Dzyaloshinskii-Moriya interaction at metallic bilayer interfaces

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In ferromagnetic and heavy metal interfaces, the Dzyaloshinskii-Moriya interaction (DMI), 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 domain walls in a Néel configuration with a given chirality. Recent measurements and theory for the interfacial DMI have opened new possibilities to obtain understanding on the origin of the DMI and its relation with the details of the electronic and atomic structures of materials.

Here, we present the systematic investigation on the interfacial DMI between 3d transition-metals (TM=Co, Fe) thin films and heavy-metals (X=Ta, W, Re, Os, Ir, P) from first principles.[1)] Calculations were performed within the generalized gradient approximation using the full-potential linearized augmented plane-wave method in a slab geometry, where the spin-spiral structures of a wave vector, q, without the spin-orbit coupling (SOC) were first treated in the generalized Bloch theorem and then the SOC was introduced by the second variational method, in which large unit cells (supercells) with lattice constants corresponding to wavelengths of commensurate spin-spiral structures were employed. The 2400 special k-points (in the chemical BZ) were used to reduce the numerical errors. The DMI parameters were estimated from the total energy with respect to the spin-spiral wavevectors.

The results predict that the DMI parameters depend significantly on the species of both the 3d and heavy metals; typical examples are shown in Fig.1, where the DMI parameter in the Co/Pt has a positive value while that in the Co/Ir has a negative one. We confirmed that for both interfaces, when the Co thickness increases the DMI parameters roughly converge to constant values although the absolute values decrease, and thus the signs of the DMI parameters do not alter with the increase of layer thickness. The results of the Co/Pt agree with experiments and suggest that the DMI originates mainly at the interfaces. We have further checked the interfacial structural dependence by comparing the obtained DMI parameters for both fcc and hcp stackings at the TM/X interfaces, and find that the DMI parameters depend on the stacking structures but the sign does not change. Our results further show that the DMI parameters are related to the orbital magnetic moments of the heavy metal elements. In the talk, we will present/discuss systematically the details of the DMI at the 3d and heavy-metal interfaces.

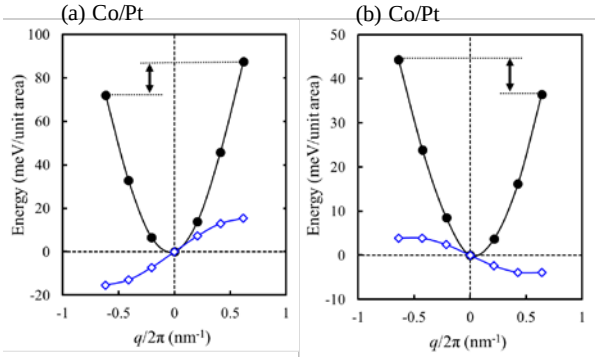

Fig.1. Formation energies of spin-spiral structures, E_{spiral}, as a function of wave number, q, for (a) Co/Pt and (b) Co/Ir interfaces. Open diamonds indicate the difference in the E_{spiral} between q states, where the gradient corresponds to the DMI parameter.

References

1) K. Yamamoto, A-M. Pradipto, K. Nawa, T. Akiyama. T. Ito, T. Ono, and K. Nakamura, AIP Advances **7**, 056302 (2017), K. Nakamura et.al., submitted.