Anatomy of Large Perpendicular Magnetic Anisotropy Energy in Co/Ni (111) multilayer

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In the past few decades, spin-transfer torque, spin-orbit torque, and voltage control magnetic random access memory have become prominent options for non-volatile memory and computing due to their low write energy, fast write speed, and practically unlimited endurance. In the three kinds of phenomena mentioned above, the magnetic property such as magnetic anisotropy plays an important role in realizing magnetization switching. In particular, high perpendicular magnetic anisotropy for thermal stability at advance technology node and high voltage controlled magnetic anisotropy (VCMA) coefficient for low write energy are needed.

In this work, we investigated the magnetic anisotropy energy (MAE) in the free-standing Co/Ni (111) multilayer as both Ni thickness dependence (t_{Ni}=1-4MLs) and number of multilayer repetition times (N=1-3) by means of a first-principles electronic structure calculation based on spin density functional theory [1]. We included both contributions to the MAE from magnetocrystalline anisotropy energy (MCAE) originating from spin-orbit coupling and shape magnetic anisotropy energy (SMAE) originating from spin dipole-dipole interaction [2]. The MCAE part was evaluated from both methods of total energy (TE) and grand-canonical force theorem (GCFT). The SMAE part was calculated by using a spin density approach (SDA). All MCAE values from the TE are well reproduced by those from the GCFT method. In N=1, the total MAE (MCAE+SMAE) for t_{Ni} showed a perpendicular MAE (PMAE) with a maximum value of 1.67 mJ/m^2 at t_{Ni}=2MLs as shown in the Fig. 1. The PMAE increases with increasing N. The series of t_{Ni}=3MLs showed a linear behavior as N dependence with an increasing ratio of 0.68 mJ/m^2, which is in good agreement with experimental measurement [3,4]. By using the GCFT, we evaluated the atom-resolved and **k**-resolved MCAEs. The atom-resolved MCAE indicates that the Co/Ni interface is the main origin of PMAE. The PMAE is mainly located at $\bar{\Gamma}$-$\bar{K}$ line in the two dimensional Brillouin zone as shown in Fig. 2. This is attributed to large components of the d-orbitals extending along the multilayer plane on Co and Ni near the Fermi energy. We also calculated the SMAE using a discrete approach (DA) and found that there is a reduction of SMAE part in the SDA, compared to the DA. This reduction originates from a prolate quadrupole component of spin density distribution. The present comprehensive study may provide a better understanding of magnetic properties in Co/Ni multilayers as widely used in spintronic devices.

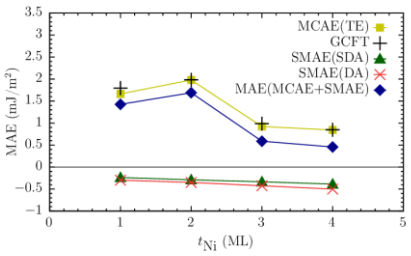

Fig. 1. MCAE, SMAE, and MAE as Ni thickness dependence.

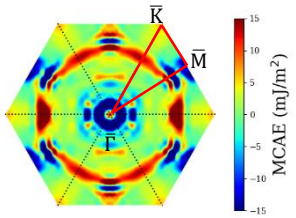

Fig. 2. **k**-resolved MCAE for N=1 and t_{Ni}=3MLs.

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