Turkish Journal of Physics

http://journals.tubitak.gov.tr/physics/

Research Article

Turk J Phys
(2020) 44: 356 – 363

doi:10.3906/fiz-1912-2

Influence of capping layer on skyrmion and domain-wall formation in Co/Pt(111)

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Received: 03.12.2019 • **Accepted/Published Online:** 27.04.2020 • **Final Version:** 31.08.2020

Abstract: In order to realize skyrmion-based next-generation logic and memory devices, investigating the impact of material parameters on skyrmion formation is essential. Capping magnetic thin layers for the purposes of both preventing oxidation and/or enhancing crystal structure has an influence on chiral spin texture of the layer. In this paper, we have carried out a systematic computational study on magnetic skyrmion and domain-wall formation in which 2-atomic layer of Co, deposited on Pt(111) substrate and capped by certain (Ta, Ir, and Pt) $5d$ elements with various thicknesses. We have determined the magnetic topography of the structures by simulations based on DFT-calculated parameters; micromagnetic Dzyaloshinskii-Moriya interaction, exchange interaction, and magnetic anisotropy coefficients. We have revealed the influence of capping material and thickness on the chiral spin texture. We anticipate that our predictions provide a rational basis for skyrmion-based devices in which skyrmions are used as logic or information element.

Key words: Chiral spin textures, magnetic skyrmions, first-principles calculations, micromagnetic simulations

1. Introduction

The precise control and stabilization of topologically protected spin structures [1–5] have attracted the interest of numerous investigators due to the diversity and potential of future spintronic devices [6–8]. Particularly, the usage of skyrmions and/or domain walls as an information carrier in cutting-edge logic and memory technology can pave the way for the production of energy efficient and compact sized devices with high magnetic stability. Chiral spin structures can emerge in magnetic materials lacking inversion symmetry. Bloch-type magnetic skyrmions have first been observed in noncentrosymmetric B20 materials under certain conditions, such as external magnetic field and low ambient temperature [9–12]. Then, ferromagnetic/heavy metal multilayers with broken inversion symmetry became popular for researchers to obtain room-temperature zero field skyrmions. Such interfaces could induce strong Dzyaloshinskii-Moriya interaction (DMI) [13,14] which could form skyrmion lattices. This strategy is partially justified by the observation of Néel-type skyrmions. However, their presence was still dependent on high magnetic fields and low temperature conditions [15–17]. Finally, researches have figured out that perpendicular magnetic anisotropy (PMA) could be used like an internal magnetic field, to abolish external magnetic field dependency of skyrmion formation. By this way, room-temperature zero field skyrmions have been formed in Pt/Co/Ta and Co/Pd multilayer thin films [12,18,19].

For the use magnetic skyrmions in nonvolatile and low-power consumption magnetic memory and logic applications, further investigations were indispensable on their stability. Especially, the creation of DMI at magnetic/nonmagnetic interfaces have been investigated by a large number of experimental and computational

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studies [20–23]. The role of Hund's first rule in DMI at $3d/5d$ interfaces is recently revealed by Belabbes et. al.; the number of valance electrons in a magnetic layer determines the DMI strength [24]. Relevant studies on DMI at Co/Pt bilayers can be found in the literature [23,25]. On the other hand, Pt/Co/nonmagnetic(NM) trilayers have become the focus of current studies, which aim to control DMI strength and sign [26,27]. Even though the influence of specific nonmagnetic layer element in Pt/Co/NM system on DMI is recently studied [28,29], revealing the effect of NM capping layer (CL) thickness have not been investigated yet. A certain capping layer thickness preventing the system from oxidation can alter the chiral magnetic properties.

In this study, we explore magnetic properties of 2-atomic layer of Co, deposited on Pt(111) substrate and capped by certain (Ta, Ir, Pt) $5d$ elements with various thicknesses. By employing Density-Functional Theory (DFT) for first-principles calculations, micromagnetic DMI (D), exchange (J) and magnetic anisotropy energy (K) coefficients are determined. We also perform micromagnetic simulations to make an interface between atomic framework and device dimensions by transforming the output of the DFT calculations to the input of micromagnetic calculations. Thus, spin textures of the structures generated by the simulations are also discussed within the scope of this paper.

