

Supporting Information for

Impact of interfacial disorder and band structure on the resonant conductance oscillation in quantum-well based magnetic tunnel junctions

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Note 1: RHEED patterns of Sample *E* at different growth steps

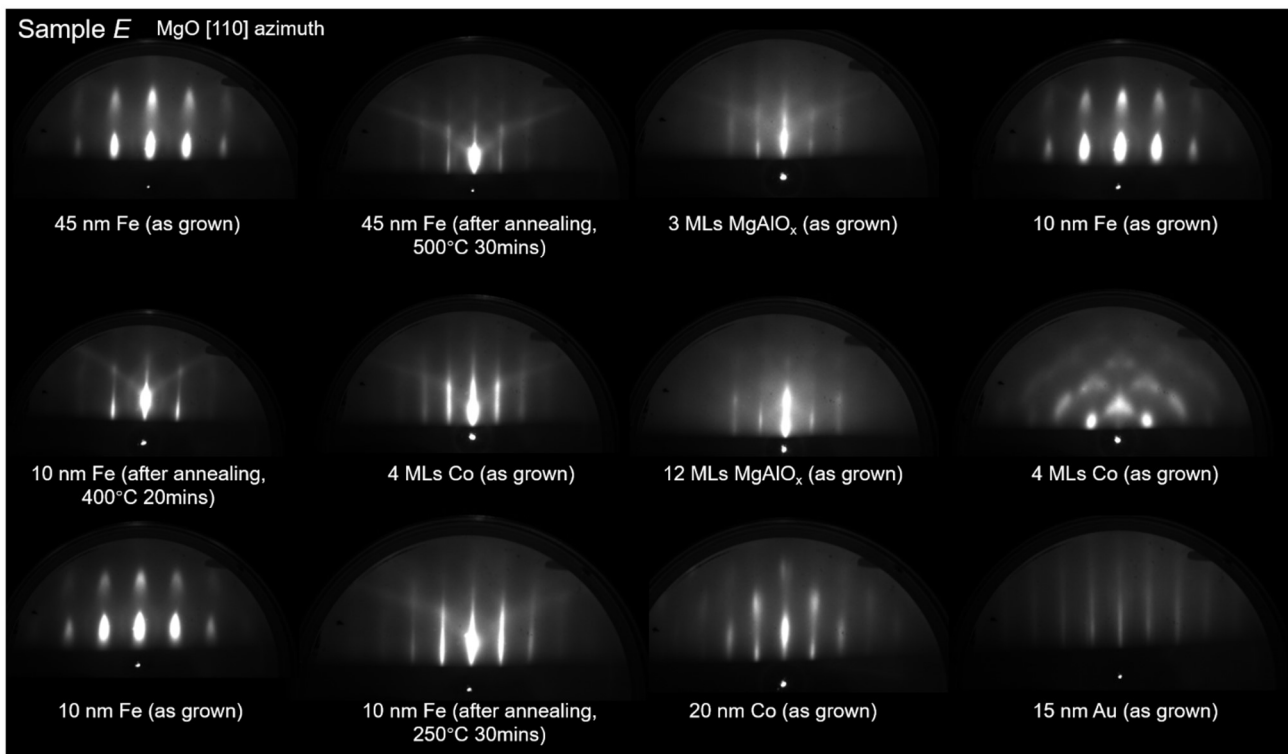


Figure S1. RHEED patterns of Sample *E* at different growth steps along the [110] azimuth of MgO substrate. The growth temperature in “as grown” state is around 30 to 80°C.

Note 2: STEM-EELS elements maps of Samples *B*, *D* and *E* with different Co insertion at Fe/MgAlO_x interface inside QW

