

Theoretical study of magnetic anisotropy in Co/h-BN heterostructures

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Ensuring reliable long-term data retention in devices such as magnetoresistive random-access memory (MRAM) requires achieving effective perpendicular magnetic anisotropy (PMA) in storage layers. The PMA engineering has relied on the ferromagnet/oxide interfaces, where cubic symmetry enhances magnetic stability and performance. On the other hand, the increasing demand for two-dimensional (2D) materials as channel materials requires the tunnel barriers materials that conform to hexagonal symmetry. Recent research predicts that the tunnel magnetoresistance ratio of the Co/h-BN heterostructure is similar to that of the Fe/MgO heterostructure¹). However, achieving high PMA in Co/h-BN heterostructure remains a significant challenge, and a research is needed to understand the mechanisms of magnetic anisotropy (MA) in these heterostructures.

In this study, we investigated the MA in Co/h-BN heterostructures by using first-principles calculations. The Co/h-BN interface is stable when Co atoms are located on N atoms as shown in Fig. 1. Figure 2 shows the calculated results of the magnetocrystalline anisotropy (MCA) and MCA with dipolar anisotropy energy for Co/h-BN heterostructures, where up to five layers of Co were stacked on top of five layers of h-BN. MCA calculations revealed that a single Co layer on h-BN layers displays a PMA of 1.86 mJ/m², comparable to that of a single Fe layer on MgO layers²), whereas a free-standing single Co layer shows in-plane MCA. In the system without considering dipolar energy, the multilayer systems retain the PMA. However, when we introduced dipolar energy, only one layer of Co maintains the PMA and for two or more layers of Co, the in-plane MA becomes stable. In the presentation, we will also discuss the mechanism of MA.

Ref:

- 1) J. Robertson *et al.*, Jpn. J. Appl. Phys., **62** (2023) SC0804.
- 2) K. Nakamura *et al.*, Phys. Rev. B **81** (2010) 220409(R).

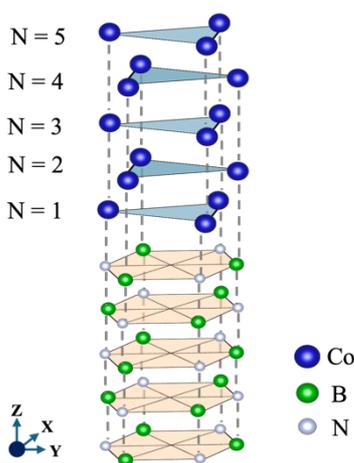


Fig. 1. Schematic illustration of Co/h-BN heterostructure where N represents the number of Co layer.

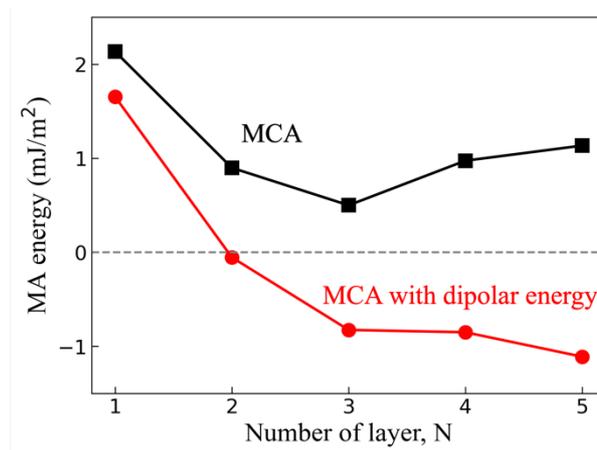


Fig. 2. Calculated MA energy as a function of the number of Co layer, N. The positive value of MA energy defines the PMA. The black and red lines represent the results of MCA and MCA with dipolar energy, respectively