Uncovering spin reorientation in magnetic heterostructures: DFT-based spin-orbit torque method

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In order to increase the storage capacity of magnetoresistive random-access memories (MRAMs), the reduction of size of memory cell requires the enhancement of the magnetic anisotropy to meet the criterion of thermal stability. The recently discovered perpendicular magnetic anisotropy (PMA) at the ferromagnetic metal/oxide and ferromagnetic metal/heavy metal interfaces plays a crucial role in MRAM applications. However, both first-principles calculated total energy and fitted experimental data remain difficult to quan-titatively evaluate the magnetic anisotropy energy (MAE), especially in magnetic heterostructures with complex interfaces between multi-layers.

An alternative solution is the so-called spin-orbit torque (SOT) method. In this study, the validity of our DFT-based self-developed JunPy [1,2] package with SOT calculation has been rigorously confirmed in two kinds of PMA systems, including iron thin films [3], and Fe/MgO/Fe magnetic tunnel junction [4]. Our results agree with the conventional MAE calculation but provide deeper insights into atomistic spin dynamics of local magnetic moments.

Our DFT-based SOT method has succeed in building up a picture to enrich the fundamental knowledge about the IMA-to-PMA transition in Cr-intercalated $CrTe_2$ layered transition metal halides. The layer-resolved SOT is essential to estimate the average surface anisotropy energy for each surface/interface, but not simply to choose a constant interfacial anisotropy as used in conventional experimental analysis.

The main advantage of our DFT-based SOT method is to provide the well-decomposed lay-er-resolved SOT and SOC-dominated spin current accumulation and the comprehensive physical under-standing in angular momentum transfer between spin and orbital, competition between SOT and spin current accumulation, and precise spin torque acting on each local magnetic moment that is crucial for the atomistic spin dynamics especially in magnetic heterostructures.

References

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