Effects of the direction of magnetic moment on magnetic and electronic properties of Co/MgO/Co magnetic tunnel junction system: First-principles calculations

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Magnetic tunnel junctions (MTJs) with crystalline insulating barrier have attracted many interests because of high tunneling magnetoresistance (TMR) ratio[1]. Since TMR is a phenomenon that resistance of a device changes depending on the directions of the magnetic moments of both ferromagnetic (FM) layers, non-collinear calculation which can alter the direction of magnetic moment of each atom is necessary. In this study, a MTJ system which consists of bcc Co FM layer and rocksalt MgO insulating barrier has been investigated with either parallel (P) and anti-parallel (AP) states of bottom (polarizer) and upper (analyzer) electrodes. The first-principles calculations were conducted with Vienna *ab-initio* simulation package code[2] using projector augmented wave method with generalized gradient approximation scheme[3].

In case of P state, high spin polarization (SP) values were represented at both FM electrodes (~91%) showing highly symmetric configuration from the center of MgO layer as shown in *Fig 1* (a). In case of AP state, high SP values were also shown in Co bottom layer, however, Co upper layer failed to represent as high SP as in P state, even showing negative SPs. It is considered that fluctuation in sign of SP is the major reason for TMR phenomenon. Magnetization along the x-axis was also calculated (*Fig 1* (b)). Interestingly, Mg showed diamagnetic behavior contrary to its magnetic ordering of bulk state: paramagnetic. Density of states (DOS) data for each slab are presented in *Fig 2*. In both cases, Co bottom layer is pinned along the +x direction, representing majority spin state is spin down state. In Co upper layer, however, majority spin state is spin up state in AP state where spin transport is prevented due to lack of the spin down state. In addition, band structure was calculated since spin transport along the z-axis ($k_{||}$=0) is significant in MTJs. Spatial distribution of magnetization vectors according to the real space coordinate was also calculated to observe how the magnetization vectors changes along the spin transport axis.

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[1] X.-G. Zhang and W.H. Butler, Phys. Rev. B **70**, 172407 (2004)
[2] G. Kress and J. Futhmüller, *Vienna Ab-initio Simulation Package* (University of Wien, Vienna, 2001).
[3] J. P. Pedrew et al., Phys. Rev. B **59**, 1758 (1992).

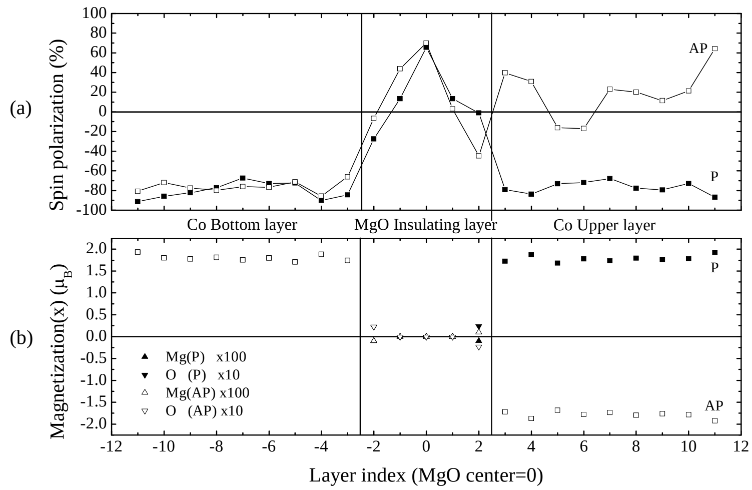

Fig 1: Spin polarization (a) and magnetization (b) along the x-axis for MTJ with bcc-Co(001) and rosksalt MgO(001).

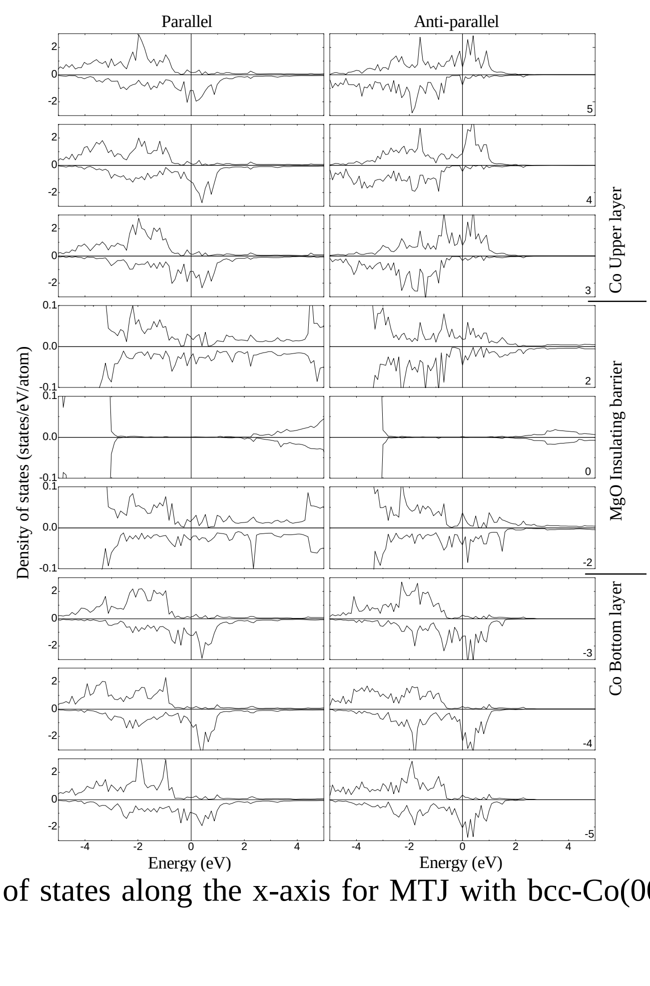

Fig 2: Density of states along the x-axis for MTJ with bcc-Co(001) and rocksalt MgO(001).