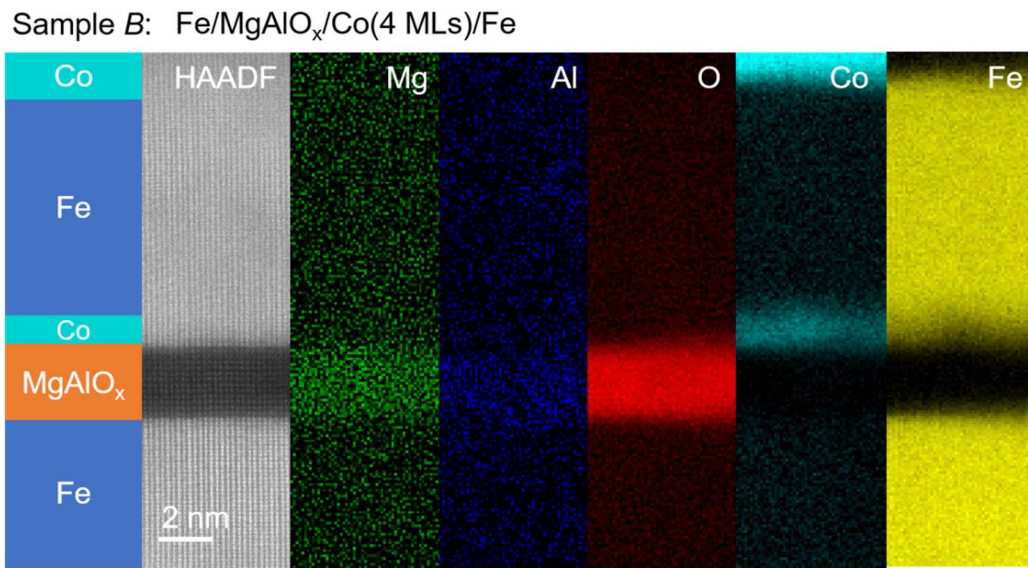


Figure S2. STEM-HAADF images and elements maps extracted from STEM-EELS measurements of Sample *B*.

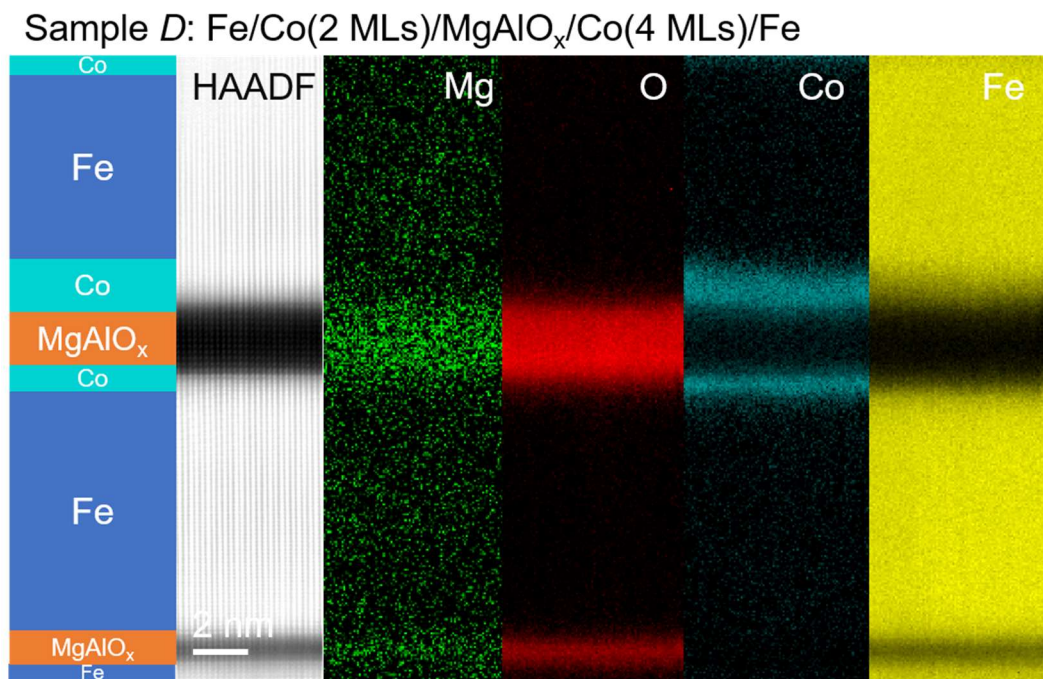


Figure S3. STEM-HAADF images and elements maps extracted from STEM-EELS measurements of Sample *D*.

