DFT-NEGF study of biaxial strain effects on Co_2FeAl-based magnetic tunnel junctions

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Spin-transfer torque-based magnetoresistive random access memory (STT-MRAM) is the most promising candidate for energy-efficient future memory. Due to its fast switching speed and nonvolatile nature, there have been numerous attempts to replace DRAM as well as L3 cache memory. Still, STT-MRAM based on perpendicular-type magnetic tunnel junction (pMTJ) encounters the issues with respect to high current density and low thermal stability for a write operation and responsible data retention, respectively. Heusler alloy has been suggested as an alternative for resolving these problems by significantly decreasing Gilbert damping constant while preserving approximately 100% spin polarization. In particular, $L2_1$ ordered Co_2FeAl (CFA)-based MTJ exhibits not only outstanding half-metallicity [1], but perpendicular magnetocrystalline anisotropy (PMA) characteristic arising from Fe-O or Co-O orbital hybridization at the interface [2].

In this research, we investigate the biaxial strain effects of CFA-based MTJ by manually adjusting in-plane bulk lattice constants (a) from -4% to +4% (from 5.57 Å to 6.03 Å), while the atoms are relaxed in the transverse direction. The CFA-MTJ structure is comprised of MgO as a tunnel barrier and two CFA layers as semi-infinite magnetic leads (Fig. 1). The geometric optimization and transport calculations were carried out with SIESTA and SMEAGOL package to perform DFT-NEGF simulations. Figs. 2 and 3 show the calculated transport characteristics in a low bias voltage range in the parallel and antiparallel configurations, respectively, demonstrating dissimilar I-V behaviors under the compressive and tensile strain. Different behaviors of I-V can be explained by analyzing transmission peaks in the vicinity of the Fermi energy. As illustrated in Figs. 4, 5 and 6, biaxial strain and bias voltage effectively translocate the transmission peaks, which in turn results in the different tendencies of tunneling magnetoresistance (TMR) upon the compressive and tensile strain (Fig. 7).

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[1] I. Galanakis et al., Phys. Rev. B 66, 174429 (2002).
[2] J. Okabayashi et al., Appl. Phys. Lett. **103**, 102402 (2013).

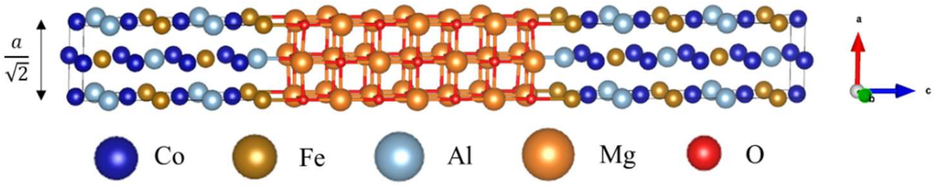

Fig. 1: Schematic crystal structure of Co_2FeAl (8ML)-MgO (9ML)-Co_2FeAl (8ML) magnetic tunnel junction structure.

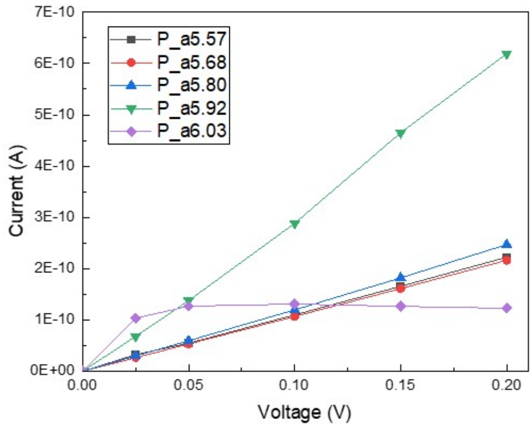

Fig. 2: I-V characteristics of parallel (P) configuration. Each symbol indicates the in-plane unit cell lattice constant (a) of Co_2FeAl from 5.57 Å to 6.03 Å.

