these systems. In order to get a better insight on this issue, we have calculated the orbital magnetic moments in the spin spiral states with the right-handed ($\frac{q}{2\pi} = +0.21$ nm^{-1}) and left-handed ($\frac{q}{2\pi} = -0.21$ nm^{-1}) magnetization rotations along the M direction in each different interface. Figure 3 shows the magnitudes of the Co orbital moments on the Pt and Ir substrates, and the corresponding induced orbital moments of the Pt and Ir atoms at the interfaces. Due to the magnetocrystalline anisotropy ascribable to the SOC, it is expected that the in-plane and out-of-plane magnetization will lead to different induced orbital moments, not only at the Co sites but also on the heavy metal sites. As a consequence, the Néel type out-of-plane rotation [Fig. 1(c)] should give rise to a periodic variation of orbital moments at different atomic positions along the spin-spiral direction. Indeed, such variation is clearly observed in our calculations. Interestingly, one can observe obvious difference between the variations induced by the left- and right-handed magnetization rotations in all systems considered in this work. In particular, the difference between the out-of-plane and in-plane orbital moments of Co due to the right-hand rotations is always larger than those due to the left-hand ones [see Figs. 3(a) and 3(c)]. Such difference is more apparent in the Co/Pt interface than in Co/Ir.

The orbital magnetic moments in the heavy metal sites [see Figs. 3(b) and 3(d)], on the other hands, show a more interesting feature. It should be noted, however, that one cannot compare the magnitude of orbital moments in Pt and Ir due to different number of the valence electrons. In the Co/Pt, while the right-hand rotation leads to apparent Pt orbital moment variation, the left-hand one practically does not alter the orbital moments [Fig. 3(b)]. The situation is completely different for the orbital moments of Ir in the Co/Ir. As both right- and left-hand rotations induce visible orbital moment variation, the alteration in the right-hand rotation is more significant than in the left-hand one [Fig. 3(d)].

Another difference is also visible when comparing the atomic positions of Pt and Ir where the maximum orbital moments can be observed. In the case of the Co/Pt, the orbital moment of Co is maximum at the out-of-plane magnetization, while at this position, the orbital moment of Pt in the right-hand rotation is minimum [Figs. 3(a) and 3(b)]. In the Co/Ir, however, the maximum values of orbital moments in Co and Ir are both found in the out-of-plane magnetization. The results show a shift in the periodic cycle of the induced orbital moment variation in Pt and Ir, the origin of which

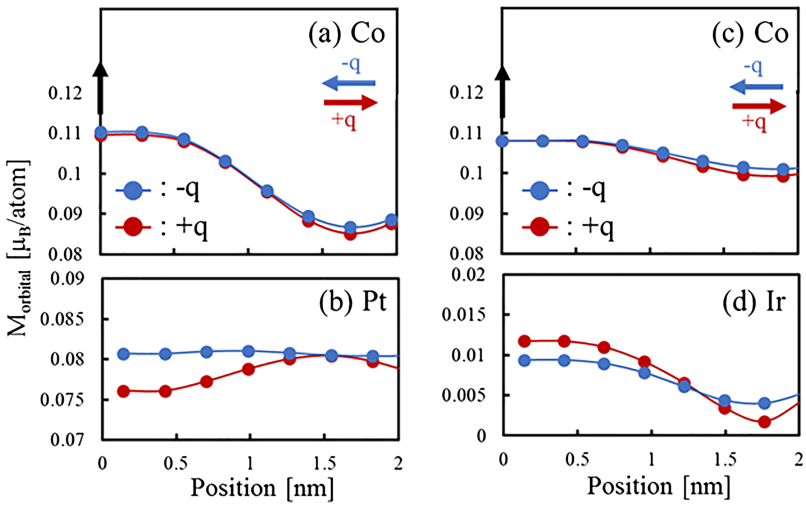

FIG. 3. The magnitude of orbital moments, M_{orbital}, of the Co and Pt (Ir) at interface as a function of the atomic positions along the M direction. (a) and (b) show orbital moments at the Co/Pt interface. The orbital moment of Co is maximum at the out-of-plane magnetization, while at this position, the orbital moment of Pt in the right-hand rotation is minimum. (c) and (d) show orbital moments at the Co/Ir interface. The orbital moments of Ir is maximum at the out-of-plane magnetization.

deserves further study. These different behaviors should contribute to the different signs of their DMI parameters.

IV. SUMMARY

We studied the DMI of the Co/heavy metal (X=Pt and Ir) interfaces by first principles calculations. The magnitude of the D depends on the Co thickness and interface structures, but the variation is small and thus the sign of the D is mainly determined by the species of the heavy metals, i.e., Pt or Ir. Moreover, the orbital moments at the interfaces are found to be sensitive to the sign of the D. The results shed more lights on the mechanisms contributing to the DMI in transition metal bilayer interfaces.

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