Sample *E*: Fe/Co(4 MLs)/MgAlO_x/Co(4 MLs)/Fe

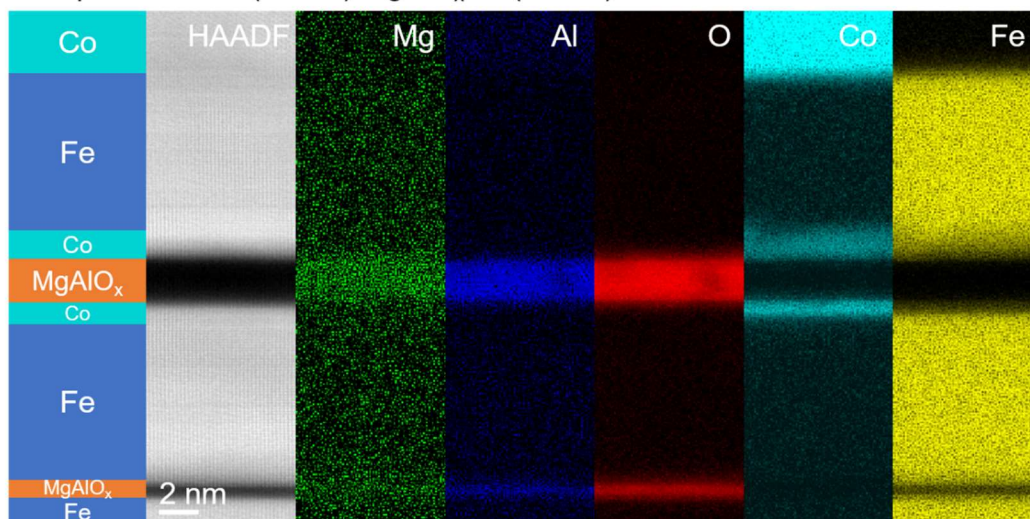


Figure S4. STEM-HAADF images and elements maps extracted from STEM-EELS measurements of Sample *E*.

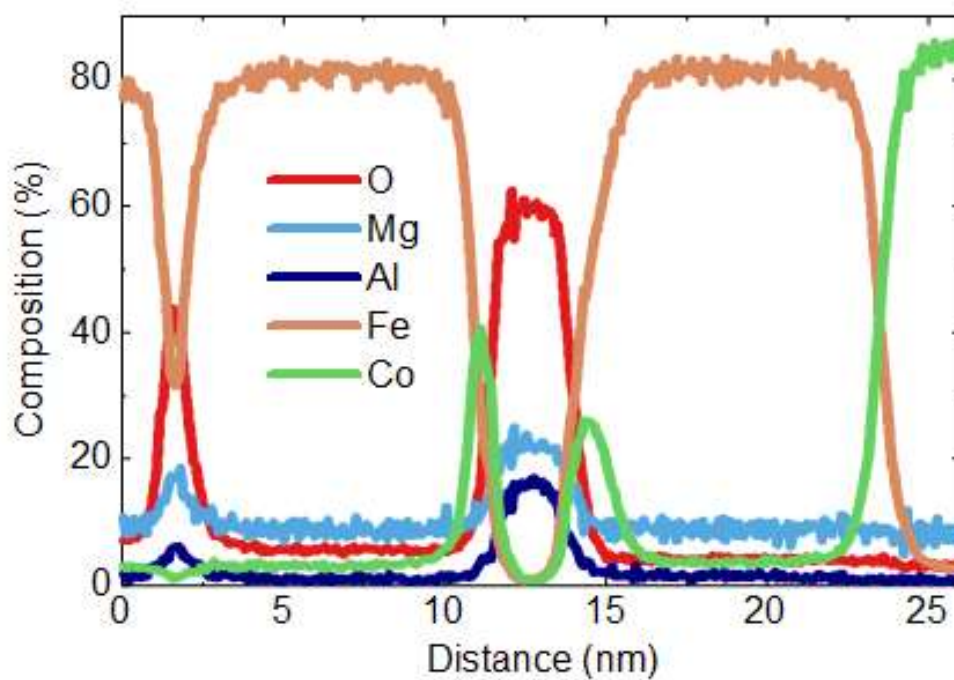


Figure S5: Atomic composition profiles extracted from STEM-EELS for Sample *E*.

