Electron correlation effects on the magnetocrystalline anisotropy of Fe/MgO interfaces with inserted transition-metal oxide monolayers

Mie University

○(M2) K. Mobayashi, A.-M. Pradipto, T. Akiyama T. Ito and K. Nakamura

E-mail: 417M616@m.mie-u.ac.jp

Establishing a data-rewriting based on electric-field induced magnetization reversal in non-volatile spin memories, materials having vertical magnetization easy axis and excellent responsiveness of the magnetocrystalline anisotropy energy (E_{MCA}) to electric field is required. Predicting physical properties from a theoretical point of view using first-principles calculations are very useful for the materials design. However, there have been concerns on the accuracy of the calculations. For example, Density Functional Theory (DFT) is known for its inability to adequately describe the electronic structures of transition-metal oxides (TMOs) due to the difficulties in the treatment of the strong interaction caused by the localized electrons. As an alternative, DFT+*U* method has become one of effective means to deal with this problem. This method describes the electronic states by introducing the screened on-site Coulomb interaction in terms of Hubbard model parameter, U_{eff}. However, various values for the U_{eff} have been reported even for the same ionic state and the same material. Since material properties are susceptible to the U_{eff} values, it is important to choose reliable ones. Previously, we have investigated the on-site Coulomb interaction in bulk 3*d* TMOs, based on constrained DFT approach[1] within a linear response theory.[2] We here extend our approach to determine the U_{eff} values for thin films of TMOs. We calculated the U_{eff} for GGA+*U* calculation on the Fe/MgO(001) thin film interfaces with inserted 3*d*, 4*d* and 5*d* TMO monolayers and investigated the E_{MCA} in these systems. Calculations were carried out based on the generalized gradient approximation[3] by using full-potential linearized augmented plane wave method.[4] The U_{eff} values were calculated from the second derivatives of the total energy, based on the constrained DFT. The E_{MCA} was derived as the difference of total energy when the magnetization easy axis is normal and along the film planes using the force theorem.[5,6] Details and discussion on the calculated E_{MCA} of the inserted 3*d*, 4*d* and 5*d* TMO systems in the GGA+*U*, will be presented.

[1] M. Cococcioni and S. de Gironcoli. *Phys. Rev. B*, **71**, 035105 (2005).

[2] K. Nawa, T. Akiyama, T. Ito *et al.*, *Phys. Rev. B*, **97**, 035117 (2018).

[3] J. P. Perdew, Kieron Burke, and Matthias Ernzerhof, *Phys. Rev. Lett.*, **77**, 3865 (1996).

[4] K. Nakamura, A. J. Freeman, L. Zhong *et al.*, *Phys. Rev. B*, **67**, 14405 (2003).

[5] M. Weinert, R. E. Watson, and J. W. Davenport, *Phys. Rev. B*, **32**, 2115 (1985).

[6] G. H. O. Daalderop, P. J. Kelly, and M. F. H. Schuurmans, *Phys. Rev. B*, **41**, 11919 (1990).