## (111)配向磁気トンネル接合における巨大磁気抵抗の理論予測 Theoretical prediction of giant tunnel magnetoresistance in (111)-oriented magnetic tunnel junctions 物材機構<sup>1</sup>, 関大システム理工<sup>2</sup> <sup>0</sup>増田 啓介<sup>1</sup>, 伊藤 博介<sup>2</sup>, 三浦 良雄<sup>1</sup> NIMS<sup>1</sup>, Kansai Univ.<sup>2</sup> <sup>o</sup>Keisuke Masuda<sup>1</sup>, Hiroyoshi Itoh<sup>2</sup>, and Yoshio Miura<sup>1</sup> E-mail: MASUDA.Keisuke@nims.go.jp

One of the most important discoveries in the field of spintronics is the observation of giant tunnel magnetoresistance (TMR) in Fe(Co)/MgO/Fe(Co)(001) magnetic tunnel junctions (MTJs) [1,2], which accelerated not only fundamental studies on TMR but also its applications to various spintronic devices. So far, such giant TMR in the (001)-oriented MTJs has been explained by the coherent tunneling mechanism based on bulk band structures [3,4]: bulk wave functions of the ferromagnetic electrode are selectively filtered by the MgO barrier and only the  $\Delta_1$  wave function with half-metallicity at the Fermi level passes through the barrier, leading to the high TMR ratio. Although this mechanism can be naturally understood, it is still unclear whether or not this is the only possibility to achieve high TMR in various types of MTJs, e.g., with different stacking direction or with different ferromagnetic electrodes and the tunnel barrier.

Here, we focus on the TMR in unconventional (111)-oriented MTJs [Fig.1(a)] and show that the interfacial effect provides resonance giant TMR in the Co/MgO/Co(111). By combining the density-functional theory and the Landauer formula, we calculated the TMR ratios in two basic (111)-oriented MTJs, Co/MgO/Co(111) and Ni/MgO/Ni(111). The obtained TMR ratios were 2130% for the Co-based MTJ and 250% for the Ni-based one. We analyzed the in-plane wave vector  $\mathbf{k}_{\parallel} = (k_x, k_y)$ resolved majority-spin conductance in the Co-based MTJ [Fig. 1(b)] to gain insight into the high TMR ratio. It is seen that the conductance has significant values in a set of  $\mathbf{k}_{\parallel}$ points surrounding  $\mathbf{k}_{\parallel}=(0,0)$ , which indicates that the TMR cannot be explained by the coherent tunneling of the bulk  $\Lambda_1$  state in analogy with the case of (001)-oriented MTJs.



Fig.1. (a) The supercell of Co/MgO/Co(111). (b) The  $\mathbf{k}_{\parallel}$  dependence of the majority-spin conductance in Co/MgO/Co(111) with parallel magnetizations of electrodes. The unit of the color bar is  $G_0=e^2/h$ .

By further analyzing the correlation between the local electronic structures and the transport properties (not shown), we found that the interfacial states are formed close to the Fermi level and the resonance of these states (interfacial resonance) gives rise to the giant TMR ratio.

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