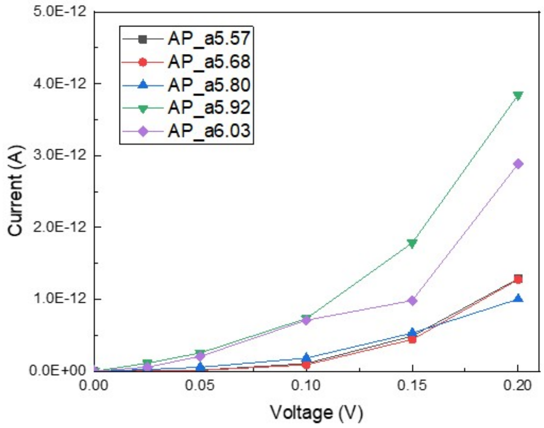

Fig. 3: I-V characteristics of antiparallel (AP) configuration for various in-plane unit cell lattice constants.

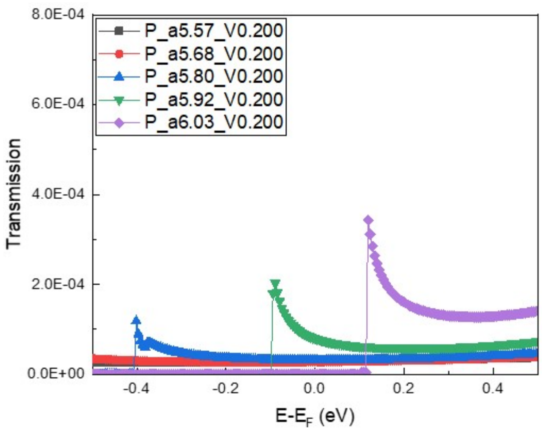

Fig. 4: Strain-induced transmission peak translocation for P configuration under 0.2V.

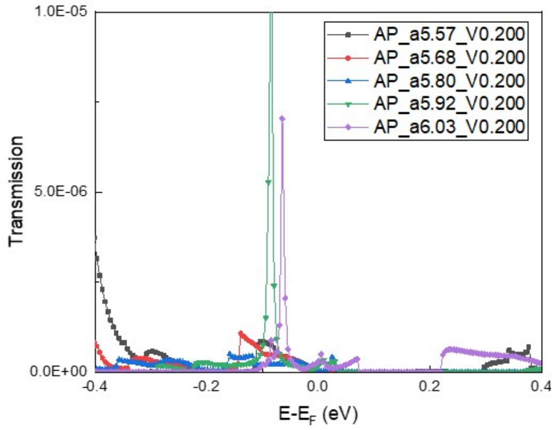

Fig. 5: Strain-induced transmission peak translocation for AP configuration under 0.2V.

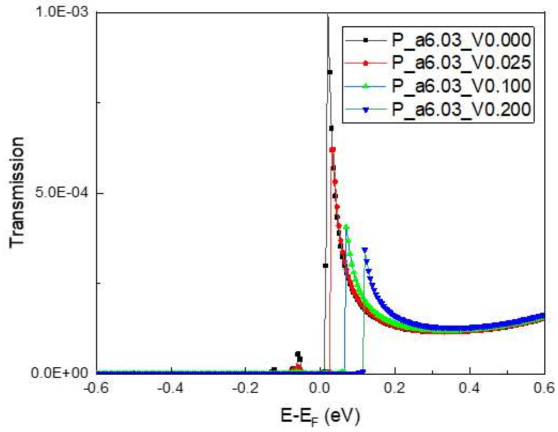

Fig. 6: Voltage-induced transmission peak translocation for P configuration under tensile strain (a = 6.03 Å).

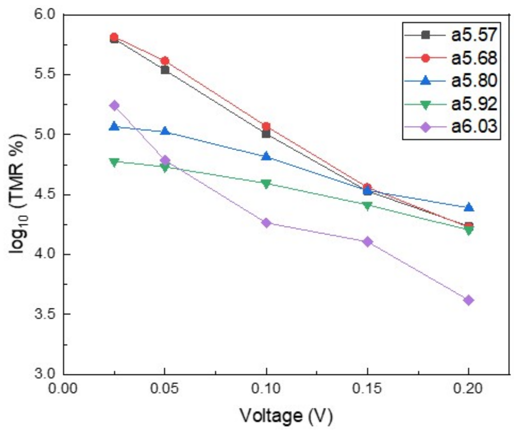

Fig. 7: Tunneling magnetoresistance (TMR) ratio is saturated under compressive strain (a = 5.57 Å and 5.68 Å), whereas degraded under tensile strain (a = 5.92 Å and 6.03 Å).