First-principles exploration of spacer thickness effects on magnetic anisotropy in CoFeB/MgO/CoFeB MTJs

Justyn Snarski-Adamski,[1] Ján Rusz,[2] and Mirosław Werwiński[1]

[1] *Institute of Molecular Physics, Polish Academy of Sciences, M. Smoluchowskiego 17, 60-179 Poznań, Poland*

[2] *Department of Physics and Astronomy, Uppsala University, Box 516, SE-751 20 Uppsala, Sweden*

Magnetic tunnel junctions (MTJs) featuring perpendicular magnetic anisotropy represent a key building block actively pursued for spintronic device applications [1]. Current state-of-the-art MTJs incorporate ultrathin CoFeB ferromagnetic layers and an MgO tunnel barrier, each nominally around 1.0 nm thick (corresponding to only a few atomic monolayers) [1]. Such reduced dimensions enable accurate 1:1 atomic-scale modeling through first-principles methods, which provide a full quantum-mechanical treatment of the electronic structure. In this study, we employ density functional theory (DFT) calculations using the FPLO code [2] to investigate CoFeB/MgO/CoFeB trilayer systems. The magnetic CoFeB layers are modeled with a thickness of approximately 0.8 nm (five atomic monolayers), while the non-magnetic MgO spacer thickness is varied across about 0.8 nm, 0.5 nm, and 0.2 nm (five, three, and one atomic monolayers, respectively). This work builds upon and extends our prior theoretical analysis of the Fe/MgO interface [3]. These computations allow us to establish the nature of the interlayer magnetic coupling (ferromagnetic/parallel versus antiferromagnetic/antiparallel) as a function of spacer thickness, as well as the preferred magnetization direction in the magnetic layers (in-plane versus perpendicular-to-plane), thereby characterizing the overall magnetic anisotropy of the system. Additionally, by evaluating the magnetic moments and charge distributions on individual atoms, we gain detailed insight into the interfacial properties at the CoFeB/MgO boundary and the CoFeB free surface. The findings enhance our fundamental understanding of existing CoFeB/MgO-based magnetic tunnel junctions and support the rational design of next-generation, higher-performance spintronic devices.

References:

[1] S. Ikeda, K. Miura, H. Yamamoto, K. Mizunuma, H.D. Gan, M. Endo, S. Kanai, J. Hayakawa, F. Matsukura, H. Ohno, A perpendicular-anisotropy CoFeB–MgO magnetic tunnel junction, Nature Mater. 9 (2010) 721–724.

[2] K. Koepernik, H. Eschrig, Full-potential nonorthogonal local-orbital minimum-basis band-structure scheme, Phys. Rev. B. 59 (1999) 1743–1757.

[3] T. Thersleff, S. Muto, M. Werwiński, J. Spiegelberg, Y. Kvashnin, B. Hjörvarsson, O. Eriksson, J. Rusz, K. Leifer, Towards sub-nanometer real-space observation of spin and orbital magnetism at the Fe/MgO interface, Sci. Rep. 7 (2017) 44802.

We acknowledge the financial support from the National Science Center of Poland under Grant Nos. DEC-2018/30/E/ST3/00267 (SONATA BIS 8) and DEC-2021/41/B/ST5/02894 (OPUS 21).