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

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The field of magnetic thin film is one of the most exciting areas in solid state research. There are many applications based on discovered novel magnetic phenomena. One of the phenomena is current induced magnetization switching so-called spin torque effect. Nowadays, this effect becomes one of the promising application on spintronic devices such as magnetic random access memories (STT-MRAM). In the implementation, magnetic film which has low damping, high perpendicular anisotropy, high spin polarization, and moderate magnetization is required to realize a faster, dense, thermally stable and low power consumption memory devices.

Co/Ni multilayer is one of the highly desirable materials for STT-MRAM. It was shown very recently that the films have a spin polarization of about 90%, which is similar to the best spintronic materials [1]. In this work, we investigated the magnetic properties of Co/Ni (111) multilayer, based on first-principles electronic structure calculation. Our system investigated is a slab model with a perfect FCC stacking, vacuum/Au(3ML)/Ni(3ML)/[Co(1ML)/Ni(3ML)]$_n$/Au(3ML)/vacuum with n = 1-3. This structure is similar to the structure in the experimental investigations [1,2]. We will discuss the details of electronic structure, magnetization, spin polarization, orbital magnetic moment, and magnetic anisotropy energy (MAE). In the MAE calculation, two kinds of contributions will be discussed. The first is magnetocrystalline anisotropy energy (MCAE) originated from spin-orbit coupling (SOC), while the second is shape anisotropy (SA) due to spin dipole-dipole interaction (SDI).

From the total energy calculation, we found that all the systems have a perpendicular MCAE (PMCAE). The PMCAE increases by increasing number of repetition layer, n. The layer resolved MCAE analysis show that the PMCAE contribution originated from Co layer, Ni interface with Co layer and an additional from Ni layer between Co layers for n = 2 and 3. Furthermore, from k-space resolved analysis, we found that most of the PMCAE is distributed along the K-Γ line in 2D Brillouin zone. This is attributed to the large d-orbital components of $|m_l|$ = 2 on Co and Ni minority spin states near the Fermi level. Next, we calculated the SA using the data of the atomic magnetic moment (AMM) or spin density approach (SDA) [2]. We found that the SA from SDA method smaller than AMM method. This difference originated from the quadrupole component of the spin magnetic moment density.

Finally, the MAE was estimated by summing up the MCAE and the SA from SDA. We found a large PMAE, which is in good agreement with experimental results in the similar structures [2]. This result is useful for a better understanding of magnetic properties in Co/Ni multilayers as potentially used in spintronic devices.

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