THE Fe/Cr INTERCHANGE INDUCES SIGN CHANGE IN VOLTAGE-CONTROL MAGNETIC ANISOTROPY

Indra PARDEDE,[1] Tomosato KANAGAWA,[1] Nurul IKHSAN,[1] Masao OBATA,[1, 2] Tatsuki ODA,[1, 2]

[1]Graduate School of Natural Science and Technology, Kanazawa University, Kakuma-machi, Kanazawa, 920- 1192, Japan
[2]Institute of Science and Engineering, Kanazawa University, Kakuma-machi, Kanazawa, 920-1192, Japan

A new perspective in utilizing additional degrees of freedom of electron, i.e spin by using the electric field (EF) get increasing attention in research activity in the recent year. Manipulation of the spin using EF effect is a promising technology on a magnetic device due to low power consumption, non-volatility, high-speed reading/writing and good compatibility with the conventional semiconductor industry technology [1]. In case of magnetic data storage, this field shows a great potential application, especially taking into account the recent initiative in internet of things, big data, artificial intelligence, and cloud computing. There are a lot of experimental works and theoretical investigations on the modulation and switching of magnetism in order to understand the mechanism and the demand for better performance. Several physical mechanisms have been proposed such as the modulation of spin-orbit interaction by charge accumulation and depletion [2,3,4], Rashba effect [5,6] voltage redox reaction [7] and electromigration [8]. Nevertheless, there are still many challenges in understanding the physics behind this phenomena and introduce several material systems including tuning strategies such as sign in EF effect. In the case of dynamic switching, the accurate magnetic switching can occur when the direction of total magnetic anisotropy changes from perpendicular to in-plane direction or vice versa purely by EF.

In this work, we systematically investigated EF effect in Fe/MgO interface systems with Cr underlayers by introducing the interchange of Cr and Fe layers. Our model using slab system, vacuum (0.79 nm)/Cr (6ML)/Fe (1ML)/Cr (1ML)/Fe (3ML)/MgO (5ML)/vacuum (0.79 nm) and vacuum (0.79 nm)/Cr (5ML)/Fe (1ML)/Cr (1ML)/Fe (1ML)/Cr (1ML)/Fe (2ML)/MgO (5ML)/vacuum (0.79 nm). We carried out first principles electronic structure calculations [9,10] which employ fully relativistic and scalar relativistic ultrasoft pseudopotentials and plane wave basis by using the generalized gradient approximation (GGA) for the exchange-correlation energy. The magnetic anisotropy energy (MAE) was calculated from the total energy difference between in-plane magnetization ([100] direction) and out-of-plane magnetization ([001] direction), MAE = $E[100] - E[001]$. In order to impose the EF, we have applied the scheme of effective screening method (ESM) developed by Otani and Sugino [11]. Some tiny number of electrons is subtracted from or added to the system for induction of the EF. The strength of EF (E) is estimated from the slope of electrostatic potential at the front of ESM.

We found an opposite sign in the modification of MAE (γ) as EF dependence, as shown in Fig. 1. Interestingly, the change of γ sign can be achieved only by increase thickness of [Fe/Cr] interchanges. This result shows that underlayer structure is very sensitive to Fe layers at the interface since EF may screen only at the interface. We attribute this a unique behavior of electronic structures in the interface resonance state of Fe/MgO. Beside concerning hybridization between the orbitals of Fe $d(3z^2\text{-}r^2)$ and O $p(z)$ which keeps the $d(3z^2\text{-}r^2)$ away from the Fermi level, Fe-Cr hybridization in the formation of antiferromagnetic (AFM) ground state may play a crucial role in electronic structure. Furthermore, a large change in the number of electron filling for 3*d* orbital spin states may correspond to the sensitivity modulation of MAE when applied EF. The EF modulation in the electronic structure around the Fermi level can be related with MAE by the using second order perturbative formula [12].

Opposite sign in the modification of MAE also found experimentally by Shiota *et al* in CoFeB/MgO with different underlayer, Ta or Ru respectively [13]. They confirmed such phenomenon by both the static magnetoresistance and voltage-induced ferromagnetic resonance measurement. Discussion for the reason of observed opposite sign is related to a different spin-orbit coupling in the underlayer, a difference in crystallinity, etc. but the origin is still an open question. Regarding this issue, a comprehensive study may be needed in order to clarify and propose some possible origin against underlayer effect. Additionally, the

Indra Pardede
pardede@cphys.s.kanazawa-u.ac.jp

MAE variation on band-filling may contribute to a fundamental understanding in the physics of EF effect, particularly, the orbital occupancy in the 3d orbitals.