2. Computational details

To reveal capping layer thickness dependency of magnetic properties of Co/Pt(111), we exploit first-principles calculations based on the density functional theory, implemented in the VASP code [30]. Generalized gradient approximation - Perdew-Burke-Ernzerhof type functional for electron-electron interactions and projector augmented wave method [31] for electron-ion interactions are used for the calculations with the cut-off energies for the plane-wave basis sets of 400 eV. Γ-centred 4 $\times$16 $\times$1 k-point sampling is employed for the Brillioiun-zone mesh. Most stable geometries are determined by structural relaxations until the forces become smaller than 0.001 ev/Å. Then, charge distribution of the structures' ground state is calculated by solving Kohn-Sham equations in the absence of spin-orbit coupling. Finally, the effect of the orientation of the magnetic moments, which is controlled by using the constrained method implemented in VASP, on the self-consistent total energy of the structure is revealed by the calculations with spin-orbit coupling. A supercell consisting of 2 atomic monolayers (ML) of Co on 8 ML of Pt is employed to form Co(2)/Pt(fcc) structure. Over the capping layers, a 6 ML-thick vacuum slab was considered along the thickness direction to avoid the interaction between the repeating slabs. The z component of the DMI vector is calculated using opposite spin chirality configurations, where the supercell contains a row of 4 atoms in the plane. Thus, the cycloid wavelength is chosen as n = 4 for convenience.

The spin textures of the systems are generated by icromagnetic simulations based on the Landau-Lifshitz-Gilbert (LLG) equation. The simulations are performed by using the Mumax^3 software [32]. The micromagnetic simulation parameters D (DMI constant), J (micromagnetic exchange constant, i.e. exchange stiffness) and K (first-order uniaxial magnetic anisotropy constant) are calculated by DFT and used in the simulations with the saturation magnetization of Co, $M_S = 1.4 \times 10^6$ A/m [7]. The simulation surface is discretized into 200 $\times$200 $\times$1 unit cells, with the cell size of 1 $\times$1 $\times$1 nm^3, which is smaller than both the minimum Néel exchange length $\lambda_{N\acute{e}el} = 2.71$ nm and the minimum Bloch exchange length $\lambda_{Bloch} = 2.39$ nm (for 1ML Ir CL).

3. Results and discussions

Working performance of the future spin-based memory and logic applications strongly leans on the chiral spin texture. The stability of such textures is dependent on the material used. However, theoretical calculations to

be carried out as a precursor to the experiments can be used to predetermine parameters such as material and thickness. These rationally designed nanostructures can achieve better performance, e.g., very high speed in a racetrack memory even at low current densities. For this purposes, we have calculated DMI, exchange and anisotropy constants of 5d(x ML)/Co(2ML)/Pt(111) structure, where 5d is the material (Ta,Ir,Pt) and x (1-3 ML) is the thickness of the capping layer.

In the first part of this section, we present the results of DMI calculations for certain capping layer materials and thicknesses in Figure 1. Thanks to their relatively high spin-orbit coupling, Pt-interfaced multilayers are one of the most widely studied material for the production of chiral spin textures. However, the capping material and thickness can disrupt the total magnitude of DMI in the system.

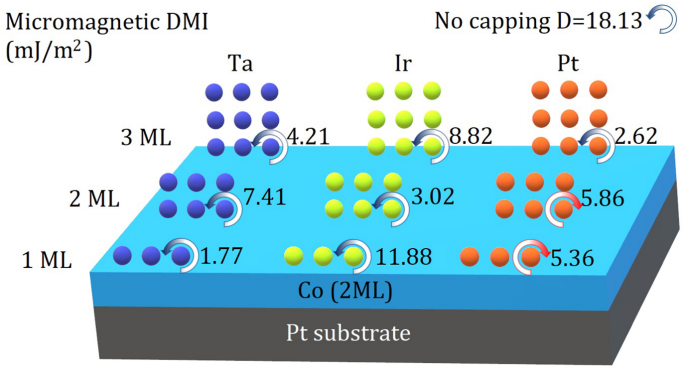

Figure 1. Micromagnetic DMI constant of Co/Pt(111) for Ta, Ir, and Pt capping layers with certain thicknesses. Blue-gradient and counter-clockwise arrows represent positive DMI values while red-gradient and clockwise arrows show negative DMI. Micromagnetic DMI constant of the Co/Pt(111) system without capping layer is also calculated as 18.13 mJ/m^2.

To uncover the effect of capping layer material and thickness on the total DMI of the system, we have calculated micromagnetic DMI coefficient (D) of the systems given in Figure 1. D constant of Co/Pt(111) system without capping layer is also calculated for comparison. First and foremost, introducing capping layer to the system alters the chirality of the system towards to the clockwise rotation and reduces the total DMI for all type of materials and thickness values of capping layers. Especially, D is remarkably small for thicker Pt capping layer because of the inversion symmetry. On the other hand, single layer of Ir achieved the highest value of DMI, which is expected since the Ir layer prefers a counter-clockwise rotation for the opposite stacking order [33,34]. Besides, for all type of the capping material, the magnitude of DMI has an oscillatory behaviour as a function of capping layer thickness. A similar behaviour was also observed in an experimental study performed by Shahbazi et. al. and was attributed to the interfacial sensitivity dependence on the heavy-metal 5d states filling as well as the alignment of Fermi levels across the ferromagnetic material/heavy-metal interface [35]. This is somewhat unexpected since second and further neighbour layers of a nonmagnetic metal from a nonmagnetic/magnetic layer interface are generally not responsible for the DMI. A possible reason for this effect is a probable relaxation of substrate induced-strain along perpendicular to the film plane, which can influence the distance between Co-Co neighbours. According to our calculations, the material and thickness of capping layer are crucial parameters for the formation of DMI. however, some other magnetic coefficients can affect chiral spin texture of the system, such as J and K.

