半導体バリア $CuInSe_2$, $CuGaSe_2$ を用いた 磁気トンネル接合におけるスピン依存伝導特性の理論解析

Theoretical study for magnetic tunneling junctions including semiconductor barriers $CuInSe_2$ and $CuGaSe_2$

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High magnetoresistance (MR) ratios and low resistance-area products (*RA*) are required for magnetic tunneling junctions (MTJs) to realize ultrahigh-density hard disk drives and Gbit-class magnetoresistive random access memories (MRAMs). Recently, Kasai *et al*. observed relatively high MR ratios keeping low *RA* in MTJs with new semiconductor barriers $CuIn_{1-x}Ga_xSe_2$ (CIGS) [1]. Inspired by this founding, we investigated transport properties of magnetic tunneling junctions (MTJs) with semiconductor barriers $CuInSe_2$ (CIS) and $CuGaSe_2$ (CGS) by means of the first-principles-based calculations and the Landauer formula. We also took into account the Coulomb repulsion *U* for the Cu 3*d* states in the barriers to investigate the band-gap dependence of the MR ratio systematically. Figure 1(a) shows a $\mathbf{k}_{//}$ dependence of the majority-spin transmittance in the Fe/CIS/Fe MTJ with parallel magnetization of Fe electrodes. We can see a sharp peak around $\mathbf{k}_{//}$=(0,0), which is a clear evidence of the coherent tunneling of the wave functions. We found from complex band structure of CIS that the Δ_1 states provide dominant contributions to this peak [2]. We confirmed that the spin-dependent coherent tunneling of the Δ_1 wave functions also occurs in the CGS-based MTJs. Figure 1(b) shows the MR ratios and *RA* values of the CIS-, CGS-, and MgO-based MTJs. We see that the MR ratios in the CGS-based MTJs are around 300%, which is much higher than those of the CIS-based MTJs around 70%. We also found that the *RA* values of the CIS- and CGS-based MTJs are much smaller than those of the MgO-based MTJs even if the MgO barrier is quite thin (~1.24 nm), which is consistent with experimental results in the CIGS-based MTJs [1].

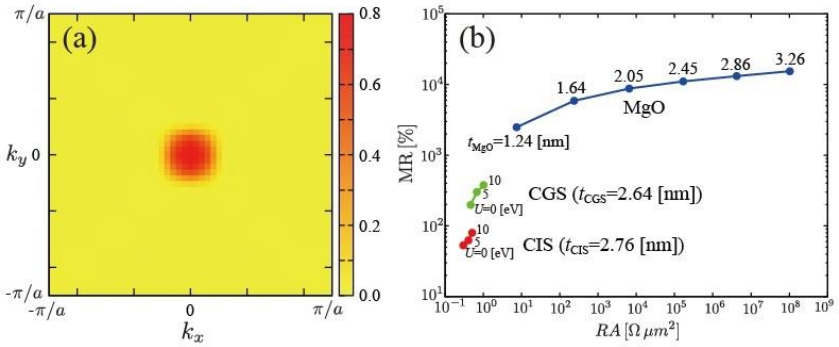

Fig. 1. (a) The $\mathbf{k}_{//}$ dependence of the majority-spin transmittance for *U*=5 eV in the CIS-based MTJ with parallel magnetization of Fe electrodes. (b) The MR ratios and RA values of the CIS-, CGS-, and MgO-based MTJs. The barrier thickness (t_{CIS},t_{CGS}, or t_{MgO}) is defined as the distance between two Fe layers closest to the barrier.

[1] S. Kasai *et al*., Appl. Phys. Lett. **109**, 032409 (2016).

[2] K. Masuda and Y. Miura, arXiv:1609.07713 (to appear in Jpn. J. Appl. Phys.).