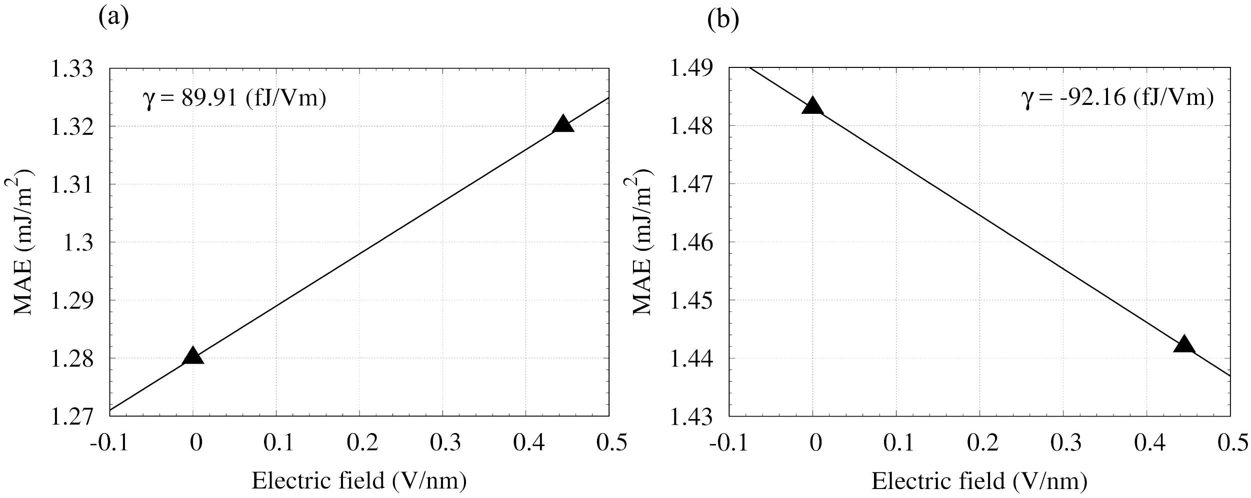

Fig. 1 EF variation of MAE in system (a). Cr (6ML)/Fe (1ML)/Cr (1ML)/Fe (3ML)/MgO (5ML) and (b) Cr (5ML)/Fe (1ML)/Cr (1ML)/Fe (1ML)/Cr (1ML)/Fe (2ML)/MgO (5ML).

This work was supported by ImPACT Program of Council for Science, Technology and Innovation (Cabinet Office, Japan Government) and by the Kanazawa University SAKIGAKE Project.

REFERENCES

[1] C. Song, B. Cui, F. Li, X. Zhou and F. Pan, Progress in Material Science. 87, 10.1016, (2017)

[2] C.-G. Duan, J. P. Velev, R. F. Sabirianov, Z. Zhu, J. Chu, S. S. Jaswal, and E. Y. Tsymbal, Phys. Rev. Lett. 101,137201 (2008).

[3] K. Nakamura, R. Shimabukuro, Y. Fujiwara, T. Akiyama, T. Ito, and A. J. Freeman, Phys. Rev. Lett. 102, 187201 (2009).

[4] M. Tsujikawa and T. Oda, Phys. Rev. Lett. 102, 247203 (2009).

[5] L. Xu and S. Zhang, J. Appl. Phys. 111, 07C501 (2012).

[6] S. E. Barnes, J. Ieda, and S. Maekawa, Sci. Rep. 4, 4105 (2013).

[7] U. Bauer, L. Yao, A. J. Tan, P. Agrawal, S. Emori, H. L. Tuller, S. van Dijken, and G. S. D. Beach, Nat. Mater. 14, 174 (2015).

[8] A. Rajanikanth, T. Hauet, F. Montaigne, S. Mangin, and S. Andrieu, Appl. Phys. Lett. 103, 062402 (2013)

[9] T. Oda, A. Pasquarello, and R. Car, Phys. Rev. Lett. 80, 3622, (1998).

[10] T. Oda and A. Hosokawa, Phys. Rev. B 72, 224428 (2005).

[11] M. Otani and O. Sugino, Phys. Rev. B 73 115407, (2006)

[12] D. S. Wang, R. Wu, and A. J. Freeman, Phys. Rev. B 47, 14932 (1993).

[13] Y. Shiota, F. Bonell, S. Miwa, N. Mizuochi, T. Shinjo, and Y. Suzuki, Appl. Phys. Lett. 103, 082410 (2013).