

First-principles calculations of tunnel magnetoresistance effect in lattice-matched magnetic tunnel junctions

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Magnetic tunnel junctions (MTJs) exhibit a large tunnel magnetoresistance (TMR) effect [1,2]. The TMR effect strongly depends on the lattice matching between magnetic and insulating layers. In a recent study, a significant TMR ratio of 631% was achieved in lattice-matched FeCo/MgO/FeCo MTJs at room temperature [3]. In this study, we investigate the tunneling transmittance and conductance of electrons, and TMR ratio in good lattice-matched MTJs using first-principles calculations.

We used Quantum ESPRESSO for first-principles calculations. The calculated structures are Fe-based MTJs, consisting of Fe/MgO/Fe, Fe/SrTiO₃/Fe, and Fe/InP/Fe, and FeCo-based MTJs, consisting of FeCo/MgO/FeCo, FeCo/SrTiO₃/FeCo, and FeCo/InP/FeCo. First, we performed structural relaxation for each MTJ in parallel magnetization. Then, we calculated the tunneling transmittance and conductance in parallel and antiparallel magnetizations using the Landauer-Büttiker method. Finally, we calculated the TMR ratio for each MTJ from the obtained conductance.

Table 1 shows the conductances G_P and G_{AP} in parallel and antiparallel magnetizations, respectively, and TMR ratio for MTJs. We obtain large TMR ratios of 8920% and 6420% in Fe/MgO/Fe and FeCo/MgO/FeCo MTJs, respectively. Figure 1 shows the k_{\parallel} -resolved conduction spectra of majority spins in parallel magnetization. The suppression of the conduction through the Δ_1 band of majority spins as well as the enhancement of the conduction through other bands leads to the decrease of TMR ratio in SrTiO₃-based and InP-based MTJs, whereas the robust conduction through the Δ_1 band of majority spins contributes to large TMR ratio in MgO-based MTJs.

Table 1: Conductance in parallel and antiparallel magnetizations, respectively, and TMR ratio for MTJs.

MTJs	G_P ($\Omega^{-1}\mu\text{m}^{-2}$)	G_{AP} ($\Omega^{-1}\mu\text{m}^{-2}$)	TMR ratio
Fe-MgO	0.508	0.00564	8920%
Fe-SrTiO ₃	51.4	15.7	229%
Fe-InP	64.9	32.6	100%
FeCo-MgO	0.673	0.0103	6420%
FeCo-SrTiO ₃	20.8	4.92	324%
FeCo-InP	41.5	8.03	416%

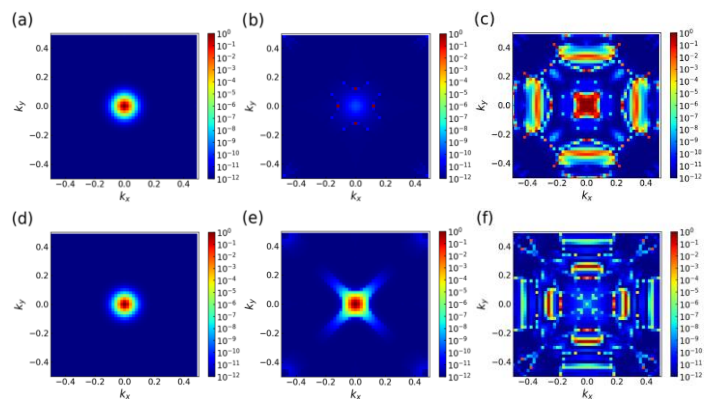


Figure 1: k_{\parallel} -resolved conduction spectra (in units of Ω^{-1}) of majority spins in parallel magnetization for (a) Fe/MgO/Fe, (b) Fe/SrTiO₃/Fe, (c) Fe/InP/Fe, (d) FeCo/MgO/FeCo, (e) FeCo/SrTiO₃/FeCo, and (f) FeCo/InP/FeCo MTJs.

[1] S. S. P. Parkin *et al.*, *Nat. Mater.* **3**, 862 (2004). [2] S. Yuasa *et al.*, *Nat. Mater.* **3**, 868 (2004).

[3] T. Scheike *et al.*, *Appl. Phys. Lett.* **112**, 112404 (2023).