Note 3: RHEED patterns and magneto-transport measurements of the control Sample *K*

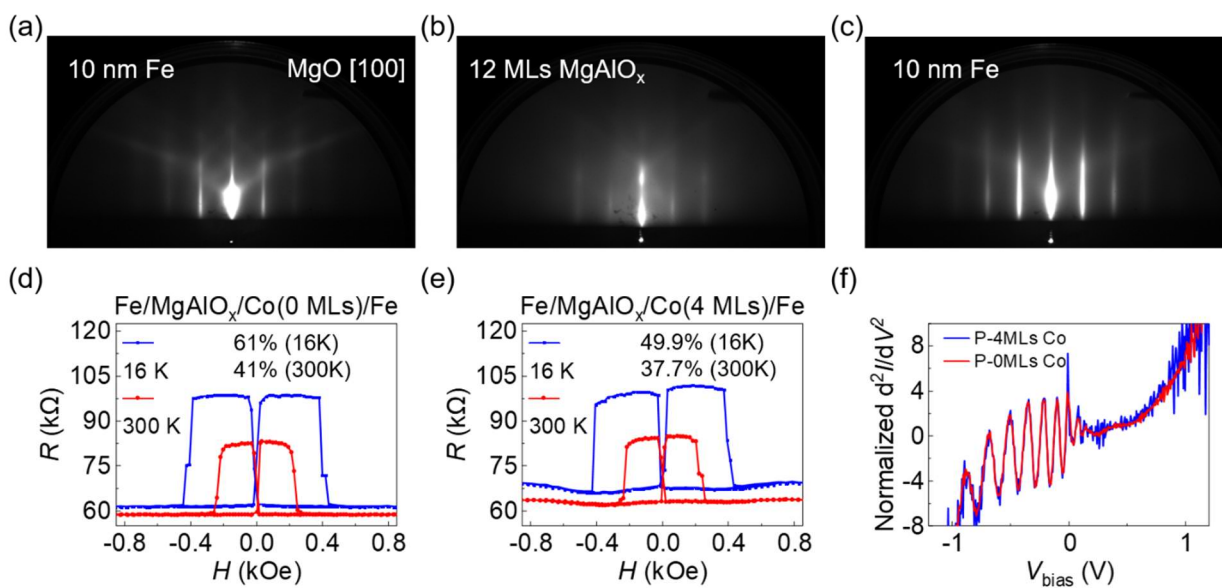


Figure S6. (a-c) RHEED patterns of the control Sample *K* at different growth steps along the [100] azimuth of MgO substrate. (a) 10 nm Fe QW after annealing at 400°C. (b) 12 MLs MgAlO_x grown at 80°C. (c) 10 nm top Fe layer after annealing at 250°C. (d,e) TMR curves measured at 16K and RT in DMTJs (d) without and (e) with Co insertion. (f) The corresponding bias dependence of normalized d^2I/dV^2 in the P state.

