$Fe/CuIn_{1-x}Ga_xSe_2$ 界面における高垂直磁気異方性の理論予測
Theoretical prediction of large perpendicular magnetic anisotropy at $Fe/CuIn_{1-x}Ga_xSe_2$ interface

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Large perpendicular magnetic anisotropy (PMA) at interfaces between ferromagnetic electrodes and tunnel barriers is an essential property in magnetic tunnel junctions (MTJs) to realize non-volatile magnetic random access memories (MRAMs). Up to now, large PMA has been observed at interfaces between Fe-based ferromagnets and oxide barriers [1,2]. However, no previous studies have reported such large interfacial PMA in the case of non-oxide barriers. Recently, Kasai *et al*. successfully fabricated a new MTJ consisting of a semiconductor barrier $CuIn_{0.8}Ga_{0.2}Se_2$ (CIGS) and ferromagnetic Heusler alloys $Co_2FeGa_{0.5}Ge_{0.5}$ [3]. In this MTJ, they observed high magnetoresistance (MR) ratios and low resistance-area products (*RA*), both of which are required properties for MRAM applications. Possible occurrence of interfacial PMA in the CIGS-based MTJ must be investigated, but no theoretical and experimental studies have addressed this issue.

In this work, we theoretically investigated interfacial magnetocrystalline anisotropy in various Fe/semiconductor heterostructures including $Fe/CuIn_{1-x}Ga_xSe_2$ by estimating their interfacial anisotropy constants K_i on the basis of the first-principles calculations. We found that most of the heterostructures show interfacial PMA. In particular, we obtained a quite large K_i of 2.305 mJ/m^2 in $Fe/CuInSe_2$, which is about 1.6 times as large as that of Fe/MgO (1.396 mJ/m^2) with a similar barrier thickness (see Fig. 1). By studying the correlation between anisotropy constants K_i and anisotropies of orbital magnetic moments at interfacial Fe atoms, we found that the PMA in the present systems can be explained by the Bruno's relation, which means that minority-spin scatterings around the Fermi level provide the dominant contribution to the PMA. We further analyzed the local density of states (LDOS) of $Fe/CuInSe_2$ and clarified that this system has favorable *d*-orbital configurations around the Fermi level to achieve large interfacial PMA [4].

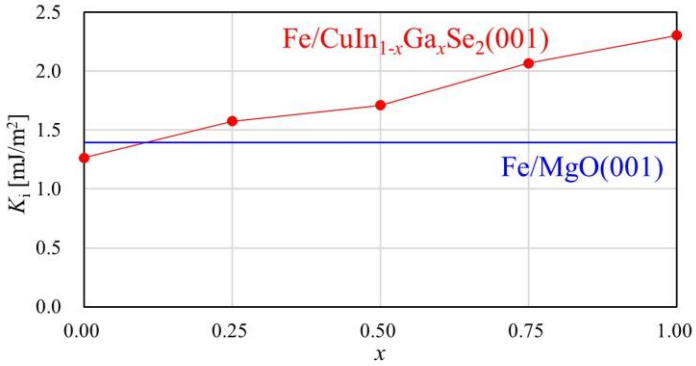

Fig. 1. Values of K_i in $Fe/CuIn_{1-x}Ga_xSe_2(001)$ obtained in this work. We also showed K_i of Fe/MgO(001) for comparison.

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