We calculated micromagnetic exchange interaction coefficient (exchange stiffness, J) of the structures, as can be seen in Figure 2. For 1 ML of capping layer, Ir CL provides slightly different J when compared to Ta

and Pt, similar to the discussion on DMI constant above. Indeed, there is a quantitative correlation between micromagnetic D and J for single layer of CL: Ta CL which comprises lowest value of D has the highest J, while Ir CL forms highest D value and lowest J. It can be understood that DMI is a kind of antisymmetric exchange interaction and it tends to oppose the parallel configuration of the direction of magnetic moments, which favoured by ferromagnetic exchange interaction. The interplay between D and J generally determines the chiral spin structure of the material, however, there is a third parameter which exerts an influence on the orientation of the spins in a system; magnetic anisotropy. Here, we should note that the physical mechanisms behind these 3 interactions are different: DMI and magnetic anisotropy are originated respectively in the first and second order in the perturbation theory while exchange interaction is originated from the Pauli exclusion principle.

Magnetic anisotropy energies of the structures are calculated and represented in Figure 3. Growth of single capping layer preserves the perpendicular magnetic anisotropy in Co/Pt(111) structure. Moreover, it is enhanced for Ta and Ir layers. For all thickness value of Ta capping layer, perpendicular magnetic anisotropy is observed. For thicker Ta and Ir capping layers, magnetic easy axis of the film is rotated along the film plane or magnetic anisotropy of the film is almost vanished. Determining all micromagnetic parameter by DFT calculations have allowed us to reveal magnetic topography of the structures by micromagnetic simulations.

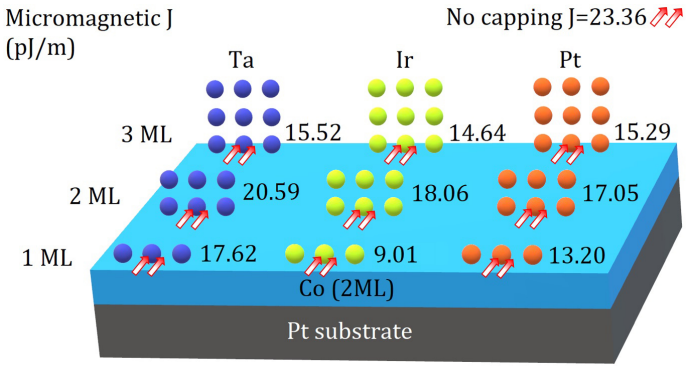

Figure 2. Micromagnetic exchange interaction coefficient (J) of Co/Pt(111) for Ta, Ir, and Pt capping layers with certain thicknesses. Arrows represent positive J values, corresponding ferromagnetic interaction for all capping layers. J constant of the Co/Pt(111) system without capping layer is also calculated as 23.36 pJ/m.

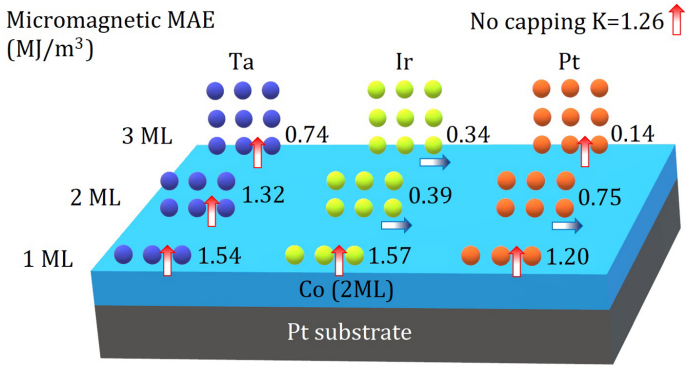

Figure 3. First-order uniaxial magnetic anisotropy constant (K) of Co/Pt(111) for Ta, Ir, and Pt capping layers with certain thicknesses. Red-gradient and out-of-plane oriented arrows represent positive K values while blue-gradient and in-plane oriented arrows shows negative K values. Micromagnetic K constant of the Co/Pt(111) system without capping layer is also calculated as 1.26 MJ/m^3.