Note 4: Symmetry-dependent band structure of bcc Fe, bcc Co and Fe₄N

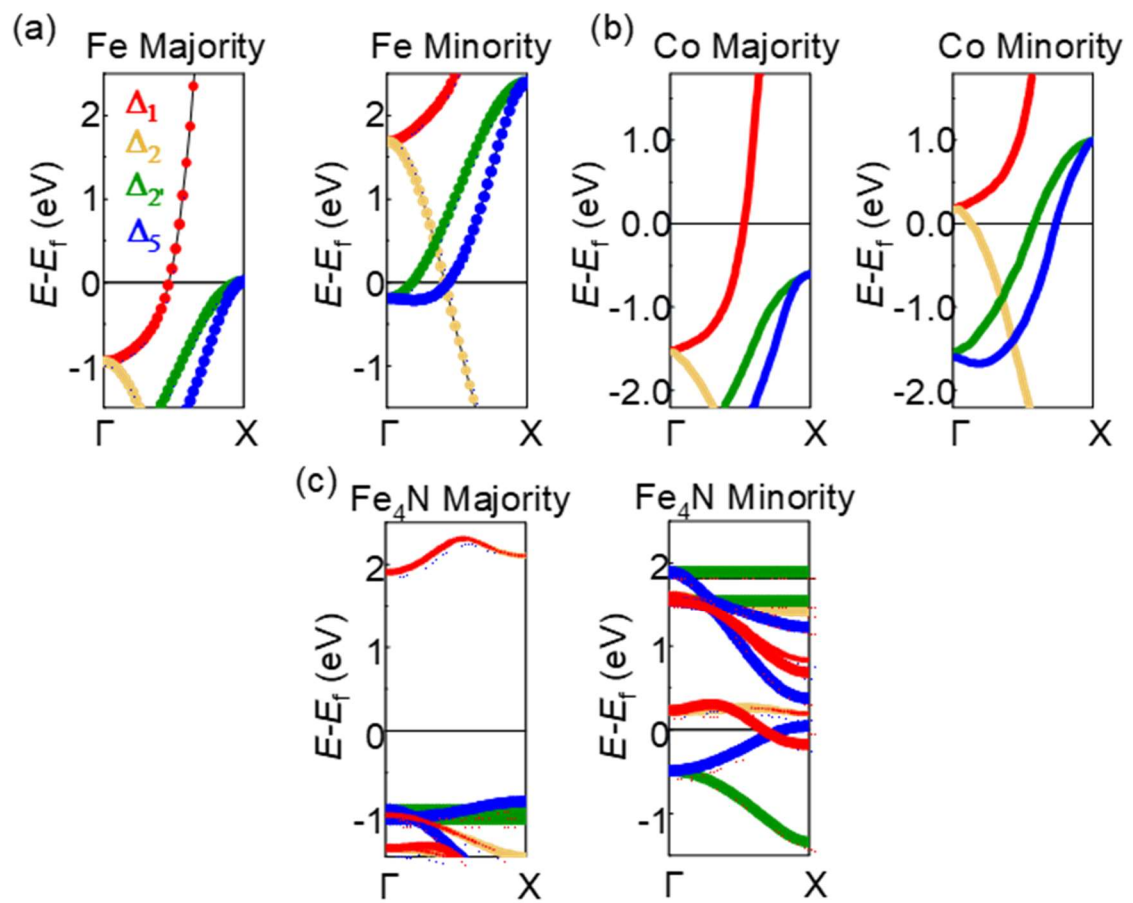


Figure S7. Symmetry and spin-resolved band structures of bulk (a) bcc Fe, (b) bcc Co and (c) Fe₄N along the transport direction ($\Gamma-X$). (a,c) are redrawn from Ma et al.¹ (b) are redrawn from Bagayako et al.²

Note 5: STEM-HAADF images and RHEED pattern of Sample C with Fe₄N top electrode

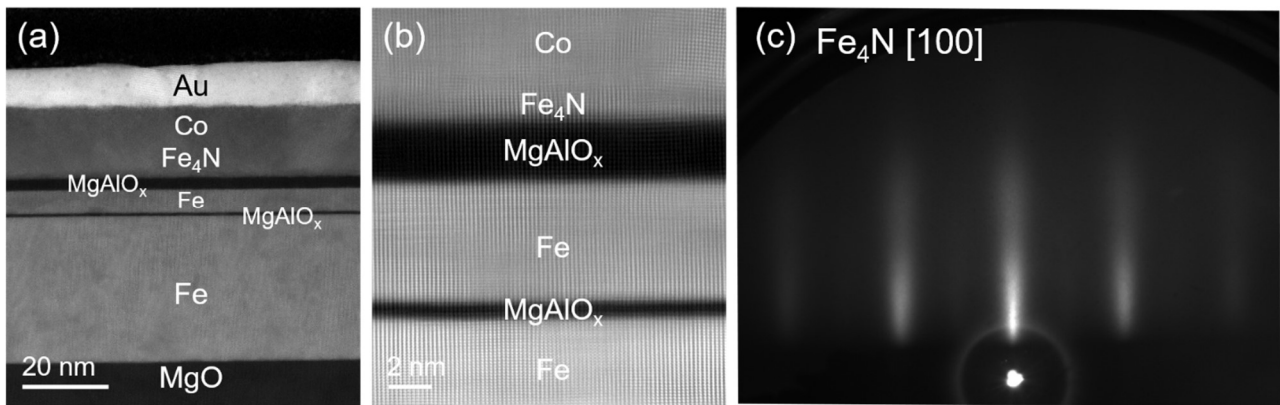


Figure S8. STEM-HAADF images with (a) low-magnification and (b) high-resolution scale. Figures are redrawn from Ma et al.¹ (c) RHEED pattern shows that Fe₄N is epitaxially grown on MgAlO_x.

