High magnetoresistance of hexagonal boron nitride-graphene heterostructure-based MTJ through excited-electron transmission

°(D1) Halimah Harfah[1], (D2) Yusuf Wicaksono[1], Gagus Ketut Sunnardianto[2,4], Muhammad Aziz Majidi[3], Koichi Kusakabe[4]

Osaka Univ. [1]; The National Research and Innovation Agency of Indonesia[2]; Univ. Indonesia[3], Hyogo Univ.[4]

E-mail: harfah.h@opt.mp.es.osaka-u.ac.jp

An ab-initio study was done of a few-layers hexagonal boron nitride (hBN) and hBN-graphene heterostructure sandwiched between Ni(111) layers. Spin-polarized density functional theory calculations and transmission probability calculations were conducted on Ni(111)/nhBN/Ni(111) with n = 2, 3, 4, and 5 as well as on Ni(111)/hBN-Gr-hBN/Ni(111). Slabs with magnetic alignment in an anti-parallel configuration (APC) and parallel configuration (PC) were considered. The pd-hybridizations at both the upper and lower interfaces between the Ni slabs and hBN stabilized the system. The Ni/nhBN/Ni magnetic tunnel junction (MTJ) was found to exhibit a high tunneling magnetoresistance (TMR) ratio at $E - E_F = 0.28$ eV for n = 2 and 0.34 eV for n > 2, which are slightly higher than the Fermi energy. The observed shifting of this high TMR ratio originates from the transmission of electrons through the surface states of the d_{z^2}-orbital of Ni atoms at interfaces which are hybridized with the p_z-orbital of N atoms. In the case of n > 2, the proximity effect causes an evanescent wave, contributing to decreasing transmission probability but increasing the TMR ratio. The highest TMR ratio was observed when Ni/3hBN/Ni MTJ was considered. However, TMR ratio and transmission probability were increased by replacing the unhybridized hBN layer of the Ni/3hBN/Ni MTJ with graphene, thus becoming Ni/hBN-Gr-hBN/Ni. A TMR ratio as high as ~1200% was observed at $E - E_F = 0.34$ eV. A specific device design is proposed, as shown in Fig. 1.b, which has a new reading mechanism by exploiting the high TMR observed at $E - E_F = 0.34$ eV.

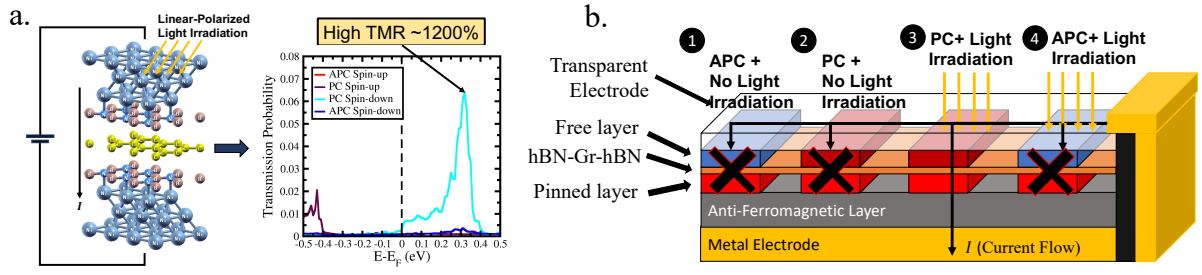

Figure 1. a. The high TMR ratio observed on Ni/hBN-Gr-hBN/Ni at E-E_F=0.34 eV *that can be realized by giving linear-polarized light irradiation on Ni slabs, b. the proposed design of a device that exploits The high performance and unique characteristics of Ni/hBN-Gr-hBN/Ni MTJ*

References: [1] H. Harfah, Y. Wicaksono, K. Kusakabe, G. K. Sunnardianto, M. A. Majidi, *Nanoscale Adv.,* 2022, 4, 117