Magnetic topography of the systems generated by micromagnetic simulations based on DFT calculated-parameters is represented in Figure 4. For single Ir CL, the magnetization conserves its labyrinth structure up to external magnetic field of 2 T. Magnetic skyrmions with thin domain walls are observed under the magnetic field of 4 T. When the Ir capping layer thickness is increased to 3 ML, labyrinth structure is still preserved in the absence of magnetic field. However, skyrmion lattice is formed under external magnetic field. The diameter of the skyrmions is getting smaller with increasing magnetic field, as expected. For Pt and Ta capping layers, ferromagnetic states, meta-stable skyrmions and labyrinth structures have been observed for certain thicknesses and magnetic field values. According to the our calculations, Co/Pt(111) structure with 3 ML Ir capping layer is a candidate material for skyrmion-based memory and logic technologies.

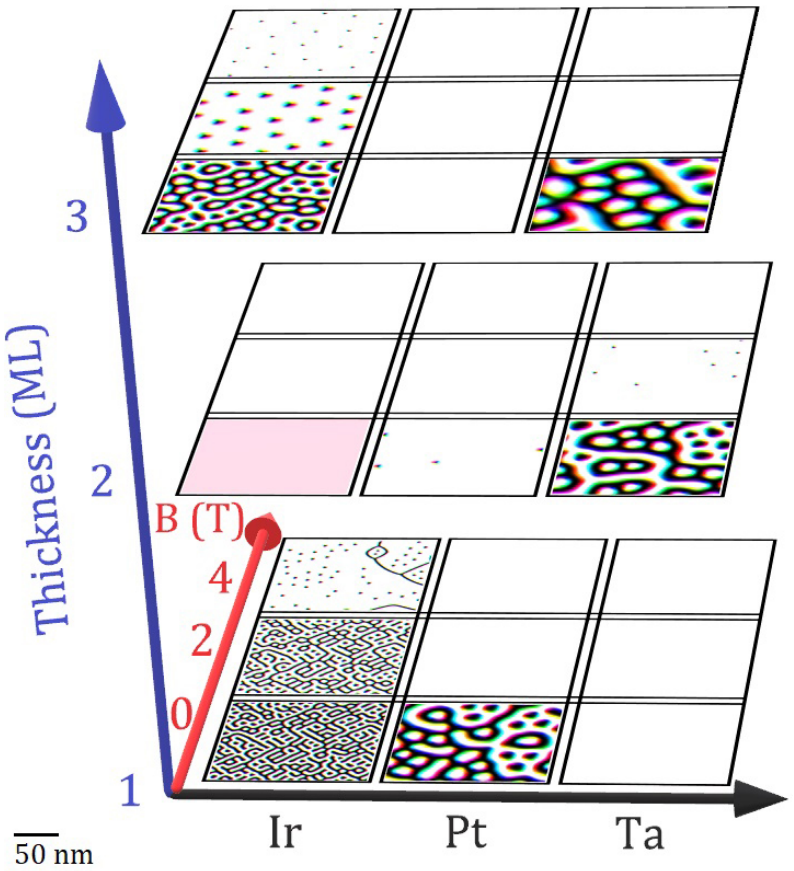

Figure 4. Low-temperature spatial magnetization of Co/Pt(111) structure with Ta, Ir, and Pt capping layers as a function of external magnetic field. White (black) colour corresponds to the simulation cells magnetized in +z (-z) direction. Other colours represent the regions have in-plane magnetization component. Scale bar: 50 nm.

4. Conclusion

In this paper, we demonstrated a comprehensive DFT and micromagnetic study on the effect of capping layer on the formation of skyrmions and domain walls in Co/Pt(111) system. Micromagnetic DMI, exchange and magnetic anisotropy parameters are determined for *5d*(x ML)/Co(2ML)/Pt(111) structure, where 5d is the material (Ta,Ir,Pt) and x (1-3 ML) is the thickness of the capping layer. The DFT-calculated parameters are

implemented to the simulations and spatial magnetization of the system is revealed. Ferromagnetic state with a few metastable skyrmions is observed in most samples. However, 3 ML-thick Ir capping layer induced the formation of skyrmion lattice under magnetic field. We anticipate that our study not only offers a rational design for the materials comprises desired chiral spin structures but also will inspire future considerations about the influence of the capping layer and nonmagnetic/magnetic layer interfaces on the creation of skyrmions and domain walls.

Acknowledgements

The numerical calculations reported in this paper were fully performed at TÜBİTAK ULAKBİM, High Performance and Grid Computing Centre (TRUBA resources). Computational analyses are performed at the Simulations and Modelling Research Lab (Simulab), Physics Department of MU. The author wishes to acknowledge I. Yavuz for fruitful discussions.

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