Note 6: Repetition measurements to confirm sub-step features in d^2I/dV^2 curves

To ensure that noise does not affect the measured signal and to confirm that the sub-steps are indeed due to the QW states, we conducted two independent measurements. The first measurement characterized the I - V curves over a range of ± 1.5 V with 20 repetitions. The second measurement covered a range of ± 0.65 V with 50 repetitions. As shown in **Fig. S9**, similar features with sub-steps are clearly observed in the averaged d^2I/dV^2 curves from both measurements. Our results confirm that the sub-steps indicated by the black arrows originate from the broadened QW states due to the chemical disorder. For verification, we have also uploaded all raw I - V curves to the website (<https://zenodo.org/records/13291346>).

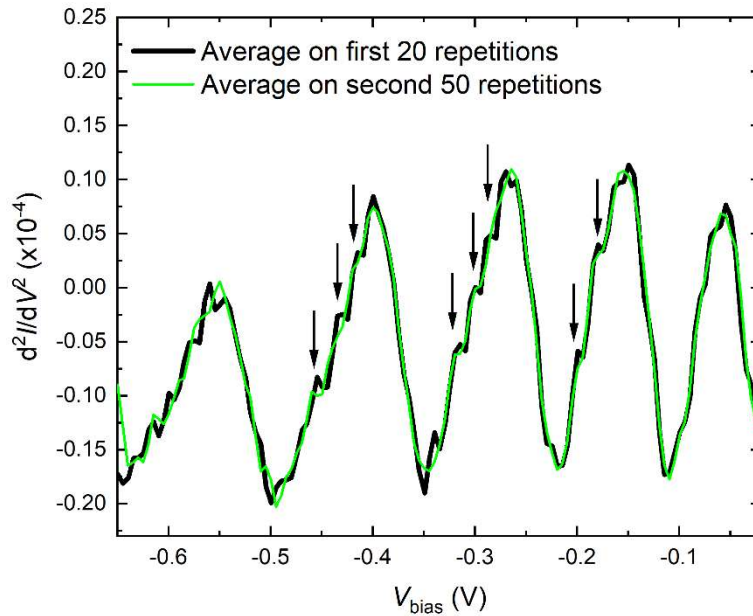


Figure S9. Experimentally measured fine structure in d^2I/dV^2 of Sample *D*. The two independent measurements show similar sub-step features that are marked by black arrows.

Note 7: RHEED patterns and intensity oscillation of Samples *F* and *G* with different Fe insertion at Fe/MgAlO_x interface in the QW

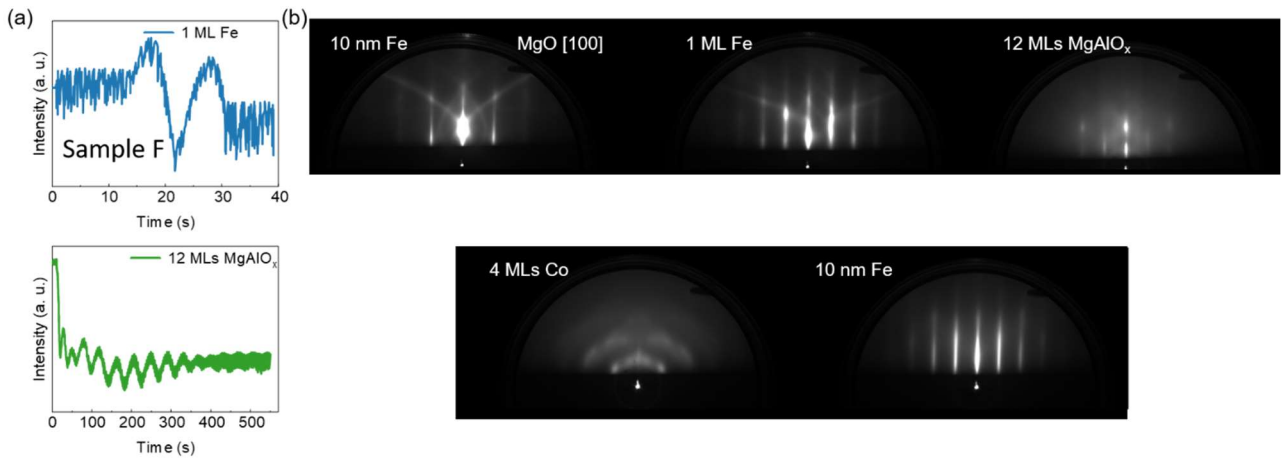


Figure S10. (a) RHEED intensity evolution of Sample *F* during the growth of 1 ML Fe (upper panel) and the growth of 12 MLs MgAlO_x (lower panel). (b) RHEED patterns of Sample *F* at different growth steps along the [100] azimuth of MgO substrate. The top 10 nm Fe was annealed at 400°C.

