Magnetocrystalline anisotropy and Dzyaloshinskii-Moriya interaction in ultrathin Co/Pd/Pt-based multilayer systems

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The interplay between inversion symmetry breaking and the spin-orbit coupling has been at the heart of the fundamental understanding of various important magnetic and transport phenomena for the spintronics application. While recent theoretical analysis shows that the magnetocrystalline anisotropy (MCA) is strongly affected by the broken inversion symmetry-induced Rashba parameter [1], by combining magnetic measurement and first principles density functional theory (DFT) studies, we provide an evidence for the MCA enhancement due to the structural inversion symmetry breaking [2]. On the other hand, broken inversion symmetry will traditionally give rise to another important phenomenon in magnetic materials, i.e. the Dzyaloshinskii-Moriya interaction (DMI). A correlation between MCA and DMI will reveal the underlying mechanisms of the MCA at systems with broken inversion symmetry. In the present work, we investigate both phenomena on Co-Pt/Pd-based multilayer systems by first principles calculations [3]. We consider three ultrathin film models, i.e. Pt/Co/Pd, Pt/Co/Pt, and Pd/Co/Pd, with increasing repetition numbers in which the inversion symmetry is supposed to retain in the latter two systems. We therefore further introduce Pt substrate layers at one side of the films to break inversion symmetry of the Pt/Co/Pt and Pd/Co/Pd systems, and study the evolution of MCA and DMI as functions of repetition number. We find that indeed by increasing the repetition number, the DMI increases monotonically in the Pt/Co/Pd case and diminishes in the other two systems, since adding more repetition numbers in Pt/Co/Pt and Pd/Co/Pd cases brings them closer to the bulk limit with inversion symmetry. On the other hand, the calculated MCA values in all systems increase with increasing repetition number, approaching the bulk values. We analyze the electronic structure and the *k*-dependent properties of all systems, and discuss the mechanisms. Details of the results will be further discussed in the presentation.

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