FIRST-PRINCIPLES STUDY FOR MAGNETIC TUNNELING JUNCTIONS WITH SEMICONDUCTOR BARRIERS $CuInSe_2$ AND $CuGaSe_2$

Keisuke MASUDA[1] and Yoshio MIURA[1,2,3,4]

1) National Institute for Materials Science (NIMS), Tsukuba, Japan, MASUDA.Keisuke@nims.go.jp
2) Kyoto Institute of Technology, Kyoto, Japan, MIURA.Yoshio@nims.go.jp
3) Center for Materials Research by Information Integration, National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba 305-0047, Japan
4) Center for Spintronics Research Network (CSRN), Graduate School of Engineering Science, Osaka University, Machikaneyama 1-3, Toyonaka, Osaka 560-8531, Japan

Magnetic tunneling junctions (MTJs), in which an insulating barrier layer is sandwiched between ferromagnetic electrodes, have attracted much attention due to their potential applications to high performance spintronic devices, such as ultrahigh-density hard disk drives (HDD) and Gbit-class non-volatile magnetic random access memories (MRAM). To realize such applications, MTJs are required to have low resistance-area products (*RA*) in addition to high magnetoresistance ratios (MR ratios). Up to the present, elaborate deposition techniques for making ultrathin MgO barriers have been established in order to decrease *RA* of MgO-based MTJs with high MR ratios [1]. However, MR ratios tend to decrease when the barrier thicknesses are reduced. Moreover, such ultrathin barriers lead to poor controllability of the MTJs. On the other hand, the use of Heusler alloys increased the MR ratios of current-perpendicular-to-plane giant magnetoresistance (CPP-GMR) devices with quite low *RA*. Although the current highest MR ratio is 80 % at room temperature [2], more improvement is needed to achieve high performance in the above-mentioned devices. Another possible way to obtain high MR ratios and low *RA* is using semiconductors as barrier layers instead of band insulators. Recently, Kasai *et al.* demonstrated that the MTJs with semiconductor barriers $CuIn_{1-x}Ga_xSe_2$ (CIGS) have high MR ratios (40 % at room temperature and 100 % at low temperature) and low *RA* (0.3-3 $\Omega\mu m^2$). We can expect high controllability and high breakdown voltage in these systems due to the sufficient thickness of CIGS (~2 nm).

In order to understand high MR ratios and low *RA* in the CIGS-based MTJs, we theoretically investigated transport properties of MTJs with semiconductor barriers, $CuInSe_2$ (CIS) and $CuGaSe_2$ (CGS), which are two terminal compounds of CIGS. For simplicity, bcc Fe is adopted as ferromagnetic electrodes in both the MTJs. On the basis of the density-functional method implemented in the Vienna *ab-initio* simulation program (VASP) [4,5], we first optimized the atomic structures of the supercells, Fe(3)/CIS(17)/Fe(3) and Fe(3)/CGS(17)/Fe(3), where each number represents the number of layers of each compound. Using the optimized supercells, we calculated transmittances of the CIS- and CGS-based MTJs by means of the quantum code ESPRESSO [6] for both cases of parallel and antiparallel magnetization of Fe electrodes. Since our system has a two-dimensional periodicity in the *xy* plane, the transmittances can be classified by an in-plane wave vector $\mathbf{k}_{//}=(k_x,k_y)$. Finally, the MR ratios and *RA* were evaluated from the calculated transmittances. In the present work, we took into account the on-site Coulomb interaction *U* in the Cu 3*d* states of both the CIS and CGS barriers to study the band-gap dependence of MR ratio and *RA* systematically.

Figure 1(a) shows the $\mathbf{k}_{//}$ dependence of the majority-spin transmittance in the CIS-based MTJ with *U*=5 eV and with parallel magnetization of Fe electrodes. We see that the transmittance has a large value around $\mathbf{k}_{//}=(0,0)$, which is a clear evidence of the coherent tunneling of wave functions [7]. By analyzing the complex band structures of the CIS-based MTJ, it was found that the Δ_1 wave functions give the dominant contributions to the total transmittance. Although not shown here, we also found that the coherent tunneling of the Δ_1 wave functions occurs in the CGS-based MTJs [8]. Figure 1(b) shows the MR ratios and *RA* values of the CIS- and CGS-based MTJs. We also show those of the MgO-based MTJs for comparison. We see that the CGS-based MTJs have larger MR ratios (~300 %) than the CIS-based MTJs. Note here that a larger Coulomb interaction *U* gives a larger band gap of the semiconductor. In addition,

Keisuke MASUDA
Masuda.Keisuke@nims.go.jp

CGS has a larger band gap than CIS for the same U. Thus, we can conclude that the MTJ with a larger band gap of the semiconductor gives a higher MR ratio. The *RA* values of the CIS- and CGS-based MTJs are nearly six orders of magnitude smaller than those of the MgO-based MTJs with similar barrier thicknesses. If the thickness of the MgO barrier is sdecreased from 3 to 1 nm, the *RA* is still larger than those of the CIS- and CGS-based MTJs. These results on the *RA* values and MR ratios are in good agreement with experimental ones on the CIGS-based MTJs [3].

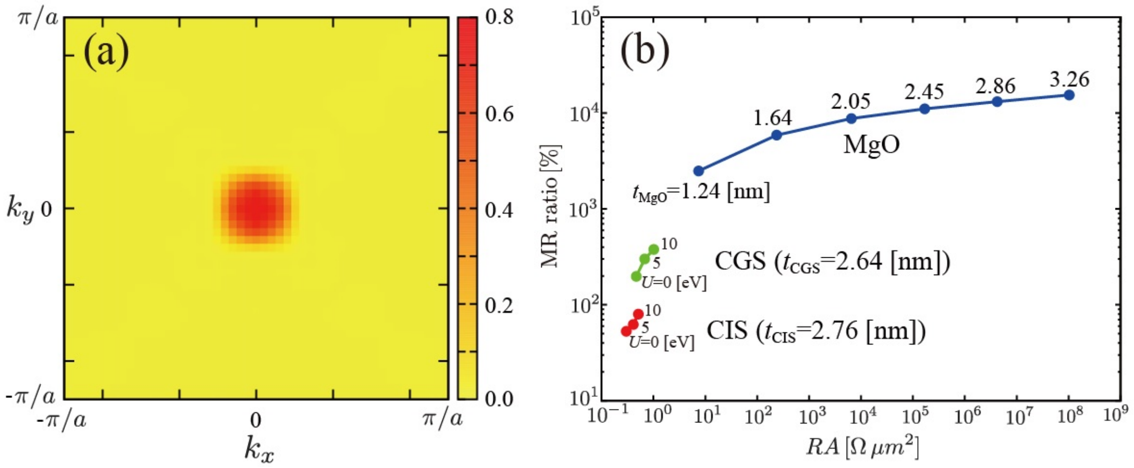

Fig. 1. (a) The $\mathbf{k}_{//}$ dependence of the majority-spin transmittance in the CIS-based MTJ with U=5 eV and with parallel magnetization of Fe electrodes. (b) The MR ratios and RA values of the CIS-, CGS-, and MgO-based MTJs. The barrier thickness (t_{CIS}, t_{CGS}, or t_{MgO}) is defined as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

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