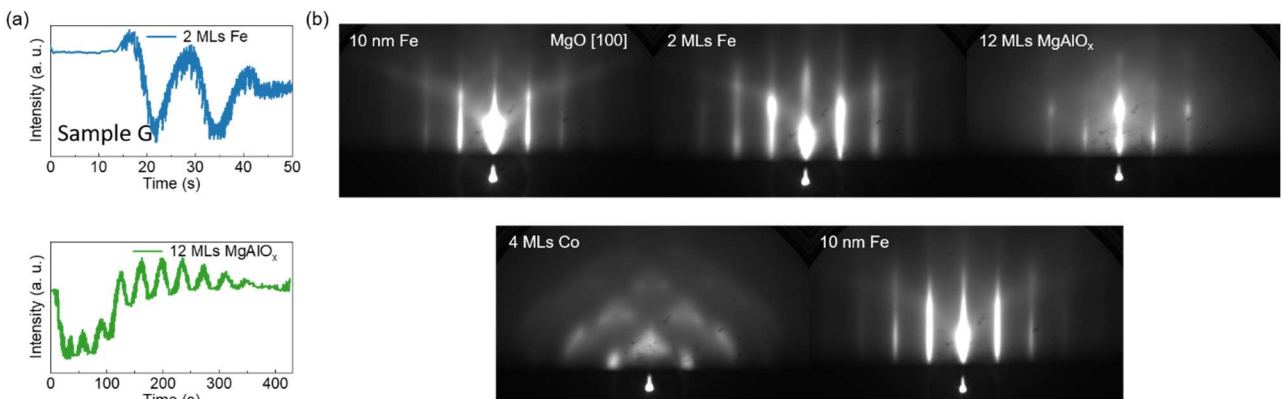


Figure S11. (a) RHEED intensity evolution of Sample *G* during the growth of 2 MLs Fe (upper panel) and the growth of 12 MLs MgAlO_x (lower panel). (b) RHEED patterns of Sample *G* at different growth steps along the [100] azimuth of MgO substrate. The top 10 nm Fe was annealed at 250°C.

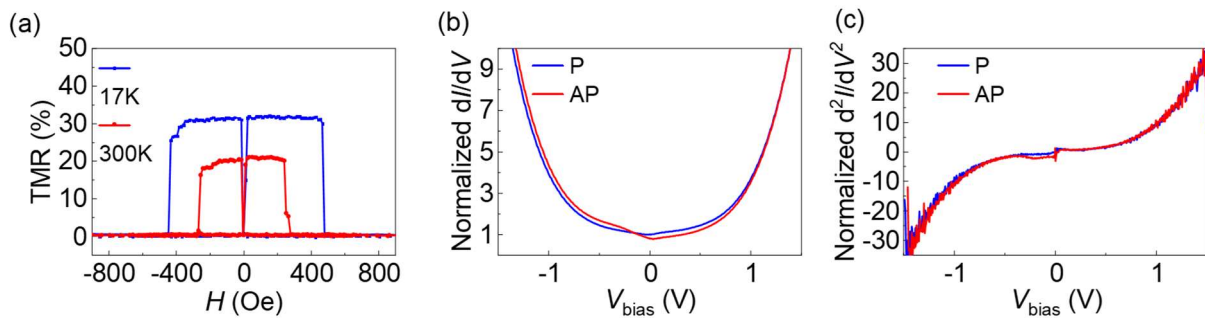


Figure S12. Magneto-transport measurements for Sample *G*. (a) TMR curves measured at 17K and RT. (b,c) Bias dependent normalized (b) dI/dV and (c) d^2I/dV^2 curves in P and AP states.

Note 8: RHEED and magneto-transport measurements on single barrier MgAlO_x MTJ with Co insertion

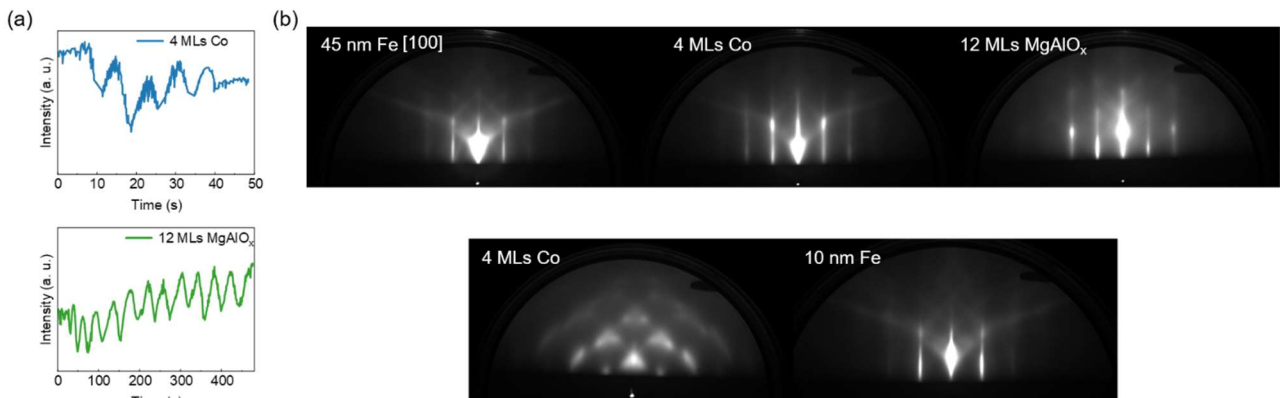


Figure S13. RHEED intensity oscillation (a) and patterns (b) of sample Fe/Co(4MLs)/MgAlO_x/Co(4MLs)/Fe MTJ at different growth steps along the [100] azimuth of MgO substrate. The top 10 nm Fe was annealed at 400°C.

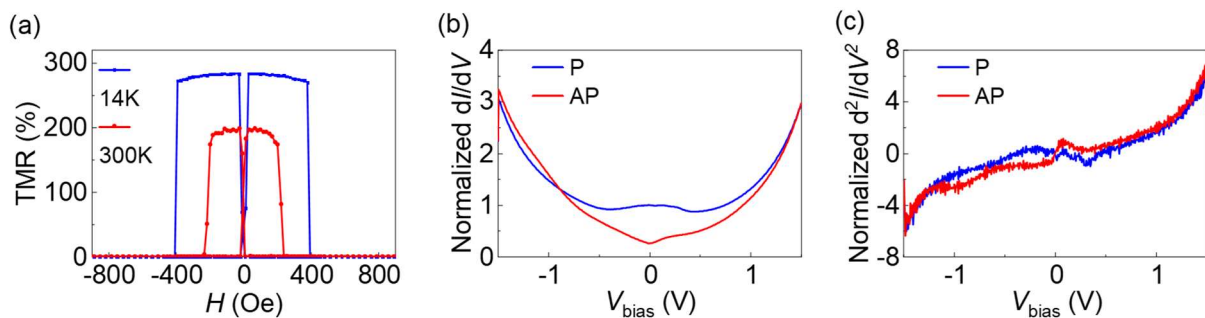


Figure S14. (a) TMR curves measured at 14K and RT in normal MTJ with Co insertion. (b,c) Bias dependent normalized (b) dI/dV and (c) d^2I/dV^2 curves in P and AP states.

References

- (1) Ma, T.; Zhu, Y.; Dainone, P. A.; Chen, T.; Devaux, X.; Wan, C.; Migot, S.; Lengaigne, G.; Vergnat, M.; Yan, Y.; Han, X.; Lu, Y. Large Sign Reversal of Tunneling Magnetoresistance in an Epitaxial Fe/MgAlOx/Fe4N Magnetic Tunnel Junction. *ACS Appl. Electron. Mater.* **2023**, *5* (11), 5954–5961. <https://doi.org/10.1021/acsaelm.3c00937>.
- (2) Bagayoko, D.; Ziegler, A.; Callaway, J. Band Structure of Bcc Cobalt. *Phys. Rev. B* **1983**, *27* (12), 7046–7049. <https://doi.org/10.1103/PhysRevB.27.7046>.